Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 07:16 AM EDT

PDB ID	:	4ERM / pdb_00004erm
Title	:	Crystal structure of the dATP inhibited E. coli class Ia ribonucleotide reductase complex at 4 Angstroms resolution
Authors	:	Zimanyi, C.M.; Drennan, C.L.
Deposited on	:	2012-04-20
Resolution	:	3.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

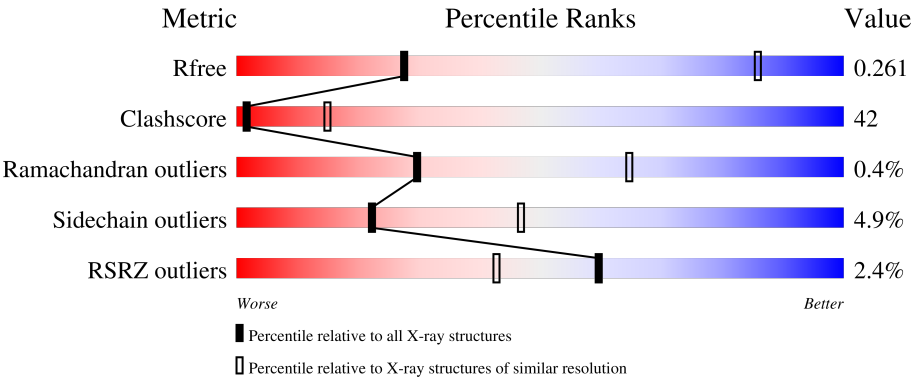
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	2% 41% 51%
1	B	761	2% 43% 49%
1	C	761	2% 43% 49%
1	D	761	2% 45% 47% 5%
2	E	375	2% 43% 47% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	375	2% 43% 50% 5%
2	G	375	3% 41% 48% 5% 5%
2	H	375	3% 44% 48% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DAT	D	802	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 35345 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

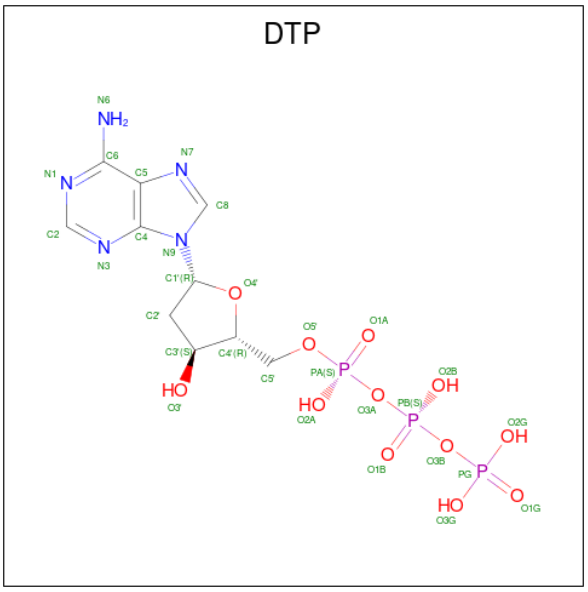
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase 1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	0	0
			5841	3710	1003	1104	24			
1	B	734	Total	C	N	O	S	0	0	0
			5845	3712	1004	1105	24			
1	C	731	Total	C	N	O	S	0	0	0
			5821	3696	1000	1101	24			
1	D	733	Total	C	N	O	S	0	0	0
			5837	3708	1002	1103	24			

- Molecule 2 is a protein called Ribonucleoside-diphosphate reductase 1 subunit beta.

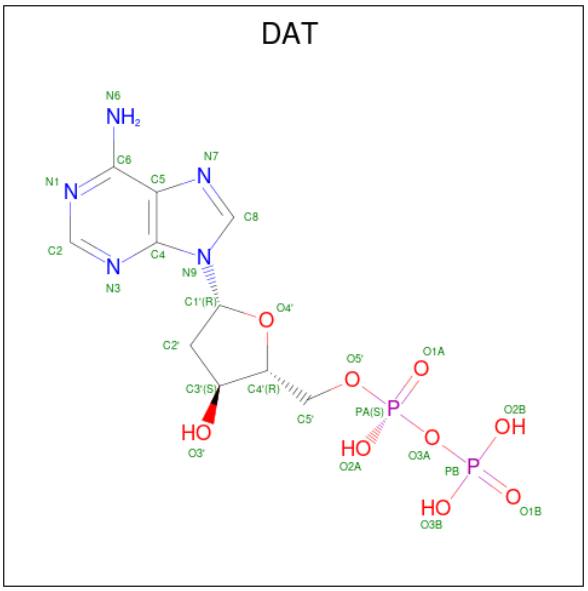
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	352	Total	C	N	O	S	0	0	0
			2885	1841	478	553	13			
2	F	356	Total	C	N	O	S	0	0	0
			2917	1861	483	560	13			
2	G	356	Total	C	N	O	S	0	0	0
			2917	1861	483	560	13			
2	H	356	Total	C	N	O	S	0	0	0
			2914	1859	482	560	13			

- Molecule 3 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$)



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is 2'-DEOXYADENOSINE-5'-DIPHOSPHATE (CCD ID: DAT) (formula: $C_{10}H_{15}N_5O_9P_2$).

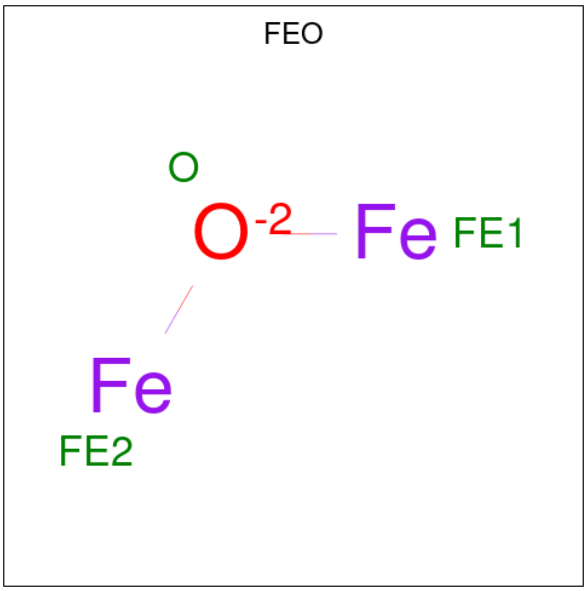


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	B	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	C	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
4	D	1	Total	C	N	O	P	0	0
			26	10	5	9	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is MU-OXO-DIIRON (CCD ID: FEO) (formula: Fe_2O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total Fe O 3 2 1	0	0
6	F	1	Total Fe O 3 2 1	0	0
6	G	1	Total Fe O 3 2 1	0	0
6	H	1	Total Fe O 3 2 1	0	0

- Molecule 7 is water.

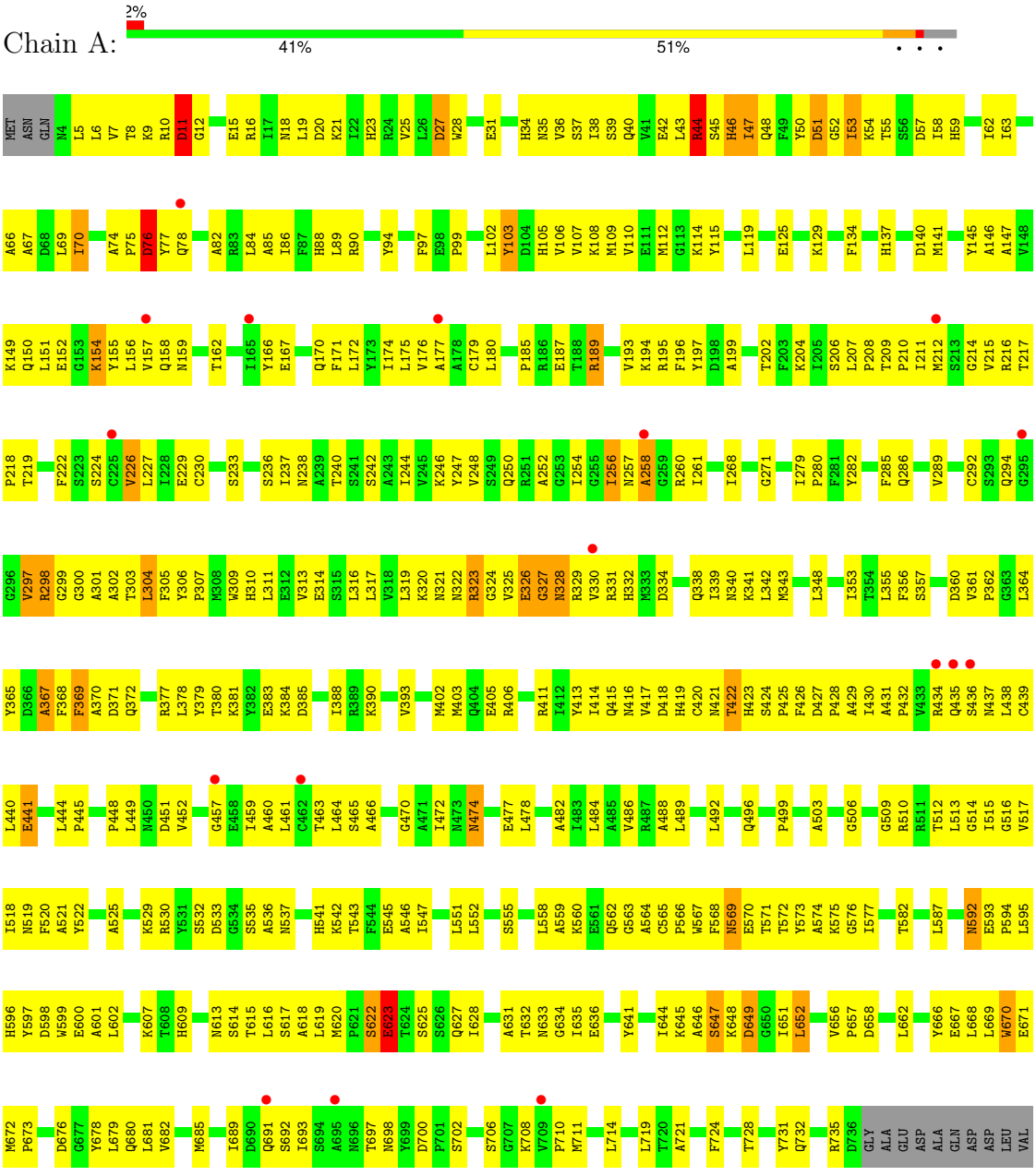
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	2	Total O 2 2	0	0
7	F	2	Total O 2 2	0	0
7	G	2	Total O 2 2	0	0
7	H	2	Total O 2 2	0	0

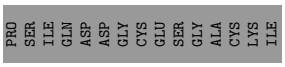
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

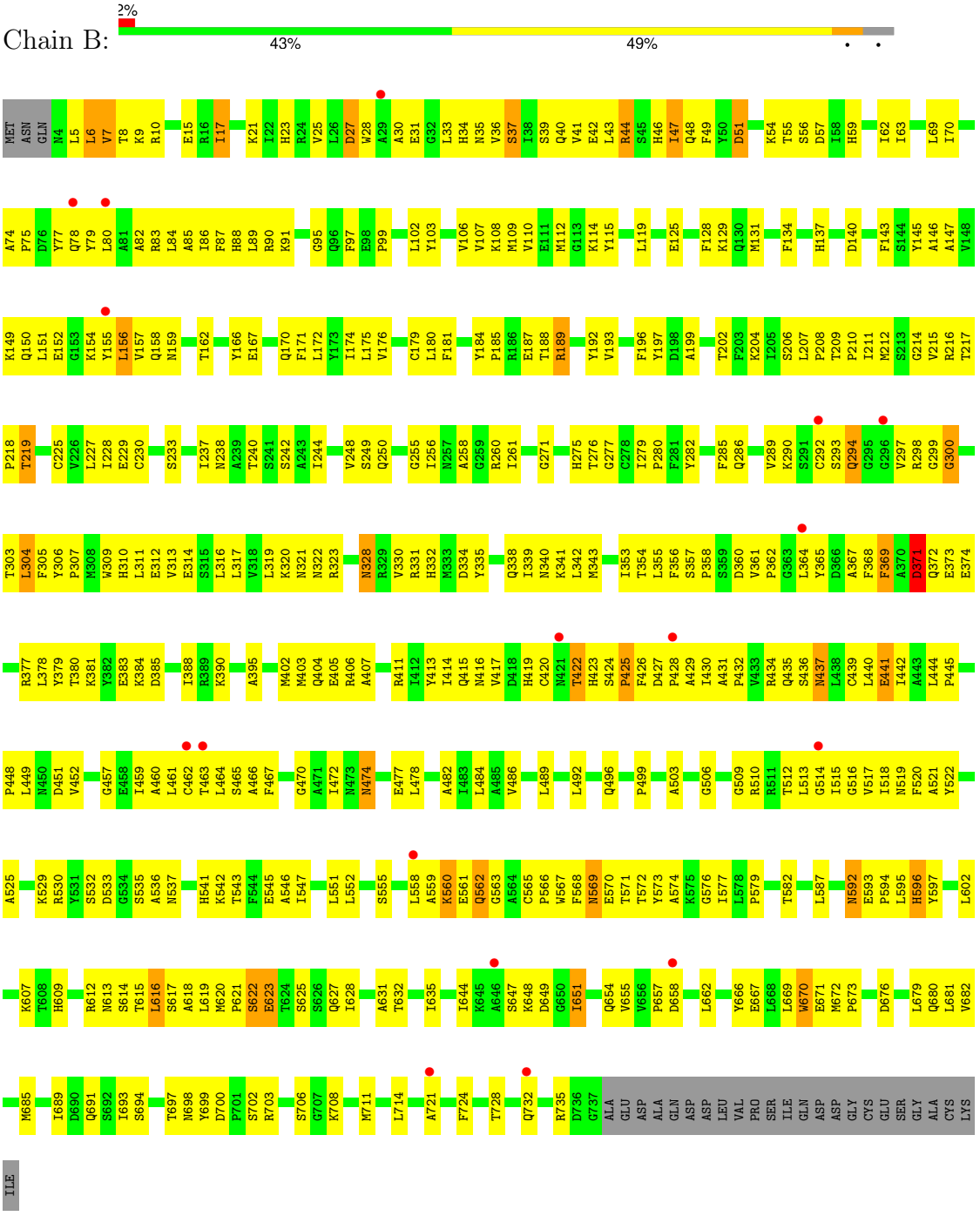
Chain A:





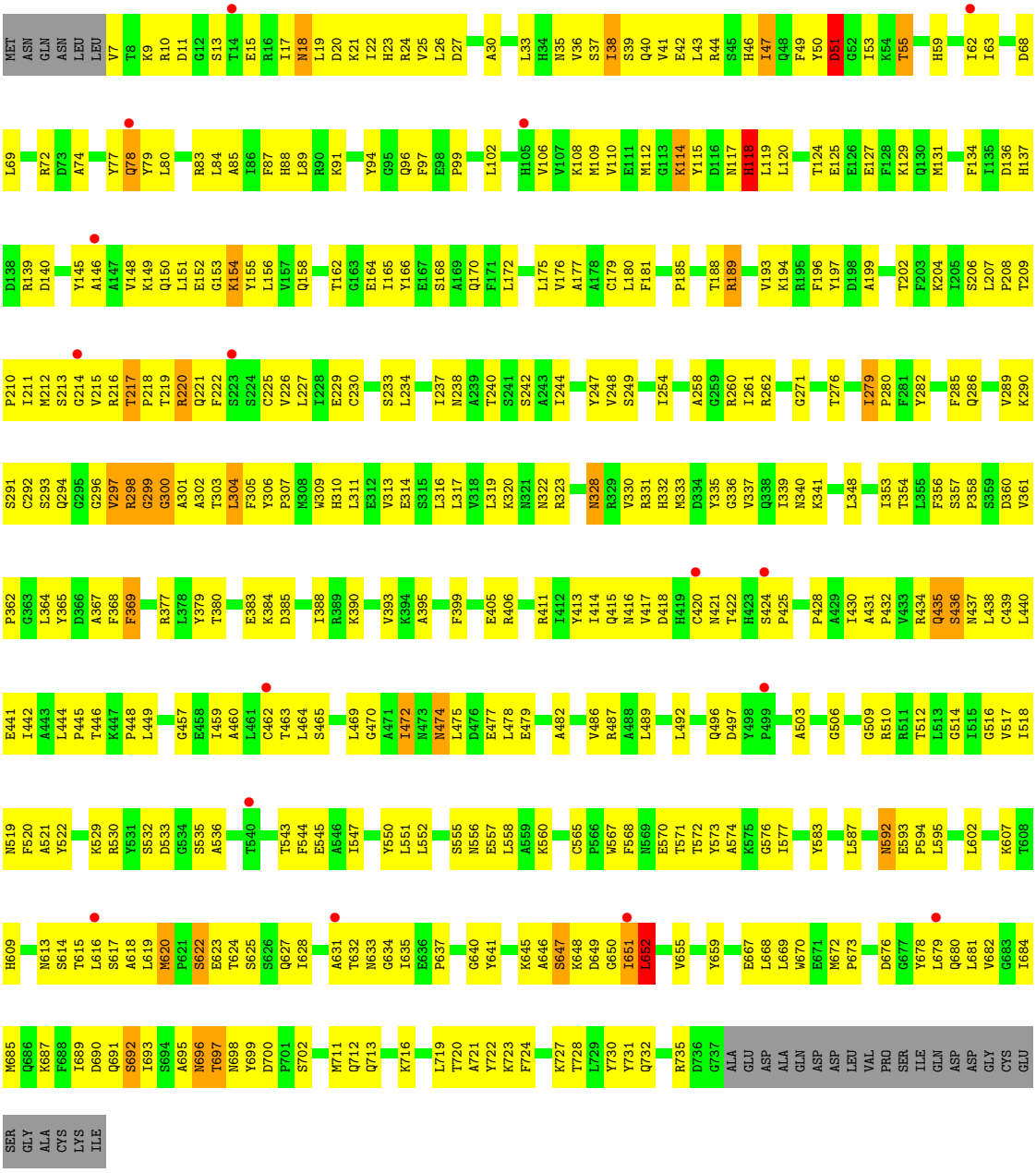
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

Chain B:



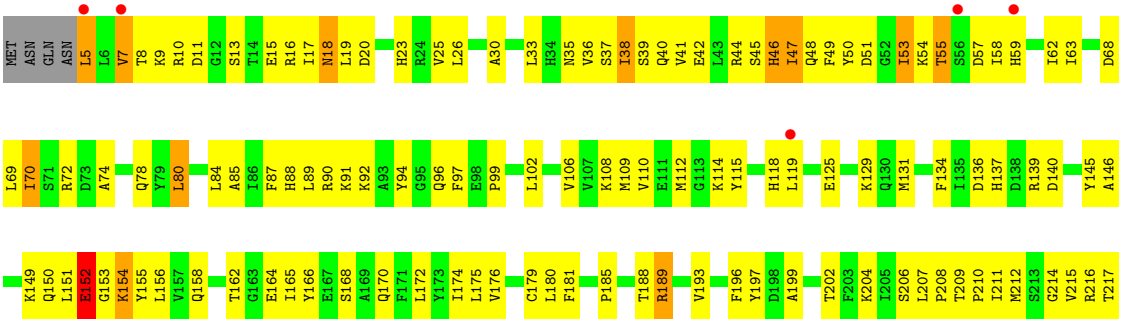
• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

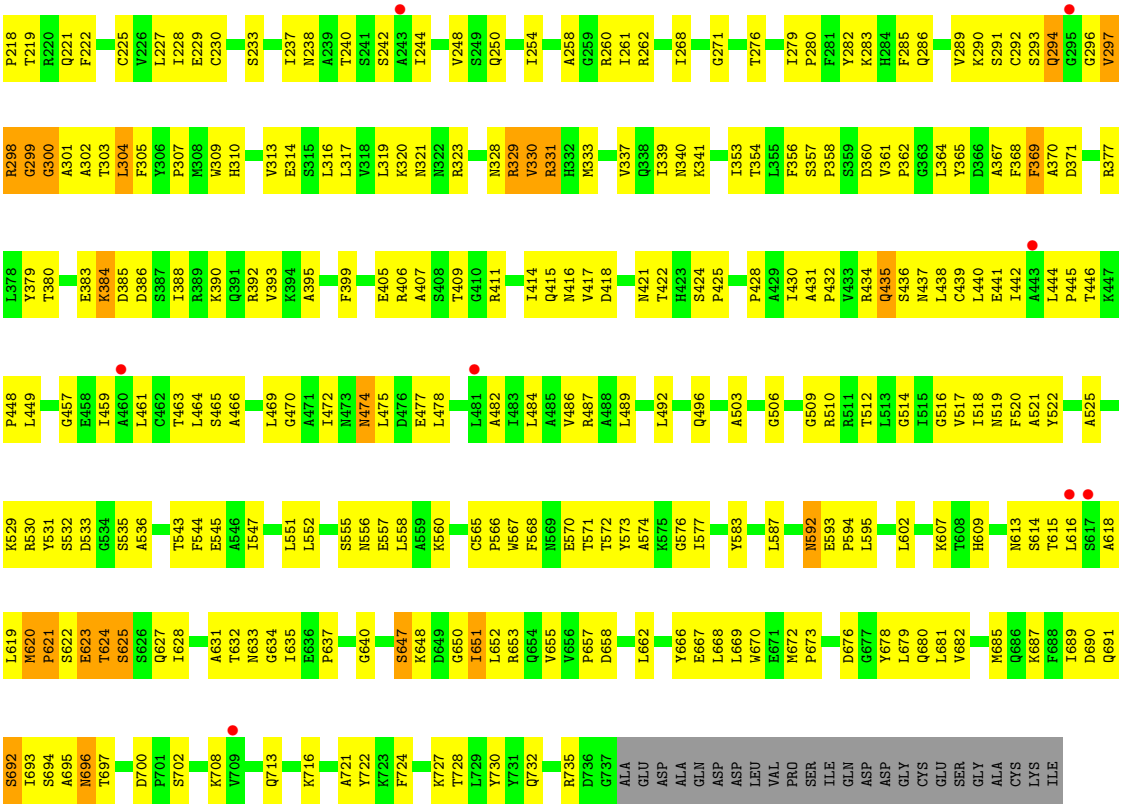
Chain C:



• Molecule 1: Ribonucleoside-diphosphate reductase 1 subunit alpha

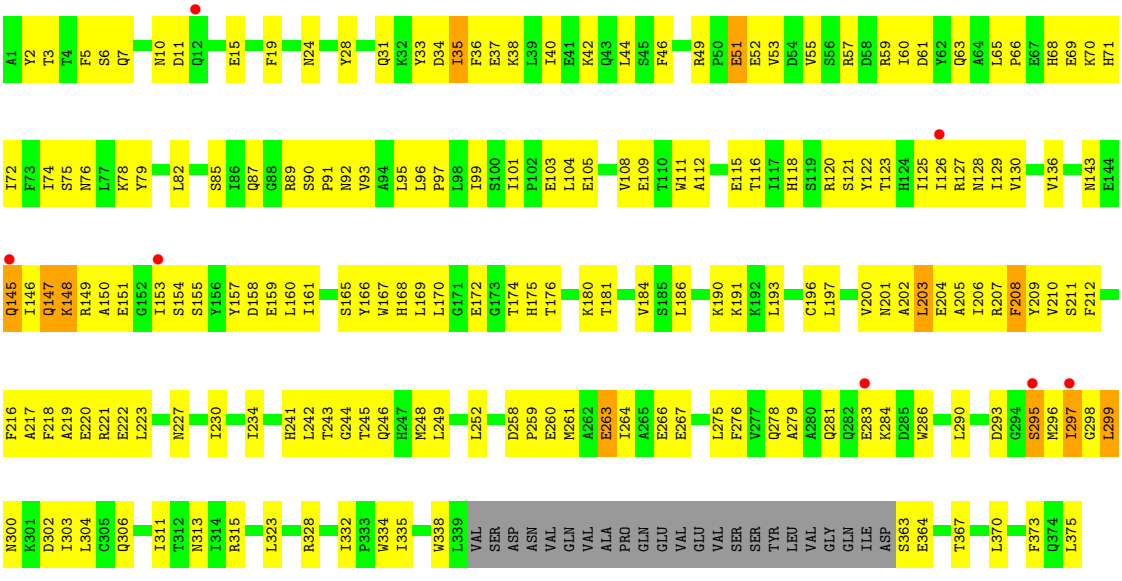
Chain D:





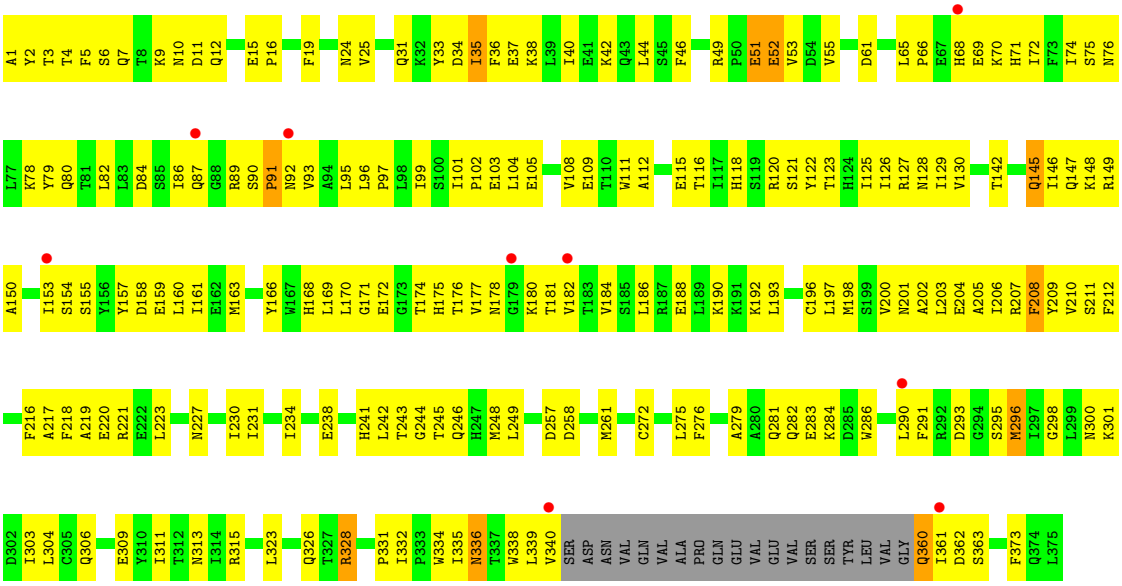
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain E:



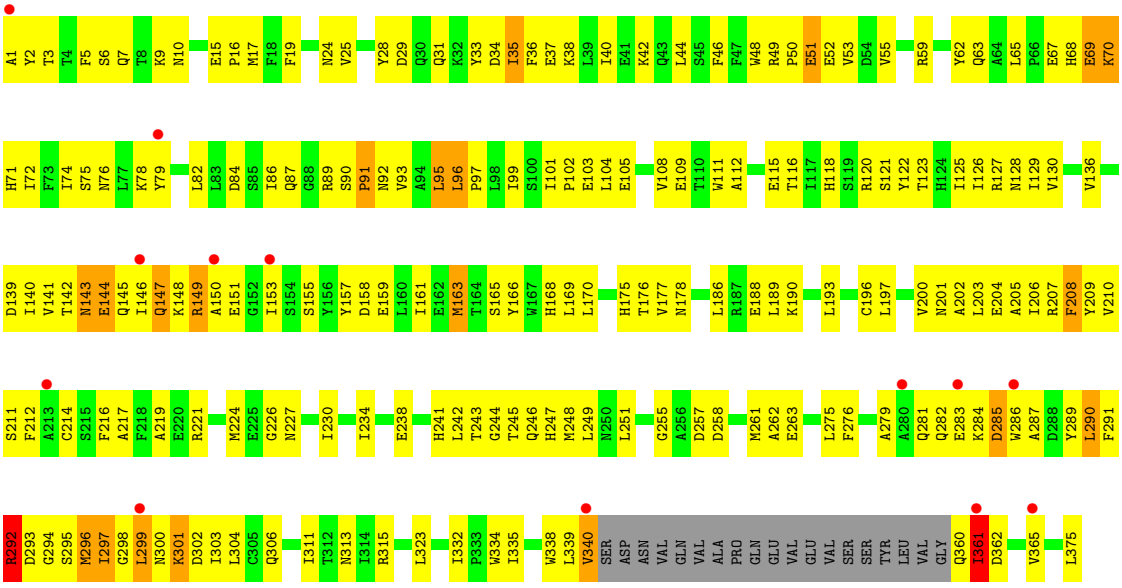
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain F:



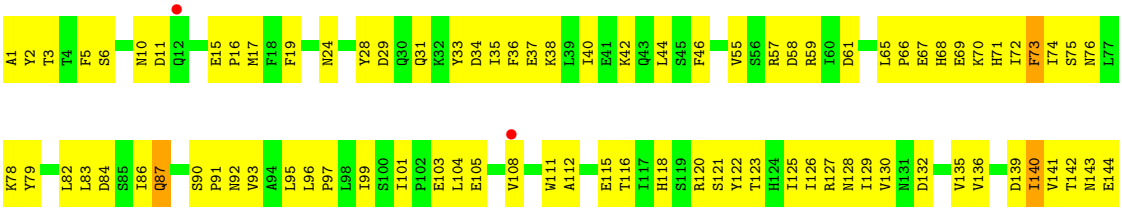
• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

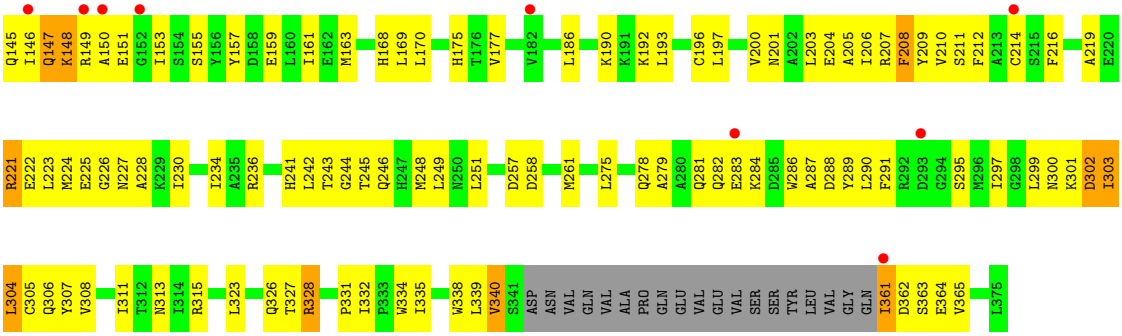
Chain G:



• Molecule 2: Ribonucleoside-diphosphate reductase 1 subunit beta

Chain H:




Q145 I146 Q147 K148 R149 A150 E151 G152 I153 S154 S155 Y156 Y157 D158 E159 L160 I161 E162 M163 H168 L169 L170 H175 T176 V177 V182 L186 K190 K191 K192 L193 C196 L197 V200 N201 A202 L203 E204 A205 I206 R207 F208 Y209 V210 S211 F212 A213 C214 S215 F216 A219 E220
R221 E222 L223 M224 E225 G226 N227 A228 K229 I230 I234 A235 R236 H241 L242 T243 G244 T245 Q246 H247 M248 L249 N250 L251 D257 D258 M261 L275 Q278 A279 A280 Q281 Q282 E283 K284 D285 W286 A287 D288 Y289 L290 F291 R292 D293 G294 S295 M296 I297 G298 L299 N300 K301 D302 I303
L304 C305 Q306 Y307 V308 I311 T312 N313 I314 R315 L323 Q326 T327 R328 P331 I332 P333 W334 I335 W338 L339 V340 S341 ASP ASN VAL GLN VAL ALA PRO GLN GLU VAL GLU VAL SER SER TYR LEU VAL GLY GLN I361 D362 S363 E364 V365 L375

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	280.47Å 155.74Å 166.92Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	30.00 – 3.95 30.00 – 3.95	Depositor EDS
% Data completeness (in resolution range)	96.1 (30.00-3.95) 95.9 (30.00-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.259 , 0.284 0.240 , 0.261	Depositor DCC
R_{free} test set	2527 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	95.3	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	35345	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAT, FEO, MG, DTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.32	1/5969 (0.0%)	0.81	20/8085 (0.2%)
1	B	0.31	1/5973 (0.0%)	0.79	11/8090 (0.1%)
1	C	0.31	0/5949	0.78	13/8057 (0.2%)
1	D	0.30	1/5965 (0.0%)	0.76	8/8079 (0.1%)
2	E	0.36	2/2949 (0.1%)	0.76	3/3998 (0.1%)
2	F	0.28	0/2981	0.72	2/4042 (0.0%)
2	G	0.30	0/2981	0.73	0/4042
2	H	0.30	0/2978	0.80	6/4038 (0.1%)
All	All	0.31	5/35745 (0.0%)	0.78	63/48431 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	203	LEU	C-N	9.06	1.47	1.33
2	E	207	ARG	C-N	-6.29	1.25	1.33
1	B	48	GLN	C-N	5.92	1.41	1.33
1	A	48	GLN	C-N	5.91	1.41	1.33
1	D	48	GLN	C-N	5.87	1.41	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	303	ILE	N-CA-C	14.37	124.21	110.42
2	H	141	VAL	N-CA-C	9.76	120.28	110.82
1	A	372	GLN	N-CA-C	8.28	120.38	111.36
2	E	203	LEU	CA-C-N	-7.39	108.12	120.68
2	E	203	LEU	C-N-CA	-7.39	108.12	120.68
1	C	118	HIS	N-CA-C	-7.35	103.27	111.28
1	A	649	ASP	N-CA-C	7.21	119.22	111.36
1	D	152	GLU	N-CA-C	-7.09	103.56	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	48	GLN	O-C-N	6.99	132.10	123.01
1	A	48	GLN	O-C-N	6.98	132.08	123.01
1	B	373	GLU	N-CA-C	6.97	118.96	111.36
1	B	48	GLN	O-C-N	6.97	132.07	123.01
1	B	623	GLU	N-CA-C	6.92	118.91	111.36
1	A	569	ASN	N-CA-C	-6.81	104.08	112.38
2	H	73	PHE	N-CA-C	6.79	118.56	111.03
2	E	367	THR	N-CA-C	6.75	118.72	111.36
1	A	323	ARG	N-CA-C	-6.72	100.49	110.23
1	C	213	SER	N-CA-C	6.71	118.39	111.14
2	H	304	LEU	N-CA-C	-6.70	103.79	112.23
1	A	326	GLU	N-CA-C	-6.67	103.21	111.75
1	C	46	HIS	N-CA-C	-6.66	102.75	111.74
1	C	214	GLY	N-CA-C	6.55	121.15	112.77
1	B	46	HIS	N-CA-C	-6.47	102.74	111.54
1	D	46	HIS	N-CA-C	-6.46	102.75	111.54
1	A	46	HIS	N-CA-C	-6.42	102.80	111.54
2	F	293	ASP	N-CA-C	6.37	118.22	111.28
1	D	214	GLY	N-CA-C	6.34	120.89	112.77
1	D	70	ILE	N-CA-C	-6.24	100.50	108.93
1	A	103	TYR	N-CA-C	6.23	118.16	111.36
1	A	299	GLY	N-CA-C	6.18	120.69	112.65
1	C	51	ASP	N-CA-C	-6.11	101.00	110.10
1	D	294	GLN	N-CA-C	-6.01	101.14	110.10
2	H	302	ASP	N-CA-C	-5.97	104.77	111.28
1	A	622	SER	N-CA-C	5.95	119.02	107.71
1	B	569	ASN	N-CA-C	-5.94	104.88	111.71
1	C	217	THR	CA-C-N	5.92	125.60	119.56
1	C	217	THR	C-N-CA	5.92	125.60	119.56
2	H	140	ILE	N-CA-C	-5.90	103.68	111.05
1	B	648	LYS	N-CA-C	5.89	117.70	111.28
1	B	425	PRO	N-CA-C	-5.85	105.75	113.65
1	C	652	LEU	N-CA-C	5.69	117.83	109.24
1	C	294	GLN	N-CA-C	-5.67	101.65	110.10
1	A	11	ASP	N-CA-C	-5.65	105.22	111.71
1	C	367	ALA	N-CA-C	-5.63	105.23	111.71
1	B	294	GLN	N-CA-C	-5.60	101.76	110.10
1	C	649	ASP	N-CA-C	5.59	117.45	111.36
1	A	44	ARG	N-CA-C	-5.49	105.30	111.28
1	A	367	ALA	N-CA-C	-5.43	105.46	111.71
1	B	622	SER	N-CA-C	5.39	118.94	107.67
1	D	624	THR	N-CA-C	5.34	117.19	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	ASP	N-CA-C	-5.33	105.40	112.34
2	F	52	GLU	N-CA-C	-5.26	105.66	111.71
1	A	647	SER	N-CA-C	5.24	116.81	108.79
1	C	279	ILE	CB-CA-C	-5.23	108.73	113.70
1	A	258	ALA	N-CA-C	-5.17	106.65	113.17
1	B	514	GLY	O-C-N	-5.12	116.04	122.70
1	A	70	ILE	N-CA-C	-5.12	102.60	109.30
1	A	623	GLU	N-CA-C	5.10	116.92	111.36
1	A	256	ILE	N-CA-C	5.10	116.16	109.58
1	A	422	THR	N-CA-C	5.08	116.90	111.36
1	C	298	ARG	N-CA-C	5.03	116.84	109.24
1	D	298	ARG	N-CA-C	5.03	116.83	109.24
1	B	371	ASP	N-CA-C	5.01	116.56	108.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5767	518	0
1	B	5845	0	5770	521	0
1	C	5821	0	5742	503	0
1	D	5837	0	5764	479	0
2	E	2885	0	2813	215	0
2	F	2917	0	2845	247	0
2	G	2917	0	2845	293	0
2	H	2914	0	2842	240	0
3	A	60	0	22	1	0
3	B	60	0	22	8	0
3	C	60	0	22	10	0
3	D	60	0	22	9	0
4	A	26	0	12	3	0
4	B	26	0	12	1	0
4	C	26	0	12	5	0
4	D	26	0	12	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	3	0	0	0	0
6	G	3	0	0	0	0
6	H	3	0	0	0	0
7	E	2	0	0	1	0
7	F	2	0	0	1	0
7	G	2	0	0	0	0
7	H	2	0	0	1	0
All	All	35345	0	34524	2901	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 42.

All (2901) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:HG21	1:B:356:PHE:CZ	1.44	1.52
1:A:646:ALA:HB2	1:A:651:ILE:CG2	1.40	1.52
1:A:646:ALA:CB	1:A:651:ILE:HG22	1.41	1.46
1:A:297:VAL:CG1	1:A:298:ARG:HG2	1.50	1.41
1:A:53:ILE:HD11	1:A:58:ILE:CD1	1.50	1.40
2:E:149:ARG:NH2	2:E:286:TRP:HB2	1.37	1.39
1:D:53:ILE:CD1	1:D:58:ILE:HD11	1.61	1.31
1:A:297:VAL:HG12	1:A:298:ARG:CG	1.61	1.30
2:E:218:PHE:CE1	2:E:296:MET:SD	2.25	1.29
1:C:696:ASN:HB2	1:C:731:TYR:O	1.32	1.28
1:B:354:THR:HG21	1:B:356:PHE:CE2	1.69	1.27
2:G:79:TYR:CE1	2:G:149:ARG:CD	2.20	1.25
1:D:53:ILE:HD11	1:D:58:ILE:CD1	1.69	1.22
1:A:215:VAL:O	1:A:216:ARG:HG2	1.37	1.22
1:D:622:SER:HB3	4:D:802:DAT:O1A	1.38	1.22
2:H:149:ARG:NH2	2:H:286:TRP:HB2	1.51	1.22
2:G:79:TYR:CE1	2:G:149:ARG:HD2	1.74	1.21
1:C:115:TYR:CE2	1:C:175:LEU:CD1	2.27	1.19
1:C:72:ARG:HG2	1:C:659:TYR:OH	1.39	1.18
1:B:419:HIS:HA	1:B:422:THR:OG1	1.43	1.18
2:G:300:ASN:H	2:G:303:ILE:CG2	1.55	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:302:ASP:O	2:H:306:GLN:HG3	1.42	1.18
2:G:149:ARG:HH11	2:G:149:ARG:HG3	1.05	1.17
1:A:53:ILE:CD1	1:A:58:ILE:HD11	1.75	1.16
2:H:299:LEU:HD11	2:H:304:LEU:HB2	1.24	1.16
1:D:19:LEU:HD12	2:G:295:SER:O	1.41	1.15
1:A:646:ALA:HA	1:A:651:ILE:HA	1.16	1.15
1:B:555:SER:CB	1:B:616:LEU:HD11	1.75	1.14
1:B:420:CYS:O	1:B:424:SER:HB2	1.47	1.13
2:E:147:GLN:HA	2:E:147:GLN:NE2	1.59	1.13
1:A:710:PRO:HA	2:F:362:ASP:HB3	1.18	1.12
1:C:115:TYR:HE2	1:C:175:LEU:HD11	1.14	1.11
1:D:442:ILE:HA	1:D:691:GLN:OE1	1.48	1.11
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.30	1.10
1:C:699:TYR:HE2	1:C:732:GLN:NE2	1.47	1.10
1:D:555:SER:CB	1:D:616:LEU:HD11	1.80	1.10
2:G:149:ARG:NH2	2:G:286:TRP:HB2	1.65	1.10
1:B:354:THR:CG2	1:B:356:PHE:CZ	2.32	1.10
1:B:356:PHE:CE1	1:B:390:LYS:HB3	1.85	1.10
1:B:6:LEU:HD23	1:B:6:LEU:H	1.02	1.10
1:C:215:VAL:O	1:C:216:ARG:HG2	1.51	1.09
1:B:5:LEU:HD22	1:B:51:ASP:HB2	1.30	1.09
1:B:555:SER:HB3	1:B:616:LEU:HD11	1.25	1.08
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.10	1.08
1:B:689:ILE:HG22	1:B:691:GLN:O	1.52	1.08
1:B:5:LEU:HD22	1:B:51:ASP:CB	1.84	1.08
1:B:542:LYS:HG3	1:B:596:HIS:NE2	1.68	1.07
1:B:699:TYR:CE2	1:B:732:GLN:NE2	2.20	1.07
2:F:149:ARG:NH2	2:F:286:TRP:HB2	1.69	1.07
1:B:466:ALA:HA	1:B:516:GLY:O	1.53	1.06
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.35	1.06
1:B:489:LEU:CD1	1:B:513:LEU:HD11	1.84	1.06
1:C:72:ARG:NH1	1:C:641:TYR:CD2	2.23	1.06
2:E:258:ASP:OD2	2:E:261:MET:HG2	1.56	1.06
2:G:49:ARG:O	2:G:52:GLU:HG2	1.56	1.06
2:H:153:ILE:HD12	2:H:203:LEU:HD12	1.36	1.06
1:C:555:SER:HB3	1:C:616:LEU:HD11	1.38	1.05
2:E:49:ARG:O	2:E:52:GLU:HG2	1.55	1.05
2:G:62:TYR:CE1	2:G:70:LYS:HG2	1.90	1.05
1:A:710:PRO:HA	2:F:362:ASP:CB	1.86	1.05
1:D:320:LYS:HE2	1:D:411:ARG:CG	1.86	1.05
1:D:708:LYS:HE2	2:G:362:ASP:HB2	1.30	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:190:LYS:HD3	2:E:261:MET:SD	1.97	1.04
1:D:175:LEU:HB2	1:D:216:ARG:HD2	1.33	1.04
1:B:354:THR:CG2	1:B:356:PHE:CE2	2.38	1.04
1:B:489:LEU:HD12	1:B:513:LEU:HD11	1.39	1.04
1:B:622:SER:HB2	1:B:625:SER:OG	1.58	1.03
2:E:260:GLU:HA	2:E:263:GLU:OE2	1.58	1.03
2:G:79:TYR:CE1	2:G:149:ARG:HD3	1.93	1.03
2:H:299:LEU:CD1	2:H:304:LEU:HB2	1.87	1.03
2:G:300:ASN:CB	2:G:303:ILE:HG22	1.88	1.03
2:H:73:PHE:CZ	2:H:224:MET:CE	2.42	1.03
1:C:72:ARG:HG2	1:C:659:TYR:CZ	1.93	1.03
1:C:474:ASN:HD21	1:C:477:GLU:HG2	1.20	1.02
1:A:53:ILE:HD11	1:A:58:ILE:CG1	1.89	1.02
2:E:297:ILE:H	2:E:297:ILE:HD12	1.20	1.02
1:A:35:ASN:HD22	1:A:74:ALA:HB2	1.21	1.02
1:D:330:VAL:O	1:D:330:VAL:HG12	1.59	1.01
2:E:153:ILE:HD12	2:E:203:LEU:HD12	1.39	1.01
1:C:469:LEU:HA	1:C:472:ILE:HD11	1.43	1.01
1:C:555:SER:CB	1:C:616:LEU:HD11	1.89	1.01
1:D:622:SER:HA	4:D:802:DAT:O2A	1.59	1.01
1:D:555:SER:HB3	1:D:616:LEU:HD11	1.37	1.01
1:A:149:LYS:HG2	1:A:652:LEU:HD22	1.42	1.00
2:F:221:ARG:NH1	2:F:296:MET:HG2	1.77	1.00
2:H:153:ILE:CD1	2:H:203:LEU:HD12	1.91	1.00
1:C:115:TYR:CE2	1:C:175:LEU:HD11	1.95	1.00
1:B:356:PHE:HE1	1:B:390:LYS:HB3	1.24	1.00
2:H:73:PHE:CE2	2:H:224:MET:CE	2.44	1.00
1:D:9:LYS:HE3	1:D:15:GLU:OE1	1.62	0.99
1:A:423:HIS:HB2	1:A:582:THR:O	1.62	0.99
1:D:320:LYS:HE2	1:D:411:ARG:HB2	1.45	0.99
1:A:149:LYS:HG2	1:A:652:LEU:CD2	1.92	0.99
1:A:419:HIS:HA	1:A:422:THR:OG1	1.61	0.98
2:F:153:ILE:HD12	2:F:203:LEU:HD12	1.44	0.98
1:B:356:PHE:CE1	1:B:390:LYS:HE3	1.98	0.98
2:E:66:PRO:HB2	2:E:68:HIS:CD2	1.98	0.98
1:A:53:ILE:HD11	1:A:58:ILE:HD11	0.99	0.98
1:B:156:LEU:HD13	1:B:167:GLU:O	1.64	0.97
1:C:413:TYR:OH	1:C:731:TYR:HE1	1.47	0.97
2:G:300:ASN:N	2:G:303:ILE:CG2	2.27	0.97
2:H:300:ASN:OD1	2:H:303:ILE:HG12	1.64	0.97
1:B:6:LEU:HD23	1:B:6:LEU:N	1.78	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:207:ARG:HH22	2:F:282:GLN:NE2	1.63	0.96
1:B:6:LEU:H	1:B:6:LEU:CD2	1.77	0.96
1:D:320:LYS:HE2	1:D:411:ARG:CB	1.95	0.96
2:H:300:ASN:ND2	2:H:303:ILE:HG13	1.81	0.96
2:G:149:ARG:HH11	2:G:149:ARG:CG	1.79	0.95
1:A:436:SER:OG	1:A:440:LEU:HA	1.66	0.95
1:A:53:ILE:CD1	1:A:58:ILE:CG1	2.45	0.95
1:A:215:VAL:O	1:A:216:ARG:CG	2.13	0.95
1:B:249:SER:HA	1:B:292:CYS:SG	2.07	0.95
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.49	0.95
2:E:205:ALA:HB1	2:E:315:ARG:HD2	1.46	0.95
1:B:6:LEU:N	1:B:6:LEU:CD2	2.30	0.95
1:C:72:ARG:NH1	1:C:641:TYR:HD2	1.58	0.95
1:A:53:ILE:CD1	1:A:58:ILE:CD1	2.40	0.94
1:D:708:LYS:HE2	2:G:362:ASP:CB	1.95	0.94
2:F:49:ARG:O	2:F:52:GLU:HG2	1.67	0.94
2:G:82:LEU:HD22	2:G:146:ILE:HG23	1.45	0.94
2:H:79:TYR:CE1	2:H:149:ARG:HD3	2.02	0.94
1:B:615:THR:HG21	1:B:691:GLN:HE21	1.33	0.94
2:G:149:ARG:NH2	2:G:286:TRP:CE3	2.36	0.94
2:G:301:LYS:HD2	2:G:301:LYS:O	1.67	0.94
2:E:153:ILE:HD12	2:E:203:LEU:CD1	1.98	0.94
1:C:151:LEU:HD23	1:C:155:TYR:CD2	2.03	0.93
1:B:151:LEU:HD23	1:B:155:TYR:CD2	2.03	0.93
1:B:23:HIS:CE1	1:B:42:GLU:OE2	2.20	0.93
1:C:699:TYR:CE2	1:C:732:GLN:NE2	2.36	0.93
1:D:329:ARG:HG2	1:D:329:ARG:HH11	1.29	0.93
1:A:50:TYR:O	1:A:53:ILE:HG22	1.69	0.93
2:G:297:ILE:HD12	2:G:297:ILE:H	1.33	0.93
1:C:155:TYR:HE2	1:C:628:ILE:HG13	1.30	0.93
2:G:79:TYR:HE1	2:G:149:ARG:CD	1.79	0.93
2:H:73:PHE:CE2	2:H:224:MET:HE2	2.04	0.92
2:E:153:ILE:CD1	2:E:203:LEU:HD12	1.98	0.92
1:D:175:LEU:CB	1:D:216:ARG:HD2	1.99	0.92
1:A:426:PHE:CE2	1:A:445:PRO:HD3	2.05	0.92
1:B:323:ARG:HB3	1:B:323:ARG:HH11	1.35	0.91
1:D:622:SER:HB3	4:D:802:DAT:PA	2.09	0.91
2:G:153:ILE:HD12	2:G:203:LEU:HD12	1.51	0.91
1:A:597:TYR:O	1:A:599:TRP:HD1	1.52	0.91
2:E:149:ARG:HH22	2:E:286:TRP:HB2	1.21	0.91
1:A:226:VAL:CG1	1:A:459:ILE:CG2	2.48	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:PHE:CE1	1:B:390:LYS:CB	2.54	0.91
1:D:5:LEU:O	1:D:16:ARG:HA	1.71	0.91
1:C:474:ASN:ND2	1:C:477:GLU:HG2	1.86	0.91
2:E:258:ASP:HB3	2:E:261:MET:HG3	1.50	0.91
2:H:153:ILE:HD12	2:H:203:LEU:CD1	2.00	0.91
2:E:79:TYR:CE1	2:E:149:ARG:HD3	2.06	0.90
2:H:87:GLN:OE1	2:H:87:GLN:HA	1.70	0.90
1:A:214:GLY:O	1:A:217:THR:HG23	1.71	0.90
1:B:297:VAL:O	1:B:297:VAL:HG12	1.71	0.90
2:H:82:LEU:HD22	2:H:146:ILE:HG23	1.52	0.90
1:A:439:CYS:SG	4:A:802:DAT:H3'	2.11	0.90
1:B:75:PRO:O	1:B:78:GLN:HG3	1.69	0.90
1:A:622:SER:HB2	1:A:625:SER:OG	1.69	0.90
2:F:176:THR:HA	2:F:180:LYS:O	1.72	0.90
1:C:155:TYR:CE2	1:C:628:ILE:HG13	2.07	0.90
1:A:369:PHE:CD2	1:A:434:ARG:HG2	2.07	0.89
1:D:19:LEU:CD1	2:G:296:MET:HA	2.03	0.89
1:D:516:GLY:CA	1:D:618:ALA:O	2.20	0.89
2:G:91:PRO:O	2:G:95:LEU:HB2	1.72	0.89
2:E:258:ASP:HB3	2:E:261:MET:CG	2.03	0.89
1:D:682:VAL:HA	1:D:685:MET:HE3	1.54	0.89
1:D:555:SER:HB2	1:D:616:LEU:HD11	1.53	0.89
1:A:226:VAL:HG13	1:A:461:LEU:CD2	2.03	0.89
2:F:175:HIS:CD2	2:G:178:ASN:HD21	1.91	0.89
2:F:82:LEU:HD21	2:F:150:ALA:HB2	1.52	0.89
2:G:153:ILE:HD12	2:G:203:LEU:CD1	2.02	0.89
2:H:145:GLN:HG2	2:H:289:TYR:CD2	2.08	0.88
1:D:18:ASN:HD21	1:D:20:ASP:HB2	1.37	0.88
2:H:149:ARG:HH22	2:H:286:TRP:HB2	1.36	0.88
1:B:175:LEU:CD1	1:B:216:ARG:HD2	2.03	0.88
2:E:149:ARG:NH2	2:E:286:TRP:CB	2.31	0.88
2:E:147:GLN:HA	2:E:147:GLN:HE21	1.34	0.88
2:G:149:ARG:HG3	2:G:149:ARG:NH1	1.87	0.88
1:A:424:SER:OG	1:A:425:PRO:HD2	1.73	0.88
1:C:647:SER:HB2	1:C:652:LEU:HD11	1.55	0.88
2:G:79:TYR:CD1	2:G:149:ARG:HD2	2.06	0.88
1:C:682:VAL:HA	1:C:685:MET:HE3	1.56	0.88
1:A:23:HIS:CD2	1:A:42:GLU:OE2	2.26	0.87
1:B:615:THR:HG21	1:B:691:GLN:NE2	1.89	0.87
1:C:115:TYR:CE2	1:C:175:LEU:HD13	2.06	0.87
1:C:516:GLY:CA	1:C:618:ALA:O	2.21	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:SER:O	1:C:691:GLN:HG2	1.73	0.87
1:A:226:VAL:HG21	1:A:247:TYR:CD2	2.09	0.87
1:C:72:ARG:HH11	1:C:641:TYR:HD2	0.92	0.87
1:A:23:HIS:HD2	1:A:42:GLU:OE2	1.56	0.86
1:D:50:TYR:O	1:D:53:ILE:CG2	2.22	0.86
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.57	0.86
1:D:208:PRO:HD2	1:D:211:ILE:HD12	1.57	0.86
2:G:153:ILE:CD1	2:G:203:LEU:HD12	2.04	0.86
2:F:153:ILE:CD1	2:F:203:LEU:HD12	2.05	0.86
1:B:356:PHE:HE1	1:B:390:LYS:HE3	1.37	0.86
2:E:5:PHE:CE1	2:E:24:ASN:HB2	2.09	0.86
2:G:291:PHE:HB3	2:G:294:GLY:O	1.75	0.86
1:B:151:LEU:CA	1:B:155:TYR:HB2	2.04	0.86
2:F:221:ARG:HH11	2:F:296:MET:HG2	1.39	0.86
2:H:287:ALA:HB2	2:H:304:LEU:HD22	1.55	0.86
1:B:519:ASN:HB2	1:B:631:ALA:HB1	1.58	0.86
2:H:5:PHE:CE1	2:H:24:ASN:HB2	2.09	0.85
1:C:72:ARG:CG	1:C:659:TYR:CZ	2.59	0.85
1:B:35:ASN:HD22	1:B:74:ALA:HB2	1.41	0.85
1:A:103:TYR:O	1:A:107:VAL:HG23	1.77	0.85
2:F:309:GLU:HB2	2:F:328:ARG:HH11	1.41	0.85
1:A:70:ILE:HD13	1:A:78:GLN:HB3	1.59	0.85
1:B:419:HIS:CA	1:B:422:THR:OG1	2.25	0.85
1:B:151:LEU:HD23	1:B:155:TYR:CB	2.07	0.85
1:A:177:ALA:CB	1:A:196:PHE:HD2	1.90	0.84
1:A:157:VAL:HG23	1:A:216:ARG:NH2	1.92	0.84
2:E:221:ARG:NH1	2:E:296:MET:HG3	1.92	0.84
2:E:252:LEU:HD22	2:E:261:MET:HE2	1.58	0.84
1:A:519:ASN:HB2	1:A:631:ALA:HB1	1.58	0.84
1:A:97:PHE:O	1:A:99:PRO:HD3	1.77	0.84
2:G:149:ARG:HH22	2:G:286:TRP:HB2	1.37	0.84
1:B:689:ILE:CG2	1:B:691:GLN:O	2.24	0.84
1:D:621:PRO:HD3	1:D:694:SER:CB	2.07	0.84
1:B:439:CYS:SG	4:B:802:DAT:H3'	2.17	0.84
1:C:9:LYS:HE3	1:C:15:GLU:CD	2.02	0.84
1:B:323:ARG:HB3	1:B:323:ARG:NH1	1.93	0.84
1:D:330:VAL:HG11	1:D:333:MET:HE3	1.59	0.84
1:A:423:HIS:CD2	1:A:423:HIS:O	2.30	0.84
1:B:407:ALA:HB3	2:H:361:ILE:HD12	1.59	0.84
1:D:286:GLN:HB2	1:D:333:MET:HE2	1.59	0.83
2:G:149:ARG:NH2	2:G:286:TRP:CB	2.40	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:SER:O	1:B:237:ILE:HG13	1.78	0.83
2:E:218:PHE:CD1	2:E:296:MET:SD	2.71	0.83
1:B:555:SER:HB2	1:B:616:LEU:HD11	1.58	0.83
1:C:151:LEU:CD2	1:C:155:TYR:HD2	1.90	0.83
1:D:708:LYS:HB2	2:G:361:ILE:HA	1.60	0.83
2:G:300:ASN:CA	2:G:303:ILE:HG22	2.08	0.83
1:B:682:VAL:HA	1:B:685:MET:HE3	1.60	0.83
1:D:708:LYS:CE	2:G:362:ASP:HB2	2.08	0.83
1:A:568:PHE:CE2	1:A:574:ALA:HB2	2.13	0.83
1:D:621:PRO:HD3	1:D:694:SER:HB2	1.57	0.83
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.61	0.83
1:A:226:VAL:HG12	1:A:459:ILE:CG2	2.09	0.83
1:D:637:PRO:HG2	1:D:669:LEU:HD13	1.61	0.83
2:G:190:LYS:HB3	2:G:261:MET:SD	2.19	0.83
1:A:53:ILE:CD1	1:A:58:ILE:HG12	2.09	0.82
1:D:320:LYS:CE	1:D:411:ARG:HG3	2.10	0.82
2:F:172:GLU:HA	2:F:184:VAL:O	1.79	0.82
1:C:474:ASN:ND2	1:C:477:GLU:CG	2.42	0.82
1:B:708:LYS:HE2	2:H:362:ASP:HB2	1.60	0.82
1:C:520:PHE:HB3	1:C:635:ILE:HA	1.60	0.82
1:D:320:LYS:CE	1:D:411:ARG:HB2	2.10	0.82
1:A:516:GLY:CA	1:A:618:ALA:O	2.27	0.82
1:A:597:TYR:O	1:A:599:TRP:CD1	2.32	0.82
1:A:134:PHE:CE2	1:A:194:LYS:HB2	2.15	0.81
1:A:682:VAL:HA	1:A:685:MET:HE3	1.62	0.81
2:G:296:MET:HE2	2:G:299:LEU:HB2	1.60	0.81
2:H:73:PHE:CZ	2:H:224:MET:HE2	2.10	0.81
1:A:35:ASN:ND2	1:A:74:ALA:HB2	1.95	0.81
1:B:155:TYR:HE2	1:B:628:ILE:HG13	1.45	0.81
1:B:430:ILE:HG21	1:B:570:GLU:HG2	1.59	0.81
1:B:542:LYS:HE2	1:B:596:HIS:NE2	1.94	0.81
1:C:290:LYS:NZ	1:C:332:HIS:HB3	1.94	0.81
1:D:286:GLN:OE1	1:D:330:VAL:HG13	1.79	0.81
2:G:300:ASN:HB3	2:G:303:ILE:HG22	1.62	0.81
1:D:320:LYS:CE	1:D:411:ARG:CG	2.58	0.81
2:G:68:HIS:O	2:G:71:HIS:HB3	1.79	0.81
1:B:699:TYR:CD2	1:B:732:GLN:NE2	2.48	0.81
1:C:439:CYS:SG	4:C:802:DAT:H3'	2.21	0.81
2:H:363:SER:O	2:H:365:VAL:HG13	1.80	0.81
2:F:361:ILE:HD12	2:F:361:ILE:O	1.80	0.81
1:D:622:SER:CB	1:D:625:SER:OG	2.29	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:327:THR:O	2:H:328:ARG:HG2	1.81	0.80
2:F:309:GLU:HB2	2:F:328:ARG:NH1	1.95	0.80
1:C:117:ASN:ND2	1:C:120:LEU:HD12	1.95	0.80
1:D:520:PHE:HB3	1:D:635:ILE:HA	1.62	0.80
1:C:215:VAL:O	1:C:216:ARG:CG	2.30	0.80
1:D:7:VAL:HG21	3:D:801:DTP:N6	1.96	0.80
1:B:151:LEU:HD23	1:B:155:TYR:HD2	1.41	0.80
1:B:340:ASN:OD1	1:B:368:PHE:HE1	1.64	0.80
2:F:155:SER:O	2:F:159:GLU:HG3	1.81	0.80
1:C:18:ASN:HD21	1:C:20:ASP:HB2	1.44	0.80
1:A:226:VAL:HG13	1:A:461:LEU:HD23	1.64	0.79
2:F:149:ARG:HH22	2:F:286:TRP:HB2	1.46	0.79
1:B:5:LEU:HB3	1:B:51:ASP:HA	1.64	0.79
2:G:300:ASN:N	2:G:303:ILE:HG22	1.95	0.79
1:A:619:LEU:HB2	1:A:693:ILE:HG23	1.64	0.79
1:B:699:TYR:HE2	1:B:732:GLN:HE21	0.86	0.79
1:A:646:ALA:CB	1:A:651:ILE:CG2	2.24	0.79
1:B:357:SER:OG	1:B:358:PRO:HD2	1.83	0.79
1:C:297:VAL:O	1:C:297:VAL:CG1	2.31	0.79
1:A:50:TYR:O	1:A:53:ILE:CG2	2.31	0.79
1:C:290:LYS:HD2	1:C:296:GLY:O	1.81	0.79
2:H:73:PHE:CE2	2:H:224:MET:HE1	2.17	0.79
1:A:257:ASN:HB2	1:A:435:GLN:OE1	1.82	0.79
1:A:115:TYR:HA	1:A:216:ARG:O	1.82	0.79
1:A:565:CYS:SG	1:A:568:PHE:HB2	2.22	0.79
2:F:175:HIS:HD2	2:G:178:ASN:ND2	1.80	0.79
1:B:699:TYR:HE2	1:B:732:GLN:NE2	1.67	0.78
1:C:696:ASN:CB	1:C:731:TYR:O	2.24	0.78
1:C:697:THR:OG1	1:C:732:GLN:CG	2.31	0.78
1:D:297:VAL:O	1:D:297:VAL:CG1	2.30	0.78
1:D:619:LEU:HD12	1:D:693:ILE:HG12	1.66	0.78
2:E:145:GLN:NE2	2:E:145:GLN:H	1.82	0.78
2:F:309:GLU:CD	2:F:328:ARG:HH12	1.91	0.78
2:H:300:ASN:ND2	2:H:303:ILE:CG1	2.46	0.78
2:G:74:ILE:HG13	2:G:78:LYS:HE3	1.66	0.78
1:D:50:TYR:O	1:D:53:ILE:HG22	1.82	0.78
1:C:425:PRO:HG3	1:C:690:ASP:HB3	1.65	0.78
1:D:290:LYS:HD2	1:D:296:GLY:O	1.83	0.78
1:A:646:ALA:HA	1:A:651:ILE:CA	2.08	0.78
1:B:248:VAL:HG11	1:B:289:VAL:HA	1.65	0.78
1:A:226:VAL:HG21	1:A:247:TYR:CG	2.19	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.65	0.78
1:D:622:SER:CA	4:D:802:DAT:O2A	2.32	0.77
2:E:66:PRO:HB2	2:E:68:HIS:NE2	1.99	0.77
2:E:147:GLN:NE2	2:E:147:GLN:CA	2.42	0.77
2:H:145:GLN:HG2	2:H:289:TYR:CE2	2.19	0.77
1:B:697:THR:OG1	1:B:732:GLN:HG3	1.83	0.77
2:F:335:ILE:O	2:F:339:LEU:HG	1.82	0.77
2:G:301:LYS:HD2	2:G:301:LYS:C	2.09	0.77
2:H:300:ASN:HD21	2:H:303:ILE:HG13	1.48	0.77
1:A:248:VAL:HG11	1:A:289:VAL:HA	1.66	0.77
1:C:286:GLN:HB2	1:C:333:MET:HE2	1.66	0.77
1:B:297:VAL:O	1:B:297:VAL:CG1	2.33	0.77
1:C:551:LEU:O	1:C:616:LEU:CD1	2.32	0.77
1:D:622:SER:HB2	1:D:625:SER:OG	1.84	0.77
2:E:218:PHE:HE1	2:E:296:MET:SD	2.02	0.77
1:B:322:ASN:HA	1:B:331:ARG:HE	1.50	0.77
1:A:420:CYS:O	1:A:424:SER:HB2	1.85	0.77
1:C:647:SER:CB	1:C:652:LEU:HD11	2.15	0.77
1:C:436:SER:HB3	1:C:440:LEU:HD13	1.67	0.77
2:G:149:ARG:NH2	2:G:286:TRP:CD2	2.53	0.77
1:B:151:LEU:CD2	1:B:155:TYR:HD2	1.98	0.76
2:F:190:LYS:HB3	2:F:261:MET:SD	2.25	0.76
2:G:217:ALA:CB	2:G:299:LEU:CD2	2.63	0.76
1:B:555:SER:HB2	1:B:616:LEU:CD1	2.15	0.76
1:C:565:CYS:SG	1:C:568:PHE:HB2	2.25	0.76
1:D:323:ARG:HB3	1:D:323:ARG:HH11	1.48	0.76
2:H:61:ASP:O	2:H:65:LEU:HG	1.86	0.76
1:A:689:ILE:HG22	1:A:691:GLN:O	1.85	0.76
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.65	0.76
1:C:40:GLN:O	1:C:44:ARG:HG2	1.85	0.76
1:A:613:ASN:HB2	1:A:616:LEU:HD21	1.68	0.76
1:C:151:LEU:HD23	1:C:155:TYR:CB	2.16	0.76
2:G:297:ILE:HD12	2:G:297:ILE:N	2.00	0.76
1:B:292:CYS:SG	1:B:292:CYS:O	2.44	0.76
1:D:330:VAL:O	1:D:330:VAL:CG1	2.32	0.76
1:D:551:LEU:O	1:D:616:LEU:CD1	2.33	0.76
1:A:430:ILE:HG21	1:A:570:GLU:HG2	1.68	0.76
1:B:214:GLY:O	1:B:217:THR:HB	1.84	0.76
1:B:519:ASN:HD21	1:B:522:TYR:HD2	1.31	0.76
2:G:300:ASN:H	2:G:303:ILE:HG23	1.50	0.76
1:D:565:CYS:SG	1:D:568:PHE:HB2	2.25	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:74:ILE:HG13	2:E:78:LYS:HE3	1.66	0.76
1:A:436:SER:HG	1:A:440:LEU:HA	1.47	0.76
1:B:209:THR:N	1:B:210:PRO:HD2	2.01	0.76
1:B:214:GLY:O	1:B:217:THR:CB	2.34	0.76
2:E:221:ARG:HH11	2:E:296:MET:CG	1.99	0.76
2:F:339:LEU:O	2:F:340:VAL:HG23	1.86	0.76
2:G:92:ASN:O	2:G:96:LEU:HB2	1.85	0.76
2:G:291:PHE:O	2:G:292:ARG:C	2.28	0.76
1:C:516:GLY:HA2	1:C:618:ALA:O	1.85	0.75
1:C:555:SER:HB2	1:C:616:LEU:HD11	1.69	0.75
2:H:140:ILE:HG22	2:H:146:ILE:HG21	1.68	0.75
1:B:555:SER:CB	1:B:616:LEU:CD1	2.61	0.75
1:D:40:GLN:O	1:D:44:ARG:HG2	1.84	0.75
2:G:157:TYR:O	2:G:161:ILE:HG13	1.87	0.75
1:A:119:LEU:HD21	1:A:179:CYS:SG	2.27	0.75
2:E:147:GLN:HE21	2:E:147:GLN:CA	1.99	0.75
2:F:5:PHE:CE1	2:F:24:ASN:O	2.38	0.75
1:B:208:PRO:C	1:B:210:PRO:HD2	2.11	0.75
2:H:82:LEU:HD22	2:H:146:ILE:CG2	2.17	0.75
2:F:174:THR:CG2	2:F:181:THR:CG2	2.64	0.75
2:F:221:ARG:NH1	2:F:296:MET:CG	2.49	0.75
2:G:79:TYR:HE1	2:G:149:ARG:HD3	1.44	0.75
1:C:323:ARG:HB3	1:C:323:ARG:HH11	1.51	0.75
1:C:519:ASN:HD21	1:C:522:TYR:HD2	1.34	0.75
1:D:623:GLU:O	1:D:627:GLN:HG3	1.87	0.75
2:F:175:HIS:HD2	2:G:178:ASN:HD21	1.33	0.75
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.66	0.75
1:D:516:GLY:HA2	1:D:618:ALA:O	1.84	0.75
2:F:5:PHE:HE1	2:F:24:ASN:O	1.67	0.75
1:D:708:LYS:HE2	2:G:362:ASP:CA	2.17	0.75
2:G:245:THR:HA	2:G:248:MET:HE3	1.67	0.75
1:B:78:GLN:OE1	1:B:655:VAL:HB	1.87	0.75
2:H:59:ARG:HB2	2:H:128:ASN:O	1.86	0.74
1:C:413:TYR:HE1	1:C:731:TYR:CD1	2.05	0.74
2:E:148:LYS:HG2	2:E:149:ARG:N	2.03	0.74
2:E:155:SER:O	2:E:159:GLU:HG3	1.87	0.74
2:F:99:ILE:HD11	2:F:108:VAL:HG21	1.69	0.74
1:A:233:SER:O	1:A:237:ILE:HG13	1.87	0.74
1:D:444:LEU:HD22	1:D:512:THR:HG21	1.67	0.74
1:A:106:VAL:O	1:A:110:VAL:HG23	1.87	0.74
1:B:426:PHE:CE2	1:B:445:PRO:HD3	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:99:ILE:HD11	2:E:108:VAL:HG21	1.69	0.74
2:F:86:ILE:HG21	2:F:153:ILE:CG2	2.17	0.74
1:C:40:GLN:OE1	1:C:44:ARG:HG3	1.88	0.74
1:D:329:ARG:HH11	1:D:329:ARG:CG	2.00	0.74
2:H:99:ILE:HD11	2:H:108:VAL:HG21	1.69	0.74
2:F:74:ILE:HG13	2:F:78:LYS:HE3	1.68	0.74
2:H:74:ILE:HG13	2:H:78:LYS:HE3	1.69	0.74
1:A:423:HIS:O	1:A:423:HIS:CG	2.38	0.74
1:A:689:ILE:CG2	1:A:691:GLN:O	2.36	0.74
1:A:152:GLU:HA	1:A:156:LEU:HD12	1.67	0.74
1:A:646:ALA:CA	1:A:651:ILE:HA	2.08	0.74
2:E:245:THR:HA	2:E:248:MET:HE3	1.70	0.74
2:F:49:ARG:O	2:F:52:GLU:CG	2.36	0.74
2:F:207:ARG:HG2	2:F:207:ARG:HH11	1.52	0.74
1:A:226:VAL:HG11	1:A:459:ILE:HG21	1.68	0.74
1:A:426:PHE:HB3	1:A:431:ALA:O	1.87	0.74
1:A:519:ASN:HD21	1:A:522:TYR:HD2	1.34	0.74
1:D:519:ASN:HD21	1:D:522:TYR:HD2	1.34	0.74
2:F:125:ILE:HG21	2:F:227:ASN:HD22	1.51	0.74
2:G:206:ILE:O	2:G:210:VAL:HG23	1.88	0.74
2:G:70:LYS:O	2:G:74:ILE:HG22	1.88	0.73
1:B:467:PHE:CE2	1:B:515:ILE:HG21	2.23	0.73
2:F:219:ALA:HB1	2:F:338:TRP:CH2	2.24	0.73
2:H:148:LYS:HG2	2:H:149:ARG:N	2.03	0.73
1:B:466:ALA:HB1	1:B:518:ILE:HG23	1.70	0.73
1:B:551:LEU:HD13	1:B:616:LEU:O	1.88	0.73
1:B:669:LEU:HD11	1:B:698:ASN:ND2	2.02	0.73
1:A:42:GLU:OE1	2:F:298:GLY:HA2	1.88	0.73
2:E:170:LEU:HD21	2:H:177:VAL:HG11	1.70	0.73
1:D:207:LEU:HB2	1:D:212:MET:HE3	1.70	0.73
1:C:322:ASN:HA	1:C:331:ARG:HE	1.53	0.73
1:D:18:ASN:ND2	1:D:20:ASP:H	1.85	0.73
1:D:708:LYS:HE3	2:G:361:ILE:C	2.13	0.73
2:G:95:LEU:HD12	2:G:108:VAL:CG2	2.18	0.73
2:G:99:ILE:HD11	2:G:108:VAL:HG21	1.68	0.73
1:B:542:LYS:HG3	1:B:596:HIS:CD2	2.24	0.73
1:D:23:HIS:CE1	1:D:42:GLU:OE2	2.41	0.73
1:D:519:ASN:HB2	1:D:631:ALA:HB1	1.69	0.73
2:E:95:LEU:O	2:E:99:ILE:HG13	1.89	0.73
2:G:297:ILE:H	2:G:297:ILE:CD1	2.01	0.73
1:C:519:ASN:HB2	1:C:631:ALA:HB1	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:622:SER:CB	4:D:802:DAT:O1A	2.30	0.73
2:H:300:ASN:CG	2:H:303:ILE:HG12	2.14	0.73
1:A:226:VAL:HG13	1:A:461:LEU:HD21	1.69	0.73
1:B:551:LEU:O	1:B:616:LEU:HD12	1.88	0.73
1:C:297:VAL:O	1:C:297:VAL:HG13	1.89	0.73
2:F:177:VAL:HG12	2:F:178:ASN:ND2	2.04	0.72
1:B:542:LYS:CG	1:B:596:HIS:NE2	2.51	0.72
2:G:82:LEU:HD22	2:G:146:ILE:CG2	2.16	0.72
1:D:18:ASN:HD22	1:D:20:ASP:N	1.88	0.72
2:G:300:ASN:HB3	2:G:303:ILE:H	1.53	0.72
1:A:559:ALA:O	1:A:563:GLY:N	2.22	0.72
1:B:423:HIS:HE1	1:B:579:PRO:HB3	1.54	0.72
2:G:163:MET:HE1	2:G:188:GLU:HB2	1.70	0.72
1:D:425:PRO:HG3	1:D:690:ASP:HB3	1.71	0.72
2:E:297:ILE:HD12	2:E:297:ILE:N	2.01	0.72
2:H:291:PHE:CZ	2:H:299:LEU:HG	2.24	0.72
1:C:730:TYR:CE2	1:C:731:TYR:CE2	2.78	0.72
2:G:62:TYR:CZ	2:G:70:LYS:HG2	2.23	0.72
1:A:89:LEU:HD21	1:A:152:GLU:HG3	1.72	0.72
1:B:5:LEU:HD13	1:B:51:ASP:N	2.05	0.72
1:C:118:HIS:CE1	1:C:119:LEU:HD23	2.24	0.72
1:D:19:LEU:HD12	2:G:295:SER:C	2.15	0.72
1:D:53:ILE:CG1	1:D:58:ILE:HD11	2.20	0.72
1:C:225:CYS:SG	1:C:462:CYS:HB3	2.29	0.72
1:C:323:ARG:HB3	1:C:323:ARG:NH1	2.05	0.72
1:C:711:MET:HB3	2:E:364:GLU:O	1.89	0.72
2:E:221:ARG:HH11	2:E:296:MET:HG3	1.55	0.72
2:H:190:LYS:HB3	2:H:261:MET:SD	2.28	0.72
1:A:324:GLY:HA3	1:A:329:ARG:CZ	2.19	0.72
1:B:517:VAL:HG11	1:B:547:ILE:HD13	1.70	0.72
1:D:689:ILE:HG22	1:D:691:GLN:O	1.90	0.72
2:F:10:ASN:HD22	2:F:15:GLU:HG3	1.55	0.72
2:G:95:LEU:HD12	2:G:108:VAL:HG22	1.70	0.72
1:B:175:LEU:HD12	1:B:216:ARG:HD2	1.71	0.71
1:A:242:SER:O	1:A:246:LYS:HG2	1.91	0.71
2:G:291:PHE:O	2:G:293:ASP:N	2.22	0.71
2:H:299:LEU:HD12	2:H:300:ASN:N	2.05	0.71
1:A:53:ILE:CG1	1:A:58:ILE:HD11	2.20	0.71
1:D:323:ARG:HB3	1:D:323:ARG:NH1	2.04	0.71
2:E:149:ARG:HH21	2:E:286:TRP:HB2	1.50	0.71
2:F:339:LEU:O	2:F:340:VAL:CB	2.37	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:803:DTP:H5'1	3:B:803:DTP:H8	1.73	0.71
1:C:44:ARG:HA	1:C:44:ARG:HE	1.54	0.71
1:C:109:MET:HE1	1:C:166:TYR:HB3	1.73	0.71
2:G:242:LEU:O	2:G:246:GLN:HG3	1.91	0.71
1:A:685:MET:O	1:A:689:ILE:HG12	1.90	0.71
1:C:23:HIS:CD2	1:C:42:GLU:OE2	2.43	0.71
1:D:25:VAL:HG11	1:D:59:HIS:HE1	1.55	0.71
2:E:145:GLN:H	2:E:145:GLN:HE21	1.35	0.71
2:H:207:ARG:HH22	2:H:282:GLN:NE2	1.88	0.71
1:B:175:LEU:HD13	1:B:216:ARG:HD2	1.71	0.71
1:B:212:MET:HA	1:B:212:MET:HE2	1.73	0.71
1:C:55:THR:HG21	3:C:801:DTP:O3A	1.91	0.71
2:E:66:PRO:CB	2:E:68:HIS:CD2	2.73	0.71
1:D:53:ILE:HD11	1:D:58:ILE:HD11	0.78	0.71
2:G:102:PRO:HD2	2:G:103:GLU:OE1	1.91	0.71
2:G:147:GLN:HA	2:G:147:GLN:NE2	2.05	0.71
1:A:619:LEU:CB	1:A:693:ILE:HG23	2.21	0.71
1:D:435:GLN:NE2	1:D:446:THR:HG21	2.06	0.71
2:H:73:PHE:CZ	2:H:224:MET:HE3	2.24	0.71
1:B:444:LEU:CD2	1:B:512:THR:HG21	2.15	0.71
1:C:697:THR:OG1	1:C:732:GLN:HG2	1.91	0.71
1:D:297:VAL:O	1:D:297:VAL:HG13	1.90	0.71
1:A:297:VAL:HG12	1:A:298:ARG:HG2	0.76	0.70
1:C:340:ASN:OD1	1:C:368:PHE:HE1	1.73	0.70
1:D:9:LYS:HE3	1:D:15:GLU:CD	2.15	0.70
1:D:19:LEU:HD11	2:G:296:MET:HA	1.73	0.70
1:D:40:GLN:OE1	1:D:44:ARG:HG3	1.91	0.70
2:F:245:THR:HA	2:F:248:MET:HE3	1.73	0.70
2:G:149:ARG:HH21	2:G:286:TRP:CB	2.02	0.70
2:H:123:THR:O	2:H:127:ARG:HG2	1.91	0.70
2:H:300:ASN:CG	2:H:303:ILE:CG1	2.64	0.70
2:G:207:ARG:HH22	2:G:282:GLN:NE2	1.89	0.70
2:H:10:ASN:HD22	2:H:15:GLU:HG3	1.56	0.70
2:H:95:LEU:O	2:H:99:ILE:HG13	1.91	0.70
1:B:206:SER:HB3	1:B:466:ALA:HB3	1.72	0.70
2:G:149:ARG:NH2	2:G:286:TRP:CG	2.59	0.70
1:A:53:ILE:HD12	1:A:58:ILE:CG1	2.21	0.70
2:E:300:ASN:H	2:E:303:ILE:CG2	2.02	0.70
2:F:206:ILE:O	2:F:210:VAL:HG23	1.92	0.70
2:F:12:GLN:NE2	2:F:25:VAL:HG13	2.06	0.70
1:A:305:PHE:CE2	1:A:436:SER:HB3	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ALA:HB1	1:A:662:LEU:HD13	1.73	0.70
1:D:212:MET:HE2	1:D:212:MET:HA	1.74	0.70
2:F:218:PHE:CE1	2:F:296:MET:SD	2.84	0.70
1:B:466:ALA:CA	1:B:516:GLY:O	2.36	0.70
2:F:219:ALA:HB1	2:F:338:TRP:CZ2	2.27	0.70
2:E:82:LEU:HD22	2:E:146:ILE:HG23	1.74	0.70
1:A:226:VAL:CG1	1:A:459:ILE:HG21	2.22	0.69
1:B:559:ALA:O	1:B:563:GLY:N	2.24	0.69
1:D:283:LYS:HG2	1:D:330:VAL:CG2	2.22	0.69
2:E:297:ILE:H	2:E:297:ILE:CD1	1.98	0.69
1:B:155:TYR:HE2	1:B:628:ILE:CG1	2.05	0.69
1:D:109:MET:HE1	1:D:166:TYR:HB3	1.75	0.69
2:E:10:ASN:HD22	2:E:15:GLU:HG3	1.57	0.69
2:F:339:LEU:O	2:F:340:VAL:HB	1.92	0.69
1:C:78:GLN:NE2	1:C:655:VAL:HB	2.06	0.69
2:G:10:ASN:HD22	2:G:15:GLU:HG3	1.55	0.69
1:B:423:HIS:CE1	1:B:579:PRO:HB3	2.27	0.69
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.27	0.69
1:B:340:ASN:CG	1:B:368:PHE:HE1	2.00	0.69
1:B:669:LEU:HD11	1:B:698:ASN:CG	2.17	0.69
1:C:442:ILE:HD12	1:C:462:CYS:SG	2.33	0.69
1:B:521:ALA:HB3	1:B:632:THR:HG21	1.73	0.69
1:A:35:ASN:HD22	1:A:74:ALA:CB	2.02	0.69
1:B:225:CYS:SG	1:B:462:CYS:HB3	2.33	0.69
1:B:551:LEU:C	1:B:616:LEU:HD12	2.17	0.69
2:F:12:GLN:HE22	2:F:25:VAL:HG13	1.58	0.69
2:F:129:ILE:HG13	2:F:130:VAL:HG13	1.75	0.69
2:G:360:GLN:O	2:G:361:ILE:HG23	1.92	0.69
1:B:568:PHE:CE2	1:B:574:ALA:HB2	2.28	0.69
1:D:18:ASN:HD22	1:D:20:ASP:H	1.41	0.69
1:B:156:LEU:CD1	1:B:167:GLU:O	2.41	0.69
1:B:23:HIS:ND1	1:B:42:GLU:OE2	2.26	0.68
1:C:176:VAL:HG22	1:C:215:VAL:HB	1.75	0.68
1:C:439:CYS:HB2	1:C:441:GLU:OE1	1.94	0.68
1:D:708:LYS:HE2	2:G:362:ASP:N	2.08	0.68
1:A:59:HIS:CD2	1:A:88:HIS:HB2	2.28	0.68
1:B:419:HIS:HA	1:B:422:THR:HG1	1.58	0.68
2:E:313:ASN:HB3	2:E:323:LEU:HD22	1.75	0.68
2:H:245:THR:HA	2:H:248:MET:HE3	1.74	0.68
1:A:53:ILE:HG13	1:A:53:ILE:O	1.92	0.68
2:F:174:THR:CG2	2:F:181:THR:HG23	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:244:GLY:O	2:G:248:MET:HG3	1.94	0.68
1:A:521:ALA:HB3	1:A:632:THR:HG21	1.75	0.68
1:A:627:GLN:HE22	1:A:645:LYS:HE2	1.58	0.68
1:C:254:ILE:HB	1:C:302:ALA:HB2	1.76	0.68
1:B:670:TRP:HA	1:B:670:TRP:CE3	2.29	0.68
1:C:292:CYS:HA	1:D:276:THR:HG21	1.75	0.68
1:D:208:PRO:HG3	1:D:464:LEU:HB2	1.76	0.68
1:D:279:ILE:HG21	1:D:328:ASN:HA	1.73	0.68
2:G:296:MET:CE	2:G:299:LEU:HD23	2.24	0.68
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.75	0.68
1:B:617:SER:O	1:B:691:GLN:HG3	1.93	0.68
1:C:368:PHE:CD2	1:C:417:VAL:HG21	2.28	0.68
1:A:560:LYS:HG2	1:A:609:HIS:CD2	2.29	0.68
1:C:175:LEU:HD12	1:C:216:ARG:HD2	1.76	0.68
1:D:282:TYR:O	1:D:333:MET:HE1	1.93	0.68
2:F:5:PHE:CD2	2:G:150:ALA:HB1	2.29	0.68
1:C:365:TYR:HE2	1:C:434:ARG:HH21	1.41	0.67
1:C:623:GLU:O	1:C:627:GLN:HG3	1.93	0.67
1:D:525:ALA:HB1	1:D:662:LEU:HD13	1.76	0.67
2:G:149:ARG:HH21	2:G:286:TRP:HB2	1.51	0.67
2:H:145:GLN:NE2	2:H:145:GLN:H	1.92	0.67
2:H:291:PHE:HZ	2:H:299:LEU:HG	1.57	0.67
1:A:258:ALA:HB1	1:A:261:ILE:HD12	1.75	0.67
1:B:44:ARG:HA	1:B:44:ARG:HE	1.58	0.67
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.74	0.67
1:B:525:ALA:HB1	1:B:662:LEU:HD13	1.76	0.67
2:F:221:ARG:HH11	2:F:296:MET:CG	2.07	0.67
2:G:55:VAL:HG23	2:G:128:ASN:ND2	2.09	0.67
2:G:62:TYR:CZ	2:G:70:LYS:HD3	2.29	0.67
2:H:206:ILE:O	2:H:210:VAL:HG23	1.94	0.67
1:A:441:GLU:HA	1:A:692:SER:O	1.94	0.67
1:B:54:LYS:HB2	1:B:57:ASP:OD2	1.95	0.67
1:D:39:SER:HA	1:D:42:GLU:CD	2.18	0.67
2:F:313:ASN:HB3	2:F:323:LEU:HD22	1.77	0.67
1:A:325:VAL:O	1:A:327:GLY:N	2.27	0.67
1:A:369:PHE:CG	1:A:434:ARG:HG2	2.29	0.67
1:B:289:VAL:HG12	1:B:300:GLY:C	2.18	0.67
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.75	0.67
2:F:339:LEU:O	2:F:340:VAL:CG2	2.42	0.67
1:A:328:ASN:H	1:A:328:ASN:HD22	1.42	0.67
1:D:185:PRO:HG2	1:D:188:THR:OG1	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:ND2	1:C:20:ASP:H	1.92	0.67
1:D:320:LYS:HB3	1:D:409:THR:HG21	1.77	0.67
1:D:248:VAL:HG11	1:D:289:VAL:HA	1.76	0.67
1:D:365:TYR:HE2	1:D:434:ARG:HH21	1.41	0.67
1:B:119:LEU:HD21	1:B:179:CYS:SG	2.35	0.67
1:B:622:SER:HB2	1:B:625:SER:HG	1.57	0.67
2:F:205:ALA:HB1	2:F:315:ARG:HD2	1.77	0.67
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.76	0.67
1:B:576:GLY:HA3	1:B:607:LYS:NZ	2.09	0.67
1:D:7:VAL:HG23	1:D:15:GLU:HG3	1.77	0.67
1:D:474:ASN:HD21	1:D:477:GLU:HG3	1.58	0.67
2:H:157:TYR:O	2:H:161:ILE:HG13	1.95	0.67
1:A:517:VAL:HG22	1:A:619:LEU:HD22	1.77	0.67
2:F:309:GLU:CB	2:F:328:ARG:NH1	2.58	0.67
2:G:205:ALA:HB1	2:G:315:ARG:HD2	1.76	0.67
1:A:325:VAL:O	1:A:326:GLU:C	2.38	0.66
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.77	0.66
1:C:340:ASN:CG	1:C:368:PHE:CE1	2.73	0.66
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.77	0.66
1:B:551:LEU:O	1:B:616:LEU:CD1	2.43	0.66
1:C:151:LEU:CD2	1:C:155:TYR:CD2	2.71	0.66
1:A:542:LYS:HE2	1:A:596:HIS:NE2	2.10	0.66
1:A:623:GLU:O	1:A:627:GLN:HG3	1.95	0.66
2:H:205:ALA:HB1	2:H:315:ARG:HD2	1.77	0.66
1:A:242:SER:OG	1:B:238:ASN:HB3	1.95	0.66
1:A:226:VAL:HG21	1:A:247:TYR:CE2	2.30	0.66
2:G:313:ASN:HB3	2:G:323:LEU:HD22	1.77	0.66
1:C:18:ASN:ND2	1:C:20:ASP:HB2	2.09	0.66
2:E:127:ARG:HH21	2:H:29:ASP:HA	1.61	0.66
1:C:38:ILE:HD13	1:C:38:ILE:N	2.10	0.66
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.78	0.66
1:C:208:PRO:HG3	1:C:464:LEU:HB2	1.77	0.66
1:C:248:VAL:HG11	1:C:289:VAL:HA	1.77	0.66
1:A:360:ASP:O	1:A:362:PRO:HD3	1.96	0.66
2:F:149:ARG:O	2:F:153:ILE:HG12	1.95	0.66
1:C:369:PHE:O	1:C:421:ASN:CG	2.39	0.66
2:H:87:GLN:O	2:H:91:PRO:CD	2.43	0.66
2:H:313:ASN:HB3	2:H:323:LEU:HD22	1.78	0.66
1:A:419:HIS:CA	1:A:422:THR:OG1	2.41	0.66
1:A:670:TRP:HA	1:A:670:TRP:CE3	2.30	0.66
1:B:444:LEU:CD2	1:B:691:GLN:HE22	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:HE2	1:C:411:ARG:HG3	1.77	0.66
1:B:617:SER:O	1:B:691:GLN:CG	2.44	0.65
1:C:413:TYR:CE1	1:C:731:TYR:CE1	2.83	0.65
2:G:296:MET:HE2	2:G:299:LEU:HD23	1.78	0.65
1:B:519:ASN:CB	1:B:631:ALA:HB1	2.26	0.65
2:F:177:VAL:HG22	2:G:177:VAL:HG22	1.78	0.65
1:C:19:LEU:HD12	2:E:295:SER:O	1.95	0.65
1:C:72:ARG:NH1	1:C:641:TYR:CE2	2.63	0.65
2:H:83:LEU:HD22	2:H:203:LEU:HD11	1.77	0.65
2:H:86:ILE:HG21	2:H:153:ILE:CG2	2.27	0.65
1:A:464:LEU:HB3	1:A:620:MET:HE2	1.78	0.65
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.78	0.65
1:D:320:LYS:CE	1:D:411:ARG:CB	2.71	0.65
2:E:205:ALA:HB1	2:E:315:ARG:CD	2.24	0.65
2:F:145:GLN:H	2:F:145:GLN:HE21	1.45	0.65
1:A:297:VAL:HG12	1:A:298:ARG:CB	2.24	0.65
1:B:5:LEU:HD22	1:B:51:ASP:HB3	1.74	0.65
1:B:228:ILE:N	1:B:435:GLN:HE22	1.94	0.65
2:F:9:LYS:HA	2:G:141:VAL:HG11	1.79	0.65
2:F:55:VAL:HG23	2:F:128:ASN:ND2	2.11	0.65
2:F:207:ARG:HH22	2:F:282:GLN:HE21	1.43	0.65
1:A:379:TYR:O	1:A:383:GLU:HG3	1.96	0.65
1:C:262:ARG:HA	1:C:358:PRO:HG2	1.76	0.65
2:F:86:ILE:HG21	2:F:153:ILE:HG21	1.76	0.65
2:H:208:PHE:CE2	7:H:602:HOH:O	2.50	0.65
1:A:519:ASN:CB	1:A:631:ALA:HB1	2.26	0.65
1:B:151:LEU:HA	1:B:155:TYR:CB	2.06	0.65
1:B:293:SER:HB3	1:B:298:ARG:O	1.97	0.65
1:B:328:ASN:HD22	1:B:328:ASN:H	1.43	0.65
1:B:356:PHE:CZ	1:B:390:LYS:HE3	2.32	0.65
1:C:9:LYS:NZ	3:C:801:DTP:N7	2.44	0.65
1:C:551:LEU:O	1:C:616:LEU:HD13	1.95	0.65
1:C:690:ASP:C	1:C:691:GLN:HE21	2.05	0.65
1:D:521:ALA:HB3	1:D:632:THR:HG21	1.79	0.65
1:D:635:ILE:HD12	1:D:685:MET:HE1	1.79	0.65
1:C:206:SER:OG	1:C:625:SER:HB2	1.97	0.65
2:F:203:LEU:HA	2:F:207:ARG:HB2	1.78	0.65
2:G:49:ARG:O	2:G:52:GLU:CG	2.41	0.65
2:G:145:GLN:HB3	2:G:286:TRP:CZ3	2.31	0.65
1:A:369:PHE:CD2	1:A:434:ARG:CG	2.80	0.65
1:C:635:ILE:HD12	1:C:685:MET:HE1	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ILE:HB	1:D:302:ALA:HB2	1.79	0.65
2:E:206:ILE:O	2:E:210:VAL:HG23	1.97	0.65
2:H:300:ASN:H	2:H:303:ILE:HB	1.62	0.65
1:B:685:MET:O	1:B:689:ILE:HG12	1.97	0.65
1:B:558:LEU:CD2	1:B:612:ARG:HG2	2.27	0.64
1:C:177:ALA:CB	1:C:196:PHE:HD2	2.10	0.64
1:D:439:CYS:HB2	1:D:441:GLU:OE1	1.96	0.64
1:B:217:THR:HG22	1:B:219:THR:HG22	1.78	0.64
1:B:670:TRP:HA	1:B:670:TRP:HE3	1.63	0.64
1:C:469:LEU:HA	1:C:472:ILE:CD1	2.24	0.64
2:G:163:MET:HB3	2:G:189:LEU:HD13	1.77	0.64
1:A:212:MET:HE2	1:A:212:MET:HA	1.79	0.64
1:C:360:ASP:O	1:C:362:PRO:HD3	1.98	0.64
1:C:669:LEU:HD12	1:C:672:MET:CE	2.27	0.64
1:D:149:LYS:HG2	1:D:652:LEU:HD21	1.78	0.64
2:E:170:LEU:CD2	2:H:177:VAL:HG11	2.28	0.64
2:E:260:GLU:CA	2:E:263:GLU:OE2	2.39	0.64
1:B:209:THR:N	1:B:210:PRO:CD	2.61	0.64
1:C:290:LYS:HZ1	1:C:332:HIS:HB3	1.60	0.64
1:D:510:ARG:NH1	1:D:567:TRP:CZ3	2.66	0.64
1:B:202:THR:OG1	1:B:204:LYS:HD3	1.97	0.64
1:D:262:ARG:HA	1:D:358:PRO:HG2	1.78	0.64
2:F:207:ARG:NH2	2:F:282:GLN:NE2	2.42	0.64
1:B:360:ASP:O	1:B:362:PRO:HD3	1.97	0.64
1:B:552:LEU:HA	1:B:616:LEU:HD12	1.80	0.64
1:D:155:TYR:OH	1:D:624:THR:HG22	1.96	0.64
2:F:3:THR:HA	2:G:158:ASP:OD1	1.98	0.64
2:G:62:TYR:CD1	2:G:65:LEU:HD12	2.33	0.64
2:G:72:ILE:CD1	2:G:296:MET:HG2	2.28	0.64
1:A:69:LEU:O	1:A:70:ILE:C	2.40	0.64
1:A:592:ASN:H	1:A:592:ASN:HD22	1.44	0.64
1:B:444:LEU:HD21	1:B:691:GLN:HE22	1.63	0.64
1:A:419:HIS:HA	1:A:422:THR:HG1	1.63	0.64
1:A:444:LEU:CD2	1:A:691:GLN:HE22	2.11	0.64
1:C:290:LYS:HZ2	1:C:332:HIS:HB3	1.60	0.64
1:D:385:ASP:OD1	1:D:388:ILE:HG12	1.97	0.64
2:E:66:PRO:HD2	2:E:69:GLU:CD	2.22	0.64
2:F:175:HIS:CD2	2:G:178:ASN:ND2	2.57	0.64
2:G:214:CYS:HA	2:G:299:LEU:HD21	1.80	0.64
1:B:78:GLN:OE1	1:B:655:VAL:CB	2.45	0.64
1:B:506:GLY:HA2	1:B:567:TRP:CZ3	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PRO:CG	1:D:464:LEU:HB2	2.28	0.64
1:D:555:SER:HB2	1:D:616:LEU:CD1	2.26	0.64
2:F:61:ASP:O	2:F:65:LEU:HG	1.98	0.64
1:B:360:ASP:HB3	1:B:388:ILE:HG23	1.80	0.64
1:B:619:LEU:HD12	1:B:693:ILE:CG1	2.28	0.64
1:C:413:TYR:OH	1:C:731:TYR:CE1	2.31	0.64
2:E:165:SER:CB	2:H:169:LEU:HD11	2.28	0.64
2:F:153:ILE:HD12	2:F:203:LEU:CD1	2.22	0.64
1:A:37:SER:HB2	2:F:331:PRO:O	1.98	0.63
1:A:75:PRO:O	1:A:77:TYR:N	2.32	0.63
1:A:576:GLY:HA3	1:A:607:LYS:NZ	2.13	0.63
1:B:368:PHE:CE2	1:B:417:VAL:HG21	2.33	0.63
1:B:669:LEU:HD12	1:B:672:MET:CE	2.27	0.63
1:D:154:LYS:HD3	1:D:209:THR:CG2	2.28	0.63
1:D:669:LEU:HD12	1:D:672:MET:CE	2.28	0.63
2:E:116:THR:O	2:E:120:ARG:HG3	1.98	0.63
2:F:82:LEU:CD1	2:G:5:PHE:CZ	2.80	0.63
2:G:149:ARG:CZ	2:G:286:TRP:CE3	2.80	0.63
1:A:149:LYS:HG2	1:A:652:LEU:HD21	1.79	0.63
1:A:461:LEU:HD11	1:A:503:ALA:HB1	1.80	0.63
1:B:40:GLN:O	1:B:44:ARG:HG2	1.97	0.63
1:B:151:LEU:HD23	1:B:155:TYR:CG	2.32	0.63
1:C:117:ASN:HD21	1:C:120:LEU:HD12	1.60	0.63
1:C:592:ASN:H	1:C:592:ASN:HD22	1.46	0.63
2:E:208:PHE:CE2	7:E:601:HOH:O	2.50	0.63
2:H:221:ARG:HB3	2:H:223:LEU:HD12	1.80	0.63
1:A:529:LYS:HB3	1:A:536:ALA:HB2	1.80	0.63
1:B:151:LEU:HD23	1:B:155:TYR:HB3	1.81	0.63
1:B:152:GLU:O	1:B:158:GLN:NE2	2.31	0.63
1:C:552:LEU:HA	1:C:616:LEU:HD12	1.80	0.63
1:D:80:LEU:HD12	1:D:80:LEU:O	1.99	0.63
2:F:339:LEU:C	2:F:340:VAL:HG23	2.23	0.63
2:G:72:ILE:HD12	2:G:296:MET:HG2	1.81	0.63
2:G:129:ILE:HG13	2:G:130:VAL:HG13	1.80	0.63
1:A:109:MET:HE1	1:A:166:TYR:HB3	1.80	0.63
1:B:305:PHE:CE2	1:B:436:SER:HB3	2.33	0.63
1:C:379:TYR:O	1:C:383:GLU:HG3	1.98	0.63
1:C:428:PRO:HA	1:C:432:PRO:HB3	1.80	0.63
1:D:18:ASN:ND2	1:D:20:ASP:HB2	2.10	0.63
2:E:129:ILE:HG13	2:E:130:VAL:HG13	1.81	0.63
1:A:214:GLY:O	1:A:217:THR:CG2	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:442:ILE:CA	1:D:691:GLN:OE1	2.36	0.63
1:A:572:THR:HB	1:A:577:ILE:HB	1.81	0.63
1:B:379:TYR:O	1:B:383:GLU:HG3	1.99	0.63
1:C:385:ASP:OD1	1:C:388:ILE:HG12	1.98	0.63
1:C:464:LEU:HB3	1:C:620:MET:HE3	1.80	0.63
1:D:155:TYR:HE2	1:D:628:ILE:HG13	1.62	0.63
1:D:640:GLY:HA2	1:D:668:LEU:HD22	1.80	0.63
1:D:658:ASP:O	1:D:662:LEU:HB2	1.99	0.63
2:E:61:ASP:O	2:E:65:LEU:HG	1.98	0.63
2:G:149:ARG:HH21	2:G:286:TRP:CG	2.17	0.63
1:B:529:LYS:HB3	1:B:536:ALA:HB2	1.80	0.63
1:B:592:ASN:HD22	1:B:592:ASN:H	1.45	0.63
1:C:444:LEU:HD22	1:C:512:THR:HG21	1.80	0.63
2:G:62:TYR:CE1	2:G:70:LYS:CG	2.76	0.63
1:B:5:LEU:HD13	1:B:51:ASP:H	1.64	0.63
1:B:613:ASN:HB2	1:B:616:LEU:CD2	2.29	0.63
2:E:149:ARG:NH1	2:E:286:TRP:HE3	1.96	0.63
2:E:191:LYS:HG2	2:E:264:ILE:HG23	1.81	0.63
2:F:300:ASN:H	2:F:303:ILE:CG2	2.12	0.63
2:G:53:VAL:HG11	2:G:230:ILE:HG13	1.81	0.63
2:H:203:LEU:HD23	2:H:203:LEU:C	2.23	0.63
1:A:532:SER:HB3	1:A:673:PRO:HD2	1.80	0.62
1:B:489:LEU:HD13	1:B:513:LEU:HD11	1.76	0.62
1:C:151:LEU:HD23	1:C:155:TYR:CG	2.33	0.62
1:D:40:GLN:HE22	1:D:44:ARG:HH11	1.46	0.62
1:A:214:GLY:O	1:A:217:THR:N	2.30	0.62
1:B:157:VAL:HG23	1:B:167:GLU:OE2	1.99	0.62
1:B:532:SER:HB3	1:B:673:PRO:HD2	1.81	0.62
1:C:55:THR:HG23	3:C:801:DTP:H5'1	1.81	0.62
1:C:637:PRO:HG2	1:C:669:LEU:HD13	1.80	0.62
1:D:428:PRO:HA	1:D:432:PRO:HB3	1.80	0.62
2:F:147:GLN:NE2	2:G:7:GLN:OE1	2.33	0.62
2:H:73:PHE:CD2	2:H:224:MET:HE2	2.34	0.62
1:A:428:PRO:HA	1:A:432:PRO:HB3	1.80	0.62
1:B:97:PHE:O	1:B:99:PRO:HD3	1.99	0.62
1:C:340:ASN:OD1	1:C:368:PHE:CE1	2.52	0.62
1:C:697:THR:CG2	1:C:732:GLN:HG3	2.29	0.62
1:D:154:LYS:HD3	1:D:209:THR:HG21	1.81	0.62
2:F:101:ILE:HB	2:F:103:GLU:OE1	2.00	0.62
2:G:217:ALA:CB	2:G:299:LEU:HD21	2.28	0.62
2:F:336:ASN:HD22	2:F:336:ASN:N	1.97	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:HD22	1:C:20:ASP:H	1.47	0.62
1:C:293:SER:HB3	1:C:298:ARG:O	1.99	0.62
1:C:406:ARG:HH21	1:C:697:THR:CG2	2.12	0.62
1:C:697:THR:OG1	1:C:732:GLN:HG3	1.97	0.62
1:D:189:ARG:O	1:D:193:VAL:HG23	2.00	0.62
1:D:474:ASN:H	1:D:474:ASN:HD22	1.46	0.62
2:E:55:VAL:HG23	2:E:128:ASN:ND2	2.14	0.62
2:G:145:GLN:HB3	2:G:286:TRP:HZ3	1.63	0.62
1:D:37:SER:HB3	1:D:40:GLN:HB2	1.82	0.62
1:D:689:ILE:CG2	1:D:691:GLN:O	2.47	0.62
2:E:53:VAL:HG11	2:E:230:ILE:HG13	1.81	0.62
2:E:258:ASP:CG	2:E:261:MET:HG2	2.24	0.62
2:H:129:ILE:HG13	2:H:130:VAL:HG13	1.81	0.62
1:A:360:ASP:HB3	1:A:388:ILE:HG23	1.81	0.62
1:B:109:MET:HE1	1:B:166:TYR:HB3	1.81	0.62
1:B:115:TYR:CD1	1:B:216:ARG:HG3	2.35	0.62
1:C:30:ALA:HA	1:C:33:LEU:HD12	1.82	0.62
1:C:435:GLN:NE2	1:C:446:THR:HG21	2.13	0.62
2:G:163:MET:HE1	2:G:188:GLU:CB	2.30	0.62
1:A:202:THR:OG1	1:A:204:LYS:HD3	2.00	0.62
1:B:464:LEU:HB3	1:B:620:MET:HE2	1.82	0.62
1:C:529:LYS:HB3	1:C:536:ALA:HB2	1.81	0.62
1:C:26:LEU:HD21	1:C:62:ILE:HD12	1.81	0.62
1:D:298:ARG:O	1:D:299:GLY:O	2.18	0.62
2:F:209:TYR:HA	2:F:212:PHE:HD2	1.65	0.62
2:G:292:ARG:HG3	2:G:293:ASP:N	2.14	0.62
1:A:279:ILE:HG21	1:A:328:ASN:HA	1.82	0.62
1:A:369:PHE:CE2	1:A:434:ARG:HG2	2.34	0.62
1:C:328:ASN:HD22	1:C:328:ASN:H	1.47	0.62
1:C:465:SER:O	1:C:620:MET:HE1	2.00	0.62
1:D:18:ASN:ND2	1:D:20:ASP:N	2.45	0.62
1:D:330:VAL:HG11	1:D:333:MET:CE	2.29	0.62
2:H:190:LYS:HD3	2:H:261:MET:SD	2.40	0.62
1:A:209:THR:N	1:A:210:PRO:HD2	2.14	0.61
1:A:555:SER:CB	1:A:616:LEU:HD11	2.31	0.61
1:A:555:SER:HB3	1:A:616:LEU:HD11	1.81	0.61
1:B:340:ASN:HB3	1:B:368:PHE:CE1	2.35	0.61
2:H:209:TYR:HA	2:H:212:PHE:HD2	1.65	0.61
1:A:9:LYS:HE3	1:A:15:GLU:OE1	2.00	0.61
1:A:238:ASN:HB3	1:B:242:SER:OG	1.99	0.61
1:B:189:ARG:O	1:B:193:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:THR:HG21	1:D:292:CYS:HA	1.82	0.61
2:F:12:GLN:OE1	2:F:102:PRO:HG3	2.00	0.61
2:F:53:VAL:HG11	2:F:230:ILE:HG13	1.83	0.61
2:H:304:LEU:O	2:H:308:VAL:HG23	2.00	0.61
1:A:176:VAL:O	1:A:180:LEU:HG	2.00	0.61
1:A:297:VAL:HG11	1:A:298:ARG:HG2	1.71	0.61
1:B:565:CYS:SG	1:B:568:PHE:HB2	2.41	0.61
1:A:340:ASN:OD1	1:A:368:PHE:HE1	1.82	0.61
1:C:317:LEU:O	1:C:405:GLU:HG3	2.00	0.61
1:D:529:LYS:HB3	1:D:536:ALA:HB2	1.82	0.61
1:D:530:ARG:HB2	1:D:533:ASP:OD2	2.00	0.61
1:D:592:ASN:HD22	1:D:592:ASN:H	1.47	0.61
1:A:568:PHE:CE2	1:A:574:ALA:CB	2.81	0.61
1:B:7:VAL:HG11	3:B:801:DTP:N1	2.16	0.61
1:B:23:HIS:O	1:B:27:ASP:HB2	2.00	0.61
1:C:530:ARG:HB2	1:C:533:ASP:OD2	2.00	0.61
1:A:215:VAL:O	1:A:216:ARG:CB	2.48	0.61
1:A:328:ASN:O	1:A:329:ARG:NH1	2.28	0.61
1:A:444:LEU:HD21	1:A:691:GLN:HE22	1.66	0.61
1:D:39:SER:HA	1:D:42:GLU:CG	2.30	0.61
2:F:170:LEU:HD21	2:G:177:VAL:HG11	1.83	0.61
2:H:1:ALA:H3	2:H:168:HIS:HB3	1.64	0.61
1:A:226:VAL:CG1	1:A:459:ILE:HG22	2.28	0.61
1:B:215:VAL:O	1:B:216:ARG:HG2	2.01	0.61
1:C:289:VAL:HG12	1:C:300:GLY:O	2.00	0.61
1:C:730:TYR:CZ	1:C:731:TYR:CE2	2.88	0.61
1:D:293:SER:HB3	1:D:298:ARG:O	2.00	0.61
1:D:436:SER:HB3	1:D:440:LEU:HD13	1.83	0.61
1:D:572:THR:HB	1:D:577:ILE:HB	1.83	0.61
2:F:335:ILE:HG23	2:F:336:ASN:HD22	1.66	0.61
2:G:95:LEU:O	2:G:99:ILE:HG13	1.99	0.61
1:A:6:LEU:HD13	1:A:16:ARG:HA	1.82	0.61
1:A:552:LEU:HD23	1:A:616:LEU:HD12	1.81	0.61
1:B:430:ILE:CG2	1:B:570:GLU:HG2	2.30	0.61
1:B:621:PRO:HD3	1:B:694:SER:CB	2.30	0.61
1:A:322:ASN:OD1	1:A:323:ARG:N	2.32	0.61
1:A:622:SER:CB	4:A:802:DAT:O2A	2.48	0.61
1:C:40:GLN:HE22	1:C:44:ARG:HH11	1.47	0.61
2:H:116:THR:O	2:H:120:ARG:HG3	2.00	0.61
1:C:18:ASN:HD22	1:C:20:ASP:N	1.97	0.61
1:C:254:ILE:O	1:C:302:ALA:HA	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:214:CYS:SG	2:H:299:LEU:HD21	2.40	0.61
1:A:177:ALA:HB2	1:A:196:PHE:HD2	1.66	0.60
1:A:322:ASN:O	1:A:323:ARG:C	2.41	0.60
1:B:289:VAL:HG12	1:B:300:GLY:O	2.00	0.60
1:C:44:ARG:HG3	1:C:69:LEU:HD21	1.82	0.60
1:C:298:ARG:O	1:C:299:GLY:O	2.18	0.60
2:G:155:SER:O	2:G:159:GLU:HG3	2.00	0.60
2:G:209:TYR:HA	2:G:212:PHE:HD2	1.65	0.60
2:H:149:ARG:HH21	2:H:286:TRP:HB2	1.57	0.60
1:A:670:TRP:HA	1:A:670:TRP:HE3	1.64	0.60
1:D:560:LYS:HG2	1:D:609:HIS:CD2	2.36	0.60
2:H:221:ARG:HB3	2:H:223:LEU:CD1	2.31	0.60
2:H:300:ASN:HD21	2:H:303:ILE:CG1	2.11	0.60
1:C:425:PRO:HG3	1:C:615:THR:HG22	1.83	0.60
1:D:202:THR:OG1	1:D:204:LYS:HD3	2.01	0.60
1:D:547:ILE:O	1:D:551:LEU:HG	2.02	0.60
2:F:335:ILE:HG23	2:F:336:ASN:ND2	2.16	0.60
1:B:323:ARG:HH11	1:B:323:ARG:CB	2.13	0.60
1:C:72:ARG:O	1:C:659:TYR:HE2	1.84	0.60
1:D:364:LEU:O	1:D:364:LEU:HD13	2.00	0.60
2:F:1:ALA:H3	2:F:168:HIS:HB3	1.65	0.60
2:G:292:ARG:HD2	2:G:293:ASP:OD1	2.01	0.60
2:H:300:ASN:O	2:H:303:ILE:HB	2.01	0.60
1:B:37:SER:HB2	2:H:331:PRO:O	2.01	0.60
1:C:474:ASN:HD22	1:C:477:GLU:HG3	1.67	0.60
2:G:24:ASN:OD1	2:G:25:VAL:N	2.34	0.60
1:C:647:SER:HB3	1:C:650:GLY:O	2.01	0.60
2:F:82:LEU:HD22	2:F:146:ILE:CG2	2.30	0.60
2:F:149:ARG:NH2	2:F:286:TRP:CB	2.56	0.60
2:F:163:MET:HE1	2:F:188:GLU:HB3	1.84	0.60
2:G:86:ILE:HG21	2:G:153:ILE:HG22	1.82	0.60
2:G:116:THR:O	2:G:120:ARG:HG3	2.01	0.60
2:H:287:ALA:CB	2:H:304:LEU:HD22	2.30	0.60
1:C:97:PHE:O	1:C:99:PRO:HD3	2.00	0.60
2:F:95:LEU:O	2:F:99:ILE:HG13	2.01	0.60
2:G:292:ARG:NE	2:G:293:ASP:OD1	2.34	0.60
2:H:95:LEU:HB2	2:H:108:VAL:HG11	1.84	0.60
1:A:357:SER:O	1:A:361:VAL:HG22	2.00	0.60
1:B:568:PHE:CE1	1:B:573:TYR:HB2	2.35	0.60
1:C:521:ALA:HB3	1:C:632:THR:HG21	1.82	0.60
1:C:560:LYS:HG2	1:C:609:HIS:CD2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:LEU:O	1:D:616:LEU:HD13	2.01	0.60
2:H:291:PHE:HZ	2:H:299:LEU:CG	2.15	0.60
1:C:472:ILE:CG2	1:C:477:GLU:HB2	2.32	0.60
2:G:285:ASP:OD2	2:G:285:ASP:C	2.44	0.60
1:A:568:PHE:O	1:A:569:ASN:C	2.45	0.60
1:C:510:ARG:NH1	1:C:567:TRP:CZ3	2.69	0.60
1:D:379:TYR:O	1:D:383:GLU:HG3	2.02	0.60
2:E:101:ILE:HB	2:E:103:GLU:OE1	2.01	0.60
2:E:258:ASP:HB3	2:E:261:MET:HG2	1.82	0.60
2:H:101:ILE:HB	2:H:103:GLU:OE1	2.01	0.60
1:A:370:ALA:HB1	1:A:428:PRO:O	2.02	0.59
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.82	0.59
1:C:189:ARG:O	1:C:193:VAL:HG23	2.02	0.59
1:C:679:LEU:HD13	1:C:721:ALA:HB2	1.83	0.59
1:C:699:TYR:HE2	1:C:732:GLN:CD	2.08	0.59
2:G:149:ARG:NH2	2:G:286:TRP:HE3	1.99	0.59
1:C:202:THR:OG1	1:C:204:LYS:HD3	2.02	0.59
1:C:240:THR:O	1:C:244:ILE:HG13	2.02	0.59
1:D:179:CYS:HB2	1:D:215:VAL:CG1	2.32	0.59
2:E:209:TYR:HA	2:E:212:PHE:HD2	1.66	0.59
2:F:227:ASN:O	2:F:231:ILE:HG12	2.03	0.59
1:A:155:TYR:CE1	1:A:209:THR:HG23	2.36	0.59
1:C:413:TYR:HE1	1:C:731:TYR:CE1	2.19	0.59
1:D:85:ALA:O	1:D:89:LEU:HG	2.02	0.59
1:D:679:LEU:HD13	1:D:721:ALA:HB2	1.84	0.59
2:F:86:ILE:HG21	2:F:153:ILE:HG22	1.83	0.59
2:G:190:LYS:HD3	2:G:261:MET:SD	2.42	0.59
1:C:208:PRO:CG	1:C:464:LEU:HB2	2.32	0.59
2:G:201:ASN:HD21	2:G:246:GLN:HG2	1.68	0.59
1:A:69:LEU:HD13	1:A:77:TYR:CZ	2.38	0.59
1:A:75:PRO:O	1:A:76:ASP:C	2.45	0.59
1:B:5:LEU:CD2	1:B:51:ASP:HB2	2.21	0.59
1:B:44:ARG:HG3	1:B:69:LEU:HD21	1.85	0.59
3:B:803:DTP:H5'1	3:B:803:DTP:C8	2.33	0.59
1:D:285:PHE:O	1:D:289:VAL:HG23	2.03	0.59
2:E:49:ARG:O	2:E:52:GLU:CG	2.41	0.59
2:G:242:LEU:HD12	2:G:243:THR:N	2.17	0.59
2:H:242:LEU:HD12	2:H:243:THR:N	2.17	0.59
1:B:59:HIS:HB2	3:B:801:DTP:H4'	1.84	0.59
1:B:340:ASN:CG	1:B:368:PHE:CE1	2.81	0.59
1:C:59:HIS:HB2	3:C:801:DTP:H4'	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:THR:HB	1:C:577:ILE:HB	1.85	0.59
1:D:254:ILE:O	1:D:302:ALA:HA	2.03	0.59
1:D:380:THR:HA	1:D:383:GLU:OE1	2.02	0.59
2:F:169:LEU:HD13	2:G:166:TYR:CE1	2.38	0.59
1:B:9:LYS:HE3	1:B:15:GLU:OE1	2.02	0.59
1:A:137:HIS:HA	1:A:170:GLN:HG3	1.84	0.59
1:A:700:ASP:OD1	1:A:735:ARG:HD3	2.02	0.59
1:D:340:ASN:OD1	1:D:368:PHE:HE1	1.86	0.59
2:E:125:ILE:HG21	2:E:227:ASN:HD22	1.68	0.59
1:A:516:GLY:HA2	1:A:618:ALA:O	2.01	0.59
1:D:172:LEU:HG	1:D:216:ARG:NH2	2.18	0.59
1:A:226:VAL:HG12	1:A:459:ILE:HG23	1.81	0.59
1:C:209:THR:N	1:C:210:PRO:HD2	2.18	0.59
1:D:209:THR:N	1:D:210:PRO:HD2	2.18	0.59
2:H:101:ILE:HG13	2:H:104:LEU:HB3	1.85	0.59
2:H:140:ILE:CG2	2:H:146:ILE:HG21	2.32	0.59
2:H:203:LEU:HA	2:H:207:ARG:HB2	1.84	0.59
1:C:474:ASN:ND2	1:C:477:GLU:HG3	2.16	0.58
1:D:30:ALA:HA	1:D:33:LEU:HD12	1.84	0.58
1:D:44:ARG:HG3	1:D:69:LEU:HD21	1.85	0.58
1:D:317:LEU:O	1:D:405:GLU:HG3	2.03	0.58
2:E:95:LEU:HB2	2:E:108:VAL:HG11	1.84	0.58
2:F:176:THR:CA	2:F:180:LYS:O	2.50	0.58
1:A:320:LYS:HE2	1:A:411:ARG:HG3	1.86	0.58
1:C:115:TYR:OH	1:C:216:ARG:HD2	2.03	0.58
1:C:472:ILE:HG22	1:C:477:GLU:CG	2.33	0.58
1:D:530:ARG:HB3	1:D:667:GLU:OE2	2.03	0.58
2:E:70:LYS:O	2:E:74:ILE:HG22	2.03	0.58
2:E:186:LEU:O	2:E:190:LYS:HG3	2.03	0.58
2:G:102:PRO:CD	2:G:103:GLU:OE1	2.50	0.58
2:G:203:LEU:HA	2:G:207:ARG:HB2	1.85	0.58
1:B:59:HIS:CD2	1:B:88:HIS:HB2	2.38	0.58
1:B:179:CYS:HB2	1:B:215:VAL:CG1	2.34	0.58
1:C:40:GLN:OE1	1:C:44:ARG:CG	2.52	0.58
1:C:368:PHE:CE2	1:C:417:VAL:HG21	2.39	0.58
1:D:313:VAL:O	1:D:317:LEU:HD23	2.03	0.58
2:F:127:ARG:HH21	2:G:29:ASP:HA	1.68	0.58
2:F:155:SER:O	2:F:159:GLU:CG	2.51	0.58
2:G:291:PHE:CB	2:G:294:GLY:O	2.50	0.58
2:H:214:CYS:SG	2:H:299:LEU:CD2	2.92	0.58
1:B:428:PRO:HA	1:B:432:PRO:HB3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:ASN:C	1:B:437:ASN:OD1	2.47	0.58
1:B:572:THR:HB	1:B:577:ILE:HB	1.85	0.58
1:D:18:ASN:HD21	1:D:20:ASP:CB	2.14	0.58
1:D:708:LYS:CE	2:G:361:ILE:C	2.76	0.58
2:F:186:LEU:O	2:F:190:LYS:HG3	2.03	0.58
2:G:291:PHE:HZ	2:G:299:LEU:HB3	1.68	0.58
2:H:99:ILE:HD13	2:H:105:GLU:HA	1.85	0.58
1:A:34:HIS:O	1:A:36:VAL:HG13	2.03	0.58
1:A:317:LEU:HD12	1:A:402:MET:HA	1.85	0.58
1:A:370:ALA:CB	1:A:428:PRO:O	2.51	0.58
1:D:175:LEU:HB2	1:D:216:ARG:CD	2.23	0.58
2:E:279:ALA:O	2:E:283:GLU:HG2	2.04	0.58
2:G:86:ILE:HG21	2:G:153:ILE:CG2	2.33	0.58
1:A:568:PHE:CE2	1:A:574:ALA:CA	2.87	0.58
1:A:646:ALA:CA	1:A:651:ILE:HG22	2.26	0.58
1:B:516:GLY:HA2	1:B:618:ALA:O	2.04	0.58
1:C:364:LEU:O	1:C:364:LEU:HD13	2.03	0.58
1:D:35:ASN:HD22	1:D:74:ALA:HB2	1.69	0.58
1:D:532:SER:CB	1:D:673:PRO:HD2	2.34	0.58
2:F:116:THR:O	2:F:120:ARG:HG3	2.02	0.58
2:H:79:TYR:CE1	2:H:149:ARG:CD	2.83	0.58
1:A:317:LEU:O	1:A:405:GLU:HG3	2.04	0.58
1:A:324:GLY:O	1:A:329:ARG:HG3	2.03	0.58
1:A:547:ILE:O	1:A:551:LEU:HG	2.03	0.58
1:B:279:ILE:HG21	1:B:328:ASN:HA	1.84	0.58
1:C:640:GLY:HA2	1:C:668:LEU:HD22	1.85	0.58
1:A:53:ILE:HD11	1:A:58:ILE:HG12	1.73	0.58
1:B:568:PHE:CE2	1:B:574:ALA:HA	2.39	0.58
1:C:415:GLN:OE1	1:C:436:SER:HB2	2.04	0.58
1:C:547:ILE:O	1:C:551:LEU:HG	2.04	0.58
2:E:242:LEU:HD12	2:E:243:THR:N	2.18	0.58
1:B:258:ALA:HB1	1:B:261:ILE:HD12	1.86	0.58
1:C:557:GLU:HA	1:C:560:LYS:HD3	1.86	0.58
2:F:92:ASN:O	2:F:96:LEU:HG	2.03	0.58
2:F:101:ILE:HG13	2:F:104:LEU:HB3	1.86	0.58
2:F:190:LYS:HD3	2:F:261:MET:SD	2.44	0.58
2:F:242:LEU:HD12	2:F:243:THR:N	2.18	0.58
2:G:292:ARG:CD	2:G:293:ASP:OD1	2.52	0.58
1:A:155:TYR:HE1	1:A:209:THR:HG23	1.69	0.58
1:B:317:LEU:O	1:B:405:GLU:HG3	2.04	0.58
1:C:441:GLU:HB2	1:C:619:LEU:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:ILE:HG21	1:C:477:GLU:HB2	1.86	0.58
1:C:474:ASN:HD22	1:C:474:ASN:H	1.51	0.58
1:D:557:GLU:HA	1:D:560:LYS:HD3	1.86	0.58
1:D:622:SER:CB	4:D:802:DAT:O2A	2.52	0.58
2:G:123:THR:O	2:G:127:ARG:HG2	2.04	0.58
1:A:559:ALA:O	1:A:563:GLY:CA	2.52	0.57
1:B:436:SER:OG	1:B:440:LEU:HA	2.04	0.57
2:E:155:SER:O	2:E:159:GLU:CG	2.52	0.57
2:F:220:GLU:OE2	2:F:338:TRP:NE1	2.27	0.57
2:G:300:ASN:N	2:G:303:ILE:HG21	2.15	0.57
1:A:189:ARG:O	1:A:193:VAL:HG23	2.04	0.57
1:B:317:LEU:HD12	1:B:402:MET:HA	1.86	0.57
1:B:320:LYS:HE2	1:B:411:ARG:HG3	1.86	0.57
1:B:439:CYS:O	1:B:440:LEU:HB2	2.04	0.57
1:C:18:ASN:ND2	1:C:20:ASP:N	2.52	0.57
1:C:415:GLN:HA	1:C:728:THR:HG22	1.86	0.57
2:E:66:PRO:CB	2:E:68:HIS:NE2	2.66	0.57
2:F:99:ILE:HD13	2:F:105:GLU:HA	1.85	0.57
2:G:144:GLU:OE1	2:G:144:GLU:HA	2.04	0.57
2:G:300:ASN:H	2:G:303:ILE:HG21	1.58	0.57
1:B:542:LYS:CE	1:B:596:HIS:NE2	2.65	0.57
1:C:106:VAL:O	1:C:110:VAL:HG23	2.04	0.57
1:C:472:ILE:HG22	1:C:477:GLU:CB	2.33	0.57
1:D:97:PHE:O	1:D:99:PRO:HD3	2.04	0.57
1:D:425:PRO:HG3	1:D:615:THR:HG22	1.85	0.57
2:E:242:LEU:O	2:E:246:GLN:HG3	2.03	0.57
2:F:66:PRO:HD2	2:F:69:GLU:CD	2.29	0.57
2:H:125:ILE:HG21	2:H:227:ASN:HD22	1.69	0.57
1:A:326:GLU:O	1:A:327:GLY:C	2.48	0.57
1:B:568:PHE:CE2	1:B:574:ALA:CA	2.87	0.57
1:D:106:VAL:O	1:D:110:VAL:HG23	2.05	0.57
2:E:193:LEU:O	2:E:197:LEU:HG	2.05	0.57
2:G:186:LEU:O	2:G:190:LYS:HG3	2.05	0.57
2:G:292:ARG:HE	2:G:293:ASP:CG	2.12	0.57
1:A:54:LYS:HB2	1:A:57:ASP:OD2	2.03	0.57
1:C:17:ILE:HD11	1:C:49:PHE:CZ	2.39	0.57
1:C:35:ASN:HD22	1:C:74:ALA:HB2	1.69	0.57
1:C:118:HIS:C	1:C:118:HIS:ND1	2.61	0.57
1:D:215:VAL:O	1:D:216:ARG:CG	2.52	0.57
1:D:329:ARG:CG	1:D:329:ARG:NH1	2.62	0.57
1:B:506:GLY:HA2	1:B:567:TRP:HZ3	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:GLU:O	1:B:703:ARG:NH2	2.37	0.57
1:B:700:ASP:OD1	1:B:735:ARG:HD3	2.04	0.57
1:C:109:MET:HE3	1:C:114:LYS:HB3	1.85	0.57
1:C:179:CYS:HB2	1:C:215:VAL:CG1	2.34	0.57
1:C:217:THR:OG1	1:C:219:THR:HG22	2.04	0.57
1:D:179:CYS:HB2	1:D:215:VAL:HG13	1.87	0.57
1:D:320:LYS:HE2	1:D:411:ARG:HG2	1.82	0.57
2:E:167:TRP:CE3	2:E:168:HIS:CD2	2.92	0.57
2:F:193:LEU:O	2:F:197:LEU:HG	2.05	0.57
2:G:1:ALA:H3	2:G:168:HIS:HB3	1.69	0.57
2:H:326:GLN:HB3	2:H:328:ARG:NH1	2.19	0.57
1:A:69:LEU:HB3	1:A:77:TYR:CD2	2.39	0.57
1:B:561:GLU:HB3	1:B:562:GLN:HE21	1.69	0.57
1:C:697:THR:HG23	1:C:732:GLN:HG3	1.87	0.57
2:F:53:VAL:HG21	2:F:230:ILE:HG12	1.85	0.57
2:F:91:PRO:HB2	2:F:112:ALA:HB2	1.86	0.57
2:H:66:PRO:HD2	2:H:69:GLU:CD	2.30	0.57
1:A:177:ALA:HB2	1:A:196:PHE:CD2	2.39	0.57
1:B:515:ILE:O	1:B:618:ALA:O	2.22	0.57
2:E:209:TYR:HA	2:E:212:PHE:CD2	2.40	0.57
2:G:1:ALA:HB3	2:G:168:HIS:HA	1.87	0.57
2:H:92:ASN:O	2:H:96:LEU:HG	2.05	0.57
2:H:209:TYR:HA	2:H:212:PHE:CD2	2.39	0.57
2:H:279:ALA:O	2:H:283:GLU:HG2	2.05	0.57
1:A:316:LEU:HA	1:A:319:LEU:HG	1.87	0.57
1:C:44:ARG:HA	1:C:44:ARG:NE	2.20	0.57
1:D:38:ILE:HD13	1:D:38:ILE:N	2.19	0.57
2:E:120:ARG:HG2	2:H:28:TYR:CE2	2.40	0.57
2:G:90:SER:HB2	2:G:91:PRO:HD3	1.87	0.57
2:H:145:GLN:NE2	2:H:145:GLN:N	2.53	0.57
2:H:145:GLN:H	2:H:145:GLN:HE21	1.50	0.57
1:A:658:ASP:O	1:A:662:LEU:HB2	2.05	0.57
1:B:179:CYS:HB2	1:B:215:VAL:HG13	1.85	0.57
1:B:461:LEU:HD11	1:B:503:ALA:HB1	1.87	0.57
2:F:1:ALA:HB3	2:F:168:HIS:HA	1.87	0.57
2:F:209:TYR:HA	2:F:212:PHE:CD2	2.40	0.57
1:B:313:VAL:O	1:B:317:LEU:HD23	2.05	0.56
1:B:670:TRP:CE2	1:B:735:ARG:HG3	2.40	0.56
1:C:532:SER:CB	1:C:673:PRO:HD2	2.35	0.56
1:D:552:LEU:HA	1:D:616:LEU:HD12	1.86	0.56
2:E:82:LEU:HD22	2:E:146:ILE:CG2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:THR:O	2:E:127:ARG:HG2	2.05	0.56
2:G:217:ALA:HB1	2:G:299:LEU:HD22	1.87	0.56
1:A:644:ILE:CG2	1:A:651:ILE:HD13	2.35	0.56
1:B:79:TYR:O	1:B:83:ARG:HG3	2.04	0.56
1:B:215:VAL:O	1:B:216:ARG:CG	2.54	0.56
1:C:583:TYR:CD2	1:C:687:LYS:HE3	2.40	0.56
2:E:92:ASN:O	2:E:96:LEU:HG	2.05	0.56
2:F:177:VAL:HA	2:G:176:THR:O	2.04	0.56
2:H:70:LYS:O	2:H:74:ILE:HG22	2.04	0.56
2:H:111:TRP:O	2:H:111:TRP:CD1	2.58	0.56
2:H:193:LEU:O	2:H:197:LEU:HG	2.05	0.56
1:A:177:ALA:CB	1:A:196:PHE:CD2	2.81	0.56
1:A:568:PHE:CD1	1:A:571:THR:OG1	2.58	0.56
1:A:669:LEU:HD11	1:A:698:ASN:ND2	2.20	0.56
1:B:155:TYR:CE2	1:B:628:ILE:HD11	2.40	0.56
1:B:290:LYS:NZ	1:B:299:GLY:O	2.29	0.56
1:B:547:ILE:O	1:B:551:LEU:HG	2.06	0.56
1:C:258:ALA:HB1	1:C:261:ILE:HD12	1.87	0.56
1:C:530:ARG:HB3	1:C:667:GLU:OE2	2.04	0.56
1:D:37:SER:CB	1:D:40:GLN:HB2	2.35	0.56
1:D:230:CYS:HB2	1:D:240:THR:HG21	1.86	0.56
1:D:293:SER:CB	1:D:298:ARG:O	2.54	0.56
1:D:320:LYS:O	1:D:321:ASN:C	2.48	0.56
1:D:516:GLY:HA3	1:D:618:ALA:O	2.05	0.56
2:F:79:TYR:CE1	2:F:149:ARG:HD2	2.40	0.56
2:G:193:LEU:O	2:G:197:LEU:HG	2.05	0.56
1:A:9:LYS:HE3	1:A:15:GLU:CD	2.29	0.56
1:A:196:PHE:HB2	1:A:484:LEU:HD11	1.86	0.56
1:C:285:PHE:O	1:C:289:VAL:HG23	2.06	0.56
1:D:722:TYR:HD2	2:G:375:LEU:HD22	1.71	0.56
2:F:95:LEU:HB2	2:F:108:VAL:HG11	1.88	0.56
2:G:35:ILE:C	2:G:35:ILE:HD13	2.31	0.56
1:A:321:ASN:HB2	1:A:405:GLU:OE1	2.06	0.56
1:B:679:LEU:HD13	1:B:721:ALA:HB2	1.86	0.56
1:C:212:MET:HE2	1:C:212:MET:HA	1.87	0.56
1:D:258:ALA:HB1	1:D:261:ILE:HD12	1.87	0.56
2:F:7:GLN:OE1	2:G:147:GLN:NE2	2.39	0.56
2:H:196:CYS:O	2:H:200:VAL:HG23	2.05	0.56
1:A:568:PHE:CD2	1:A:574:ALA:HB2	2.41	0.56
1:D:152:GLU:HA	1:D:156:LEU:HD12	1.87	0.56
1:D:568:PHE:CE2	1:D:574:ALA:HB2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:TYR:CD1	2:F:170:LEU:HD12	2.41	0.56
2:F:174:THR:HG22	2:F:181:THR:HG23	1.87	0.56
2:G:217:ALA:HB1	2:G:299:LEU:CD2	2.34	0.56
1:A:365:TYR:HE2	1:A:434:ARG:HH21	1.54	0.56
1:B:322:ASN:HA	1:B:331:ARG:NE	2.18	0.56
1:B:621:PRO:HG3	1:B:694:SER:HB3	1.87	0.56
1:C:155:TYR:CE2	1:C:628:ILE:CG1	2.85	0.56
1:D:622:SER:CB	4:D:802:DAT:PA	2.90	0.56
1:D:696:ASN:H	1:D:696:ASN:HD22	1.53	0.56
2:E:99:ILE:HD13	2:E:105:GLU:HA	1.88	0.56
2:H:91:PRO:HB2	2:H:112:ALA:HB2	1.87	0.56
1:A:7:VAL:HG22	1:A:15:GLU:O	2.06	0.56
1:A:411:ARG:NH1	1:A:731:TYR:CZ	2.74	0.56
1:B:8:THR:HB	1:B:54:LYS:HA	1.87	0.56
1:B:354:THR:CB	1:B:356:PHE:CE2	2.89	0.56
1:C:18:ASN:HD21	1:C:20:ASP:CB	2.17	0.56
1:C:72:ARG:HG2	1:C:659:TYR:HH	1.63	0.56
1:D:320:LYS:NZ	1:D:411:ARG:HG3	2.21	0.56
2:F:336:ASN:N	2:F:336:ASN:ND2	2.54	0.56
2:H:86:ILE:HG21	2:H:153:ILE:HG22	1.87	0.56
2:H:149:ARG:NH1	2:H:286:TRP:HE3	2.03	0.56
1:A:474:ASN:H	1:A:474:ASN:HD22	1.54	0.56
1:B:474:ASN:H	1:B:474:ASN:HD22	1.54	0.56
1:C:151:LEU:HD21	1:C:155:TYR:HD2	1.68	0.56
2:E:101:ILE:HG13	2:E:104:LEU:HB3	1.86	0.56
2:F:5:PHE:CE1	2:F:24:ASN:C	2.84	0.56
2:G:149:ARG:CG	2:G:149:ARG:NH1	2.47	0.56
2:G:279:ALA:O	2:G:283:GLU:HG2	2.06	0.56
1:A:525:ALA:CB	1:A:662:LEU:HD13	2.36	0.56
1:B:42:GLU:HB3	2:H:297:ILE:HG23	1.87	0.56
1:B:106:VAL:O	1:B:110:VAL:HG23	2.05	0.56
1:B:151:LEU:CD2	1:B:155:TYR:CD2	2.78	0.56
1:B:413:TYR:HB3	1:B:440:LEU:HD21	1.86	0.56
1:B:669:LEU:HA	1:B:672:MET:HE2	1.88	0.56
1:C:555:SER:HB2	1:C:616:LEU:CD1	2.36	0.56
1:D:669:LEU:HD12	1:D:672:MET:HE2	1.86	0.56
2:F:82:LEU:HD22	2:F:146:ILE:HG23	1.88	0.56
2:F:242:LEU:O	2:F:246:GLN:HG3	2.06	0.56
2:G:125:ILE:HG21	2:G:227:ASN:HD22	1.71	0.56
2:H:242:LEU:O	2:H:246:GLN:HG3	2.06	0.56
1:A:322:ASN:HA	1:A:331:ARG:HE	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLY:HA3	1:A:329:ARG:NH2	2.22	0.55
1:C:37:SER:CB	1:C:40:GLN:HB2	2.35	0.55
1:D:44:ARG:HA	1:D:44:ARG:HE	1.71	0.55
2:G:3:THR:HG21	2:G:6:SER:HA	1.88	0.55
1:A:256:ILE:HB	1:A:304:LEU:HG	1.88	0.55
1:A:426:PHE:CZ	1:A:445:PRO:HD3	2.39	0.55
1:A:470:GLY:HA3	1:A:519:ASN:ND2	2.21	0.55
1:B:658:ASP:O	1:B:662:LEU:HB2	2.06	0.55
1:C:114:LYS:HD3	1:C:114:LYS:N	2.20	0.55
1:C:146:ALA:O	1:C:150:GLN:HG2	2.07	0.55
1:C:369:PHE:HB3	1:C:421:ASN:HD21	1.71	0.55
1:C:518:ILE:HG22	1:C:622:SER:OG	2.06	0.55
1:D:289:VAL:HG12	1:D:300:GLY:O	2.05	0.55
2:G:209:TYR:HA	2:G:212:PHE:CD2	2.41	0.55
1:C:230:CYS:HB2	1:C:240:THR:HG21	1.87	0.55
1:C:380:THR:HA	1:C:383:GLU:OE1	2.06	0.55
1:C:700:ASP:OD1	1:C:735:ARG:HD3	2.05	0.55
2:F:12:GLN:NE2	2:F:25:VAL:CG1	2.68	0.55
2:E:91:PRO:HB2	2:E:112:ALA:HB2	1.88	0.55
1:A:105:HIS:O	1:A:109:MET:HG2	2.06	0.55
1:C:356:PHE:HE1	1:C:390:LYS:HE3	1.70	0.55
1:C:551:LEU:C	1:C:616:LEU:HD12	2.31	0.55
2:F:154:SER:O	2:F:158:ASP:OD2	2.24	0.55
1:A:419:HIS:CA	1:A:422:THR:HG1	2.17	0.55
1:B:215:VAL:O	1:B:216:ARG:CB	2.55	0.55
1:B:440:LEU:HD23	1:B:728:THR:HB	1.87	0.55
1:C:439:CYS:SG	4:C:802:DAT:H8	2.47	0.55
1:C:699:TYR:CE2	1:C:732:GLN:CD	2.83	0.55
1:D:115:TYR:HA	1:D:217:THR:HA	1.88	0.55
2:H:186:LEU:O	2:H:190:LYS:HG3	2.06	0.55
1:C:690:ASP:HB2	1:C:691:GLN:HE21	1.72	0.55
1:D:5:LEU:O	1:D:16:ARG:CA	2.51	0.55
1:A:152:GLU:O	1:A:158:GLN:NE2	2.39	0.55
1:A:175:LEU:CD1	1:A:216:ARG:HD2	2.36	0.55
1:B:568:PHE:O	1:B:569:ASN:C	2.49	0.55
1:D:407:ALA:HA	1:D:732:GLN:OE1	2.07	0.55
2:E:165:SER:HB2	2:H:169:LEU:HD11	1.88	0.55
1:A:206:SER:OG	1:A:625:SER:HB2	2.07	0.55
1:A:439:CYS:O	1:A:440:LEU:HB2	2.05	0.55
1:A:711:MET:HB2	2:F:362:ASP:O	2.05	0.55
1:B:137:HIS:HA	1:B:170:GLN:HG3	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:TYR:CD1	1:C:216:ARG:O	2.60	0.55
1:D:7:VAL:HG23	1:D:15:GLU:CG	2.37	0.55
1:D:25:VAL:HG11	1:D:59:HIS:CE1	2.40	0.55
1:D:26:LEU:HD21	1:D:62:ILE:HD12	1.89	0.55
1:D:320:LYS:HZ1	1:D:411:ARG:HG3	1.71	0.55
1:D:356:PHE:HE1	1:D:390:LYS:HE3	1.72	0.55
2:F:123:THR:O	2:F:127:ARG:HG2	2.06	0.55
1:A:305:PHE:CD1	1:A:435:GLN:NE2	2.74	0.55
1:B:279:ILE:HB	1:B:280:PRO:HD3	1.89	0.55
1:C:510:ARG:HB2	1:C:614:SER:OG	2.07	0.55
1:D:240:THR:O	1:D:244:ILE:HG13	2.06	0.55
2:F:70:LYS:O	2:F:74:ILE:HG22	2.06	0.55
2:G:103:GLU:OE1	2:G:103:GLU:N	2.39	0.55
2:G:339:LEU:O	2:G:340:VAL:HG13	2.07	0.55
2:H:66:PRO:O	2:H:69:GLU:N	2.38	0.55
1:A:53:ILE:HD12	1:A:58:ILE:HG12	1.83	0.54
1:A:324:GLY:HA3	1:A:329:ARG:NE	2.22	0.54
1:A:679:LEU:HD13	1:A:721:ALA:HB2	1.88	0.54
1:C:151:LEU:HD23	1:C:155:TYR:HB2	1.87	0.54
1:D:229:GLU:HB2	1:D:435:GLN:OE1	2.07	0.54
1:D:233:SER:O	1:D:237:ILE:HG13	2.07	0.54
1:D:279:ILE:HB	1:D:280:PRO:HD3	1.89	0.54
2:E:53:VAL:HG21	2:E:230:ILE:HG12	1.89	0.54
2:H:221:ARG:O	2:H:222:GLU:HB2	2.06	0.54
1:A:415:GLN:HA	1:A:728:THR:HG22	1.88	0.54
1:A:615:THR:HG21	1:A:691:GLN:HE21	1.72	0.54
1:B:39:SER:O	1:B:43:LEU:HG	2.07	0.54
1:C:439:CYS:O	1:C:440:LEU:HB2	2.06	0.54
1:D:23:HIS:HE1	1:D:42:GLU:CD	2.15	0.54
1:D:551:LEU:C	1:D:616:LEU:HD12	2.32	0.54
2:E:90:SER:HB2	2:E:91:PRO:HD3	1.89	0.54
2:G:296:MET:O	2:G:297:ILE:C	2.50	0.54
1:A:109:MET:HG3	1:A:115:TYR:CE2	2.42	0.54
1:B:217:THR:CG2	1:B:218:PRO:HD2	2.37	0.54
1:C:40:GLN:HE22	1:C:44:ARG:NH1	2.06	0.54
1:C:233:SER:HA	3:C:803:DTP:O5'	2.08	0.54
1:C:279:ILE:HB	1:C:280:PRO:HD3	1.89	0.54
1:C:330:VAL:HG11	1:C:333:MET:HE3	1.87	0.54
1:D:109:MET:HB3	1:D:114:LYS:HB2	1.89	0.54
1:A:177:ALA:HB1	1:A:196:PHE:HD2	1.70	0.54
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:SER:CB	1:C:298:ARG:O	2.56	0.54
1:C:313:VAL:O	1:C:317:LEU:HD23	2.06	0.54
2:F:87:GLN:O	2:F:115:GLU:HG3	2.07	0.54
2:H:258:ASP:OD2	2:H:261:MET:HG2	2.07	0.54
1:A:313:VAL:O	1:A:317:LEU:HD23	2.08	0.54
1:C:291:SER:O	1:D:276:THR:HG21	2.08	0.54
1:C:519:ASN:ND2	1:C:522:TYR:HB3	2.22	0.54
1:D:151:LEU:HD23	1:D:155:TYR:HD2	1.73	0.54
1:D:510:ARG:NH1	1:D:567:TRP:CE3	2.76	0.54
2:E:74:ILE:O	2:E:78:LYS:HG3	2.07	0.54
2:F:89:ARG:NE	2:G:105:GLU:OE2	2.35	0.54
2:F:208:PHE:CE2	7:F:601:HOH:O	2.53	0.54
1:A:151:LEU:HD23	1:A:155:TYR:CB	2.38	0.54
1:A:645:LYS:O	1:A:652:LEU:N	2.28	0.54
1:C:153:GLY:O	1:C:158:GLN:NE2	2.41	0.54
1:C:430:ILE:HG21	1:C:570:GLU:HG2	1.89	0.54
2:E:175:HIS:O	2:E:181:THR:HA	2.07	0.54
2:F:10:ASN:ND2	2:F:15:GLU:HG3	2.23	0.54
2:F:174:THR:HA	2:F:182:VAL:O	2.08	0.54
2:G:332:ILE:O	2:G:335:ILE:HG22	2.08	0.54
1:B:316:LEU:HA	1:B:319:LEU:HG	1.89	0.54
1:C:669:LEU:HA	1:C:672:MET:HE2	1.88	0.54
1:D:80:LEU:HD12	1:D:80:LEU:C	2.32	0.54
1:D:441:GLU:O	1:D:691:GLN:HB3	2.07	0.54
2:F:207:ARG:HG2	2:F:207:ARG:NH1	2.18	0.54
1:A:224:SER:O	1:A:252:ALA:HA	2.08	0.54
1:A:282:TYR:CD2	1:A:304:LEU:HD13	2.43	0.54
1:B:214:GLY:O	1:B:217:THR:N	2.39	0.54
1:C:9:LYS:HB2	1:C:13:SER:HB3	1.90	0.54
1:C:282:TYR:CD2	1:C:304:LEU:HD13	2.43	0.54
1:C:316:LEU:HA	1:C:319:LEU:HG	1.90	0.54
1:C:413:TYR:CZ	1:C:731:TYR:CE1	2.96	0.54
1:D:23:HIS:HE1	1:D:42:GLU:OE2	1.90	0.54
1:A:85:ALA:O	1:A:89:LEU:HG	2.07	0.54
1:A:516:GLY:HA3	1:A:618:ALA:O	2.07	0.54
1:A:568:PHE:CE1	1:A:571:THR:OG1	2.61	0.54
1:B:54:LYS:HE3	1:B:57:ASP:OD2	2.08	0.54
1:B:289:VAL:O	1:B:300:GLY:HA3	2.08	0.54
1:C:172:LEU:HG	1:C:216:ARG:CZ	2.37	0.54
2:E:96:LEU:HB2	2:E:97:PRO:HD3	1.90	0.54
2:F:66:PRO:O	2:F:69:GLU:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:THR:HG21	2:H:6:SER:HA	1.90	0.54
2:H:55:VAL:HG12	2:H:226:GLY:C	2.32	0.54
1:A:519:ASN:HB2	1:A:631:ALA:CB	2.35	0.54
1:A:598:ASP:C	1:A:598:ASP:OD1	2.51	0.54
1:B:70:ILE:HG23	1:B:78:GLN:HG2	1.89	0.54
1:B:172:LEU:O	1:B:176:VAL:HG23	2.08	0.54
1:B:486:VAL:HG13	1:B:513:LEU:CD2	2.38	0.54
1:B:615:THR:CG2	1:B:691:GLN:HE21	2.13	0.54
1:C:369:PHE:CD2	1:C:434:ARG:HG2	2.42	0.54
1:D:9:LYS:HB2	1:D:13:SER:HB3	1.90	0.54
1:D:50:TYR:O	1:D:53:ILE:HG23	2.03	0.54
1:D:146:ALA:O	1:D:150:GLN:HG2	2.08	0.54
2:F:207:ARG:HH22	2:F:282:GLN:HE22	1.48	0.54
1:A:279:ILE:HB	1:A:280:PRO:HD3	1.89	0.53
1:B:37:SER:OG	1:B:40:GLN:HB2	2.08	0.53
1:B:619:LEU:HD12	1:B:693:ILE:CD1	2.38	0.53
1:B:623:GLU:O	1:B:627:GLN:HG3	2.07	0.53
1:C:176:VAL:O	1:C:180:LEU:HG	2.08	0.53
1:D:78:GLN:NE2	1:D:655:VAL:HB	2.23	0.53
1:D:360:ASP:O	1:D:362:PRO:HD3	2.08	0.53
1:D:583:TYR:CD2	1:D:687:LYS:HE3	2.43	0.53
2:F:3:THR:CG2	2:F:5:PHE:O	2.56	0.53
2:F:90:SER:HB2	2:F:91:PRO:HD3	1.89	0.53
2:H:90:SER:HB2	2:H:91:PRO:HD3	1.90	0.53
1:A:418:ASP:O	1:A:422:THR:HG23	2.07	0.53
1:B:282:TYR:CD2	1:B:304:LEU:HD13	2.44	0.53
1:B:340:ASN:OD1	1:B:343:MET:HG2	2.09	0.53
1:C:59:HIS:O	1:C:63:ILE:HG13	2.08	0.53
1:C:262:ARG:HA	1:C:358:PRO:CG	2.38	0.53
1:C:516:GLY:HA3	1:C:618:ALA:O	2.05	0.53
1:D:320:LYS:HA	1:D:331:ARG:HA	1.89	0.53
2:F:145:GLN:H	2:F:145:GLN:NE2	2.04	0.53
1:B:78:GLN:CD	1:B:655:VAL:HB	2.33	0.53
1:B:459:ILE:HB	1:B:503:ALA:HA	1.91	0.53
1:B:530:ARG:HB2	1:B:533:ASP:OD2	2.08	0.53
1:C:229:GLU:HB2	1:C:435:GLN:OE1	2.08	0.53
1:D:525:ALA:CB	1:D:662:LEU:HD13	2.37	0.53
2:H:1:ALA:HB3	2:H:168:HIS:HA	1.89	0.53
1:A:411:ARG:NH1	1:A:731:TYR:CE1	2.76	0.53
1:A:568:PHE:CE1	1:A:573:TYR:HB2	2.44	0.53
1:B:59:HIS:O	1:B:62:ILE:HG12	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:ARG:O	1:B:299:GLY:C	2.52	0.53
1:C:185:PRO:HG2	1:C:188:THR:OG1	2.08	0.53
2:E:160:LEU:HD21	2:E:193:LEU:HD23	1.91	0.53
2:F:35:ILE:HD13	2:F:35:ILE:C	2.33	0.53
2:G:217:ALA:CB	2:G:299:LEU:HD22	2.38	0.53
1:A:613:ASN:HB2	1:A:616:LEU:CD2	2.35	0.53
1:B:356:PHE:CE1	1:B:390:LYS:CE	2.85	0.53
1:B:361:VAL:HG23	1:B:361:VAL:O	2.07	0.53
1:B:470:GLY:HA3	1:B:519:ASN:ND2	2.23	0.53
1:C:357:SER:OG	1:C:358:PRO:HD2	2.09	0.53
1:C:645:LYS:HD2	1:C:646:ALA:N	2.23	0.53
1:C:696:ASN:HD22	1:C:696:ASN:H	1.55	0.53
1:D:465:SER:O	1:D:620:MET:HE1	2.09	0.53
1:D:568:PHE:CE1	1:D:573:TYR:HB2	2.43	0.53
2:H:73:PHE:CE1	2:H:224:MET:HE2	2.43	0.53
2:H:155:SER:O	2:H:159:GLU:HG3	2.09	0.53
1:A:18:ASN:OD1	1:A:20:ASP:HB2	2.08	0.53
2:E:68:HIS:O	2:E:71:HIS:HB3	2.09	0.53
2:F:9:LYS:HD2	2:G:142:THR:CG2	2.39	0.53
1:A:530:ARG:HB3	1:A:667:GLU:OE2	2.09	0.53
1:A:568:PHE:CE2	1:A:574:ALA:HA	2.43	0.53
1:B:77:TYR:HD1	1:B:80:LEU:HD23	1.73	0.53
1:B:369:PHE:HD1	1:B:417:VAL:HB	1.74	0.53
1:B:486:VAL:HG13	1:B:513:LEU:HD22	1.91	0.53
1:B:568:PHE:CE2	1:B:574:ALA:CB	2.92	0.53
1:C:9:LYS:HE3	1:C:15:GLU:CG	2.39	0.53
1:C:482:ALA:O	1:C:486:VAL:HG23	2.09	0.53
1:C:699:TYR:HE2	1:C:732:GLN:HE21	1.45	0.53
1:D:316:LEU:HA	1:D:319:LEU:HG	1.90	0.53
1:D:482:ALA:O	1:D:486:VAL:HG23	2.09	0.53
2:F:51:GLU:N	2:F:51:GLU:OE1	2.41	0.53
2:G:101:ILE:HG13	2:G:104:LEU:HB3	1.91	0.53
2:G:149:ARG:HH22	2:G:286:TRP:HE3	1.55	0.53
1:A:466:ALA:HA	1:A:516:GLY:O	2.09	0.53
1:B:7:VAL:HG11	3:B:801:DTP:C6	2.39	0.53
1:B:78:GLN:OE1	1:B:655:VAL:CG2	2.57	0.53
1:B:208:PRO:CB	1:B:210:PRO:HD2	2.39	0.53
1:D:59:HIS:O	1:D:63:ILE:HG13	2.09	0.53
2:E:165:SER:O	2:E:169:LEU:HG	2.09	0.53
2:E:169:LEU:HD12	2:H:169:LEU:HD12	1.90	0.53
2:G:91:PRO:HB2	2:G:112:ALA:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:153:ILE:HD12	2:G:203:LEU:HD11	1.86	0.53
2:G:217:ALA:HB2	2:G:299:LEU:HD21	1.90	0.53
1:C:35:ASN:ND2	1:C:74:ALA:HB2	2.23	0.53
1:C:153:GLY:HA2	1:C:158:GLN:HE22	1.73	0.53
2:F:121:SER:O	2:F:125:ILE:HG13	2.09	0.53
2:G:197:LEU:HB2	2:G:249:LEU:HD21	1.91	0.53
2:H:74:ILE:O	2:H:78:LYS:HG3	2.09	0.53
2:H:327:THR:C	2:H:328:ARG:HG2	2.34	0.53
2:H:332:ILE:HB	2:H:334:TRP:NE1	2.24	0.53
1:A:529:LYS:HD2	1:A:535:SER:O	2.09	0.53
1:B:115:TYR:HA	1:B:216:ARG:O	2.09	0.53
1:B:240:THR:O	1:B:244:ILE:HG13	2.09	0.53
1:B:519:ASN:ND2	1:B:522:TYR:HB3	2.24	0.53
1:C:11:ASP:OD2	1:C:13:SER:HB3	2.09	0.53
1:C:320:LYS:HE2	1:C:411:ARG:CG	2.38	0.53
1:C:568:PHE:CE1	1:C:573:TYR:HB2	2.44	0.53
1:D:131:MET:HA	1:D:134:PHE:CD2	2.44	0.53
1:D:282:TYR:CD2	1:D:304:LEU:HD13	2.44	0.53
1:D:708:LYS:CE	2:G:362:ASP:N	2.71	0.53
2:E:87:GLN:NE2	2:E:157:TYR:OH	2.33	0.53
2:H:19:PHE:CE2	2:H:190:LYS:HG2	2.44	0.53
2:H:84:ASP:HA	2:H:87:GLN:HB2	1.91	0.53
2:H:203:LEU:HD23	2:H:203:LEU:O	2.09	0.53
1:A:59:HIS:O	1:A:62:ILE:HG12	2.09	0.52
1:B:441:GLU:HB2	1:B:619:LEU:O	2.09	0.52
1:B:525:ALA:CB	1:B:662:LEU:HD13	2.39	0.52
1:C:233:SER:O	1:C:237:ILE:HG13	2.09	0.52
1:C:328:ASN:HD22	1:C:328:ASN:N	2.05	0.52
1:D:658:ASP:OD2	1:D:662:LEU:HG	2.09	0.52
2:F:309:GLU:CB	2:F:328:ARG:HH11	2.16	0.52
2:G:69:GLU:CD	2:G:221:ARG:HH12	2.17	0.52
2:G:105:GLU:O	2:G:109:GLU:HG3	2.08	0.52
1:A:229:GLU:OE2	1:A:448:PRO:HD3	2.09	0.52
1:A:676:ASP:O	1:A:680:GLN:HB2	2.10	0.52
1:B:436:SER:HG	1:B:440:LEU:HA	1.74	0.52
1:B:568:PHE:CD2	1:B:574:ALA:HB2	2.43	0.52
1:B:576:GLY:HA3	1:B:607:LYS:HZ3	1.73	0.52
1:C:279:ILE:HG21	1:C:328:ASN:HA	1.92	0.52
1:C:436:SER:CB	1:C:440:LEU:HD13	2.36	0.52
1:D:519:ASN:ND2	1:D:522:TYR:HB3	2.24	0.52
1:D:519:ASN:CB	1:D:631:ALA:HB1	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3:THR:HG21	2:E:6:SER:HA	1.90	0.52
2:E:35:ILE:C	2:E:35:ILE:HD13	2.33	0.52
1:B:670:TRP:CZ2	1:B:735:ARG:HA	2.45	0.52
1:C:85:ALA:O	1:C:89:LEU:HG	2.10	0.52
1:C:330:VAL:HB	1:C:335:TYR:OH	2.09	0.52
1:C:722:TYR:HD2	2:E:375:LEU:HD22	1.74	0.52
1:D:320:LYS:CB	1:D:409:THR:HG21	2.39	0.52
2:G:76:ASN:HD21	2:G:211:SER:HA	1.74	0.52
1:B:78:GLN:OE1	1:B:655:VAL:HG23	2.09	0.52
1:D:19:LEU:CD1	2:G:296:MET:CA	2.81	0.52
1:D:613:ASN:HB2	1:D:616:LEU:CD2	2.40	0.52
1:D:685:MET:O	1:D:689:ILE:HG12	2.09	0.52
2:E:196:CYS:O	2:E:200:VAL:HG23	2.10	0.52
2:H:76:ASN:HD21	2:H:211:SER:HA	1.73	0.52
2:H:332:ILE:O	2:H:335:ILE:HG22	2.08	0.52
1:A:356:PHE:HE1	1:A:390:LYS:HE3	1.75	0.52
1:A:403:MET:HE3	1:A:714:LEU:HB3	1.91	0.52
1:B:403:MET:HE3	1:B:714:LEU:HB3	1.91	0.52
1:C:357:SER:O	1:C:361:VAL:HG22	2.10	0.52
1:C:472:ILE:CG2	1:C:477:GLU:CB	2.88	0.52
2:E:121:SER:O	2:E:125:ILE:HG13	2.09	0.52
2:G:121:SER:O	2:G:125:ILE:HG13	2.10	0.52
1:A:214:GLY:O	1:A:215:VAL:C	2.51	0.52
1:B:229:GLU:OE2	1:B:448:PRO:HD3	2.08	0.52
1:D:439:CYS:SG	4:D:802:DAT:H3'	2.50	0.52
1:D:622:SER:OG	1:D:625:SER:OG	2.27	0.52
2:E:123:THR:HG21	2:H:28:TYR:H	1.75	0.52
1:A:39:SER:OG	2:F:332:ILE:HG22	2.10	0.52
1:B:49:PHE:HE2	2:H:297:ILE:HD11	1.75	0.52
1:B:208:PRO:CG	1:B:464:LEU:HB2	2.39	0.52
1:B:217:THR:HG23	1:B:218:PRO:HD2	1.92	0.52
1:C:131:MET:HA	1:C:134:PHE:CD2	2.44	0.52
1:C:369:PHE:CG	1:C:434:ARG:HG2	2.44	0.52
1:C:441:GLU:O	1:C:691:GLN:HB3	2.09	0.52
1:C:510:ARG:NH1	1:C:567:TRP:CE3	2.78	0.52
1:C:678:TYR:HE1	1:C:695:ALA:HB1	1.75	0.52
1:D:472:ILE:HD13	1:D:478:LEU:HD21	1.92	0.52
1:D:696:ASN:H	1:D:696:ASN:ND2	2.08	0.52
1:D:700:ASP:OD1	1:D:735:ARG:HD3	2.09	0.52
2:E:42:LYS:HE3	2:E:46:PHE:HZ	1.74	0.52
2:E:258:ASP:CB	2:E:261:MET:HG2	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:259:PRO:O	2:E:263:GLU:OE2	2.28	0.52
2:G:79:TYR:CZ	2:G:149:ARG:HD3	2.44	0.52
2:G:96:LEU:N	2:G:97:PRO:CD	2.73	0.52
1:C:19:LEU:CD1	2:E:295:SER:O	2.57	0.52
1:D:283:LYS:HG2	1:D:330:VAL:HG23	1.91	0.52
1:D:367:ALA:O	1:D:371:ASP:O	2.27	0.52
1:D:647:SER:HB2	1:D:652:LEU:HD11	1.92	0.52
2:F:31:GLN:HG2	2:F:37:GLU:HB2	1.92	0.52
2:F:120:ARG:HG2	2:G:28:TYR:CE2	2.45	0.52
2:G:304:LEU:HD23	2:G:304:LEU:C	2.35	0.52
1:A:420:CYS:O	1:A:424:SER:CB	2.57	0.52
1:B:9:LYS:HA	1:B:55:THR:CG2	2.40	0.52
1:B:51:ASP:C	1:B:51:ASP:OD2	2.52	0.52
1:B:356:PHE:CE1	1:B:390:LYS:HB2	2.43	0.52
1:B:367:ALA:O	1:B:371:ASP:O	2.28	0.52
1:C:17:ILE:HD11	1:C:49:PHE:CE1	2.45	0.52
1:D:470:GLY:HA3	1:D:519:ASN:ND2	2.25	0.52
2:F:74:ILE:O	2:F:78:LYS:HG3	2.10	0.52
2:H:86:ILE:HG21	2:H:153:ILE:HG21	1.91	0.52
1:A:240:THR:O	1:A:244:ILE:HG13	2.09	0.52
1:A:286:GLN:CD	1:A:332:HIS:HB2	2.35	0.52
1:A:568:PHE:O	1:A:570:GLU:N	2.43	0.52
1:A:617:SER:OG	1:A:689:ILE:HA	2.10	0.52
1:C:449:LEU:HG	1:C:457:GLY:HA3	1.92	0.52
1:D:152:GLU:O	1:D:158:GLN:NE2	2.43	0.52
2:H:299:LEU:HD11	2:H:304:LEU:CB	2.16	0.52
1:A:5:LEU:C	1:A:6:LEU:HD22	2.35	0.51
1:A:425:PRO:HG3	1:A:615:THR:HG22	1.92	0.51
1:A:530:ARG:HB2	1:A:533:ASP:OD2	2.10	0.51
1:A:627:GLN:HE22	1:A:645:LYS:CE	2.23	0.51
1:B:6:LEU:N	1:B:6:LEU:HD22	2.24	0.51
1:B:516:GLY:CA	1:B:618:ALA:O	2.59	0.51
1:B:576:GLY:HA3	1:B:607:LYS:HZ1	1.74	0.51
1:C:149:LYS:HG2	1:C:652:LEU:CD2	2.39	0.51
1:C:340:ASN:HB3	1:C:368:PHE:CZ	2.45	0.51
1:C:437:ASN:O	1:C:440:LEU:HD22	2.10	0.51
1:C:689:ILE:HG22	1:C:691:GLN:O	2.10	0.51
1:D:172:LEU:O	1:D:176:VAL:HG23	2.10	0.51
1:D:320:LYS:HD3	1:D:409:THR:HG21	1.91	0.51
1:D:464:LEU:HB3	1:D:620:MET:CE	2.41	0.51
2:E:174:THR:HG23	2:E:181:THR:CG2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:55:VAL:HA	2:H:58:ASP:OD1	2.10	0.51
1:A:155:TYR:HE1	1:A:209:THR:HA	1.75	0.51
1:A:322:ASN:ND2	1:A:323:ARG:NH1	2.59	0.51
1:A:519:ASN:HA	1:A:632:THR:OG1	2.11	0.51
1:A:568:PHE:O	1:A:571:THR:N	2.40	0.51
1:A:622:SER:HB3	4:A:802:DAT:O2A	2.10	0.51
1:B:233:SER:HA	3:B:803:DTP:H3'	1.92	0.51
1:C:286:GLN:CD	1:C:332:HIS:HB2	2.36	0.51
1:C:301:ALA:HB3	1:C:438:LEU:CD2	2.40	0.51
1:C:439:CYS:HA	1:C:730:TYR:CE1	2.44	0.51
1:C:685:MET:O	1:C:689:ILE:HG12	2.09	0.51
1:D:151:LEU:HD23	1:D:155:TYR:CD2	2.45	0.51
1:A:134:PHE:CZ	1:A:194:LYS:HD2	2.45	0.51
1:B:380:THR:HA	1:B:383:GLU:OE1	2.11	0.51
1:B:676:ASP:O	1:B:680:GLN:HB2	2.10	0.51
1:C:301:ALA:HB3	1:C:438:LEU:HD21	1.93	0.51
1:C:340:ASN:CG	1:C:368:PHE:HE1	2.15	0.51
1:D:357:SER:O	1:D:361:VAL:HG22	2.10	0.51
2:F:9:LYS:HD2	2:G:142:THR:HG23	1.92	0.51
2:F:76:ASN:HD21	2:F:211:SER:HA	1.75	0.51
2:F:96:LEU:HB2	2:F:97:PRO:HD3	1.91	0.51
2:H:35:ILE:HG23	2:H:36:PHE:N	2.26	0.51
1:A:230:CYS:HB2	1:A:240:THR:HG21	1.93	0.51
1:A:361:VAL:HG23	1:A:361:VAL:O	2.10	0.51
1:C:492:LEU:O	1:C:496:GLN:HG2	2.11	0.51
1:D:222:PHE:CD2	1:D:492:LEU:HD11	2.45	0.51
1:D:592:ASN:HD22	1:D:592:ASN:N	2.07	0.51
2:G:31:GLN:HG2	2:G:37:GLU:HB2	1.92	0.51
1:A:367:ALA:O	1:A:371:ASP:O	2.28	0.51
1:D:7:VAL:HG21	3:D:801:DTP:HN62	1.71	0.51
1:D:551:LEU:O	1:D:616:LEU:HD12	2.10	0.51
2:E:2:TYR:HE2	2:H:93:VAL:HG11	1.75	0.51
2:E:300:ASN:CG	2:E:303:ILE:HG22	2.35	0.51
2:E:332:ILE:O	2:E:335:ILE:HG22	2.09	0.51
2:F:3:THR:HA	2:G:158:ASP:CG	2.36	0.51
2:F:42:LYS:HE3	2:F:46:PHE:HZ	1.75	0.51
2:F:196:CYS:O	2:F:200:VAL:HG23	2.10	0.51
2:G:10:ASN:ND2	2:G:15:GLU:HG3	2.24	0.51
2:G:62:TYR:CZ	2:G:70:LYS:CG	2.92	0.51
2:G:216:PHE:HB3	2:G:338:TRP:NE1	2.25	0.51
2:H:96:LEU:HB2	2:H:97:PRO:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:121:SER:O	2:H:125:ILE:HG13	2.11	0.51
2:H:326:GLN:NE2	2:H:328:ARG:NH1	2.59	0.51
1:A:370:ALA:HA	1:A:428:PRO:HB3	1.93	0.51
1:B:63:ILE:HG12	1:B:84:LEU:HB3	1.93	0.51
1:C:72:ARG:HG3	1:C:659:TYR:CZ	2.44	0.51
1:D:442:ILE:HG23	1:D:691:GLN:OE1	2.11	0.51
2:E:76:ASN:HD21	2:E:211:SER:HA	1.76	0.51
2:E:258:ASP:CB	2:E:261:MET:CG	2.85	0.51
2:G:62:TYR:HD1	2:G:65:LEU:HD12	1.72	0.51
2:H:31:GLN:HG2	2:H:37:GLU:HB2	1.91	0.51
1:A:440:LEU:HD23	1:A:728:THR:HB	1.93	0.51
1:A:592:ASN:HD22	1:A:592:ASN:N	2.05	0.51
1:B:423:HIS:CD2	1:B:423:HIS:O	2.63	0.51
1:B:644:ILE:HG23	1:B:651:ILE:HG22	1.92	0.51
1:D:309:TRP:CZ3	1:D:364:LEU:HD12	2.45	0.51
1:D:437:ASN:O	1:D:440:LEU:HD22	2.10	0.51
2:E:303:ILE:HA	2:E:306:GLN:NE2	2.26	0.51
1:B:489:LEU:CB	1:B:513:LEU:HD11	2.40	0.51
1:B:619:LEU:HD12	1:B:693:ILE:HD13	1.93	0.51
1:C:305:PHE:HE2	1:C:440:LEU:HD11	1.76	0.51
2:F:203:LEU:C	2:F:203:LEU:HD23	2.36	0.51
2:F:279:ALA:O	2:F:283:GLU:HG2	2.10	0.51
2:G:42:LYS:HE3	2:G:46:PHE:HZ	1.75	0.51
1:A:115:TYR:HD1	1:A:216:ARG:O	1.94	0.51
1:A:279:ILE:HD13	1:A:328:ASN:HB2	1.93	0.51
1:A:326:GLU:O	1:A:328:ASN:N	2.44	0.51
1:A:568:PHE:CZ	1:A:574:ALA:N	2.79	0.51
1:A:669:LEU:HD12	1:A:672:MET:HE2	1.91	0.51
1:B:230:CYS:HB2	1:B:240:THR:HG21	1.92	0.51
1:D:23:HIS:HE1	1:D:42:GLU:OE1	1.94	0.51
1:A:180:LEU:HD13	1:A:488:ALA:HB1	1.92	0.51
1:A:568:PHE:C	1:A:570:GLU:N	2.67	0.51
1:A:670:TRP:CE2	1:A:735:ARG:HG3	2.46	0.51
1:B:474:ASN:HD21	1:B:477:GLU:HG3	1.76	0.51
1:B:482:ALA:O	1:B:486:VAL:HG23	2.11	0.51
1:B:619:LEU:HB2	1:B:693:ILE:HA	1.93	0.51
1:C:59:HIS:CD2	1:C:88:HIS:HB2	2.46	0.51
2:G:74:ILE:O	2:G:78:LYS:HG3	2.11	0.51
2:G:90:SER:HB3	2:G:157:TYR:CD1	2.46	0.51
2:G:245:THR:O	2:G:249:LEU:HG	2.11	0.51
2:G:258:ASP:OD2	2:G:261:MET:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:291:PHE:O	2:G:294:GLY:N	2.38	0.51
1:A:50:TYR:H	1:A:53:ILE:HG21	1.75	0.50
1:B:423:HIS:HE1	1:B:579:PRO:CB	2.21	0.50
1:C:115:TYR:CZ	1:C:175:LEU:CD1	2.88	0.50
1:C:712:GLN:HE22	2:E:370:LEU:HG	1.76	0.50
1:D:35:ASN:ND2	1:D:74:ALA:HB2	2.25	0.50
1:D:377:ARG:HG2	1:D:377:ARG:HH11	1.75	0.50
1:D:637:PRO:CG	1:D:669:LEU:HD13	2.39	0.50
2:F:207:ARG:NH2	2:F:282:GLN:HE22	2.07	0.50
2:G:19:PHE:CE2	2:G:190:LYS:HG2	2.46	0.50
2:G:143:ASN:HB3	2:G:146:ILE:HG12	1.93	0.50
2:G:186:LEU:HG	2:G:190:LYS:HE3	1.93	0.50
2:G:291:PHE:C	2:G:293:ASP:N	2.67	0.50
2:H:125:ILE:HG12	2:H:230:ILE:HD12	1.94	0.50
1:A:226:VAL:HG21	1:A:247:TYR:CD1	2.45	0.50
1:B:34:HIS:O	1:B:36:VAL:HG13	2.11	0.50
1:B:306:TYR:OH	1:B:317:LEU:HD22	2.12	0.50
1:B:334:ASP:OD1	1:B:411:ARG:HB3	2.11	0.50
1:C:474:ASN:HD22	1:C:474:ASN:N	2.07	0.50
1:C:568:PHE:CE2	1:C:574:ALA:HB2	2.45	0.50
1:D:40:GLN:HE22	1:D:44:ARG:NH1	2.09	0.50
1:D:532:SER:HB3	1:D:673:PRO:HD2	1.93	0.50
2:E:19:PHE:CE2	2:E:190:LYS:HG2	2.46	0.50
2:E:79:TYR:CE1	2:E:149:ARG:CD	2.87	0.50
2:F:19:PHE:CE2	2:F:190:LYS:HG2	2.46	0.50
1:B:82:ALA:O	1:B:86:ILE:HG12	2.11	0.50
1:B:489:LEU:CB	1:B:513:LEU:CD1	2.89	0.50
2:H:301:LYS:O	2:H:302:ASP:C	2.53	0.50
1:A:86:ILE:O	1:A:90:ARG:HG2	2.12	0.50
1:A:681:LEU:O	1:A:685:MET:HG3	2.10	0.50
1:A:706:SER:HB2	1:A:708:LYS:HG2	1.94	0.50
1:B:356:PHE:CD1	1:B:390:LYS:HB3	2.42	0.50
1:B:529:LYS:HD2	1:B:535:SER:O	2.11	0.50
1:D:7:VAL:CG2	1:D:15:GLU:O	2.59	0.50
2:E:127:ARG:NH2	2:H:29:ASP:HA	2.27	0.50
2:E:186:LEU:HG	2:E:190:LYS:HE3	1.92	0.50
2:E:191:LYS:HG2	2:E:264:ILE:CG2	2.40	0.50
2:F:166:TYR:CE1	2:G:169:LEU:HD13	2.46	0.50
2:G:62:TYR:CZ	2:G:70:LYS:CD	2.94	0.50
1:A:380:THR:HA	1:A:383:GLU:OE1	2.11	0.50
1:A:568:PHE:HE2	1:A:574:ALA:HA	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ILE:HD13	1:B:328:ASN:HB2	1.93	0.50
1:C:303:THR:O	1:C:305:PHE:CE1	2.64	0.50
1:D:217:THR:HB	1:D:218:PRO:CD	2.41	0.50
1:D:340:ASN:HB3	1:D:368:PHE:CE1	2.46	0.50
1:D:430:ILE:HG21	1:D:570:GLU:HG2	1.93	0.50
2:F:125:ILE:HG12	2:F:230:ILE:HD12	1.94	0.50
2:F:174:THR:HG23	2:F:181:THR:HG22	1.93	0.50
1:A:303:THR:OG1	1:A:438:LEU:HD12	2.12	0.50
1:A:633:ASN:OD1	1:A:633:ASN:O	2.30	0.50
1:A:669:LEU:HD11	1:A:698:ASN:CG	2.36	0.50
1:B:404:GLN:HA	2:H:361:ILE:HD11	1.92	0.50
1:B:519:ASN:HB2	1:B:631:ALA:CB	2.34	0.50
1:B:568:PHE:CD1	1:B:571:THR:OG1	2.64	0.50
1:B:711:MET:HB2	2:H:363:SER:HA	1.94	0.50
1:C:377:ARG:HG2	1:C:377:ARG:HH11	1.76	0.50
1:C:723:LYS:HG3	2:E:375:LEU:O	2.10	0.50
1:D:7:VAL:HG22	1:D:15:GLU:O	2.11	0.50
2:E:33:TYR:HB3	2:E:35:ILE:HG22	1.93	0.50
2:F:123:THR:HG21	2:G:28:TYR:H	1.76	0.50
2:F:186:LEU:HG	2:F:190:LYS:HE3	1.92	0.50
2:H:300:ASN:OD1	2:H:303:ILE:CG1	2.48	0.50
1:A:8:THR:HB	1:A:54:LYS:HA	1.93	0.50
1:A:426:PHE:CD2	1:A:445:PRO:HD3	2.45	0.50
1:A:576:GLY:HA3	1:A:607:LYS:HZ1	1.76	0.50
1:B:437:ASN:HB3	1:B:442:ILE:HB	1.93	0.50
1:C:249:SER:HB2	3:D:803:DTP:N6	2.26	0.50
1:D:449:LEU:HG	1:D:457:GLY:HA3	1.93	0.50
2:F:304:LEU:C	2:F:304:LEU:HD23	2.37	0.50
2:G:140:ILE:HG22	2:G:146:ILE:HG21	1.94	0.50
2:H:186:LEU:HG	2:H:190:LYS:HE3	1.94	0.50
1:A:598:ASP:OD1	1:A:598:ASP:O	2.30	0.50
1:A:670:TRP:CZ2	1:A:735:ARG:HA	2.46	0.50
1:B:530:ARG:HB3	1:B:667:GLU:OE2	2.11	0.50
1:C:39:SER:HB3	2:E:298:GLY:O	2.12	0.50
1:C:406:ARG:NH2	1:C:697:THR:CG2	2.75	0.50
1:D:115:TYR:HD1	1:D:217:THR:HG22	1.76	0.50
1:D:149:LYS:HG2	1:D:652:LEU:CD2	2.40	0.50
2:H:363:SER:O	2:H:364:GLU:C	2.54	0.50
1:A:306:TYR:OH	1:A:317:LEU:HD22	2.12	0.50
1:B:559:ALA:O	1:B:563:GLY:CA	2.60	0.50
1:B:568:PHE:CZ	1:B:574:ALA:N	2.80	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:HIS:HA	1:C:170:GLN:HG3	1.94	0.50
1:C:162:THR:OG1	1:C:164:GLU:HG3	2.12	0.50
1:C:519:ASN:CB	1:C:631:ALA:HB1	2.38	0.50
1:D:94:TYR:C	1:D:96:GLN:H	2.19	0.50
1:D:357:SER:OG	1:D:358:PRO:HD2	2.12	0.50
2:G:42:LYS:HE3	2:G:46:PHE:CZ	2.47	0.50
2:G:291:PHE:CZ	2:G:299:LEU:HB3	2.46	0.50
1:A:54:LYS:HE3	1:A:57:ASP:OD2	2.12	0.49
1:A:340:ASN:OD1	1:A:343:MET:HG2	2.12	0.49
1:A:644:ILE:HG21	1:A:651:ILE:HD13	1.94	0.49
1:B:515:ILE:HD12	1:B:551:LEU:HD22	1.94	0.49
1:C:42:GLU:OE1	2:E:298:GLY:HA2	2.12	0.49
1:D:176:VAL:O	1:D:180:LEU:HG	2.12	0.49
1:D:439:CYS:HA	1:D:730:TYR:CE1	2.47	0.49
2:F:157:TYR:O	2:F:161:ILE:HG13	2.11	0.49
2:H:67:GLU:HG3	2:H:68:HIS:N	2.27	0.49
2:H:163:MET:SD	2:H:192:LYS:HG3	2.51	0.49
1:A:519:ASN:ND2	1:A:522:TYR:HB3	2.28	0.49
1:B:286:GLN:CD	1:B:332:HIS:HB2	2.37	0.49
1:C:17:ILE:CD1	1:C:49:PHE:CE1	2.95	0.49
1:D:341:LYS:O	1:D:341:LYS:HD3	2.13	0.49
1:D:506:GLY:HA2	1:D:567:TRP:CZ3	2.46	0.49
1:D:510:ARG:HB2	1:D:614:SER:OG	2.11	0.49
1:D:678:TYR:HE1	1:D:695:ALA:HB1	1.76	0.49
2:E:31:GLN:HG2	2:E:37:GLU:HB2	1.92	0.49
2:F:175:HIS:CG	2:G:178:ASN:HD21	2.28	0.49
2:F:303:ILE:HA	2:F:306:GLN:NE2	2.27	0.49
2:H:287:ALA:O	2:H:291:PHE:CD2	2.64	0.49
1:B:509:GLY:HA3	1:B:567:TRP:CE3	2.46	0.49
1:C:669:LEU:HD11	1:C:698:ASN:ND2	2.27	0.49
2:E:42:LYS:HE3	2:E:46:PHE:CZ	2.47	0.49
2:G:62:TYR:HA	2:G:65:LEU:HG	1.94	0.49
2:G:196:CYS:O	2:G:200:VAL:HG23	2.12	0.49
2:H:244:GLY:O	2:H:248:MET:HG3	2.13	0.49
1:A:208:PRO:CG	1:A:464:LEU:HB2	2.42	0.49
1:B:621:PRO:CG	1:B:694:SER:HB3	2.42	0.49
1:C:176:VAL:HA	1:C:215:VAL:CG1	2.42	0.49
1:D:5:LEU:N	1:D:51:ASP:OD1	2.45	0.49
1:D:301:ALA:HB3	1:D:438:LEU:HD21	1.94	0.49
2:E:153:ILE:HD12	2:E:203:LEU:HD11	1.89	0.49
2:F:175:HIS:HB3	2:G:178:ASN:HD21	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:VAL:HG21	2:G:230:ILE:HG12	1.93	0.49
2:H:59:ARG:O	2:H:59:ARG:HG2	2.12	0.49
1:A:459:ILE:HB	1:A:503:ALA:HA	1.95	0.49
1:A:474:ASN:HD21	1:A:477:GLU:HG3	1.77	0.49
1:C:615:THR:HG21	1:C:691:GLN:HE22	1.77	0.49
1:C:692:SER:OG	1:C:727:LYS:HB2	2.11	0.49
1:C:722:TYR:CE2	2:E:375:LEU:HD13	2.47	0.49
1:D:40:GLN:OE1	1:D:44:ARG:CG	2.60	0.49
1:D:55:THR:HG21	3:D:801:DTP:O3A	2.13	0.49
1:D:439:CYS:O	1:D:440:LEU:HB2	2.11	0.49
2:E:304:LEU:HD23	2:E:304:LEU:C	2.37	0.49
2:G:125:ILE:HG12	2:G:230:ILE:HD12	1.94	0.49
2:H:42:LYS:HE3	2:H:46:PHE:HZ	1.77	0.49
2:H:153:ILE:HD11	2:H:203:LEU:HD12	1.88	0.49
2:H:288:ASP:HB2	2:H:301:LYS:HE3	1.93	0.49
1:A:37:SER:OG	1:A:40:GLN:HB2	2.13	0.49
1:B:7:VAL:O	1:B:7:VAL:CG2	2.60	0.49
1:B:519:ASN:HA	1:B:632:THR:OG1	2.12	0.49
1:C:529:LYS:HD2	1:C:535:SER:O	2.12	0.49
1:D:529:LYS:HD2	1:D:535:SER:O	2.12	0.49
2:G:90:SER:HB3	2:G:157:TYR:CE1	2.48	0.49
2:H:87:GLN:OE1	2:H:87:GLN:CA	2.54	0.49
2:H:90:SER:HB3	2:H:157:TYR:CD1	2.48	0.49
1:A:28:TRP:O	1:A:31:GLU:HB2	2.13	0.49
1:A:369:PHE:HD1	1:A:417:VAL:HB	1.77	0.49
1:A:689:ILE:HG22	1:A:691:GLN:H	1.78	0.49
1:B:293:SER:O	1:B:294:GLN:C	2.54	0.49
1:C:134:PHE:HD1	1:C:194:LYS:HZ3	1.60	0.49
1:C:215:VAL:O	1:C:216:ARG:CB	2.60	0.49
1:C:532:SER:HB3	1:C:673:PRO:HD2	1.93	0.49
1:D:474:ASN:HD22	1:D:474:ASN:N	2.06	0.49
2:E:148:LYS:HG2	2:E:149:ARG:H	1.77	0.49
2:F:68:HIS:CE1	2:F:69:GLU:HG3	2.48	0.49
2:F:197:LEU:HB2	2:F:249:LEU:HD21	1.95	0.49
2:G:255:GLY:CA	2:G:262:ALA:HB2	2.42	0.49
2:H:10:ASN:HD22	2:H:15:GLU:CG	2.24	0.49
2:H:10:ASN:ND2	2:H:15:GLU:HG3	2.24	0.49
1:A:196:PHE:HA	1:A:484:LEU:HD21	1.95	0.49
1:A:415:GLN:HE21	1:A:417:VAL:HG12	1.78	0.49
1:B:125:GLU:HG2	1:B:129:LYS:HE2	1.95	0.49
1:B:228:ILE:N	1:B:435:GLN:NE2	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:VAL:CG1	1:B:300:GLY:C	2.85	0.49
1:B:618:ALA:HA	1:B:691:GLN:HB2	1.94	0.49
1:C:225:CYS:HB3	4:C:802:DAT:H2'1	1.94	0.49
1:C:309:TRP:CZ3	1:C:364:LEU:HD12	2.48	0.49
1:D:176:VAL:HA	1:D:215:VAL:CG1	2.41	0.49
2:G:33:TYR:HB3	2:G:35:ILE:HG22	1.94	0.49
2:H:92:ASN:HA	2:H:96:LEU:HG	1.95	0.49
2:H:300:ASN:O	2:H:301:LYS:C	2.56	0.49
1:B:21:LYS:O	1:B:25:VAL:HG23	2.12	0.49
1:B:256:ILE:HB	1:B:304:LEU:HG	1.93	0.49
1:B:568:PHE:HE2	1:B:574:ALA:HA	1.75	0.49
1:B:644:ILE:CG2	1:B:651:ILE:CG2	2.90	0.49
1:D:7:VAL:N	1:D:15:GLU:O	2.23	0.49
1:D:63:ILE:HG12	1:D:84:LEU:HB3	1.95	0.49
2:G:203:LEU:HD23	2:G:203:LEU:C	2.37	0.49
1:A:19:LEU:CD1	2:F:295:SER:O	2.61	0.49
1:A:258:ALA:C	1:A:260:ARG:H	2.20	0.49
1:A:418:ASP:O	1:A:422:THR:OG1	2.20	0.49
1:A:430:ILE:CG2	1:A:570:GLU:HG2	2.42	0.49
1:B:131:MET:HA	1:B:134:PHE:CD2	2.47	0.49
1:C:78:GLN:HE22	1:C:655:VAL:HB	1.78	0.49
1:C:276:THR:HG21	1:D:291:SER:O	2.13	0.49
1:C:613:ASN:HB2	1:C:616:LEU:CD2	2.43	0.49
2:E:40:ILE:O	2:E:44:LEU:HG	2.13	0.49
2:E:300:ASN:H	2:E:303:ILE:HG22	1.78	0.49
2:F:92:ASN:HA	2:F:96:LEU:HG	1.95	0.49
2:F:171:GLY:O	2:F:184:VAL:HB	2.13	0.49
2:F:203:LEU:HA	2:F:207:ARG:HD2	1.95	0.49
2:H:142:THR:O	2:H:143:ASN:C	2.56	0.49
1:A:435:GLN:HG3	1:A:436:SER:N	2.28	0.48
1:C:406:ARG:HH21	1:C:697:THR:HG21	1.75	0.48
1:C:551:LEU:C	1:C:616:LEU:CD1	2.85	0.48
1:C:696:ASN:H	1:C:696:ASN:ND2	2.10	0.48
1:D:262:ARG:HA	1:D:358:PRO:CG	2.42	0.48
2:F:10:ASN:HD22	2:F:15:GLU:CG	2.24	0.48
2:F:42:LYS:HE3	2:F:46:PHE:CZ	2.48	0.48
2:G:93:VAL:CG1	2:G:161:ILE:HD13	2.43	0.48
1:A:21:LYS:O	1:A:25:VAL:HG23	2.13	0.48
1:A:159:ASN:HB3	1:A:162:THR:OG1	2.13	0.48
1:A:179:CYS:HB2	1:A:215:VAL:CG1	2.42	0.48
1:B:85:ALA:O	1:B:89:LEU:HG	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:HG12	1:C:84:LEU:HB3	1.95	0.48
1:C:119:LEU:HD21	1:C:179:CYS:SG	2.53	0.48
1:C:470:GLY:HA3	1:C:519:ASN:ND2	2.27	0.48
2:F:3:THR:HG23	2:F:5:PHE:C	2.38	0.48
1:A:334:ASP:OD1	1:A:411:ARG:HB3	2.13	0.48
1:A:472:ILE:HD13	1:A:478:LEU:HD21	1.95	0.48
1:A:599:TRP:C	1:A:601:ALA:N	2.67	0.48
1:B:217:THR:CG2	1:B:219:THR:HG22	2.43	0.48
1:B:328:ASN:HD22	1:B:328:ASN:N	2.04	0.48
1:B:413:TYR:HB3	1:B:440:LEU:CD2	2.42	0.48
1:C:297:VAL:O	1:C:297:VAL:HG12	2.13	0.48
1:D:297:VAL:O	1:D:297:VAL:HG12	2.12	0.48
1:D:415:GLN:HA	1:D:728:THR:HG22	1.94	0.48
2:E:93:VAL:HG11	2:H:2:TYR:HE2	1.78	0.48
2:F:125:ILE:HG21	2:F:227:ASN:ND2	2.22	0.48
2:F:126:ILE:O	2:F:129:ILE:HG12	2.12	0.48
2:F:309:GLU:CD	2:F:328:ARG:NH1	2.67	0.48
2:G:35:ILE:HG23	2:G:36:PHE:N	2.27	0.48
2:G:84:ASP:HA	2:G:87:GLN:HB2	1.93	0.48
2:G:197:LEU:CB	2:G:249:LEU:HD21	2.43	0.48
1:A:69:LEU:CD1	1:A:77:TYR:CE1	2.96	0.48
1:A:517:VAL:HG22	1:A:619:LEU:CD2	2.44	0.48
1:B:79:TYR:CD1	1:B:143:PHE:O	2.67	0.48
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.95	0.48
1:C:23:HIS:HD2	1:C:42:GLU:OE2	1.92	0.48
1:C:94:TYR:C	1:C:96:GLN:H	2.20	0.48
1:C:172:LEU:HD23	1:C:172:LEU:C	2.38	0.48
1:C:341:LYS:O	1:C:341:LYS:HD3	2.14	0.48
1:C:413:TYR:CZ	1:C:731:TYR:HE1	2.27	0.48
1:D:37:SER:OG	1:D:40:GLN:HB2	2.13	0.48
2:F:258:ASP:OD2	2:F:261:MET:HG2	2.13	0.48
2:H:326:GLN:HE21	2:H:328:ARG:HH12	1.60	0.48
1:A:411:ARG:NH1	1:A:731:TYR:OH	2.46	0.48
1:B:102:LEU:O	1:B:106:VAL:HG23	2.13	0.48
1:B:356:PHE:HE1	1:B:390:LYS:CB	2.05	0.48
1:D:415:GLN:OE1	1:D:436:SER:HB2	2.13	0.48
2:G:289:TYR:CG	2:G:289:TYR:O	2.66	0.48
1:A:268:ILE:HD13	3:A:803:DTP:C8	2.43	0.48
1:B:114:LYS:O	1:B:218:PRO:HD3	2.14	0.48
1:B:466:ALA:CB	1:B:518:ILE:HG23	2.42	0.48
1:C:276:THR:HB	3:C:803:DTP:H2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASN:HD22	1:C:592:ASN:N	2.07	0.48
2:F:40:ILE:O	2:F:44:LEU:HG	2.13	0.48
2:H:55:VAL:HG23	2:H:128:ASN:ND2	2.29	0.48
2:H:225:GLU:O	2:H:228:ALA:HB3	2.13	0.48
1:A:9:LYS:HA	1:A:55:THR:CG2	2.44	0.48
1:A:348:LEU:HD21	1:A:719:LEU:HD13	1.96	0.48
1:A:510:ARG:HB2	1:A:614:SER:OG	2.14	0.48
1:A:512:THR:HG22	1:A:614:SER:HB2	1.95	0.48
1:A:633:ASN:OD1	1:A:636:GLU:HB2	2.14	0.48
1:A:710:PRO:HA	2:F:362:ASP:HB2	1.87	0.48
1:B:40:GLN:OE1	1:B:44:ARG:HG3	2.13	0.48
1:B:146:ALA:O	1:B:150:GLN:HG2	2.13	0.48
1:C:317:LEU:HD11	1:C:337:VAL:HG21	1.96	0.48
1:D:303:THR:O	1:D:305:PHE:CE1	2.66	0.48
2:G:217:ALA:HB2	2:G:299:LEU:CD2	2.43	0.48
1:A:146:ALA:O	1:A:150:GLN:HG2	2.14	0.48
1:A:644:ILE:CG2	1:A:651:ILE:HB	2.44	0.48
1:D:301:ALA:HB3	1:D:438:LEU:CD2	2.43	0.48
1:D:339:ILE:HD13	1:D:399:PHE:HE1	1.78	0.48
1:D:492:LEU:O	1:D:496:GLN:HG2	2.13	0.48
1:D:519:ASN:HA	1:D:632:THR:OG1	2.14	0.48
2:F:33:TYR:HB3	2:F:35:ILE:HG22	1.94	0.48
2:H:197:LEU:HB2	2:H:249:LEU:HD21	1.94	0.48
1:A:19:LEU:HD12	2:F:295:SER:C	2.39	0.48
1:A:69:LEU:HD12	1:A:77:TYR:CE1	2.48	0.48
1:A:564:ALA:HB2	1:A:609:HIS:O	2.14	0.48
1:B:362:PRO:C	1:B:364:LEU:H	2.21	0.48
1:C:9:LYS:HD2	1:C:15:GLU:OE1	2.14	0.48
1:C:234:LEU:HG	3:C:803:DTP:H2'2	1.96	0.48
1:C:700:ASP:OD2	1:C:702:SER:HB2	2.14	0.48
1:D:309:TRP:CH2	1:D:364:LEU:HD12	2.48	0.48
1:D:517:VAL:HG22	1:D:619:LEU:HD22	1.95	0.48
2:H:90:SER:HB3	2:H:157:TYR:CE1	2.48	0.48
1:A:517:VAL:HG11	1:A:547:ILE:HD13	1.96	0.48
1:B:145:TYR:O	1:B:149:LYS:HB2	2.14	0.48
1:B:700:ASP:OD2	1:B:702:SER:HB2	2.13	0.48
1:C:229:GLU:OE2	1:C:448:PRO:HD3	2.14	0.48
1:C:506:GLY:HA2	1:C:567:TRP:CZ3	2.49	0.48
1:D:59:HIS:HB2	3:D:801:DTP:H4'	1.95	0.48
1:D:293:SER:OG	1:D:298:ARG:O	2.30	0.48
2:E:87:GLN:O	2:E:91:PRO:CD	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:172:GLU:HA	2:E:184:VAL:O	2.14	0.48
2:G:51:GLU:OE1	2:G:51:GLU:N	2.47	0.48
2:G:303:ILE:HA	2:G:306:GLN:NE2	2.29	0.48
2:H:148:LYS:HG2	2:H:149:ARG:H	1.77	0.48
1:A:313:VAL:HG13	1:A:314:GLU:N	2.29	0.47
1:A:546:ALA:HB2	1:A:597:TYR:HE2	1.79	0.47
1:B:51:ASP:OD2	1:B:51:ASP:O	2.32	0.47
1:B:286:GLN:OE1	1:B:330:VAL:HG13	2.14	0.47
1:B:510:ARG:NH1	1:B:567:TRP:CZ3	2.82	0.47
1:C:17:ILE:HD12	1:C:49:PHE:CD1	2.49	0.47
1:C:357:SER:HB3	1:C:360:ASP:OD2	2.14	0.47
1:C:730:TYR:CE2	1:C:731:TYR:CD2	3.02	0.47
2:E:10:ASN:ND2	2:E:15:GLU:HG3	2.25	0.47
2:F:174:THR:HG23	2:F:181:THR:CG2	2.44	0.47
2:F:275:LEU:HD13	2:F:275:LEU:C	2.38	0.47
2:G:35:ILE:HD11	2:G:247:HIS:CD2	2.49	0.47
2:H:42:LYS:HE3	2:H:46:PHE:CZ	2.49	0.47
2:H:118:HIS:CE1	2:H:234:ILE:HG23	2.49	0.47
1:A:482:ALA:O	1:A:486:VAL:HG23	2.14	0.47
1:C:10:ARG:HD3	1:C:91:LYS:HB3	1.94	0.47
1:D:431:ALA:HB1	1:D:445:PRO:HG2	1.94	0.47
1:D:530:ARG:HD2	1:D:533:ASP:OD2	2.14	0.47
2:E:165:SER:HB3	2:H:169:LEU:HD11	1.95	0.47
2:E:197:LEU:HB2	2:E:249:LEU:HD21	1.95	0.47
2:G:62:TYR:OH	2:G:70:LYS:HD3	2.14	0.47
1:A:226:VAL:HG11	1:A:247:TYR:CE2	2.49	0.47
1:A:286:GLN:OE1	1:A:330:VAL:HG13	2.14	0.47
1:A:380:THR:O	1:A:384:LYS:HD3	2.13	0.47
1:B:109:MET:HG3	1:B:115:TYR:CE2	2.49	0.47
1:B:356:PHE:CZ	1:B:390:LYS:CE	2.97	0.47
1:C:33:LEU:HB2	1:C:36:VAL:HG21	1.94	0.47
1:D:152:GLU:HG3	1:D:153:GLY:N	2.25	0.47
1:D:487:ARG:NH1	1:D:558:LEU:HD13	2.30	0.47
2:E:143:ASN:CG	2:E:146:ILE:HG12	2.40	0.47
2:F:166:TYR:HD1	2:F:170:LEU:HD12	1.79	0.47
2:F:332:ILE:O	2:F:335:ILE:HG22	2.15	0.47
2:H:40:ILE:O	2:H:44:LEU:HG	2.14	0.47
1:A:657:PRO:HG2	1:A:666:TYR:OH	2.14	0.47
1:B:39:SER:OG	2:H:332:ILE:HG22	2.14	0.47
1:B:380:THR:O	1:B:384:LYS:HD3	2.14	0.47
1:B:621:PRO:HD3	1:B:694:SER:OG	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ALA:HA	1:D:428:PRO:HB3	1.96	0.47
2:G:5:PHE:CE1	2:G:24:ASN:O	2.67	0.47
2:H:111:TRP:CD1	2:H:111:TRP:C	2.91	0.47
1:A:75:PRO:C	1:A:77:TYR:N	2.69	0.47
1:A:244:ILE:O	1:A:248:VAL:HG13	2.15	0.47
1:D:215:VAL:O	1:D:216:ARG:HG2	2.14	0.47
1:D:361:VAL:HB	1:D:364:LEU:CB	2.45	0.47
2:E:203:LEU:HD23	2:E:203:LEU:C	2.39	0.47
2:H:301:LYS:HE2	2:H:305:CYS:SG	2.54	0.47
2:H:326:GLN:NE2	2:H:328:ARG:HH12	2.12	0.47
1:A:38:ILE:HD13	1:A:38:ILE:N	2.29	0.47
1:A:384:LYS:N	1:A:384:LYS:HD2	2.30	0.47
1:A:593:GLU:OE1	1:A:594:PRO:HD2	2.15	0.47
1:B:313:VAL:HG13	1:B:314:GLU:N	2.29	0.47
1:C:59:HIS:HD2	1:C:88:HIS:HB2	1.79	0.47
1:C:289:VAL:CG1	1:C:300:GLY:O	2.62	0.47
1:D:172:LEU:C	1:D:172:LEU:HD23	2.40	0.47
1:D:229:GLU:OE2	1:D:448:PRO:HD3	2.14	0.47
2:E:72:ILE:O	2:E:290:LEU:HD11	2.14	0.47
2:F:93:VAL:HG11	2:G:2:TYR:CE2	2.49	0.47
2:G:296:MET:HE1	2:G:299:LEU:HD23	1.95	0.47
1:A:140:ASP:OD1	1:A:170:GLN:HG2	2.13	0.47
1:A:250:GLN:HE22	1:A:499:PRO:HG3	1.79	0.47
1:A:338:GLN:HE21	1:A:415:GLN:NE2	2.13	0.47
1:B:115:TYR:OH	1:B:167:GLU:OE1	2.29	0.47
1:B:151:LEU:HD23	1:B:155:TYR:HB2	1.94	0.47
1:B:176:VAL:O	1:B:180:LEU:HG	2.14	0.47
1:B:208:PRO:HG3	1:B:464:LEU:HB2	1.96	0.47
1:B:228:ILE:C	1:B:435:GLN:HE22	2.23	0.47
1:B:407:ALA:CB	2:H:361:ILE:HD12	2.39	0.47
1:B:472:ILE:HD13	1:B:478:LEU:HD21	1.96	0.47
1:B:510:ARG:HB2	1:B:614:SER:OG	2.15	0.47
1:C:102:LEU:O	1:C:106:VAL:HG23	2.15	0.47
1:C:340:ASN:HB3	1:C:368:PHE:CE1	2.49	0.47
1:C:530:ARG:HD2	1:C:533:ASP:OD2	2.14	0.47
1:D:155:TYR:HE2	1:D:628:ILE:CG1	2.27	0.47
1:D:227:LEU:HB3	1:D:435:GLN:NE2	2.30	0.47
1:D:339:ILE:O	1:D:416:ASN:HA	2.15	0.47
2:E:59:ARG:O	2:E:63:GLN:HG2	2.15	0.47
2:E:118:HIS:CE1	2:E:234:ILE:HG23	2.50	0.47
2:E:221:ARG:O	2:E:222:GLU:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:MET:SD	2:F:192:LYS:HG3	2.54	0.47
2:G:95:LEU:HB3	2:G:108:VAL:HG11	1.97	0.47
2:G:118:HIS:CE1	2:G:234:ILE:HG23	2.50	0.47
2:G:275:LEU:HD13	2:G:275:LEU:C	2.40	0.47
1:A:7:VAL:HG12	1:A:53:ILE:HG12	1.97	0.47
1:A:10:ARG:HH22	1:A:88:HIS:CE1	2.32	0.47
1:A:125:GLU:HG2	1:A:129:LYS:HE2	1.96	0.47
1:A:171:PHE:HA	1:A:174:ILE:HG22	1.95	0.47
1:A:532:SER:CB	1:A:673:PRO:HD2	2.45	0.47
1:B:427:ASP:OD1	1:B:429:ALA:HB3	2.15	0.47
1:B:510:ARG:NH1	1:B:567:TRP:CE3	2.83	0.47
1:B:613:ASN:HB2	1:B:616:LEU:HD21	1.97	0.47
1:D:17:ILE:HD11	1:D:49:PHE:CE1	2.50	0.47
1:D:102:LEU:O	1:D:106:VAL:HG23	2.15	0.47
2:E:306:GLN:HB3	2:E:328:ARG:HH11	1.80	0.47
2:F:208:PHE:CD2	2:F:238:GLU:OE1	2.68	0.47
2:G:40:ILE:O	2:G:44:LEU:HG	2.15	0.47
2:G:96:LEU:N	2:G:97:PRO:HD2	2.30	0.47
1:A:700:ASP:OD2	1:A:702:SER:HB2	2.14	0.47
1:B:285:PHE:O	1:B:289:VAL:HG23	2.15	0.47
1:B:340:ASN:HD21	1:B:342:LEU:HB3	1.80	0.47
1:B:449:LEU:HG	1:B:457:GLY:HA3	1.95	0.47
1:D:225:CYS:CB	1:D:437:ASN:HD22	2.27	0.47
2:E:95:LEU:HD12	2:E:108:VAL:HG13	1.96	0.47
2:F:35:ILE:HG23	2:F:36:PHE:N	2.29	0.47
2:H:275:LEU:C	2:H:275:LEU:HD13	2.40	0.47
1:A:285:PHE:O	1:A:289:VAL:HG23	2.14	0.47
1:A:545:GLU:OE2	1:A:596:HIS:N	2.48	0.47
1:A:599:TRP:O	1:A:600:GLU:C	2.57	0.47
1:B:9:LYS:HE3	1:B:15:GLU:CD	2.39	0.47
1:B:40:GLN:HE22	1:B:44:ARG:HH11	1.61	0.47
1:B:414:ILE:HD12	1:B:414:ILE:N	2.30	0.47
1:B:419:HIS:CA	1:B:422:THR:HG1	2.22	0.47
1:C:691:GLN:HE21	1:C:691:GLN:N	2.13	0.47
1:D:88:HIS:O	1:D:92:LYS:HG3	2.14	0.47
1:D:115:TYR:CD1	1:D:216:ARG:O	2.67	0.47
1:D:356:PHE:CE1	1:D:390:LYS:HE3	2.50	0.47
2:E:275:LEU:C	2:E:275:LEU:HD13	2.39	0.47
2:F:9:LYS:CA	2:G:141:VAL:HG11	2.45	0.47
2:H:302:ASP:C	2:H:306:GLN:HE21	2.23	0.47
1:B:25:VAL:O	1:B:28:TRP:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLN:HE21	1:B:415:GLN:NE2	2.14	0.46
1:B:419:HIS:C	1:B:422:THR:HG1	2.22	0.46
1:B:442:ILE:HG23	1:B:691:GLN:OE1	2.15	0.46
1:C:17:ILE:HG13	3:C:801:DTP:H2	1.97	0.46
1:C:512:THR:HG22	1:C:614:SER:HB2	1.97	0.46
1:C:681:LEU:O	1:C:685:MET:HG3	2.14	0.46
1:D:109:MET:HE1	1:D:166:TYR:CB	2.45	0.46
1:D:320:LYS:HD3	1:D:409:THR:CB	2.45	0.46
1:D:512:THR:HG22	1:D:614:SER:HB2	1.97	0.46
1:A:599:TRP:O	1:A:602:LEU:N	2.49	0.46
1:B:59:HIS:HD2	1:B:88:HIS:HB2	1.79	0.46
1:B:552:LEU:CA	1:B:616:LEU:HD12	2.45	0.46
1:B:706:SER:HB2	1:B:708:LYS:HG2	1.96	0.46
1:C:150:GLN:O	1:C:154:LYS:HG3	2.15	0.46
1:D:78:GLN:HE22	1:D:655:VAL:HB	1.80	0.46
1:D:633:ASN:HD22	1:D:633:ASN:N	2.13	0.46
2:E:166:TYR:CZ	2:H:169:LEU:HD22	2.50	0.46
2:G:285:ASP:OD2	2:G:286:TRP:N	2.48	0.46
1:A:301:ALA:HB3	1:A:438:LEU:HD22	1.98	0.46
1:A:362:PRO:C	1:A:364:LEU:H	2.24	0.46
1:A:369:PHE:CG	1:A:434:ARG:CG	2.97	0.46
1:B:568:PHE:O	1:B:571:THR:N	2.46	0.46
1:C:37:SER:OG	1:C:40:GLN:HB2	2.15	0.46
1:C:568:PHE:CD1	1:C:571:THR:OG1	2.67	0.46
1:C:730:TYR:CZ	1:C:731:TYR:CZ	3.03	0.46
1:D:137:HIS:HA	1:D:170:GLN:HG3	1.97	0.46
1:D:441:GLU:HB2	1:D:619:LEU:O	2.15	0.46
1:D:670:TRP:HA	1:D:670:TRP:HE3	1.80	0.46
2:E:35:ILE:HG23	2:E:36:PHE:N	2.29	0.46
2:E:125:ILE:HG12	2:E:230:ILE:HD12	1.97	0.46
2:G:10:ASN:HD22	2:G:15:GLU:CG	2.24	0.46
2:G:95:LEU:CB	2:G:108:VAL:HG11	2.45	0.46
2:G:292:ARG:NE	2:G:293:ASP:CG	2.73	0.46
1:A:175:LEU:HD12	1:A:216:ARG:HD2	1.97	0.46
1:A:297:VAL:HG12	1:A:298:ARG:N	2.25	0.46
1:A:413:TYR:HB3	1:A:440:LEU:HD21	1.97	0.46
1:B:86:ILE:O	1:B:90:ARG:HG2	2.16	0.46
1:B:568:PHE:CE1	1:B:571:THR:OG1	2.69	0.46
1:C:414:ILE:HD12	1:C:414:ILE:N	2.30	0.46
1:C:425:PRO:CG	1:C:615:THR:HG22	2.44	0.46
1:D:217:THR:CB	1:D:218:PRO:CD	2.93	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:2:TYR:HB2	2:F:168:HIS:ND1	2.31	0.46
1:A:385:ASP:OD1	1:A:388:ILE:HG12	2.16	0.46
1:A:465:SER:OG	1:A:489:LEU:HD21	2.16	0.46
1:A:506:GLY:HA2	1:A:567:TRP:CZ3	2.49	0.46
1:B:474:ASN:HD22	1:B:474:ASN:N	2.13	0.46
1:B:541:HIS:O	1:B:545:GLU:HB2	2.16	0.46
1:B:592:ASN:H	1:B:592:ASN:ND2	2.13	0.46
1:B:669:LEU:HD12	1:B:672:MET:HE1	1.98	0.46
1:C:59:HIS:HB2	3:C:801:DTP:C5'	2.45	0.46
1:C:519:ASN:HA	1:C:632:THR:OG1	2.14	0.46
2:F:118:HIS:CE1	2:F:234:ILE:HG23	2.50	0.46
2:F:169:LEU:HD22	2:G:166:TYR:CZ	2.51	0.46
2:G:193:LEU:C	2:G:193:LEU:HD13	2.40	0.46
2:G:297:ILE:N	2:G:297:ILE:CD1	2.69	0.46
2:H:3:THR:HG23	2:H:5:PHE:C	2.41	0.46
1:A:414:ILE:N	1:A:414:ILE:HD12	2.30	0.46
1:A:576:GLY:HA3	1:A:607:LYS:HZ3	1.78	0.46
1:A:592:ASN:H	1:A:592:ASN:ND2	2.13	0.46
1:B:307:PRO:HB2	1:B:309:TRP:NE1	2.31	0.46
1:C:41:VAL:HG22	1:C:69:LEU:HD12	1.97	0.46
1:C:50:TYR:O	1:C:51:ASP:C	2.56	0.46
1:C:339:ILE:O	1:C:416:ASN:HA	2.16	0.46
1:D:414:ILE:N	1:D:414:ILE:HD12	2.30	0.46
1:D:697:THR:OG1	1:D:732:GLN:HG3	2.15	0.46
2:E:51:GLU:OE1	2:E:51:GLU:N	2.48	0.46
2:G:300:ASN:HB2	2:G:303:ILE:HG22	1.89	0.46
1:B:305:PHE:CZ	1:B:436:SER:HB3	2.51	0.46
1:C:633:ASN:O	1:C:634:GLY:C	2.58	0.46
1:C:651:ILE:O	1:C:652:LEU:HD23	2.15	0.46
1:D:151:LEU:HD23	1:D:155:TYR:HB2	1.97	0.46
2:E:57:ARG:O	2:E:60:ILE:HG22	2.16	0.46
2:F:205:ALA:HB1	2:F:315:ARG:CD	2.46	0.46
2:G:205:ALA:HB1	2:G:315:ARG:CD	2.46	0.46
2:H:2:TYR:HB2	2:H:168:HIS:ND1	2.30	0.46
2:H:59:ARG:HH11	2:H:59:ARG:HG3	1.81	0.46
2:H:204:GLU:OE2	2:H:241:HIS:HB3	2.16	0.46
2:H:335:ILE:O	2:H:339:LEU:HD23	2.15	0.46
1:A:67:ALA:O	1:A:70:ILE:HG13	2.15	0.46
1:A:134:PHE:CE1	1:A:194:LYS:HD2	2.50	0.46
1:A:208:PRO:HG3	1:A:464:LEU:HB2	1.96	0.46
1:A:545:GLU:OE1	1:A:595:LEU:HA	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLU:O	1:B:316:LEU:HG	2.16	0.46
1:B:385:ASP:OD1	1:B:388:ILE:HG12	2.16	0.46
1:B:593:GLU:OE1	1:B:594:PRO:HD2	2.15	0.46
1:B:621:PRO:HD3	1:B:694:SER:HB2	1.96	0.46
1:C:109:MET:HE1	1:C:166:TYR:CB	2.44	0.46
1:D:155:TYR:HE1	1:D:209:THR:HG23	1.81	0.46
2:E:2:TYR:CE2	2:H:93:VAL:HG11	2.50	0.46
2:E:34:ASP:O	2:E:38:LYS:HG3	2.16	0.46
2:E:149:ARG:HH22	2:E:286:TRP:CB	2.09	0.46
2:F:127:ARG:NH2	2:G:29:ASP:HA	2.30	0.46
1:A:449:LEU:HG	1:A:457:GLY:HA3	1.97	0.46
1:A:509:GLY:O	1:A:566:PRO:HD2	2.15	0.46
1:B:449:LEU:N	1:B:449:LEU:HD12	2.30	0.46
1:C:115:TYR:CE1	1:C:216:ARG:HG3	2.51	0.46
1:C:459:ILE:HB	1:C:503:ALA:HA	1.98	0.46
1:D:196:PHE:HB2	1:D:484:LEU:HD11	1.97	0.46
1:D:377:ARG:HG2	1:D:377:ARG:NH1	2.31	0.46
1:D:384:LYS:O	1:D:386:ASP:OD2	2.33	0.46
1:D:424:SER:OG	1:D:425:PRO:HD2	2.16	0.46
1:D:556:ASN:C	1:D:556:ASN:HD22	2.24	0.46
2:F:72:ILE:O	2:F:290:LEU:HD11	2.16	0.46
2:F:122:TYR:O	2:F:126:ILE:HG13	2.15	0.46
2:G:281:GLN:NE2	2:G:284:LYS:HD2	2.30	0.46
2:H:299:LEU:HD12	2:H:300:ASN:H	1.80	0.46
1:A:307:PRO:HB2	1:A:309:TRP:NE1	2.31	0.46
1:B:77:TYR:CD1	1:B:80:LEU:HD23	2.50	0.46
1:B:255:GLY:O	1:B:435:GLN:NE2	2.49	0.46
1:B:340:ASN:CB	1:B:368:PHE:CE1	2.99	0.46
1:D:42:GLU:OE1	2:G:298:GLY:HA2	2.16	0.46
1:D:532:SER:HB2	1:D:673:PRO:HD2	1.97	0.46
1:D:681:LEU:O	1:D:685:MET:HG3	2.16	0.46
1:D:700:ASP:OD2	1:D:702:SER:HB2	2.16	0.46
2:E:244:GLY:O	2:E:248:MET:HG3	2.15	0.46
1:A:10:ARG:HG2	1:A:10:ARG:HH11	1.81	0.45
1:B:293:SER:CB	1:B:298:ARG:O	2.64	0.45
1:C:42:GLU:OE1	2:E:298:GLY:CA	2.64	0.45
1:C:217:THR:HB	1:C:218:PRO:HD2	1.96	0.45
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.98	0.45
1:C:517:VAL:HG22	1:C:619:LEU:HD22	1.98	0.45
1:D:613:ASN:HB2	1:D:616:LEU:HD23	1.98	0.45
1:D:640:GLY:CA	1:D:668:LEU:HD22	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:670:TRP:HA	1:D:670:TRP:CE3	2.51	0.45
2:F:84:ASP:OD2	2:F:118:HIS:CB	2.64	0.45
2:F:174:THR:HG21	2:F:181:THR:CG2	2.46	0.45
2:F:175:HIS:O	2:F:182:VAL:N	2.29	0.45
2:G:86:ILE:HD13	2:G:153:ILE:HB	1.98	0.45
2:G:204:GLU:OE2	2:G:241:HIS:HB3	2.17	0.45
2:G:287:ALA:HA	2:G:290:LEU:HB2	1.98	0.45
1:A:19:LEU:HD12	2:F:295:SER:O	2.14	0.45
1:A:108:LYS:O	1:A:112:MET:HG3	2.15	0.45
1:A:644:ILE:HG23	1:A:651:ILE:HD13	1.98	0.45
1:B:384:LYS:HD2	1:B:384:LYS:N	2.31	0.45
1:B:644:ILE:HD12	1:B:644:ILE:N	2.31	0.45
1:B:669:LEU:HD12	1:B:672:MET:HE2	1.97	0.45
1:C:25:VAL:HG11	1:C:59:HIS:HE1	1.80	0.45
1:C:322:ASN:HA	1:C:331:ARG:NE	2.28	0.45
1:C:464:LEU:CD1	4:C:802:DAT:H4'	2.46	0.45
2:E:93:VAL:HG11	2:H:2:TYR:CE2	2.51	0.45
2:E:115:GLU:OE1	2:E:115:GLU:HA	2.17	0.45
2:E:176:THR:HA	2:E:180:LYS:O	2.15	0.45
2:E:281:GLN:NE2	2:E:284:LYS:HD2	2.31	0.45
1:A:6:LEU:HD22	1:A:6:LEU:N	2.32	0.45
1:A:427:ASP:OD1	1:A:429:ALA:HB3	2.16	0.45
1:A:449:LEU:HD12	1:A:449:LEU:N	2.31	0.45
1:B:28:TRP:O	1:B:31:GLU:HB2	2.15	0.45
1:C:696:ASN:HD22	1:C:696:ASN:N	2.13	0.45
1:D:8:THR:HB	1:D:54:LYS:HA	1.98	0.45
1:D:449:LEU:HD12	1:D:449:LEU:N	2.32	0.45
1:D:593:GLU:OE1	1:D:594:PRO:HD2	2.16	0.45
1:D:669:LEU:HA	1:D:672:MET:HE2	1.98	0.45
2:E:202:ALA:HB2	2:E:276:PHE:CE1	2.52	0.45
2:H:170:LEU:HD13	2:H:175:HIS:HB2	1.98	0.45
1:B:509:GLY:O	1:B:566:PRO:HD2	2.16	0.45
1:B:532:SER:CB	1:B:673:PRO:HD2	2.46	0.45
1:B:587:LEU:HD21	1:B:724:PHE:O	2.17	0.45
1:B:681:LEU:O	1:B:685:MET:HG3	2.15	0.45
1:D:94:TYR:C	1:D:96:GLN:N	2.73	0.45
1:D:115:TYR:CD1	1:D:217:THR:HG22	2.50	0.45
2:E:157:TYR:O	2:E:161:ILE:HG13	2.17	0.45
2:H:103:GLU:OE1	2:H:103:GLU:N	2.49	0.45
1:A:282:TYR:CE2	1:A:304:LEU:HD13	2.51	0.45
1:B:79:TYR:HD1	1:B:143:PHE:O	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:CE2	1:B:628:ILE:CD1	2.99	0.45
1:B:415:GLN:HE21	1:B:417:VAL:HG12	1.82	0.45
1:C:568:PHE:CE1	1:C:571:THR:OG1	2.68	0.45
2:G:101:ILE:HB	2:G:103:GLU:OE1	2.16	0.45
1:A:10:ARG:O	1:A:11:ASP:C	2.58	0.45
1:A:670:TRP:CD2	1:A:735:ARG:HD2	2.51	0.45
1:B:560:LYS:HG3	1:B:609:HIS:CD2	2.51	0.45
1:C:690:ASP:C	1:C:691:GLN:NE2	2.72	0.45
1:D:119:LEU:HD21	1:D:179:CYS:SG	2.57	0.45
1:D:436:SER:CB	1:D:440:LEU:HD13	2.46	0.45
2:E:193:LEU:HD13	2:E:193:LEU:C	2.42	0.45
2:F:204:GLU:OE2	2:F:241:HIS:HB3	2.15	0.45
2:G:332:ILE:HG22	2:G:334:TRP:HE1	1.82	0.45
2:H:115:GLU:OE1	2:H:115:GLU:HA	2.17	0.45
1:A:697:THR:OG1	1:A:732:GLN:HG3	2.16	0.45
1:B:354:THR:CG2	1:B:356:PHE:CE1	2.97	0.45
1:B:444:LEU:HD21	1:B:691:GLN:NE2	2.31	0.45
1:B:607:LYS:HG2	1:B:607:LYS:O	2.17	0.45
1:C:438:LEU:HD23	4:C:802:DAT:C8	2.47	0.45
1:C:449:LEU:HD12	1:C:449:LEU:N	2.32	0.45
1:D:294:GLN:C	1:D:296:GLY:H	2.24	0.45
1:D:313:VAL:HG13	1:D:314:GLU:N	2.31	0.45
2:F:219:ALA:CB	2:F:338:TRP:CZ2	2.97	0.45
2:G:202:ALA:HB2	2:G:276:PHE:CE1	2.51	0.45
2:H:5:PHE:CD1	2:H:24:ASN:HB2	2.51	0.45
1:A:513:LEU:HG	1:A:613:ASN:ND2	2.32	0.45
1:B:181:PHE:CE1	1:B:192:TYR:HB3	2.52	0.45
1:B:546:ALA:HB2	1:B:597:TYR:HE2	1.81	0.45
1:C:424:SER:OG	1:C:425:PRO:HD2	2.17	0.45
1:C:670:TRP:HA	1:C:670:TRP:HE3	1.82	0.45
1:C:692:SER:OG	1:C:727:LYS:CB	2.65	0.45
1:D:109:MET:HE3	1:D:114:LYS:HB3	1.98	0.45
1:D:215:VAL:O	1:D:216:ARG:CB	2.64	0.45
1:D:268:ILE:HD13	3:D:803:DTP:C8	2.47	0.45
1:D:369:PHE:O	1:D:421:ASN:CG	2.60	0.45
2:E:204:GLU:OE1	2:E:241:HIS:HB3	2.16	0.45
2:E:263:GLU:O	2:E:267:GLU:HG3	2.17	0.45
2:F:300:ASN:CG	2:F:303:ILE:HG22	2.42	0.45
2:H:72:ILE:O	2:H:290:LEU:HD11	2.17	0.45
1:A:82:ALA:HB2	1:A:145:TYR:N	2.31	0.45
1:A:413:TYR:HB3	1:A:440:LEU:CD2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:TYR:CE2	1:B:628:ILE:HG13	2.37	0.45
1:B:616:LEU:HD23	1:B:616:LEU:N	2.31	0.45
1:D:7:VAL:HG12	1:D:53:ILE:HD13	1.99	0.45
1:D:364:LEU:HD13	1:D:364:LEU:C	2.42	0.45
1:D:676:ASP:O	1:D:680:GLN:HB2	2.17	0.45
2:F:244:GLY:O	2:F:248:MET:HG3	2.17	0.45
2:F:281:GLN:NE2	2:F:284:LYS:HD2	2.31	0.45
2:G:34:ASP:O	2:G:38:LYS:HG3	2.17	0.45
2:H:281:GLN:NE2	2:H:284:LYS:HD2	2.32	0.45
1:A:34:HIS:C	1:A:36:VAL:N	2.75	0.45
1:B:489:LEU:HB2	1:B:513:LEU:CD1	2.47	0.45
1:B:568:PHE:HE1	1:B:573:TYR:HB2	1.79	0.45
1:C:108:LYS:O	1:C:112:MET:HG3	2.16	0.45
1:C:260:ARG:HG2	1:C:365:TYR:CE2	2.51	0.45
1:C:651:ILE:H	1:C:651:ILE:HG13	1.44	0.45
1:D:45:SER:O	1:D:46:HIS:C	2.59	0.45
1:D:297:VAL:HG12	1:D:298:ARG:HG2	1.99	0.45
1:D:474:ASN:H	1:D:474:ASN:ND2	2.14	0.45
2:E:92:ASN:HA	2:E:96:LEU:HG	1.98	0.45
2:F:68:HIS:O	2:F:71:HIS:HB3	2.18	0.45
1:A:339:ILE:O	1:A:416:ASN:HA	2.17	0.44
1:B:415:GLN:HA	1:B:728:THR:HG22	1.98	0.44
1:C:377:ARG:HG2	1:C:377:ARG:NH1	2.31	0.44
1:C:418:ASP:O	1:C:422:THR:HG23	2.18	0.44
1:C:477:GLU:O	1:C:478:LEU:C	2.60	0.44
1:C:552:LEU:CA	1:C:616:LEU:HD12	2.47	0.44
1:D:125:GLU:HG2	1:D:129:LYS:HE2	1.99	0.44
1:D:317:LEU:HD11	1:D:337:VAL:HG21	1.98	0.44
1:D:551:LEU:C	1:D:616:LEU:CD1	2.90	0.44
1:D:568:PHE:CE1	1:D:571:THR:OG1	2.70	0.44
2:F:202:ALA:HB2	2:F:276:PHE:CE1	2.52	0.44
1:A:141:MET:N	1:A:141:MET:SD	2.91	0.44
1:A:406:ARG:HH11	1:A:406:ARG:HG3	1.82	0.44
1:A:599:TRP:O	1:A:601:ALA:N	2.51	0.44
1:B:465:SER:OG	1:B:489:LEU:HD21	2.17	0.44
1:C:136:ASP:OD1	1:C:139:ARG:HG3	2.17	0.44
1:C:145:TYR:O	1:C:149:LYS:HB2	2.17	0.44
1:C:309:TRP:CH2	1:C:364:LEU:HD12	2.52	0.44
1:C:328:ASN:N	1:C:328:ASN:ND2	2.65	0.44
1:C:406:ARG:NH2	1:C:697:THR:HG23	2.32	0.44
1:C:430:ILE:HG21	1:C:570:GLU:CG	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:GLU:OE1	2:G:298:GLY:CA	2.65	0.44
2:E:10:ASN:HD22	2:E:15:GLU:CG	2.25	0.44
2:E:66:PRO:O	2:E:69:GLU:N	2.50	0.44
2:F:69:GLU:CD	2:F:221:ARG:HH12	2.25	0.44
2:H:193:LEU:HD13	2:H:193:LEU:C	2.42	0.44
1:B:159:ASN:HB3	1:B:162:THR:OG1	2.17	0.44
1:B:244:ILE:O	1:B:248:VAL:HG13	2.18	0.44
1:C:242:SER:OG	1:D:238:ASN:HB3	2.17	0.44
1:D:39:SER:HA	1:D:42:GLU:HG2	1.99	0.44
1:D:418:ASP:O	1:D:422:THR:HG23	2.17	0.44
1:D:506:GLY:HA2	1:D:567:TRP:HZ3	1.81	0.44
2:E:69:GLU:CD	2:E:221:ARG:HH12	2.25	0.44
2:F:3:THR:HG21	2:F:6:SER:HA	2.00	0.44
2:F:115:GLU:OE1	2:F:115:GLU:HA	2.18	0.44
2:H:145:GLN:HB3	2:H:286:TRP:CZ3	2.52	0.44
1:A:75:PRO:O	1:A:78:GLN:HG2	2.17	0.44
1:A:463:THR:HB	1:A:513:LEU:HD22	1.99	0.44
1:A:592:ASN:N	1:A:592:ASN:ND2	2.65	0.44
1:B:23:HIS:HE1	1:B:42:GLU:OE2	1.87	0.44
1:B:413:TYR:C	1:B:414:ILE:HD12	2.42	0.44
1:C:576:GLY:HA3	1:C:607:LYS:NZ	2.32	0.44
1:C:593:GLU:OE1	1:C:594:PRO:HD2	2.16	0.44
1:C:619:LEU:HD12	1:C:693:ILE:CG1	2.41	0.44
1:C:670:TRP:HA	1:C:670:TRP:CE3	2.52	0.44
1:D:206:SER:HB2	1:D:518:ILE:HD13	1.99	0.44
1:D:406:ARG:HD2	1:D:414:ILE:HD11	1.99	0.44
1:D:509:GLY:HA3	1:D:567:TRP:CE3	2.52	0.44
2:E:3:THR:HG23	2:E:5:PHE:C	2.43	0.44
2:E:145:GLN:NE2	2:E:145:GLN:N	2.58	0.44
2:F:79:TYR:CE1	2:F:149:ARG:CD	2.99	0.44
2:F:84:ASP:OD2	2:F:118:HIS:HB3	2.17	0.44
2:H:34:ASP:O	2:H:38:LYS:HG3	2.16	0.44
2:H:122:TYR:O	2:H:126:ILE:HG13	2.17	0.44
1:A:426:PHE:CZ	1:A:445:PRO:CD	3.00	0.44
1:A:464:LEU:HA	1:A:514:GLY:O	2.18	0.44
1:A:492:LEU:O	1:A:496:GLN:HG2	2.18	0.44
1:A:607:LYS:HG2	1:A:607:LYS:O	2.17	0.44
1:B:140:ASP:OD1	1:B:170:GLN:HG2	2.17	0.44
1:B:356:PHE:HE1	1:B:390:LYS:CE	2.20	0.44
1:B:552:LEU:HD23	1:B:616:LEU:HG	1.98	0.44
1:B:619:LEU:CD1	1:B:693:ILE:HG23	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:PRO:HG2	1:B:666:TYR:OH	2.17	0.44
1:D:261:ILE:O	1:D:358:PRO:HG3	2.18	0.44
1:D:520:PHE:CB	1:D:635:ILE:HA	2.40	0.44
2:E:149:ARG:NH1	2:E:286:TRP:CE3	2.81	0.44
2:E:201:ASN:HD21	2:E:246:GLN:HG2	1.82	0.44
2:F:335:ILE:HG12	2:F:339:LEU:HD11	2.00	0.44
2:H:79:TYR:CZ	2:H:149:ARG:HD3	2.51	0.44
2:H:205:ALA:HB1	2:H:315:ARG:CD	2.46	0.44
1:A:25:VAL:O	1:A:28:TRP:HB3	2.17	0.44
1:A:59:HIS:O	1:A:63:ILE:HG13	2.17	0.44
1:A:70:ILE:HD13	1:A:78:GLN:CB	2.38	0.44
1:A:364:LEU:HD13	1:A:364:LEU:O	2.18	0.44
1:A:413:TYR:C	1:A:414:ILE:HD12	2.43	0.44
1:A:622:SER:HB2	1:A:625:SER:HG	1.78	0.44
1:A:627:GLN:NE2	1:A:645:LYS:HE2	2.28	0.44
1:B:197:TYR:C	1:B:199:ALA:H	2.26	0.44
1:B:627:GLN:HG2	1:B:654:GLN:OE1	2.18	0.44
1:C:125:GLU:HG2	1:C:129:LYS:HE2	1.99	0.44
1:C:469:LEU:HD12	1:C:520:PHE:HA	1.98	0.44
1:C:669:LEU:HD12	1:C:672:MET:HE2	1.98	0.44
1:D:108:LYS:O	1:D:112:MET:HG3	2.18	0.44
1:D:510:ARG:NH1	1:D:567:TRP:HZ3	2.15	0.44
1:D:576:GLY:HA3	1:D:607:LYS:NZ	2.33	0.44
2:G:122:TYR:O	2:G:126:ILE:HG13	2.17	0.44
2:H:139:ASP:O	2:H:140:ILE:C	2.59	0.44
1:A:34:HIS:C	1:A:36:VAL:H	2.24	0.44
1:A:114:LYS:O	1:A:218:PRO:HD3	2.17	0.44
1:B:103:TYR:O	1:B:107:VAL:HG23	2.17	0.44
1:C:420:CYS:O	1:C:424:SER:HB2	2.18	0.44
1:C:520:PHE:CB	1:C:635:ILE:HA	2.39	0.44
1:C:556:ASN:C	1:C:556:ASN:HD22	2.25	0.44
1:C:583:TYR:CB	1:C:687:LYS:HG3	2.48	0.44
1:C:722:TYR:HE2	2:E:375:LEU:HD13	1.81	0.44
1:D:115:TYR:HB3	1:D:216:ARG:O	2.17	0.44
1:D:197:TYR:C	1:D:199:ALA:H	2.26	0.44
2:F:93:VAL:HG11	2:G:2:TYR:HE2	1.83	0.44
2:F:193:LEU:HD13	2:F:193:LEU:C	2.42	0.44
2:F:201:ASN:HD21	2:F:246:GLN:HG2	1.83	0.44
2:G:2:TYR:HB2	2:G:168:HIS:ND1	2.32	0.44
2:G:62:TYR:HB2	2:G:224:MET:HE1	1.99	0.44
2:H:311:ILE:O	2:H:315:ARG:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:C	1:A:484:LEU:HD21	2.43	0.44
1:A:214:GLY:O	1:A:217:THR:CB	2.65	0.44
1:A:301:ALA:HB3	1:A:438:LEU:CD2	2.48	0.44
1:A:513:LEU:HG	1:A:613:ASN:HD22	1.83	0.44
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.99	0.44
1:B:108:LYS:O	1:B:112:MET:HG3	2.18	0.44
1:B:225:CYS:CB	1:B:437:ASN:HD22	2.30	0.44
1:B:537:ASN:HD21	1:B:680:GLN:HG2	1.83	0.44
1:B:545:GLU:OE1	1:B:595:LEU:HA	2.18	0.44
1:C:140:ASP:OD1	1:C:170:GLN:HG2	2.17	0.44
1:C:313:VAL:HG13	1:C:314:GLU:N	2.31	0.44
1:D:150:GLN:HA	1:D:150:GLN:OE1	2.18	0.44
1:D:185:PRO:O	1:D:189:ARG:N	2.51	0.44
1:D:260:ARG:HG2	1:D:365:TYR:CE2	2.53	0.44
1:D:307:PRO:HG2	1:D:310:HIS:HB2	2.00	0.44
1:D:463:THR:HG22	1:D:489:LEU:HD22	1.99	0.44
1:D:633:ASN:O	1:D:634:GLY:C	2.61	0.44
2:E:78:LYS:HE2	2:E:136:VAL:HG13	1.99	0.44
2:E:212:PHE:HB3	2:E:216:PHE:CE2	2.53	0.44
2:H:66:PRO:O	2:H:67:GLU:C	2.60	0.44
2:H:299:LEU:HD13	2:H:304:LEU:HB2	1.89	0.44
1:A:633:ASN:O	1:A:634:GLY:C	2.59	0.44
1:B:423:HIS:O	1:B:423:HIS:CG	2.70	0.44
1:C:509:GLY:HA3	1:C:567:TRP:CE3	2.52	0.44
1:D:145:TYR:O	1:D:149:LYS:HB2	2.18	0.44
2:G:95:LEU:HD12	2:G:108:VAL:HG21	1.97	0.44
2:G:292:ARG:CD	2:G:293:ASP:CG	2.90	0.44
1:A:155:TYR:CE1	1:A:209:THR:HA	2.52	0.43
1:A:463:THR:HG22	1:A:489:LEU:HD22	2.00	0.43
1:B:353:ILE:HG13	1:B:395:ALA:HB2	2.00	0.43
1:B:377:ARG:HG2	1:B:377:ARG:HH11	1.83	0.43
1:C:303:THR:HG21	1:C:413:TYR:HD2	1.83	0.43
1:C:339:ILE:HD13	1:C:399:PHE:HE1	1.82	0.43
1:C:356:PHE:CE1	1:C:390:LYS:HE3	2.51	0.43
1:D:90:ARG:HH21	1:D:140:ASP:CG	2.27	0.43
1:D:165:ILE:HG22	1:D:166:TYR:N	2.32	0.43
1:D:474:ASN:ND2	1:D:477:GLU:HG3	2.30	0.43
2:E:79:TYR:CZ	2:E:149:ARG:HD3	2.50	0.43
2:F:74:ILE:HG23	2:F:75:SER:N	2.33	0.43
2:H:149:ARG:NH1	2:H:286:TRP:CE3	2.86	0.43
2:H:236:ARG:HA	2:H:340:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:O	1:A:46:HIS:C	2.59	0.43
1:A:50:TYR:O	1:A:51:ASP:C	2.61	0.43
1:A:258:ALA:O	1:A:260:ARG:N	2.51	0.43
1:A:418:ASP:C	1:A:422:THR:HG1	2.20	0.43
1:A:669:LEU:HD12	1:A:672:MET:CE	2.48	0.43
1:B:59:HIS:O	1:B:63:ILE:HG13	2.18	0.43
1:B:463:THR:HG22	1:B:489:LEU:HD22	2.00	0.43
1:C:85:ALA:HB3	1:C:148:VAL:HG11	2.00	0.43
1:C:177:ALA:HB2	1:C:196:PHE:HD2	1.83	0.43
1:C:244:ILE:O	1:C:248:VAL:HG13	2.18	0.43
1:C:475:LEU:CD2	1:C:543:THR:HG23	2.48	0.43
1:D:207:LEU:HD12	1:D:212:MET:HE3	2.00	0.43
1:A:364:LEU:HD23	1:A:378:LEU:HB2	2.00	0.43
1:A:719:LEU:HB3	2:F:373:PHE:CE2	2.53	0.43
1:B:424:SER:OG	1:B:425:PRO:HD2	2.18	0.43
1:B:558:LEU:HD21	1:B:612:ARG:HG2	2.00	0.43
1:C:22:ILE:HG12	3:C:801:DTP:H1'	2.00	0.43
1:C:77:TYR:CD1	1:C:80:LEU:HD23	2.54	0.43
1:C:220:ARG:HD3	1:C:220:ARG:HA	1.67	0.43
1:D:10:ARG:HD3	1:D:91:LYS:HB3	2.00	0.43
1:D:469:LEU:HD12	1:D:520:PHE:HA	2.00	0.43
1:D:544:PHE:CE2	1:D:685:MET:HG2	2.53	0.43
2:F:111:TRP:HH2	2:F:200:VAL:HG11	1.83	0.43
2:G:93:VAL:HG11	2:G:161:ILE:HD13	1.99	0.43
2:G:140:ILE:CG2	2:G:146:ILE:HG21	2.48	0.43
2:G:292:ARG:NE	2:G:293:ASP:OD2	2.50	0.43
1:A:149:LYS:CG	1:A:652:LEU:HD22	2.32	0.43
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.99	0.43
1:A:222:PHE:CD2	1:A:492:LEU:HD11	2.53	0.43
1:A:292:CYS:HA	1:B:276:THR:HG21	2.00	0.43
1:B:172:LEU:HG	1:B:216:ARG:NH1	2.33	0.43
1:B:545:GLU:OE2	1:B:596:HIS:N	2.51	0.43
1:B:568:PHE:C	1:B:570:GLU:N	2.72	0.43
1:C:552:LEU:HB2	1:C:602:LEU:HD21	1.99	0.43
1:C:568:PHE:HE1	1:C:573:TYR:HB2	1.82	0.43
1:C:583:TYR:CE2	1:C:687:LYS:HE3	2.53	0.43
1:D:42:GLU:HB2	2:G:297:ILE:CG2	2.48	0.43
1:D:54:LYS:HE3	1:D:57:ASP:OD2	2.19	0.43
1:D:136:ASP:OD1	1:D:139:ARG:HG3	2.18	0.43
1:D:438:LEU:HD23	4:D:802:DAT:H8	1.99	0.43
1:D:442:ILE:CD1	1:D:691:GLN:OE1	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:ASN:HB3	1:D:730:TYR:HB3	2.00	0.43
2:E:122:TYR:O	2:E:126:ILE:HG13	2.17	0.43
2:E:126:ILE:O	2:E:130:VAL:HG22	2.18	0.43
2:G:243:THR:HG22	2:G:247:HIS:CD2	2.52	0.43
1:A:321:ASN:OD1	1:A:322:ASN:OD1	2.36	0.43
1:B:424:SER:O	1:B:425:PRO:C	2.59	0.43
1:B:492:LEU:O	1:B:496:GLN:HG2	2.19	0.43
1:B:513:LEU:O	1:B:615:THR:O	2.36	0.43
1:B:592:ASN:ND2	1:B:592:ASN:N	2.65	0.43
1:C:79:TYR:O	1:C:83:ARG:HG3	2.18	0.43
1:C:181:PHE:O	1:C:189:ARG:HG3	2.18	0.43
1:C:282:TYR:O	1:C:333:MET:HE1	2.19	0.43
1:C:696:ASN:HB3	1:C:730:TYR:HB3	2.00	0.43
1:D:208:PRO:HG2	1:D:464:LEU:HB2	1.98	0.43
2:E:5:PHE:CD2	2:H:150:ALA:HB1	2.54	0.43
2:E:28:TYR:CE2	2:H:120:ARG:HG2	2.53	0.43
2:H:212:PHE:HB3	2:H:216:PHE:CE2	2.52	0.43
2:H:332:ILE:O	2:H:332:ILE:HG13	2.19	0.43
1:A:185:PRO:HB2	1:A:187:GLU:CD	2.44	0.43
1:A:406:ARG:HD2	1:A:414:ILE:HD11	2.01	0.43
1:A:516:GLY:N	1:A:618:ALA:O	2.52	0.43
1:B:250:GLN:HE22	1:B:499:PRO:HG3	1.84	0.43
1:B:670:TRP:CD2	1:B:735:ARG:HD2	2.53	0.43
1:C:18:ASN:HD22	1:C:18:ASN:C	2.27	0.43
1:C:21:LYS:O	1:C:24:ARG:HB3	2.18	0.43
1:C:431:ALA:HB1	1:C:445:PRO:HG2	2.00	0.43
1:D:33:LEU:HB2	1:D:36:VAL:HG21	1.99	0.43
1:D:69:LEU:O	1:D:70:ILE:C	2.60	0.43
1:D:162:THR:OG1	1:D:164:GLU:HG3	2.19	0.43
1:D:461:LEU:HD11	1:D:503:ALA:HB1	2.01	0.43
1:D:474:ASN:N	1:D:474:ASN:ND2	2.67	0.43
1:D:708:LYS:CE	2:G:362:ASP:CA	2.92	0.43
2:F:103:GLU:OE1	2:F:103:GLU:N	2.51	0.43
2:G:74:ILE:HG23	2:G:75:SER:N	2.34	0.43
2:H:126:ILE:O	2:H:129:ILE:HG12	2.18	0.43
1:A:23:HIS:O	1:A:27:ASP:HB2	2.19	0.43
1:A:89:LEU:CD2	1:A:152:GLU:HG3	2.45	0.43
1:A:258:ALA:C	1:A:260:ARG:N	2.76	0.43
1:A:377:ARG:HG2	1:A:377:ARG:HH11	1.84	0.43
1:A:474:ASN:HD22	1:A:474:ASN:N	2.13	0.43
1:B:185:PRO:HG2	1:B:188:THR:OG1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:LEU:O	1:C:176:VAL:HG23	2.19	0.43
1:C:175:LEU:HD13	1:C:216:ARG:HB2	2.00	0.43
1:D:41:VAL:HG22	1:D:69:LEU:HD12	1.99	0.43
1:D:442:ILE:HD13	1:D:691:GLN:OE1	2.18	0.43
1:D:583:TYR:CE2	1:D:687:LYS:HE3	2.53	0.43
2:E:302:ASP:O	2:E:306:GLN:HG3	2.19	0.43
2:G:203:LEU:HA	2:G:207:ARG:HD2	2.00	0.43
2:G:207:ARG:HG2	2:G:207:ARG:HH11	1.84	0.43
2:H:201:ASN:HD21	2:H:246:GLN:HG2	1.84	0.43
1:A:69:LEU:HB3	1:A:77:TYR:CE2	2.54	0.43
1:A:209:THR:N	1:A:210:PRO:CD	2.81	0.43
1:B:568:PHE:O	1:B:570:GLU:N	2.51	0.43
1:C:222:PHE:CD2	1:C:492:LEU:HD11	2.54	0.43
1:C:633:ASN:HD22	1:C:633:ASN:N	2.16	0.43
1:D:221:GLN:OE1	1:D:250:GLN:HG2	2.19	0.43
1:D:552:LEU:HB2	1:D:602:LEU:HD21	2.00	0.43
2:F:175:HIS:HB3	2:G:178:ASN:ND2	2.33	0.43
2:G:170:LEU:HD13	2:G:175:HIS:HB2	2.01	0.43
2:H:78:LYS:HE2	2:H:136:VAL:HG13	2.01	0.43
1:A:451:ASP:CG	1:A:452:VAL:N	2.77	0.43
1:A:506:GLY:HA2	1:A:567:TRP:HZ3	1.83	0.43
1:B:47:ILE:C	1:B:47:ILE:HD13	2.44	0.43
1:B:260:ARG:HG2	1:B:365:TYR:CE2	2.54	0.43
1:B:437:ASN:OD1	1:B:439:CYS:N	2.52	0.43
1:C:94:TYR:C	1:C:96:GLN:N	2.76	0.43
1:C:676:ASP:O	1:C:680:GLN:HB2	2.18	0.43
1:D:175:LEU:HB3	1:D:216:ARG:CB	2.49	0.43
1:D:244:ILE:O	1:D:248:VAL:HG13	2.19	0.43
1:D:307:PRO:HB2	1:D:309:TRP:NE1	2.33	0.43
1:D:428:PRO:O	1:D:432:PRO:HB3	2.19	0.43
1:D:475:LEU:CD2	1:D:543:THR:HG23	2.48	0.43
2:E:11:ASP:O	2:E:15:GLU:HG2	2.18	0.43
2:E:332:ILE:HB	2:E:334:TRP:NE1	2.34	0.43
2:F:145:GLN:NE2	2:F:145:GLN:N	2.67	0.43
2:G:332:ILE:HB	2:G:334:TRP:NE1	2.34	0.43
2:H:157:TYR:OH	2:H:200:VAL:HG22	2.19	0.43
1:A:297:VAL:CG1	1:A:298:ARG:CG	2.46	0.43
1:B:229:GLU:O	1:B:448:PRO:HA	2.19	0.43
1:B:519:ASN:ND2	1:B:522:TYR:HD2	2.08	0.43
1:D:522:TYR:CE1	1:D:662:LEU:HD12	2.54	0.43
1:D:622:SER:HB2	1:D:625:SER:HG	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:TRP:HE3	2:E:168:HIS:CD2	2.36	0.43
2:E:204:GLU:CD	2:E:241:HIS:HB3	2.44	0.43
2:F:4:THR:HG21	2:G:157:TYR:HB3	1.99	0.43
2:F:311:ILE:O	2:F:315:ARG:HG2	2.19	0.43
2:G:59:ARG:O	2:G:63:GLN:HG2	2.19	0.43
1:A:207:LEU:HA	1:A:208:PRO:HD3	1.94	0.42
1:A:227:LEU:HD12	1:A:227:LEU:N	2.34	0.42
1:A:708:LYS:CB	2:F:360:GLN:O	2.66	0.42
1:C:306:TYR:OH	1:C:317:LEU:HD22	2.19	0.42
1:C:307:PRO:HB2	1:C:309:TRP:NE1	2.33	0.42
1:C:587:LEU:HD21	1:C:724:PHE:O	2.19	0.42
1:D:11:ASP:OD2	1:D:13:SER:HB3	2.18	0.42
1:D:181:PHE:O	1:D:189:ARG:HG3	2.18	0.42
2:E:219:ALA:HB1	2:E:338:TRP:CH2	2.53	0.42
2:F:300:ASN:N	2:F:303:ILE:CG2	2.82	0.42
1:A:425:PRO:O	1:A:572:THR:HG23	2.19	0.42
1:A:552:LEU:HB2	1:A:602:LEU:HD21	2.01	0.42
1:B:406:ARG:HG3	1:B:406:ARG:HH11	1.84	0.42
1:C:7:VAL:HG12	1:C:53:ILE:HG22	2.01	0.42
1:C:175:LEU:HB3	1:C:216:ARG:HB2	2.01	0.42
1:C:261:ILE:O	1:C:358:PRO:HG3	2.19	0.42
1:D:320:LYS:NZ	1:D:411:ARG:CB	2.82	0.42
1:D:464:LEU:HA	1:D:514:GLY:O	2.19	0.42
2:G:165:SER:O	2:G:169:LEU:HG	2.20	0.42
1:A:50:TYR:H	1:A:53:ILE:CG2	2.32	0.42
1:A:321:ASN:OD1	1:A:322:ASN:N	2.52	0.42
1:B:10:ARG:HH22	1:B:88:HIS:CE1	2.37	0.42
1:B:10:ARG:HD2	3:B:801:DTP:O3G	2.19	0.42
1:B:181:PHE:O	1:B:184:TYR:HB2	2.20	0.42
1:B:339:ILE:O	1:B:416:ASN:HA	2.19	0.42
1:B:465:SER:HB2	1:B:515:ILE:HG12	1.99	0.42
1:C:212:MET:O	1:C:216:ARG:NH1	2.32	0.42
1:C:220:ARG:HG3	1:C:497:ASP:OD2	2.19	0.42
1:C:441:GLU:HA	1:C:692:SER:O	2.20	0.42
1:D:23:HIS:CE1	1:D:42:GLU:CD	2.96	0.42
1:D:40:GLN:HE22	1:D:44:ARG:HD2	1.85	0.42
1:D:633:ASN:N	1:D:633:ASN:ND2	2.67	0.42
2:E:65:LEU:HD21	2:E:223:LEU:HD13	2.01	0.42
2:E:74:ILE:HG23	2:E:75:SER:N	2.34	0.42
2:E:121:SER:HB2	2:E:230:ILE:HG21	2.00	0.42
2:F:157:TYR:OH	2:F:200:VAL:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:339:LEU:C	2:G:340:VAL:HG22	2.44	0.42
1:A:172:LEU:C	1:A:172:LEU:HD23	2.44	0.42
1:A:353:ILE:O	1:A:393:VAL:HG22	2.19	0.42
1:B:378:LEU:O	1:B:381:LYS:HB3	2.19	0.42
1:C:9:LYS:CE	1:C:15:GLU:CD	2.82	0.42
1:C:238:ASN:HB3	1:D:242:SER:OG	2.18	0.42
1:D:353:ILE:HG13	1:D:395:ALA:HB2	2.01	0.42
1:D:425:PRO:CG	1:D:615:THR:HG22	2.50	0.42
1:D:556:ASN:O	1:D:560:LYS:HG3	2.19	0.42
1:D:568:PHE:HE1	1:D:573:TYR:HB2	1.84	0.42
1:D:647:SER:HB3	1:D:650:GLY:O	2.19	0.42
2:E:3:THR:OG1	2:E:5:PHE:O	2.28	0.42
2:H:74:ILE:HG23	2:H:75:SER:N	2.34	0.42
2:H:307:TYR:HA	2:H:331:PRO:HG3	2.01	0.42
1:A:307:PRO:HG2	1:A:310:HIS:HB2	2.02	0.42
1:A:633:ASN:OD1	1:A:636:GLU:CB	2.68	0.42
1:B:41:VAL:HG22	1:B:69:LEU:HD12	2.01	0.42
1:B:225:CYS:HB3	1:B:437:ASN:HD22	1.84	0.42
1:B:442:ILE:HD12	1:B:462:CYS:SG	2.60	0.42
1:C:47:ILE:HD13	1:C:47:ILE:C	2.44	0.42
1:C:118:HIS:ND1	1:C:119:LEU:N	2.67	0.42
1:C:464:LEU:HA	1:C:514:GLY:O	2.19	0.42
1:D:47:ILE:C	1:D:47:ILE:HD13	2.44	0.42
1:D:651:ILE:H	1:D:651:ILE:HG13	1.65	0.42
1:D:713:GLN:NE2	1:D:716:LYS:HD3	2.35	0.42
2:H:87:GLN:O	2:H:91:PRO:HD2	2.18	0.42
2:H:221:ARG:CB	2:H:223:LEU:HD12	2.49	0.42
1:A:47:ILE:HD13	1:A:47:ILE:C	2.44	0.42
1:A:151:LEU:HD23	1:A:155:TYR:HB2	2.02	0.42
1:A:328:ASN:HD22	1:A:328:ASN:N	2.04	0.42
1:A:509:GLY:HA3	1:A:567:TRP:CE3	2.55	0.42
1:B:171:PHE:HA	1:B:174:ILE:HG22	2.01	0.42
1:B:172:LEU:HD23	1:B:172:LEU:C	2.45	0.42
1:B:307:PRO:HG2	1:B:310:HIS:HB2	2.00	0.42
1:B:423:HIS:HB2	1:B:582:THR:O	2.20	0.42
1:B:451:ASP:CG	1:B:452:VAL:N	2.77	0.42
1:B:474:ASN:HD22	1:B:474:ASN:C	2.28	0.42
1:C:354:THR:HG21	1:C:356:PHE:CZ	2.55	0.42
1:C:487:ARG:NH1	1:C:558:LEU:HD13	2.34	0.42
1:C:532:SER:HB2	1:C:673:PRO:HD2	2.00	0.42
1:C:545:GLU:OE1	1:C:595:LEU:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:ASN:HB2	1:C:616:LEU:HD23	2.01	0.42
1:D:118:HIS:ND1	1:D:118:HIS:C	2.78	0.42
1:D:152:GLU:CG	1:D:153:GLY:N	2.82	0.42
1:D:320:LYS:CE	1:D:409:THR:HB	2.49	0.42
1:D:341:LYS:HD3	1:D:341:LYS:C	2.45	0.42
1:D:531:TYR:N	1:D:531:TYR:CD1	2.88	0.42
2:E:332:ILE:HG22	2:E:334:TRP:HE1	1.83	0.42
2:F:332:ILE:HG22	2:F:334:TRP:HE1	1.83	0.42
2:G:115:GLU:HA	2:G:115:GLU:OE1	2.19	0.42
2:H:219:ALA:HB1	2:H:338:TRP:CH2	2.55	0.42
2:H:221:ARG:HH21	2:H:297:ILE:HD12	1.83	0.42
1:A:63:ILE:HG12	1:A:84:LEU:HB3	2.00	0.42
1:A:175:LEU:HD13	1:A:216:ARG:HD2	2.01	0.42
1:A:233:SER:OG	1:A:236:SER:CB	2.68	0.42
1:A:587:LEU:HD21	1:A:724:PHE:O	2.18	0.42
1:B:207:LEU:HA	1:B:208:PRO:HD3	1.93	0.42
1:B:208:PRO:HG2	1:B:464:LEU:HB2	2.01	0.42
1:B:227:LEU:N	1:B:227:LEU:HD12	2.34	0.42
1:B:354:THR:HB	1:B:356:PHE:CE2	2.55	0.42
1:B:552:LEU:HB2	1:B:602:LEU:HD21	2.01	0.42
1:C:80:LEU:O	1:C:84:LEU:HG	2.19	0.42
1:C:114:LYS:O	1:C:115:TYR:HD1	2.02	0.42
1:C:197:TYR:C	1:C:199:ALA:H	2.26	0.42
1:D:19:LEU:CD1	2:G:295:SER:O	2.35	0.42
1:D:568:PHE:CE2	1:D:574:ALA:HA	2.54	0.42
2:G:111:TRP:HH2	2:G:200:VAL:HG11	1.84	0.42
2:H:132:ASP:OD2	2:H:135:VAL:HG23	2.20	0.42
1:A:197:TYR:C	1:A:199:ALA:H	2.26	0.42
1:A:369:PHE:HB3	1:A:421:ASN:HD21	1.85	0.42
1:B:17:ILE:HD11	1:B:49:PHE:CE1	2.55	0.42
1:B:309:TRP:CZ3	1:B:364:LEU:HD12	2.55	0.42
1:B:685:MET:HB2	1:B:693:ILE:CD1	2.50	0.42
1:C:27:ASP:OD1	1:C:38:ILE:HG13	2.20	0.42
1:C:568:PHE:CE2	1:C:574:ALA:HA	2.54	0.42
1:C:583:TYR:CD1	1:C:583:TYR:C	2.98	0.42
1:D:70:ILE:HD12	1:D:653:ARG:HB2	2.02	0.42
1:D:175:LEU:CB	1:D:216:ARG:CD	2.86	0.42
1:D:568:PHE:C	1:D:570:GLU:N	2.78	0.42
2:G:216:PHE:HB3	2:G:338:TRP:CD1	2.55	0.42
1:A:171:PHE:HA	1:A:174:ILE:CG2	2.49	0.42
1:A:206:SER:HB2	1:A:518:ILE:HD13	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ARG:HG2	1:A:365:TYR:CE2	2.55	0.42
1:A:320:LYS:HE2	1:A:411:ARG:CG	2.50	0.42
1:A:369:PHE:HB3	1:A:421:ASN:ND2	2.35	0.42
1:B:147:ALA:CB	1:B:628:ILE:HA	2.49	0.42
1:B:275:HIS:CD2	1:B:277:GLY:H	2.38	0.42
1:B:365:TYR:HE2	1:B:434:ARG:HH21	1.66	0.42
1:B:419:HIS:C	1:B:422:THR:OG1	2.62	0.42
1:D:276:THR:HG22	3:D:803:DTP:H2	2.01	0.42
1:D:293:SER:O	1:D:294:GLN:C	2.62	0.42
2:F:3:THR:HG21	2:F:5:PHE:O	2.20	0.42
2:G:92:ASN:OD1	2:G:109:GLU:HA	2.19	0.42
2:G:96:LEU:HB2	2:G:97:PRO:HD3	2.02	0.42
2:H:17:MET:HE1	2:H:251:LEU:HB2	2.02	0.42
2:H:33:TYR:HB3	2:H:35:ILE:HG22	2.02	0.42
2:H:78:LYS:NZ	2:H:139:ASP:OD2	2.42	0.42
2:H:236:ARG:HA	2:H:340:VAL:CG2	2.49	0.42
1:A:40:GLN:O	1:A:44:ARG:HB2	2.20	0.42
1:A:214:GLY:O	1:A:217:THR:OG1	2.38	0.42
1:A:340:ASN:HD21	1:A:342:LEU:HB3	1.85	0.42
1:A:641:TYR:O	1:A:656:VAL:HG13	2.19	0.42
1:B:128:PHE:HA	1:B:131:MET:HE3	2.00	0.42
1:B:206:SER:OG	1:B:625:SER:HB2	2.19	0.42
1:B:248:VAL:O	1:B:292:CYS:SG	2.78	0.42
1:C:176:VAL:HA	1:C:215:VAL:HG11	2.01	0.42
1:C:293:SER:OG	1:C:298:ARG:O	2.35	0.42
1:C:474:ASN:ND2	1:C:474:ASN:N	2.67	0.42
1:C:713:GLN:NE2	1:C:716:LYS:HD3	2.35	0.42
1:D:140:ASP:OD1	1:D:170:GLN:HG2	2.20	0.42
1:D:276:THR:CG2	3:D:803:DTP:H2	2.50	0.42
1:D:283:LYS:NZ	1:D:329:ARG:O	2.53	0.42
1:D:354:THR:OG1	1:D:392:ARG:NH1	2.53	0.42
1:D:466:ALA:HA	1:D:516:GLY:O	2.20	0.42
1:D:565:CYS:HA	1:D:566:PRO:HD3	1.95	0.42
1:D:583:TYR:CB	1:D:687:LYS:HG3	2.50	0.42
1:D:692:SER:OG	1:D:727:LYS:HB2	2.20	0.42
2:E:66:PRO:O	2:E:69:GLU:HB2	2.20	0.42
2:F:142:THR:HG23	2:G:9:LYS:HD2	2.02	0.42
2:G:139:ASP:O	2:G:140:ILE:C	2.63	0.42
1:A:214:GLY:C	1:A:217:THR:HG23	2.43	0.41
1:A:541:HIS:O	1:A:545:GLU:HB2	2.19	0.41
1:A:682:VAL:HG13	1:A:693:ILE:HD12	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ASN:H	1:B:474:ASN:ND2	2.18	0.41
1:C:544:PHE:HA	1:C:547:ILE:HD12	2.02	0.41
1:C:684:ILE:O	1:C:687:LYS:HB3	2.20	0.41
1:D:368:PHE:CE2	1:D:417:VAL:HG21	2.55	0.41
2:F:34:ASP:O	2:F:38:LYS:HG3	2.20	0.41
2:F:177:VAL:HG11	2:G:170:LEU:CD2	2.50	0.41
2:F:242:LEU:HD12	2:F:242:LEU:C	2.45	0.41
2:G:55:VAL:HA	2:G:226:GLY:HA3	2.00	0.41
2:G:78:LYS:HE2	2:G:136:VAL:HG13	2.02	0.41
2:G:360:GLN:O	2:G:361:ILE:CG2	2.65	0.41
1:A:19:LEU:HD12	2:F:295:SER:OG	2.21	0.41
1:A:44:ARG:O	1:A:46:HIS:CD2	2.74	0.41
1:A:217:THR:OG1	1:A:219:THR:HG22	2.21	0.41
1:A:668:LEU:O	1:A:671:GLU:HB3	2.20	0.41
1:B:303:THR:HG22	1:B:305:PHE:CE1	2.56	0.41
1:C:151:LEU:CD2	1:C:155:TYR:CB	2.94	0.41
1:C:303:THR:HB	1:C:305:PHE:CE1	2.55	0.41
1:C:413:TYR:HH	1:C:731:TYR:HE1	0.64	0.41
1:C:568:PHE:C	1:C:570:GLU:N	2.78	0.41
1:D:361:VAL:HB	1:D:364:LEU:HB2	2.01	0.41
2:F:65:LEU:HD21	2:F:223:LEU:HD13	2.02	0.41
2:F:207:ARG:HG2	2:F:283:GLU:OE2	2.19	0.41
2:G:157:TYR:OH	2:G:200:VAL:HG22	2.19	0.41
2:G:242:LEU:HD12	2:G:242:LEU:C	2.45	0.41
2:G:311:ILE:O	2:G:315:ARG:HG2	2.20	0.41
2:H:203:LEU:C	2:H:203:LEU:CD2	2.93	0.41
1:A:229:GLU:O	1:A:448:PRO:HA	2.20	0.41
1:A:307:PRO:HB2	1:A:309:TRP:CD1	2.55	0.41
1:A:489:LEU:HD12	1:A:515:ILE:HD11	2.01	0.41
1:A:543:THR:O	1:A:547:ILE:HG13	2.20	0.41
1:B:406:ARG:HD2	1:B:414:ILE:HD11	2.00	0.41
1:B:422:THR:O	1:B:582:THR:HB	2.19	0.41
1:B:615:THR:C	1:B:616:LEU:HD23	2.45	0.41
1:C:307:PRO:HG2	1:C:310:HIS:HB2	2.01	0.41
2:F:16:PRO:HA	2:F:257:ASP:OD1	2.21	0.41
2:F:332:ILE:HB	2:F:334:TRP:NE1	2.35	0.41
2:G:17:MET:HE1	2:G:251:LEU:HB2	2.01	0.41
2:H:11:ASP:O	2:H:15:GLU:HG2	2.20	0.41
2:H:16:PRO:HA	2:H:257:ASP:OD1	2.20	0.41
2:H:111:TRP:O	2:H:115:GLU:HG2	2.19	0.41
2:H:242:LEU:HD12	2:H:242:LEU:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:OH	1:A:171:PHE:CD2	2.66	0.41
1:A:474:ASN:HD22	1:A:474:ASN:C	2.28	0.41
1:B:87:PHE:C	1:B:87:PHE:CD1	2.98	0.41
1:C:43:LEU:HD13	2:E:220:GLU:HG3	2.03	0.41
1:C:117:ASN:O	1:C:118:HIS:C	2.60	0.41
1:C:341:LYS:HD3	1:C:341:LYS:C	2.45	0.41
1:C:479:GLU:HB2	1:C:550:TYR:CE1	2.55	0.41
2:H:144:GLU:HA	2:H:147:GLN:HB2	2.03	0.41
2:H:207:ARG:HG2	2:H:207:ARG:HH11	1.84	0.41
1:A:216:ARG:HG2	1:A:216:ARG:HH11	1.86	0.41
1:A:678:TYR:HD1	1:A:679:LEU:HD23	1.85	0.41
1:B:199:ALA:O	1:B:204:LYS:HB2	2.21	0.41
1:B:426:PHE:HB3	1:B:431:ALA:O	2.20	0.41
1:C:152:GLU:HA	1:C:156:LEU:HD12	2.02	0.41
1:C:310:HIS:ND1	1:C:311:LEU:N	2.69	0.41
1:C:413:TYR:CE1	1:C:731:TYR:CD1	2.95	0.41
1:C:720:THR:HA	2:E:373:PHE:CZ	2.55	0.41
1:D:354:THR:HG21	1:D:356:PHE:CZ	2.56	0.41
1:D:437:ASN:OD1	1:D:441:GLU:OE1	2.39	0.41
1:D:545:GLU:OE1	1:D:595:LEU:HA	2.20	0.41
2:F:121:SER:HB2	2:F:230:ILE:HG21	2.02	0.41
2:G:302:ASP:O	2:G:306:GLN:HG3	2.21	0.41
1:A:66:ALA:HA	1:A:69:LEU:HG	2.01	0.41
1:A:378:LEU:O	1:A:381:LYS:HB3	2.21	0.41
1:A:558:LEU:HD11	1:A:562:GLN:NE2	2.36	0.41
1:B:17:ILE:HG12	3:B:801:DTP:N1	2.35	0.41
1:B:207:LEU:HD12	1:B:212:MET:HE3	2.01	0.41
1:B:282:TYR:CE2	1:B:304:LEU:HD13	2.56	0.41
1:C:353:ILE:HG13	1:C:395:ALA:HB2	2.01	0.41
1:D:94:TYR:OH	1:D:168:SER:HB3	2.21	0.41
1:D:179:CYS:SG	1:D:216:ARG:HA	2.60	0.41
2:E:90:SER:HB3	2:E:157:TYR:CE1	2.55	0.41
2:F:11:ASP:O	2:F:15:GLU:HG2	2.21	0.41
2:F:92:ASN:OD1	2:F:109:GLU:HA	2.20	0.41
2:F:212:PHE:HB3	2:F:216:PHE:CE2	2.55	0.41
2:F:291:PHE:CD2	2:F:301:LYS:N	2.88	0.41
2:G:16:PRO:HA	2:G:257:ASP:OD1	2.21	0.41
1:A:103:TYR:CE2	1:A:125:GLU:HG3	2.56	0.41
1:A:150:GLN:O	1:A:154:LYS:HG3	2.20	0.41
1:A:369:PHE:O	1:A:421:ASN:CB	2.68	0.41
1:B:320:LYS:HE2	1:B:411:ARG:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PRO:O	1:C:189:ARG:N	2.54	0.41
1:C:618:ALA:HB2	1:C:691:GLN:HG3	2.03	0.41
1:D:7:VAL:HG21	3:D:801:DTP:C6	2.51	0.41
1:D:10:ARG:CD	1:D:91:LYS:HB3	2.50	0.41
1:D:353:ILE:O	1:D:393:VAL:HG22	2.20	0.41
2:E:7:GLN:OE1	2:H:147:GLN:NE2	2.47	0.41
2:F:160:LEU:HD21	2:F:193:LEU:HD23	2.01	0.41
2:G:296:MET:HE2	2:G:299:LEU:CD2	2.48	0.41
2:H:79:TYR:O	2:H:82:LEU:HB3	2.20	0.41
1:A:537:ASN:HD21	1:A:680:GLN:HG2	1.86	0.41
1:B:40:GLN:OE1	1:B:44:ARG:CG	2.68	0.41
1:B:364:LEU:O	1:B:364:LEU:HD13	2.19	0.41
1:B:551:LEU:HB3	1:B:616:LEU:HB3	2.02	0.41
1:C:80:LEU:O	1:C:80:LEU:HD12	2.21	0.41
1:C:94:TYR:OH	1:C:168:SER:HB3	2.21	0.41
1:C:406:ARG:HD2	1:C:414:ILE:HD11	2.02	0.41
1:D:87:PHE:CD1	1:D:87:PHE:C	2.99	0.41
1:D:227:LEU:HD12	1:D:227:LEU:N	2.35	0.41
2:E:103:GLU:OE1	2:E:103:GLU:N	2.52	0.41
2:E:261:MET:HE3	2:E:261:MET:HB3	1.99	0.41
2:G:89:ARG:HG3	2:G:90:SER:N	2.36	0.41
1:A:75:PRO:C	1:A:77:TYR:H	2.29	0.41
1:A:147:ALA:CB	1:A:628:ILE:HA	2.51	0.41
1:A:156:LEU:HD22	1:A:167:GLU:O	2.20	0.41
1:A:157:VAL:HG23	1:A:216:ARG:HH21	1.77	0.41
1:A:256:ILE:HG22	1:A:304:LEU:HD21	2.03	0.41
1:A:418:ASP:O	1:A:422:THR:CG2	2.69	0.41
1:A:444:LEU:HD21	1:A:691:GLN:NE2	2.34	0.41
1:B:91:LYS:O	1:B:95:GLY:HA2	2.21	0.41
1:B:185:PRO:HB2	1:B:187:GLU:CD	2.46	0.41
1:B:307:PRO:HB2	1:B:309:TRP:CD1	2.56	0.41
1:B:371:ASP:HB3	1:B:374:GLU:HB3	2.02	0.41
1:B:576:GLY:O	1:B:577:ILE:HD13	2.20	0.41
1:B:621:PRO:CG	1:B:694:SER:CB	2.99	0.41
1:C:124:THR:HG1	1:C:127:GLU:HG3	1.85	0.41
1:C:221:GLN:O	1:C:222:PHE:CD1	2.74	0.41
1:C:226:VAL:HG11	1:C:247:TYR:CD2	2.56	0.41
1:C:364:LEU:HD13	1:C:364:LEU:C	2.45	0.41
1:C:472:ILE:HG22	1:C:477:GLU:HG3	2.02	0.41
1:C:478:LEU:O	1:C:479:GLU:C	2.64	0.41
1:C:592:ASN:N	1:C:592:ASN:ND2	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:GLN:HE22	1:C:716:LYS:HD3	1.84	0.41
1:D:7:VAL:HG12	1:D:53:ILE:CD1	2.51	0.41
1:D:155:TYR:CE2	1:D:628:ILE:HG13	2.50	0.41
1:D:174:ILE:HG23	1:D:175:LEU:N	2.36	0.41
1:D:321:ASN:O	1:D:329:ARG:HD2	2.21	0.41
1:D:587:LEU:HD21	1:D:724:PHE:O	2.21	0.41
1:D:657:PRO:HG2	1:D:666:TYR:OH	2.20	0.41
2:E:5:PHE:CD1	2:E:24:ASN:HB2	2.54	0.41
2:E:143:ASN:HB3	2:E:146:ILE:CG1	2.51	0.41
2:E:147:GLN:NE2	2:E:150:ALA:HB3	2.35	0.41
2:E:165:SER:O	2:E:169:LEU:CG	2.69	0.41
2:E:217:ALA:HB2	2:E:299:LEU:CD2	2.51	0.41
2:E:242:LEU:HD12	2:E:242:LEU:C	2.46	0.41
2:E:311:ILE:O	2:E:315:ARG:HG2	2.20	0.41
2:F:245:THR:O	2:F:249:LEU:HG	2.21	0.41
2:G:24:ASN:OD1	2:G:25:VAL:HG12	2.21	0.41
2:G:208:PHE:CG	2:G:238:GLU:OE1	2.74	0.41
2:G:247:HIS:O	2:G:251:LEU:HG	2.20	0.41
2:H:327:THR:C	2:H:328:ARG:CG	2.94	0.41
1:A:199:ALA:O	1:A:204:LYS:HB2	2.21	0.41
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.03	0.41
1:A:411:ARG:CZ	1:A:731:TYR:CE1	3.04	0.41
1:A:474:ASN:H	1:A:474:ASN:ND2	2.17	0.41
1:B:451:ASP:CG	1:B:452:VAL:H	2.29	0.41
1:C:87:PHE:CD1	1:C:87:PHE:C	2.99	0.41
1:C:444:LEU:HB2	1:C:460:ALA:HB1	2.02	0.41
1:D:228:ILE:CG2	1:D:240:THR:HG23	2.51	0.41
1:D:713:GLN:HE22	1:D:716:LYS:HD3	1.85	0.41
2:F:71:HIS:ND1	2:F:71:HIS:C	2.79	0.41
2:F:217:ALA:CB	2:F:296:MET:HE1	2.50	0.41
1:A:451:ASP:CG	1:A:452:VAL:H	2.28	0.40
1:B:44:ARG:HA	1:B:44:ARG:NE	2.31	0.40
1:B:196:PHE:HB2	1:B:484:LEU:HD11	2.03	0.40
1:B:309:TRP:CD1	1:B:309:TRP:H	2.39	0.40
1:B:489:LEU:HD13	1:B:513:LEU:CD1	2.48	0.40
1:B:543:THR:O	1:B:547:ILE:HG13	2.21	0.40
1:B:621:PRO:HG3	1:B:694:SER:CB	2.52	0.40
1:C:227:LEU:HD12	1:C:227:LEU:N	2.36	0.40
1:C:309:TRP:CD1	1:C:309:TRP:H	2.39	0.40
1:C:336:GLY:HA2	1:C:413:TYR:O	2.21	0.40
1:C:519:ASN:HD21	1:C:522:TYR:HB3	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:544:PHE:CE2	1:C:685:MET:HG2	2.56	0.40
1:D:9:LYS:HA	1:D:9:LYS:HD3	1.79	0.40
1:D:459:ILE:HB	1:D:503:ALA:HA	2.02	0.40
1:D:583:TYR:CD1	1:D:583:TYR:C	2.99	0.40
2:E:92:ASN:OD1	2:E:109:GLU:HA	2.22	0.40
2:F:90:SER:HB3	2:F:157:TYR:CE1	2.56	0.40
2:G:219:ALA:HB1	2:G:338:TRP:CZ2	2.55	0.40
2:H:68:HIS:O	2:H:71:HIS:HB3	2.21	0.40
1:A:102:LEU:O	1:A:106:VAL:HG23	2.21	0.40
1:A:427:ASP:OD2	1:A:575:LYS:NZ	2.52	0.40
1:B:364:LEU:HD23	1:B:378:LEU:HB2	2.03	0.40
1:B:464:LEU:HD22	1:B:620:MET:HE3	2.03	0.40
1:C:353:ILE:O	1:C:393:VAL:HG22	2.21	0.40
2:E:85:SER:O	2:E:89:ARG:NH1	2.55	0.40
2:F:76:ASN:O	2:F:80:GLN:HG3	2.21	0.40
2:F:198:MET:HE2	2:F:272:CYS:HB3	2.04	0.40
2:H:203:LEU:HA	2:H:207:ARG:HD2	2.03	0.40
1:A:10:ARG:C	1:A:12:GLY:N	2.74	0.40
1:A:546:ALA:HB2	1:A:597:TYR:CE2	2.56	0.40
1:B:36:VAL:O	1:B:36:VAL:HG23	2.22	0.40
1:B:330:VAL:HB	1:B:335:TYR:OH	2.22	0.40
1:C:149:LYS:HG2	1:C:652:LEU:HD21	2.02	0.40
1:D:613:ASN:HB2	1:D:616:LEU:HD21	2.04	0.40
2:E:154:SER:O	2:E:158:ASP:OD2	2.39	0.40
2:E:166:TYR:CE2	2:H:169:LEU:HD22	2.56	0.40
2:G:121:SER:HB2	2:G:230:ILE:HG21	2.03	0.40
2:H:245:THR:O	2:H:249:LEU:HG	2.22	0.40
1:A:530:ARG:HD2	1:A:533:ASP:OD2	2.22	0.40
1:B:321:ASN:ND2	1:B:323:ARG:O	2.54	0.40
1:C:209:THR:N	1:C:210:PRO:CD	2.85	0.40
1:C:348:LEU:HD21	1:C:719:LEU:HD13	2.04	0.40
1:C:442:ILE:CD1	1:C:462:CYS:SG	3.04	0.40
1:D:199:ALA:O	1:D:204:LYS:HB2	2.21	0.40
1:D:543:THR:O	1:D:547:ILE:HG13	2.21	0.40
2:G:48:TRP:CZ3	2:G:50:PRO:HG3	2.57	0.40
2:H:3:THR:OG1	2:H:5:PHE:O	2.29	0.40
1:A:254:ILE:O	1:A:302:ALA:HA	2.22	0.40
1:A:565:CYS:HA	1:A:566:PRO:HD3	1.94	0.40
1:B:5:LEU:HB3	1:B:51:ASP:CA	2.44	0.40
1:B:7:VAL:O	1:B:7:VAL:HG22	2.21	0.40
1:B:41:VAL:HG22	1:B:69:LEU:CD1	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLN:HA	1:C:150:GLN:OE1	2.21	0.40
1:C:165:ILE:HG22	1:C:166:TYR:N	2.36	0.40
1:C:478:LEU:HD13	1:C:547:ILE:HA	2.03	0.40
1:C:506:GLY:HA2	1:C:567:TRP:HZ3	1.85	0.40
1:C:556:ASN:O	1:C:560:LYS:HG3	2.22	0.40
1:C:667:GLU:OE1	1:C:672:MET:HG2	2.21	0.40
2:E:111:TRP:HH2	2:E:200:VAL:HG11	1.85	0.40
2:E:165:SER:HB2	2:H:169:LEU:HD21	2.03	0.40
2:E:275:LEU:O	2:E:278:GLN:HB3	2.21	0.40
2:H:275:LEU:O	2:H:278:GLN:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	731/761 (96%)	687 (94%)	40 (6%)	4 (0%)	24	60
1	B	732/761 (96%)	693 (95%)	37 (5%)	2 (0%)	36	69
1	C	729/761 (96%)	690 (95%)	36 (5%)	3 (0%)	30	65
1	D	731/761 (96%)	694 (95%)	33 (4%)	4 (0%)	24	60
2	E	348/375 (93%)	336 (97%)	12 (3%)	0	100	100
2	F	352/375 (94%)	338 (96%)	13 (4%)	1 (0%)	36	69
2	G	352/375 (94%)	336 (96%)	13 (4%)	3 (1%)	14	48
2	H	352/375 (94%)	339 (96%)	13 (4%)	0	100	100
All	All	4327/4544 (95%)	4113 (95%)	197 (5%)	17 (0%)	30	65

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	GLY
1	A	300	GLY
1	B	300	GLY
1	C	299	GLY
1	C	300	GLY
1	D	299	GLY
1	D	300	GLY
1	A	327	GLY
1	A	271	GLY
1	B	271	GLY
1	C	271	GLY
1	D	271	GLY
2	G	292	ARG
1	D	621	PRO
2	F	91	PRO
2	G	91	PRO
2	G	361	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/651 (97%)	601 (96%)	28 (4%)	24	48
1	B	629/651 (97%)	597 (95%)	32 (5%)	21	46
1	C	626/651 (96%)	594 (95%)	32 (5%)	21	46
1	D	628/651 (96%)	596 (95%)	32 (5%)	21	46
2	E	319/340 (94%)	305 (96%)	14 (4%)	25	49
2	F	323/340 (95%)	312 (97%)	11 (3%)	32	55
2	G	323/340 (95%)	297 (92%)	26 (8%)	11	35
2	H	323/340 (95%)	312 (97%)	11 (3%)	32	55
All	All	3800/3964 (96%)	3614 (95%)	186 (5%)	22	47

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	27	ASP
1	A	43	LEU
1	A	44	ARG
1	A	47	ILE
1	A	51	ASP
1	A	53	ILE
1	A	76	ASP
1	A	154	LYS
1	A	189	ARG
1	A	226	VAL
1	A	294	GLN
1	A	297	VAL
1	A	298	ARG
1	A	304	LEU
1	A	328	ASN
1	A	341	LYS
1	A	369	PHE
1	A	437	ASN
1	A	441	GLU
1	A	474	ASN
1	A	592	ASN
1	A	623	GLU
1	A	647	SER
1	A	648	LYS
1	A	649	ASP
1	A	652	LEU
1	A	670	TRP
1	B	6	LEU
1	B	7	VAL
1	B	17	ILE
1	B	27	ASP
1	B	37	SER
1	B	44	ARG
1	B	47	ILE
1	B	51	ASP
1	B	56	SER
1	B	154	LYS
1	B	156	LEU
1	B	189	ARG
1	B	219	THR
1	B	304	LEU
1	B	328	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	LYS
1	B	369	PHE
1	B	371	ASP
1	B	372	GLN
1	B	422	THR
1	B	437	ASN
1	B	441	GLU
1	B	474	ASN
1	B	560	LYS
1	B	562	GLN
1	B	592	ASN
1	B	596	HIS
1	B	616	LEU
1	B	647	SER
1	B	649	ASP
1	B	651	ILE
1	B	670	TRP
1	C	18	ASN
1	C	38	ILE
1	C	47	ILE
1	C	51	ASP
1	C	55	THR
1	C	68	ASP
1	C	78	GLN
1	C	114	LYS
1	C	118	HIS
1	C	154	LYS
1	C	189	ARG
1	C	220	ARG
1	C	297	VAL
1	C	304	LEU
1	C	328	ASN
1	C	369	PHE
1	C	384	LYS
1	C	435	GLN
1	C	436	SER
1	C	472	ILE
1	C	474	ASN
1	C	592	ASN
1	C	620	MET
1	C	622	SER
1	C	624	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	647	SER
1	C	648	LYS
1	C	651	ILE
1	C	652	LEU
1	C	692	SER
1	C	696	ASN
1	C	697	THR
1	D	5	LEU
1	D	7	VAL
1	D	18	ASN
1	D	38	ILE
1	D	47	ILE
1	D	53	ILE
1	D	55	THR
1	D	68	ASP
1	D	72	ARG
1	D	80	LEU
1	D	152	GLU
1	D	154	LYS
1	D	189	ARG
1	D	219	THR
1	D	297	VAL
1	D	304	LEU
1	D	329	ARG
1	D	330	VAL
1	D	331	ARG
1	D	369	PHE
1	D	384	LYS
1	D	435	GLN
1	D	474	ASN
1	D	592	ASN
1	D	620	MET
1	D	623	GLU
1	D	625	SER
1	D	647	SER
1	D	648	LYS
1	D	651	ILE
1	D	692	SER
1	D	696	ASN
2	E	35	ILE
2	E	51	GLU
2	E	145	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	147	GLN
2	E	148	LYS
2	E	151	GLU
2	E	208	PHE
2	E	263	GLU
2	E	266	GLU
2	E	293	ASP
2	E	295	SER
2	E	297	ILE
2	E	299	LEU
2	E	363	SER
2	F	35	ILE
2	F	51	GLU
2	F	145	GLN
2	F	148	LYS
2	F	208	PHE
2	F	296	MET
2	F	326	GLN
2	F	328	ARG
2	F	336	ASN
2	F	360	GLN
2	F	363	SER
2	G	35	ILE
2	G	51	GLU
2	G	67	GLU
2	G	69	GLU
2	G	70	LYS
2	G	95	LEU
2	G	96	LEU
2	G	143	ASN
2	G	144	GLU
2	G	147	GLN
2	G	148	LYS
2	G	149	ARG
2	G	151	GLU
2	G	163	MET
2	G	208	PHE
2	G	263	GLU
2	G	285	ASP
2	G	290	LEU
2	G	292	ARG
2	G	296	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	297	ILE
2	G	299	LEU
2	G	301	LYS
2	G	340	VAL
2	G	361	ILE
2	G	365	VAL
2	H	57	ARG
2	H	87	GLN
2	H	147	GLN
2	H	148	LYS
2	H	151	GLU
2	H	208	PHE
2	H	221	ARG
2	H	295	SER
2	H	328	ARG
2	H	340	VAL
2	H	361	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (159) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	35	ASN
1	A	40	GLN
1	A	46	HIS
1	A	59	HIS
1	A	105	HIS
1	A	117	ASN
1	A	130	GLN
1	A	137	HIS
1	A	150	GLN
1	A	158	GLN
1	A	191	GLN
1	A	328	ASN
1	A	332	HIS
1	A	415	GLN
1	A	423	HIS
1	A	474	ASN
1	A	562	GLN
1	A	592	ASN
1	A	613	ASN
1	A	627	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	630	ASN
1	A	691	GLN
1	A	713	GLN
1	B	34	HIS
1	B	35	ASN
1	B	59	HIS
1	B	117	ASN
1	B	170	GLN
1	B	257	ASN
1	B	275	HIS
1	B	328	ASN
1	B	332	HIS
1	B	415	GLN
1	B	423	HIS
1	B	435	GLN
1	B	474	ASN
1	B	562	GLN
1	B	592	ASN
1	B	613	ASN
1	B	630	ASN
1	B	633	ASN
1	B	691	GLN
1	B	712	GLN
1	B	732	GLN
1	C	18	ASN
1	C	23	HIS
1	C	35	ASN
1	C	59	HIS
1	C	117	ASN
1	C	118	HIS
1	C	130	GLN
1	C	150	GLN
1	C	158	GLN
1	C	170	GLN
1	C	191	GLN
1	C	275	HIS
1	C	328	ASN
1	C	338	GLN
1	C	474	ASN
1	C	538	ASN
1	C	562	GLN
1	C	592	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	609	HIS
1	C	627	GLN
1	C	630	ASN
1	C	633	ASN
1	C	680	GLN
1	C	691	GLN
1	C	696	ASN
1	C	698	ASN
1	C	712	GLN
1	C	713	GLN
1	D	18	ASN
1	D	23	HIS
1	D	35	ASN
1	D	59	HIS
1	D	105	HIS
1	D	117	ASN
1	D	130	GLN
1	D	150	GLN
1	D	158	GLN
1	D	170	GLN
1	D	321	ASN
1	D	338	GLN
1	D	437	ASN
1	D	474	ASN
1	D	538	ASN
1	D	562	GLN
1	D	592	ASN
1	D	609	HIS
1	D	633	ASN
1	D	680	GLN
1	D	686	GLN
1	D	696	ASN
1	D	713	GLN
2	E	21	GLN
2	E	31	GLN
2	E	68	HIS
2	E	80	GLN
2	E	145	GLN
2	E	147	GLN
2	E	201	ASN
2	E	247	HIS
2	E	281	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	282	GLN
2	E	306	GLN
2	E	313	ASN
2	E	326	GLN
2	E	336	ASN
2	E	372	ASN
2	F	7	GLN
2	F	12	GLN
2	F	21	GLN
2	F	30	GLN
2	F	31	GLN
2	F	68	HIS
2	F	80	GLN
2	F	87	GLN
2	F	124	HIS
2	F	145	GLN
2	F	147	GLN
2	F	175	HIS
2	F	201	ASN
2	F	247	HIS
2	F	281	GLN
2	F	282	GLN
2	F	313	ASN
2	F	336	ASN
2	F	372	ASN
2	G	21	GLN
2	G	30	GLN
2	G	31	GLN
2	G	80	GLN
2	G	87	GLN
2	G	147	GLN
2	G	178	ASN
2	G	201	ASN
2	G	247	HIS
2	G	281	GLN
2	G	282	GLN
2	G	313	ASN
2	G	326	GLN
2	G	336	ASN
2	G	360	GLN
2	G	372	ASN
2	H	21	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	30	GLN
2	H	31	GLN
2	H	128	ASN
2	H	145	GLN
2	H	201	ASN
2	H	281	GLN
2	H	282	GLN
2	H	306	GLN
2	H	313	ASN
2	H	326	GLN
2	H	336	ASN
2	H	372	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	FEO	E	501	2,7	0,2,2	-	-	-		
4	DAT	C	802	-	27,28,28	2.05	11 (40%)	41,43,43	1.98	10 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	FEO	F	501	2,7	0,2,2	-	-	-		
4	DAT	B	802	-	27,28,28	1.99	10 (37%)	41,43,43	2.03	10 (24%)
4	DAT	A	802	-	27,28,28	1.99	11 (40%)	41,43,43	2.22	12 (29%)
3	DTP	D	801	-	31,32,32	1.75	6 (19%)	46,50,50	1.73	10 (21%)
6	FEO	G	501	2,7	0,2,2	-	-	-		
3	DTP	B	803	5	31,32,32	1.73	6 (19%)	46,50,50	1.72	10 (21%)
3	DTP	C	803	5	31,32,32	1.72	6 (19%)	46,50,50	1.72	10 (21%)
3	DTP	C	801	-	31,32,32	1.75	6 (19%)	46,50,50	1.73	10 (21%)
4	DAT	D	802	-	27,28,28	1.99	10 (37%)	41,43,43	1.97	12 (29%)
3	DTP	A	803	5	31,32,32	1.72	6 (19%)	46,50,50	1.68	10 (21%)
6	FEO	H	501	2,7	0,2,2	-	-	-		
3	DTP	D	803	5	31,32,32	1.73	7 (22%)	46,50,50	1.73	10 (21%)
3	DTP	B	801	-	31,32,32	1.78	8 (25%)	46,50,50	1.73	10 (21%)
3	DTP	A	801	-	31,32,32	1.75	6 (19%)	46,50,50	1.73	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DAT	C	802	-	-	3/16/28/28	0/3/3/3
4	DAT	B	802	-	-	9/16/28/28	0/3/3/3
4	DAT	A	802	-	-	1/16/28/28	0/3/3/3
3	DTP	D	801	-	-	4/22/34/34	0/3/3/3
3	DTP	B	803	5	-	1/22/34/34	0/3/3/3
3	DTP	C	803	5	-	4/22/34/34	0/3/3/3
3	DTP	C	801	-	-	4/22/34/34	0/3/3/3
4	DAT	D	802	-	-	5/16/28/28	0/3/3/3
3	DTP	A	803	5	-	1/22/34/34	0/3/3/3
3	DTP	D	803	5	-	4/22/34/34	0/3/3/3
3	DTP	B	801	-	-	6/22/34/34	0/3/3/3
3	DTP	A	801	-	-	4/22/34/34	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	DAT	PA-O3A	-5.75	1.53	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	DAT	PA-O3A	-5.67	1.53	1.59
4	B	802	DAT	PA-O3A	-5.62	1.53	1.59
4	D	802	DAT	PA-O3A	-5.62	1.53	1.59
3	A	803	DTP	C6-N6	5.06	1.47	1.34
3	B	803	DTP	C6-N6	5.04	1.47	1.34
3	C	801	DTP	C6-N6	5.04	1.47	1.34
3	B	801	DTP	C6-N6	5.04	1.47	1.34
3	A	801	DTP	C6-N6	5.02	1.47	1.34
3	D	801	DTP	C6-N6	5.01	1.47	1.34
3	D	803	DTP	C6-N6	5.00	1.47	1.34
3	C	803	DTP	C6-N6	5.00	1.47	1.34
3	C	803	DTP	O3'-C3'	-4.08	1.34	1.43
3	B	801	DTP	O3'-C3'	-4.05	1.34	1.43
3	D	803	DTP	O3'-C3'	-4.04	1.34	1.43
3	B	803	DTP	O3'-C3'	-4.00	1.35	1.43
3	A	801	DTP	O3'-C3'	-3.94	1.35	1.43
3	D	801	DTP	O3'-C3'	-3.92	1.35	1.43
3	C	801	DTP	O3'-C3'	-3.92	1.35	1.43
3	A	803	DTP	O3'-C3'	-3.92	1.35	1.43
4	B	802	DAT	PB-O1B	3.53	1.61	1.50
4	D	802	DAT	PB-O1B	3.51	1.61	1.50
4	A	802	DAT	PB-O1B	3.49	1.61	1.50
4	C	802	DAT	PB-O1B	3.48	1.61	1.50
3	B	801	DTP	C5'-C4'	-3.01	1.42	1.51
3	B	803	DTP	C5'-C4'	-2.97	1.42	1.51
3	C	803	DTP	C5'-C4'	-2.96	1.42	1.51
3	D	803	DTP	C5'-C4'	-2.95	1.42	1.51
3	C	801	DTP	C5'-C4'	-2.92	1.42	1.51
3	A	801	DTP	C5'-C4'	-2.92	1.42	1.51
3	D	801	DTP	C5'-C4'	-2.89	1.42	1.51
3	A	803	DTP	C5'-C4'	-2.85	1.43	1.51
4	C	802	DAT	O4'-C1'	-2.82	1.36	1.42
3	B	801	DTP	O5'-C5'	-2.78	1.34	1.44
4	C	802	DAT	C3'-C4'	-2.78	1.45	1.53
3	D	801	DTP	O5'-C5'	-2.76	1.34	1.44
3	C	801	DTP	O5'-C5'	-2.75	1.34	1.44
3	B	803	DTP	O5'-C5'	-2.75	1.34	1.44
3	C	803	DTP	O5'-C5'	-2.75	1.34	1.44
3	A	801	DTP	O5'-C5'	-2.74	1.34	1.44
4	B	802	DAT	C3'-C4'	-2.74	1.45	1.53
3	D	803	DTP	O5'-C5'	-2.74	1.34	1.44
4	A	802	DAT	C3'-C4'	-2.73	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	803	DTP	O5'-C5'	-2.73	1.34	1.44
3	C	801	DTP	C3'-C4'	-2.71	1.45	1.53
3	D	801	DTP	C3'-C4'	-2.70	1.45	1.53
3	A	801	DTP	C3'-C4'	-2.68	1.45	1.53
3	B	801	DTP	C2'-C3'	-2.68	1.46	1.52
3	A	801	DTP	C2'-C3'	-2.67	1.46	1.52
3	C	803	DTP	C2'-C3'	-2.66	1.46	1.52
3	D	801	DTP	C2'-C3'	-2.65	1.46	1.52
3	C	801	DTP	C2'-C3'	-2.65	1.46	1.52
3	A	803	DTP	C2'-C3'	-2.65	1.46	1.52
3	B	803	DTP	C2'-C3'	-2.64	1.46	1.52
4	D	802	DAT	C3'-C4'	-2.60	1.46	1.53
3	D	803	DTP	C2'-C3'	-2.60	1.46	1.52
3	B	801	DTP	PA-O3A	-2.40	1.56	1.59
4	B	802	DAT	C5-N7	-2.39	1.34	1.39
4	C	802	DAT	O5'-C5'	-2.38	1.35	1.44
3	B	801	DTP	C3'-C4'	-2.38	1.46	1.53
4	D	802	DAT	O4'-C4'	2.35	1.50	1.45
4	D	802	DAT	C5-N7	-2.35	1.34	1.39
4	B	802	DAT	O5'-C5'	-2.34	1.35	1.44
4	D	802	DAT	O5'-C5'	-2.31	1.35	1.44
4	A	802	DAT	C5-N7	-2.31	1.34	1.39
4	B	802	DAT	C8-N9	-2.31	1.33	1.37
4	C	802	DAT	C5-N7	-2.30	1.34	1.39
4	A	802	DAT	C8-N7	2.30	1.36	1.31
4	A	802	DAT	O5'-C5'	-2.30	1.35	1.44
4	C	802	DAT	C8-N7	2.27	1.36	1.31
4	A	802	DAT	O4'-C4'	2.26	1.50	1.45
4	D	802	DAT	C2'-C1'	-2.25	1.46	1.52
3	A	803	DTP	PA-O3A	-2.25	1.57	1.59
4	C	802	DAT	C8-N9	-2.24	1.33	1.37
4	B	802	DAT	C8-N7	2.23	1.36	1.31
4	D	802	DAT	C8-N9	-2.22	1.33	1.37
3	B	803	DTP	PA-O3A	-2.22	1.57	1.59
4	B	802	DAT	PB-O3B	-2.18	1.46	1.54
4	A	802	DAT	PB-O3B	-2.17	1.46	1.54
4	A	802	DAT	C2'-C1'	-2.17	1.46	1.52
4	C	802	DAT	C2'-C1'	-2.16	1.46	1.52
4	D	802	DAT	C8-N7	2.16	1.35	1.31
3	D	803	DTP	PA-O3A	-2.16	1.57	1.59
4	D	802	DAT	PB-O3B	-2.16	1.46	1.54
4	C	802	DAT	PB-O3B	-2.14	1.46	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	802	DAT	C8-N9	-2.14	1.33	1.37
4	B	802	DAT	O4'-C4'	2.12	1.49	1.45
4	B	802	DAT	C2'-C1'	-2.11	1.46	1.52
4	C	802	DAT	O4'-C4'	2.11	1.49	1.45
3	B	801	DTP	PB-O3B	-2.10	1.57	1.59
3	C	803	DTP	PA-O3A	-2.07	1.57	1.59
3	D	803	DTP	C3'-C4'	-2.06	1.47	1.53
4	A	802	DAT	C6-N6	2.00	1.39	1.34

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	802	DAT	O4'-C1'-N9	7.04	120.60	107.96
4	D	802	DAT	C5-C4-N3	-5.49	119.16	126.72
4	C	802	DAT	C5-C4-N3	-5.46	119.19	126.72
4	A	802	DAT	C5-C4-N3	-5.44	119.23	126.72
4	B	802	DAT	C5-C4-N3	-5.40	119.28	126.72
3	D	803	DTP	C5-C4-N3	-5.34	119.37	126.72
3	B	801	DTP	C5-C4-N3	-5.33	119.38	126.72
3	C	803	DTP	C5-C4-N3	-5.32	119.39	126.72
3	D	801	DTP	C5-C4-N3	-5.31	119.40	126.72
3	A	801	DTP	C5-C4-N3	-5.31	119.40	126.72
3	C	801	DTP	C5-C4-N3	-5.30	119.42	126.72
3	B	803	DTP	C5-C4-N3	-5.28	119.45	126.72
3	A	803	DTP	C5-C4-N3	-5.21	119.55	126.72
4	A	802	DAT	N3-C2-N1	-4.63	121.57	128.58
4	C	802	DAT	N3-C2-N1	-4.60	121.61	128.58
4	B	802	DAT	N3-C2-N1	-4.56	121.68	128.58
4	B	802	DAT	O4'-C1'-N9	4.49	116.04	107.96
4	D	802	DAT	N3-C2-N1	-4.48	121.81	128.58
4	B	802	DAT	N3-C4-N9	4.37	134.61	127.17
4	D	802	DAT	N3-C4-N9	4.33	134.52	127.17
4	C	802	DAT	N3-C4-N9	4.28	134.45	127.17
4	A	802	DAT	N3-C4-N9	4.25	134.39	127.17
3	D	803	DTP	N3-C4-N9	3.82	133.66	127.17
3	D	801	DTP	N3-C4-N9	3.80	133.63	127.17
3	C	801	DTP	N3-C4-N9	3.80	133.63	127.17
3	A	801	DTP	N3-C4-N9	3.80	133.63	127.17
4	C	802	DAT	O4'-C1'-N9	3.78	114.75	107.96
3	A	803	DTP	N3-C4-N9	3.78	133.59	127.17
3	B	801	DTP	N3-C4-N9	3.75	133.55	127.17
4	D	802	DAT	O4'-C1'-N9	3.75	114.69	107.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	803	DTP	N3-C4-N9	3.74	133.53	127.17
3	B	803	DTP	N3-C4-N9	3.73	133.51	127.17
3	B	801	DTP	O4'-C1'-N9	3.69	114.59	107.96
4	A	802	DAT	C2-N3-C4	3.56	120.52	111.83
4	C	802	DAT	C2-N3-C4	3.52	120.42	111.83
4	A	802	DAT	N9-C8-N7	-3.49	108.98	113.94
4	B	802	DAT	C2-N3-C4	3.49	120.35	111.83
4	D	802	DAT	C2-N3-C4	3.48	120.34	111.83
3	C	803	DTP	O4'-C1'-N9	3.47	114.20	107.96
3	D	803	DTP	O4'-C1'-N9	3.47	114.19	107.96
4	D	802	DAT	N9-C8-N7	-3.45	109.04	113.94
4	C	802	DAT	N9-C8-N7	-3.45	109.05	113.94
4	B	802	DAT	N9-C8-N7	-3.44	109.05	113.94
3	D	801	DTP	N3-C2-N1	-3.40	123.44	128.58
3	C	803	DTP	N3-C2-N1	-3.39	123.45	128.58
3	C	801	DTP	N3-C2-N1	-3.38	123.46	128.58
3	B	801	DTP	N3-C2-N1	-3.38	123.47	128.58
3	A	801	DTP	N3-C2-N1	-3.38	123.47	128.58
3	D	803	DTP	N3-C2-N1	-3.37	123.48	128.58
3	B	803	DTP	N3-C2-N1	-3.35	123.50	128.58
3	B	803	DTP	O4'-C1'-N9	3.33	113.95	107.96
3	D	801	DTP	O4'-C1'-N9	3.31	113.91	107.96
3	C	801	DTP	O4'-C1'-N9	3.30	113.89	107.96
3	C	801	DTP	N9-C8-N7	-3.29	109.26	113.94
3	A	803	DTP	N3-C2-N1	-3.29	123.60	128.58
3	A	801	DTP	O4'-C1'-N9	3.29	113.87	107.96
3	A	803	DTP	N9-C8-N7	-3.29	109.27	113.94
3	A	801	DTP	N9-C8-N7	-3.28	109.29	113.94
3	D	803	DTP	N9-C8-N7	-3.27	109.29	113.94
3	D	801	DTP	N9-C8-N7	-3.27	109.29	113.94
3	C	803	DTP	N9-C8-N7	-3.23	109.35	113.94
3	B	801	DTP	N9-C8-N7	-3.23	109.35	113.94
3	B	803	DTP	N9-C8-N7	-3.22	109.37	113.94
3	D	801	DTP	C2-N3-C4	3.14	119.49	111.83
3	C	801	DTP	C2-N3-C4	3.12	119.44	111.83
3	A	801	DTP	C2-N3-C4	3.11	119.44	111.83
3	B	801	DTP	C2-N3-C4	3.10	119.41	111.83
3	C	803	DTP	C2-N3-C4	3.09	119.39	111.83
3	B	803	DTP	C2-N3-C4	3.09	119.38	111.83
3	D	803	DTP	C2-N3-C4	3.09	119.37	111.83
3	A	803	DTP	C2-N3-C4	3.02	119.20	111.83
4	B	802	DAT	C4-N9-C8	3.02	108.91	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	DTP	C5-N7-C8	2.98	108.14	103.45
3	B	803	DTP	C5-N7-C8	2.97	108.12	103.45
3	D	803	DTP	C5-N7-C8	2.97	108.11	103.45
3	C	803	DTP	C5-N7-C8	2.96	108.10	103.45
4	C	802	DAT	C4-N9-C8	2.96	108.84	105.74
4	A	802	DAT	C4-N9-C8	2.95	108.83	105.74
3	B	801	DTP	C5-N7-C8	2.92	108.05	103.45
4	D	802	DAT	C4-N9-C8	2.92	108.80	105.74
3	C	801	DTP	C5-N7-C8	2.90	108.01	103.45
3	D	801	DTP	C5-N7-C8	2.90	108.00	103.45
3	A	801	DTP	C5-N7-C8	2.89	108.00	103.45
3	A	803	DTP	O5'-C5'-C4'	2.88	118.81	108.99
3	B	801	DTP	C4-C5-N7	-2.84	107.33	110.58
3	B	803	DTP	C4-C5-N7	-2.84	107.33	110.58
3	A	803	DTP	O4'-C1'-N9	2.83	113.05	107.96
3	C	803	DTP	C4-C5-N7	-2.82	107.36	110.58
3	D	803	DTP	C4-C5-N7	-2.79	107.40	110.58
3	A	801	DTP	C4-C5-N7	-2.78	107.40	110.58
3	C	801	DTP	C4-C5-N7	-2.78	107.40	110.58
3	D	801	DTP	C4-C5-N7	-2.78	107.40	110.58
3	A	803	DTP	C4-C5-N7	-2.76	107.43	110.58
4	A	802	DAT	O5'-C5'-C4'	2.64	117.98	108.99
3	D	801	DTP	O5'-C5'-C4'	2.64	117.98	108.99
3	A	801	DTP	O5'-C5'-C4'	2.63	117.96	108.99
4	D	802	DAT	C5-N7-C8	2.63	107.59	103.45
3	C	801	DTP	O5'-C5'-C4'	2.63	117.95	108.99
3	D	803	DTP	O5'-C5'-C4'	2.63	117.94	108.99
3	C	803	DTP	O5'-C5'-C4'	2.62	117.93	108.99
4	A	802	DAT	C5-N7-C8	2.62	107.57	103.45
3	B	803	DTP	O5'-C5'-C4'	2.60	117.85	108.99
4	B	802	DAT	C5-N7-C8	2.57	107.49	103.45
4	C	802	DAT	O5'-C5'-C4'	2.56	117.72	108.99
4	C	802	DAT	C5-N7-C8	2.55	107.45	103.45
4	A	802	DAT	O4'-C4'-C5'	2.51	117.38	109.33
3	C	801	DTP	C4-N9-C8	2.51	108.37	105.74
3	A	801	DTP	C4-N9-C8	2.48	108.34	105.74
3	D	801	DTP	C4-N9-C8	2.48	108.34	105.74
4	D	802	DAT	O5'-C5'-C4'	2.47	117.40	108.99
3	A	803	DTP	C4-N9-C8	2.44	108.30	105.74
3	B	801	DTP	O5'-C5'-C4'	2.44	117.29	108.99
4	B	802	DAT	O5'-C5'-C4'	2.40	117.17	108.99
3	D	803	DTP	C4-N9-C8	2.37	108.22	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	DTP	C4-N9-C8	2.34	108.20	105.74
3	B	803	DTP	C4-N9-C8	2.28	108.13	105.74
3	C	803	DTP	C4-N9-C8	2.26	108.11	105.74
4	B	802	DAT	O4'-C4'-C5'	2.19	116.34	109.33
4	D	802	DAT	O4'-C4'-C5'	2.10	116.07	109.33
4	A	802	DAT	C2'-C1'-N9	-2.08	109.73	114.63
4	A	802	DAT	C4-C5-N7	-2.06	108.23	110.58
4	D	802	DAT	C4-C5-N7	-2.04	108.25	110.58
4	D	802	DAT	C2'-C1'-N9	-2.03	109.85	114.63
4	C	802	DAT	O4'-C4'-C5'	2.01	115.77	109.33

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	DTP	C5'-O5'-PA-O1A
3	A	801	DTP	C5'-O5'-PA-O2A
3	A	801	DTP	C5'-O5'-PA-O3A
3	A	803	DTP	PB-O3B-PG-O3G
3	B	801	DTP	C5'-O5'-PA-O2A
3	B	801	DTP	C5'-O5'-PA-O3A
3	C	801	DTP	C5'-O5'-PA-O1A
3	C	801	DTP	C5'-O5'-PA-O2A
3	C	801	DTP	C5'-O5'-PA-O3A
3	C	803	DTP	O4'-C4'-C5'-O5'
3	D	801	DTP	C5'-O5'-PA-O1A
3	D	801	DTP	C5'-O5'-PA-O2A
3	D	801	DTP	C5'-O5'-PA-O3A
4	A	802	DAT	C4'-C5'-O5'-PA
4	B	802	DAT	O4'-C1'-N9-C4
4	C	802	DAT	PA-O3A-PB-O3B
4	B	802	DAT	C3'-C4'-C5'-O5'
4	D	802	DAT	C3'-C4'-C5'-O5'
3	C	803	DTP	C3'-C4'-C5'-O5'
4	C	802	DAT	O4'-C4'-C5'-O5'
4	D	802	DAT	O4'-C4'-C5'-O5'
4	B	802	DAT	O4'-C4'-C5'-O5'
4	C	802	DAT	C3'-C4'-C5'-O5'
3	D	803	DTP	O4'-C4'-C5'-O5'
3	D	803	DTP	C3'-C4'-C5'-O5'
3	B	801	DTP	O4'-C4'-C5'-O5'
4	B	802	DAT	O4'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	801	DTP	PG-O3B-PB-O2B
3	C	801	DTP	PG-O3B-PB-O2B
3	D	801	DTP	PG-O3B-PB-O2B
3	B	801	DTP	C5'-O5'-PA-O1A
3	D	803	DTP	C5'-O5'-PA-O1A
3	D	803	DTP	C5'-O5'-PA-O3A
4	B	802	DAT	C5'-O5'-PA-O1A
4	B	802	DAT	C4'-C5'-O5'-PA
4	D	802	DAT	C4'-C5'-O5'-PA
3	B	801	DTP	PA-O3A-PB-O2B
4	B	802	DAT	PA-O3A-PB-O1B
3	C	803	DTP	PG-O3B-PB-O1B
4	B	802	DAT	PA-O3A-PB-O2B
4	B	802	DAT	PA-O3A-PB-O3B
4	D	802	DAT	PA-O3A-PB-O3B
3	B	801	DTP	PA-O3A-PB-O1B
3	B	803	DTP	PG-O3B-PB-O2B
3	C	803	DTP	PB-O3A-PA-O2A
4	D	802	DAT	C2'-C1'-N9-C4

There are no ring outliers.

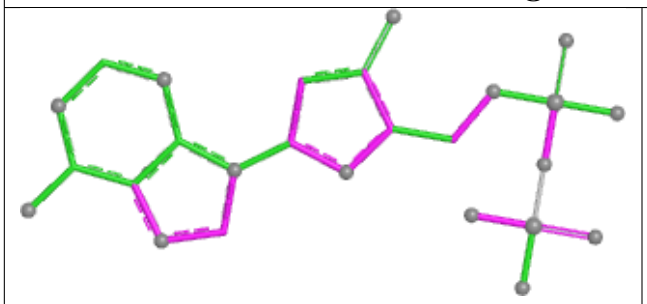
11 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	802	DAT	5	0
4	B	802	DAT	1	0
4	A	802	DAT	3	0
3	D	801	DTP	5	0
3	B	803	DTP	3	0
3	C	803	DTP	3	0
3	C	801	DTP	7	0
4	D	802	DAT	9	0
3	A	803	DTP	1	0
3	D	803	DTP	4	0
3	B	801	DTP	5	0

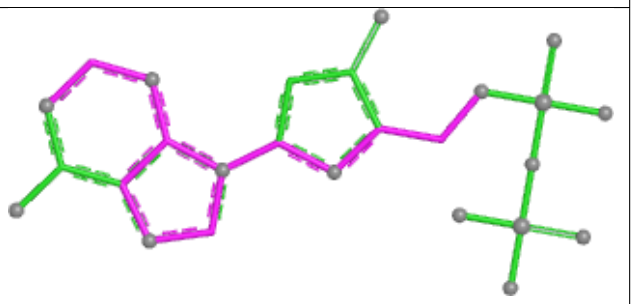
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

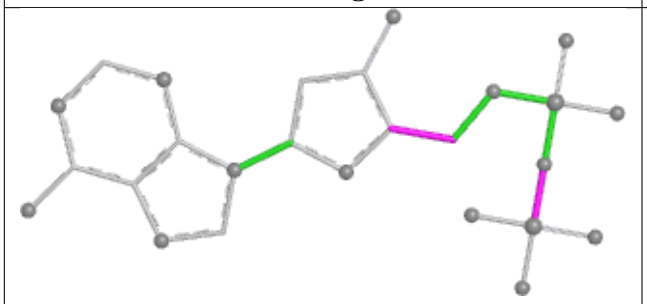
Ligand DAT C 802



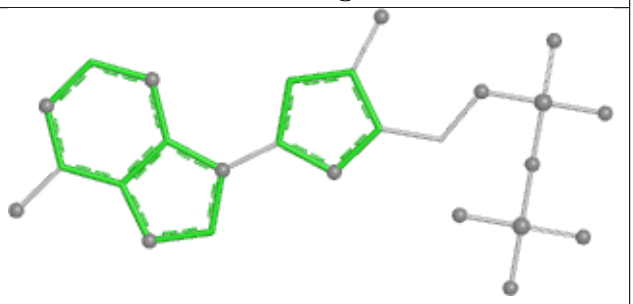
Bond lengths



Bond angles

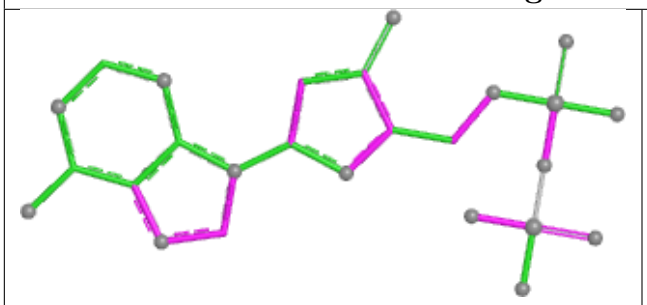


Torsions

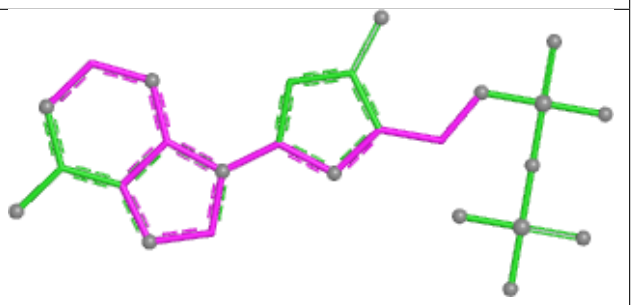


Rings

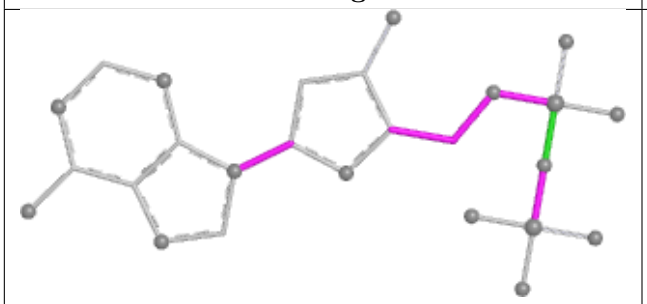
Ligand DAT B 802



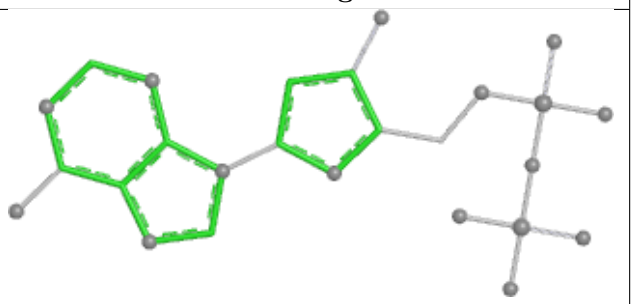
Bond lengths



Bond angles

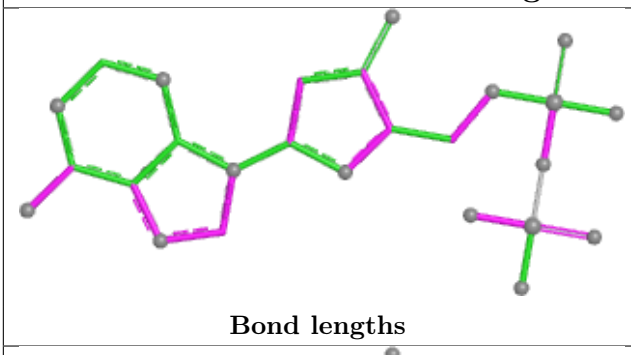


Torsions

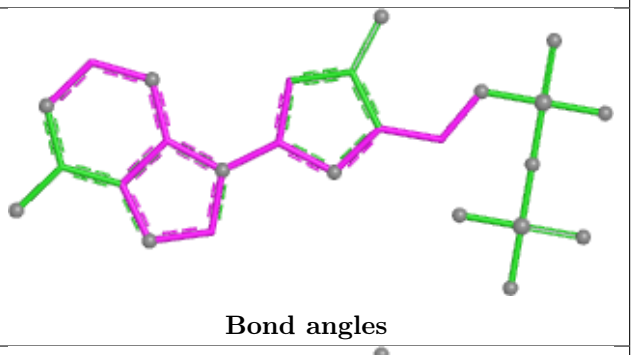


Rings

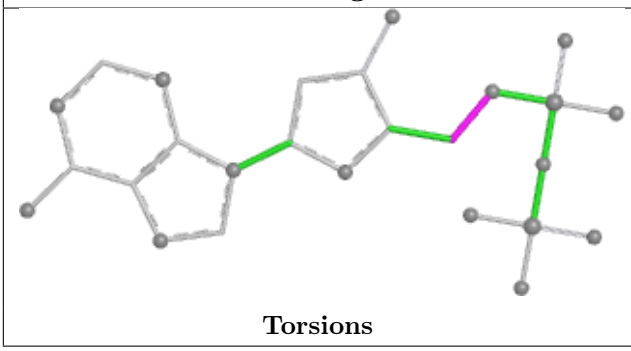
Ligand DAT A 802



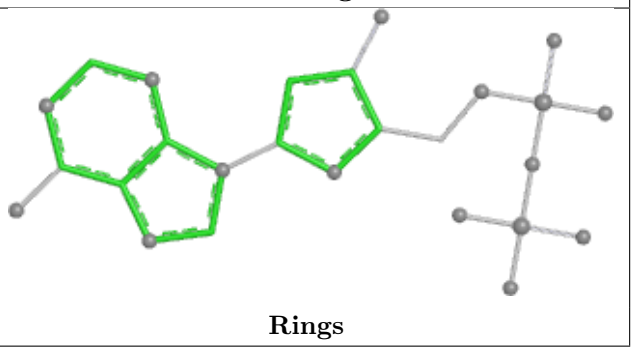
Bond lengths



Bond angles

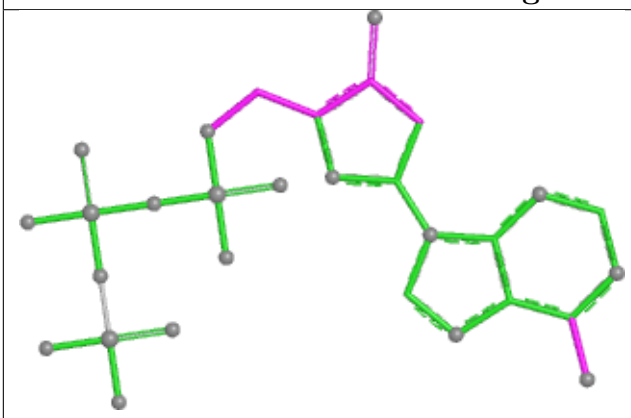


Torsions

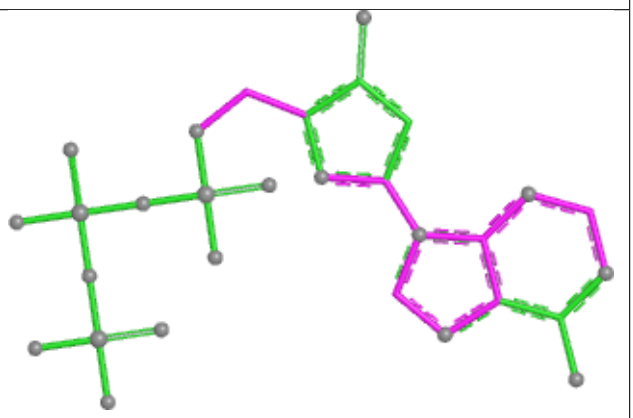


Rings

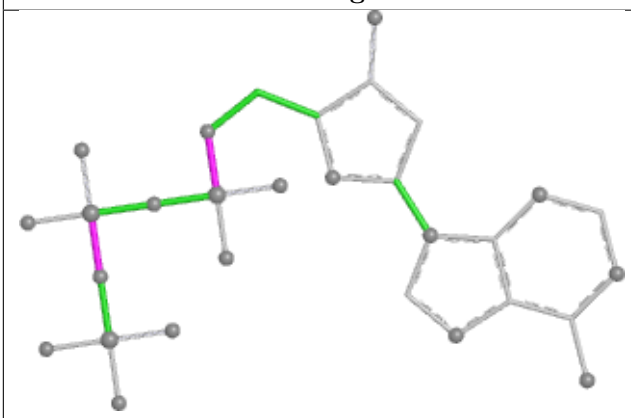
Ligand DTP D 801



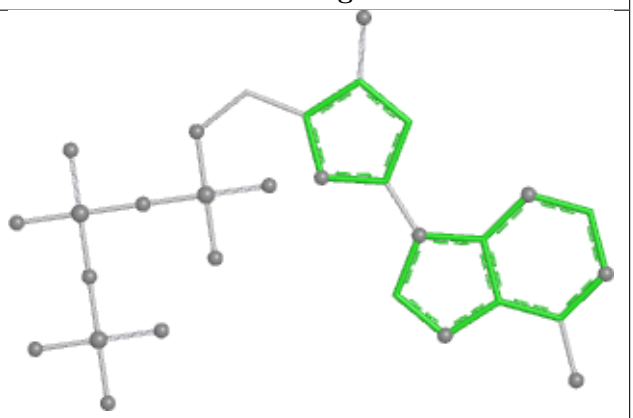
Bond lengths



Bond angles

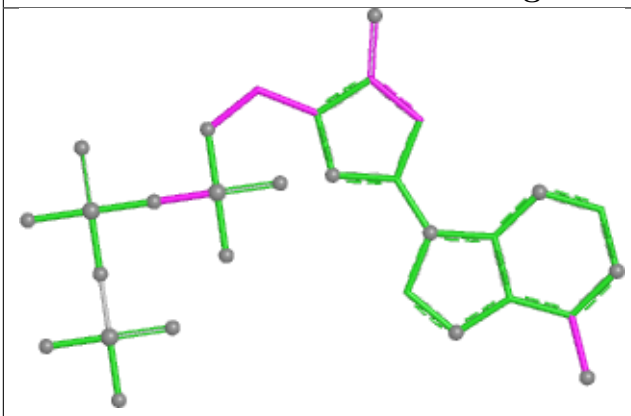


Torsions

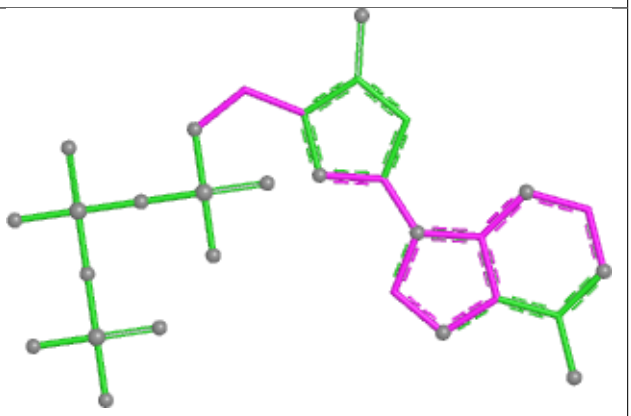


Rings

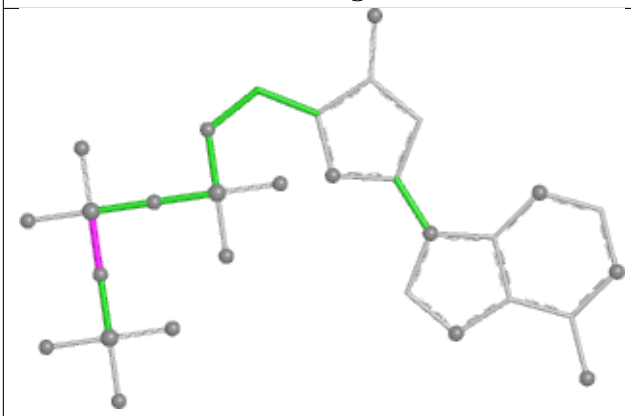
Ligand DTP B 803



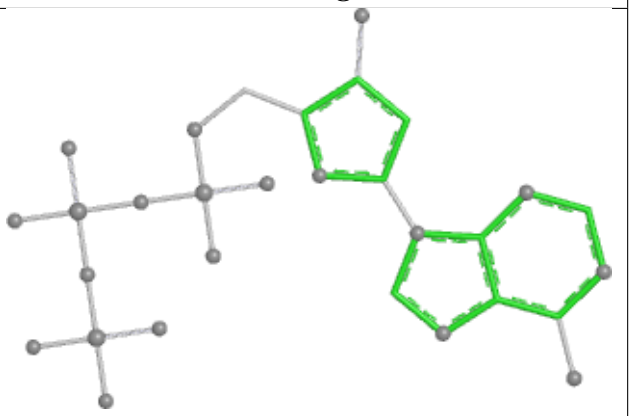
Bond lengths



Bond angles

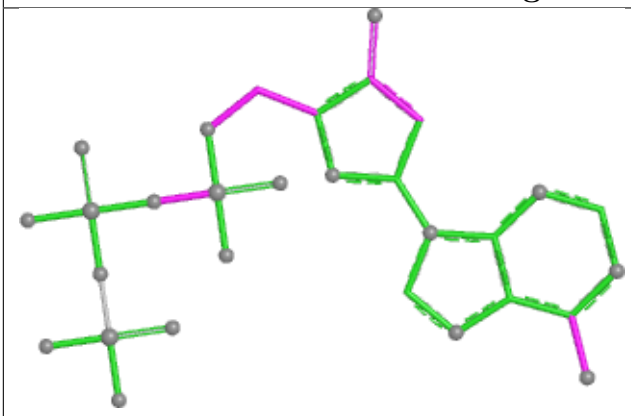


Torsions

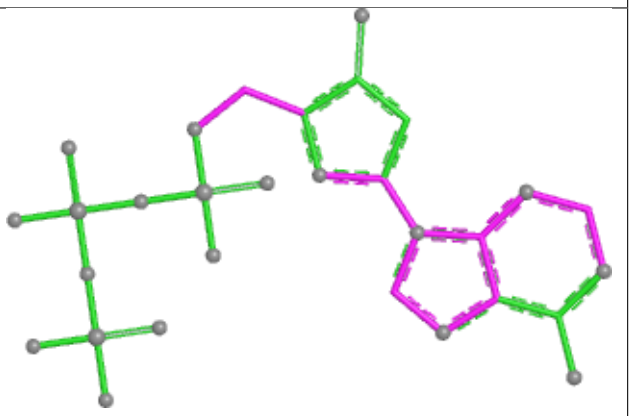


Rings

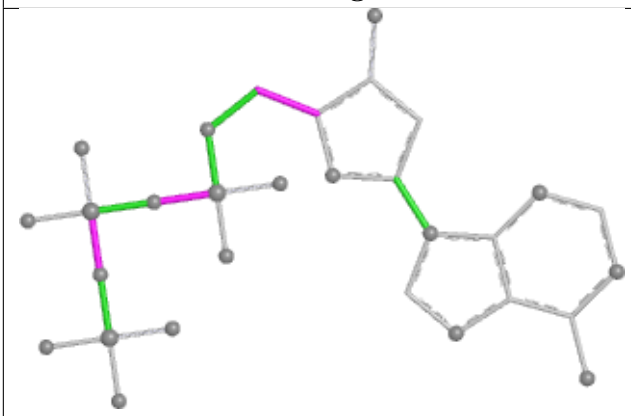
Ligand DTP C 803



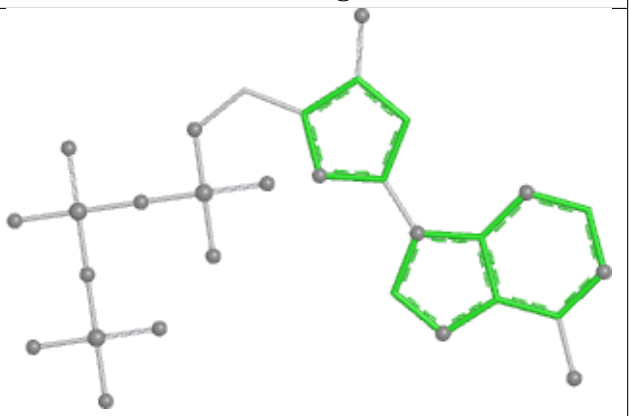
Bond lengths



Bond angles

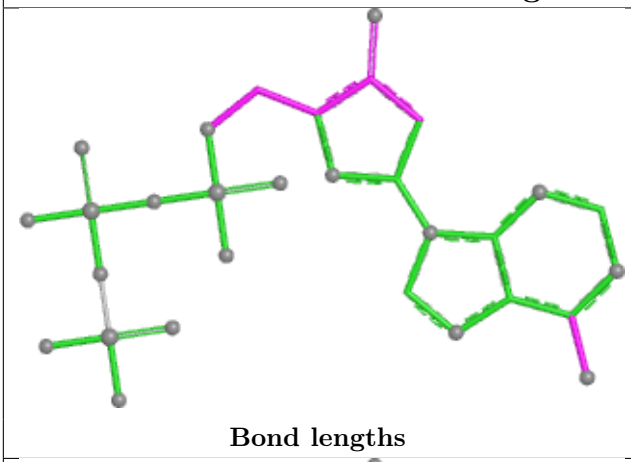


Torsions

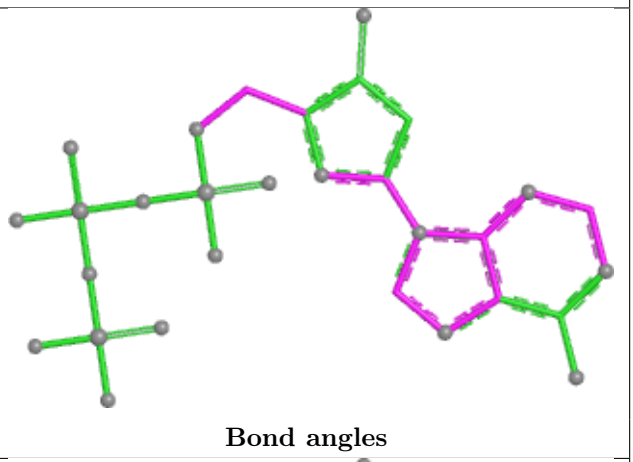


Rings

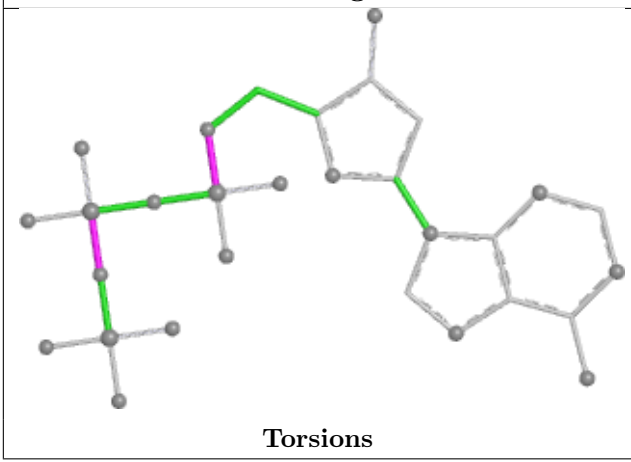
Ligand DTP C 801



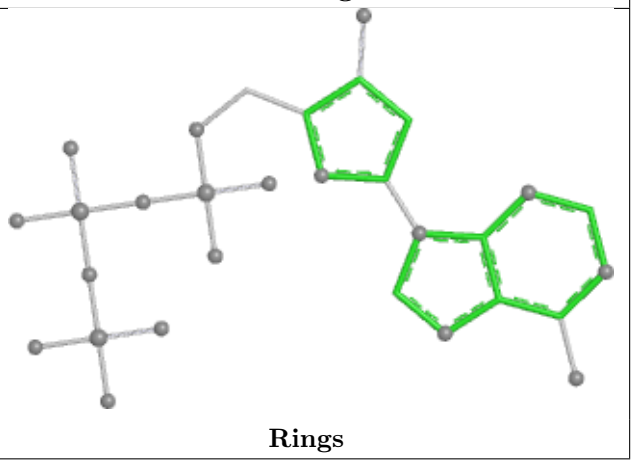
Bond lengths



Bond angles

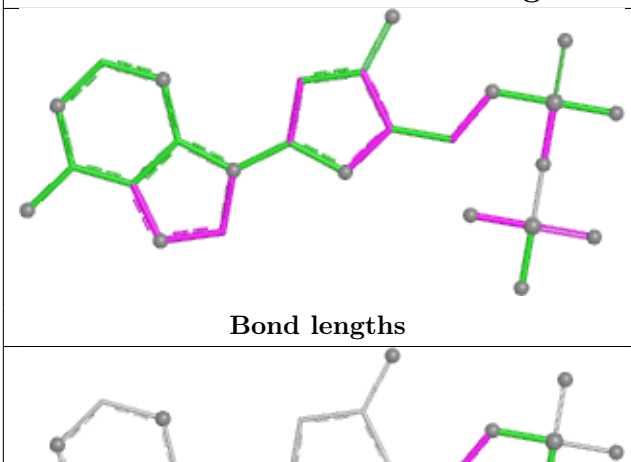


Torsions

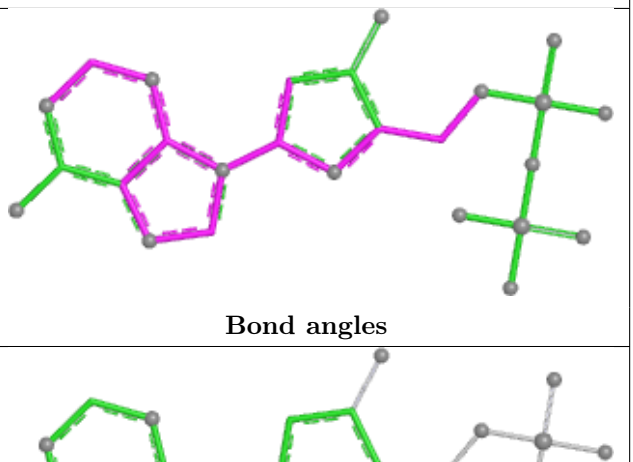


Rings

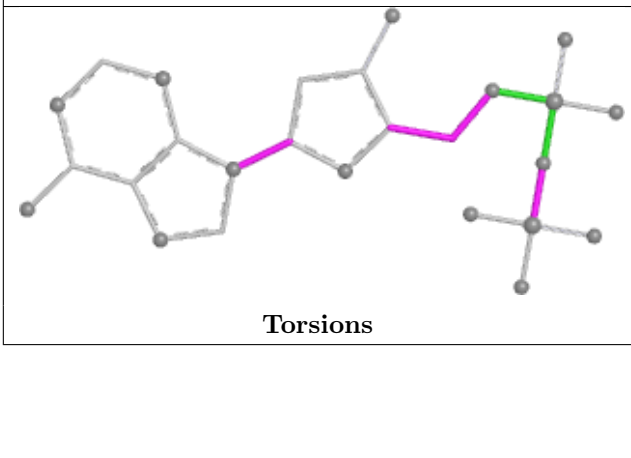
Ligand DAT D 802



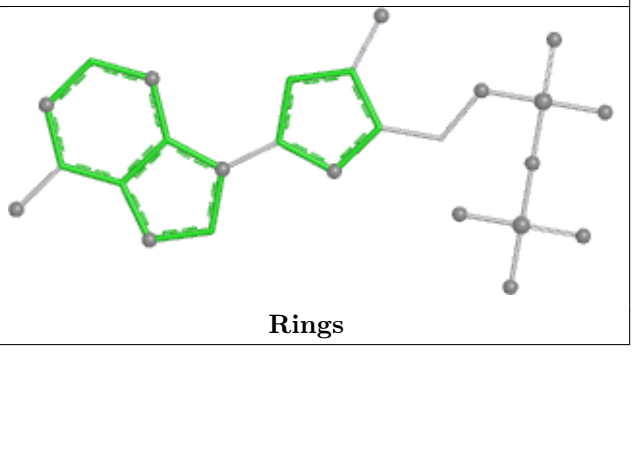
Bond lengths



Bond angles

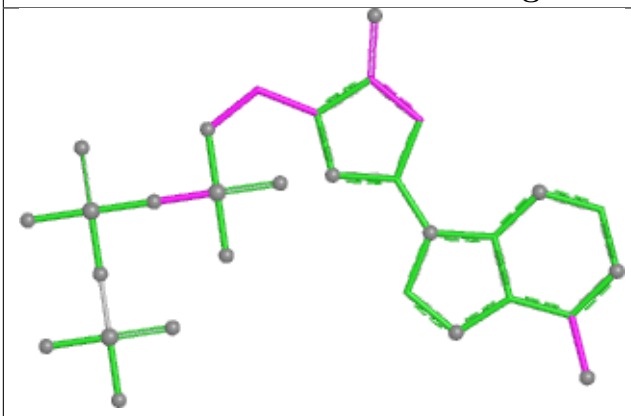


Torsions

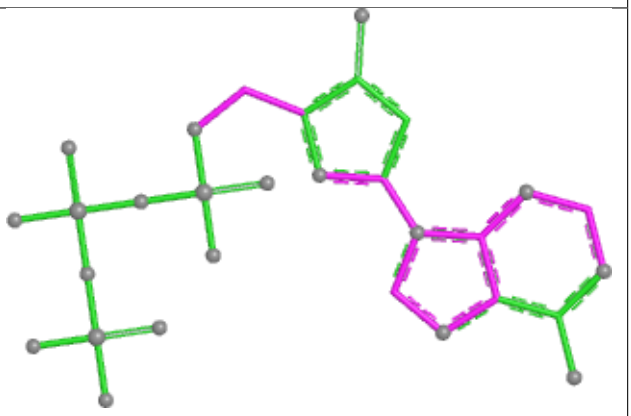


Rings

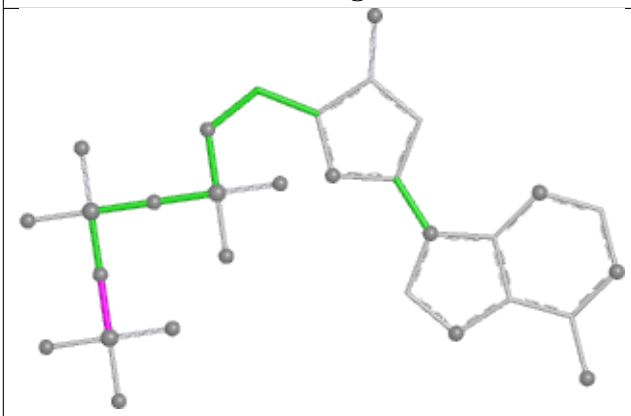
Ligand DTP A 803



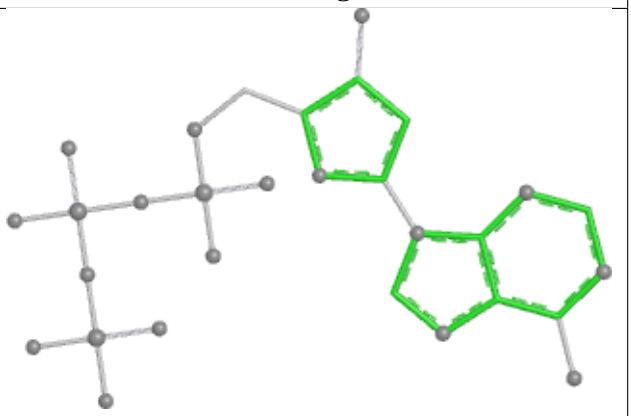
Bond lengths



Bond angles

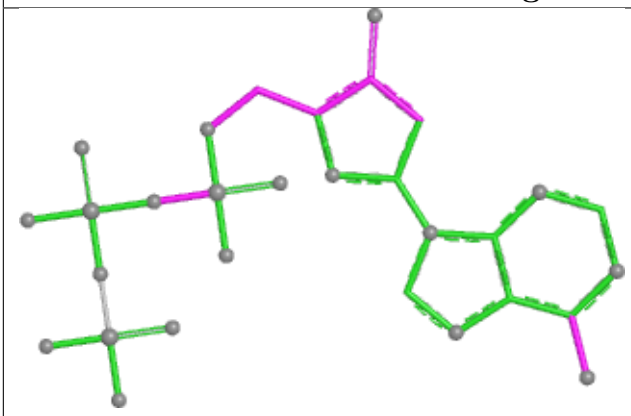


Torsions

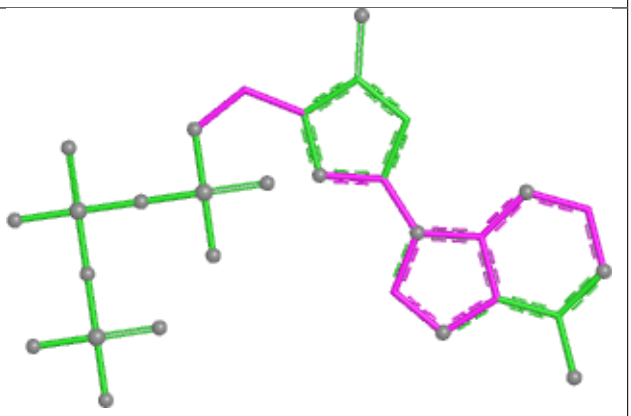


Rings

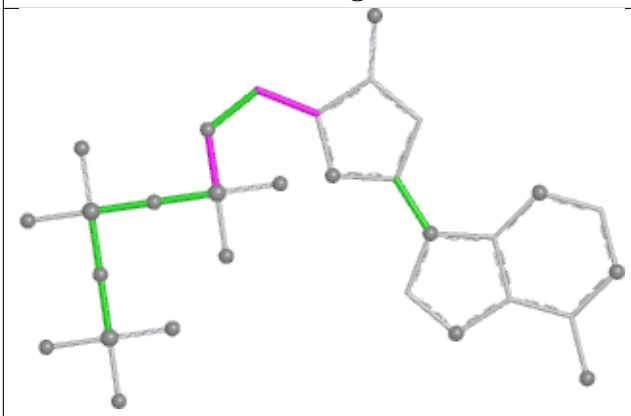
Ligand DTP D 803



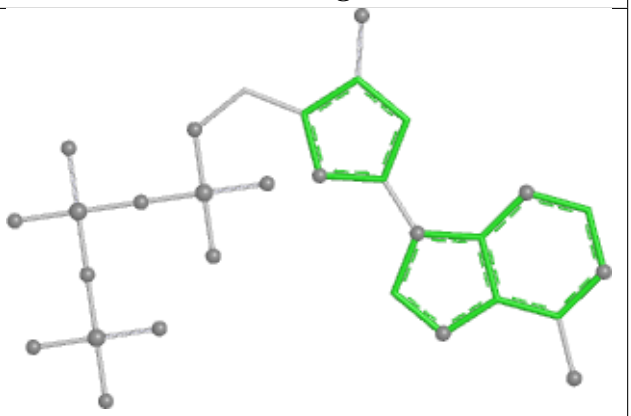
Bond lengths



Bond angles

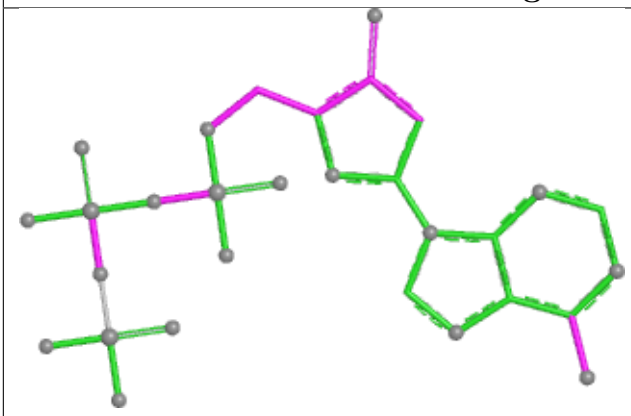


Torsions

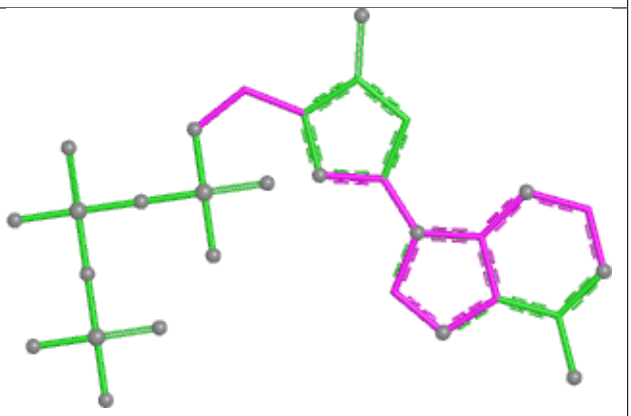


Rings

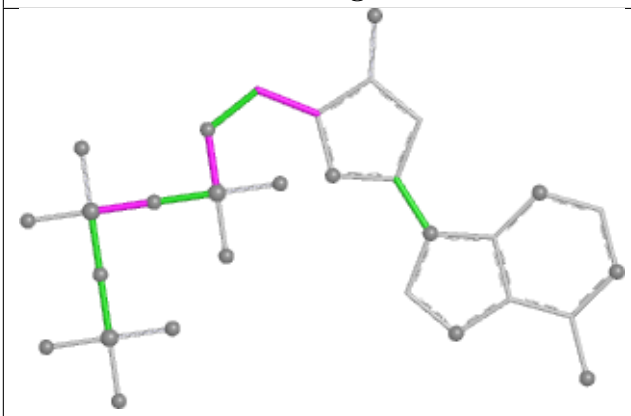
Ligand DTP B 801



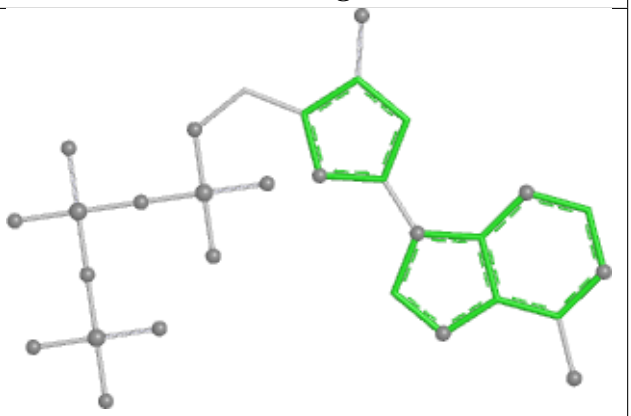
Bond lengths



Bond angles

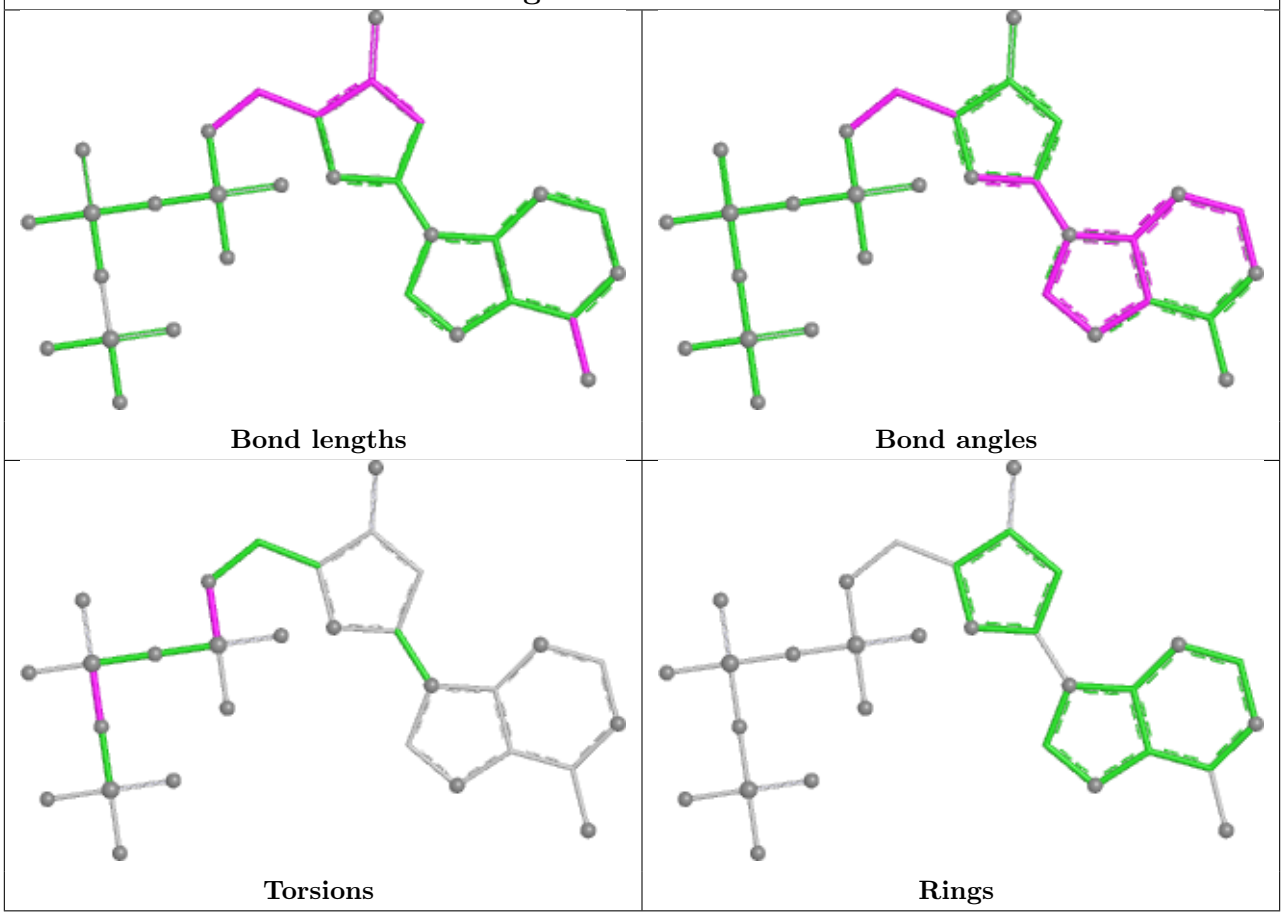


Torsions



Rings

Ligand DTP A 801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	733/761 (96%)	0.43	17 (2%)	61	43	56, 95, 121, 142	0
1	B	734/761 (96%)	0.46	17 (2%)	61	43	59, 101, 127, 151	0
1	C	731/761 (96%)	0.50	16 (2%)	62	44	101, 130, 150, 160	0
1	D	733/761 (96%)	0.48	13 (1%)	67	48	89, 128, 151, 163	0
2	E	352/375 (93%)	0.49	7 (1%)	65	46	72, 117, 154, 176	0
2	F	356/375 (94%)	0.47	9 (2%)	58	41	55, 91, 131, 158	0
2	G	356/375 (94%)	0.45	13 (3%)	45	33	59, 97, 145, 192	0
2	H	356/375 (94%)	0.41	11 (3%)	51	36	65, 98, 145, 174	0
All	All	4351/4544 (95%)	0.46	103 (2%)	59	43	55, 110, 146, 192	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	153	ILE	4.0
2	F	153	ILE	3.8
1	B	78	GLN	3.6
1	B	292	CYS	3.5
1	A	462	CYS	3.1
1	A	457	GLY	3.0
2	H	150	ALA	3.0
1	C	616	LEU	3.0
2	F	87	GLN	3.0
2	G	283	GLU	3.0
1	D	443	ALA	3.0
2	H	149	ARG	2.9
2	H	283	GLU	2.9
1	B	514	GLY	2.9
1	B	421	ASN	2.9
1	D	295	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	12	GLN	2.9
2	G	361	ILE	2.9
1	C	540	THR	2.8
1	A	295	GLY	2.8
1	D	5	LEU	2.8
1	D	56	SER	2.8
1	B	364	LEU	2.8
1	A	78	GLN	2.8
1	C	146	ALA	2.8
2	G	150	ALA	2.7
2	E	297	ILE	2.7
1	B	646	ALA	2.6
2	F	361	ILE	2.6
1	D	119	LEU	2.6
2	F	340	VAL	2.6
2	G	365	VAL	2.6
1	C	499	PRO	2.6
2	G	280	ALA	2.5
2	G	299	LEU	2.5
1	C	62	ILE	2.5
2	F	179	GLY	2.5
1	A	435	GLN	2.4
1	A	709	VAL	2.4
2	G	286	TRP	2.4
1	B	29	ALA	2.4
2	E	295	SER	2.4
1	A	157	VAL	2.4
1	B	558	LEU	2.3
2	F	182	VAL	2.3
1	A	225	CYS	2.3
2	H	108	VAL	2.3
2	H	182	VAL	2.3
1	A	436	SER	2.3
1	C	424	SER	2.3
2	G	340	VAL	2.3
1	A	212	MET	2.3
2	E	145	GLN	2.3
2	H	152	GLY	2.3
1	D	59	HIS	2.3
1	B	658	ASP	2.3
1	D	481	LEU	2.3
1	D	7	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	80	LEU	2.2
1	C	420	CYS	2.2
2	H	293	ASP	2.2
2	E	153	ILE	2.2
1	B	721	ALA	2.2
2	H	12	GLN	2.2
1	D	616	LEU	2.2
2	G	79	TYR	2.2
2	E	283	GLU	2.2
2	H	146	ILE	2.2
1	B	732	GLN	2.2
1	C	462	CYS	2.2
2	G	213	ALA	2.2
1	A	695	ALA	2.1
1	C	679	LEU	2.2
1	D	460	ALA	2.1
2	G	1	ALA	2.1
2	H	214	CYS	2.1
2	H	361	ILE	2.1
1	C	78	GLN	2.1
1	C	105	HIS	2.1
2	E	126	ILE	2.1
1	A	434	ARG	2.1
1	C	223	SER	2.1
1	C	651	ILE	2.1
1	A	330	VAL	2.1
1	B	428	PRO	2.1
1	A	177	ALA	2.1
1	D	243	ALA	2.1
2	F	92	ASN	2.1
1	B	155	TYR	2.1
2	F	290	LEU	2.1
1	D	617	SER	2.1
1	A	691	GLN	2.1
1	B	296	GLY	2.1
2	G	146	ILE	2.1
1	C	631	ALA	2.1
1	C	214	GLY	2.0
1	B	462	CYS	2.0
2	F	68	HIS	2.0
1	C	14	THR	2.0
1	D	709	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	165	ILE	2.0
1	B	463	THR	2.0
1	A	258	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

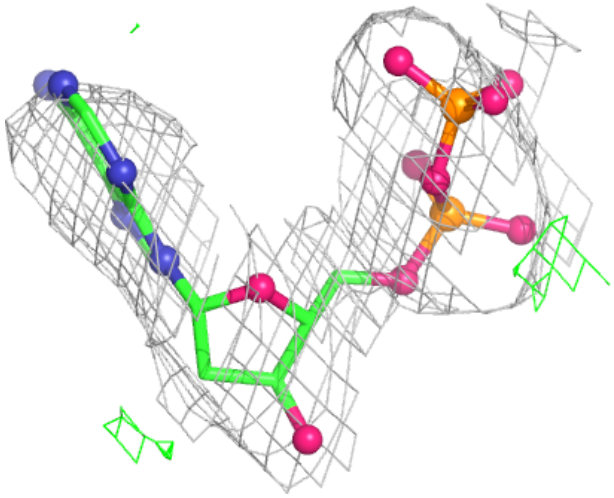
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

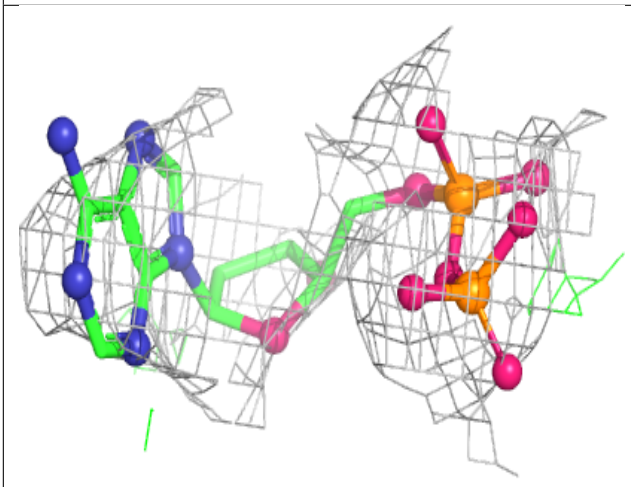
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	804	1/1	0.43	0.24	94,94,94,94	0
5	MG	B	804	1/1	0.48	0.21	94,94,94,94	0
5	MG	C	804	1/1	0.51	0.20	123,123,123,123	0
5	MG	D	804	1/1	0.60	0.19	118,118,118,118	0
4	DAT	C	802	26/26	0.76	0.13	156,156,156,156	0
4	DAT	D	802	26/26	0.79	0.14	156,156,156,156	0
4	DAT	B	802	26/26	0.80	0.14	149,149,149,149	0
3	DTP	C	801	30/30	0.81	0.14	175,175,175,175	0
3	DTP	D	801	30/30	0.82	0.15	140,140,140,140	0
4	DAT	A	802	26/26	0.88	0.12	126,126,126,126	0
3	DTP	B	801	30/30	0.89	0.14	111,111,111,111	0
3	DTP	C	803	30/30	0.91	0.07	123,123,123,123	0
3	DTP	A	801	30/30	0.91	0.12	124,124,124,124	0
3	DTP	D	803	30/30	0.92	0.08	118,118,118,118	0
3	DTP	B	803	30/30	0.94	0.07	94,94,94,94	0
3	DTP	A	803	30/30	0.95	0.08	94,94,94,94	0
6	FEO	G	501	3/3	0.98	0.06	78,78,78,78	0
6	FEO	F	501	3/3	0.99	0.05	61,61,61,61	0
6	FEO	E	501	3/3	0.99	0.04	89,89,89,89	0
6	FEO	H	501	3/3	0.99	0.03	69,69,69,69	0

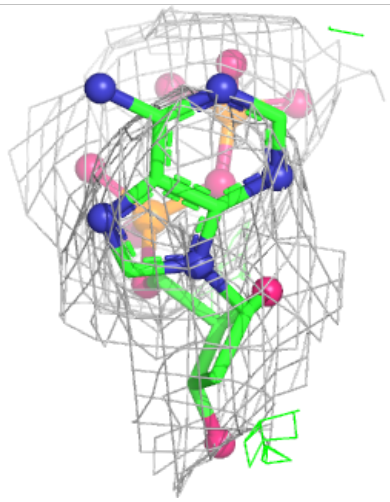
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DAT C 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

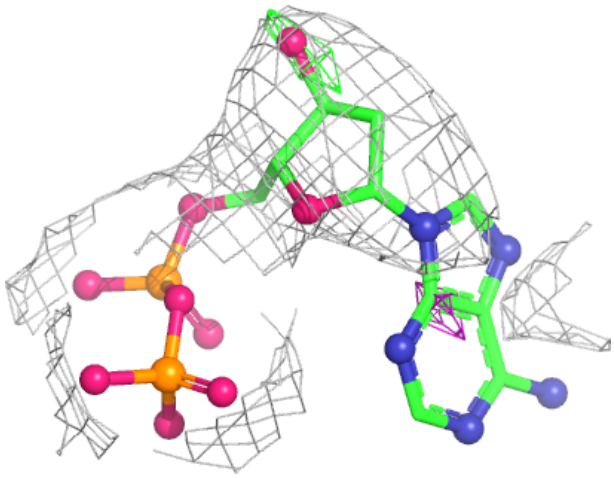


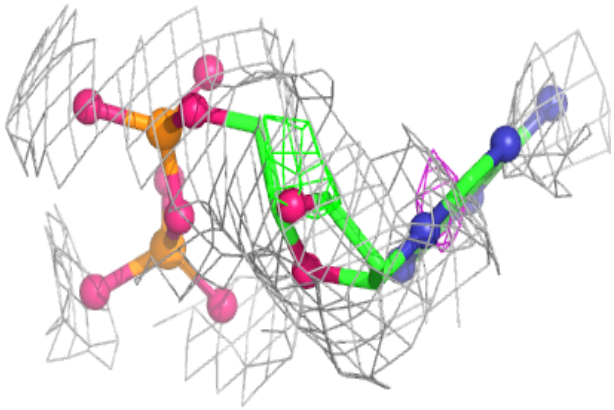


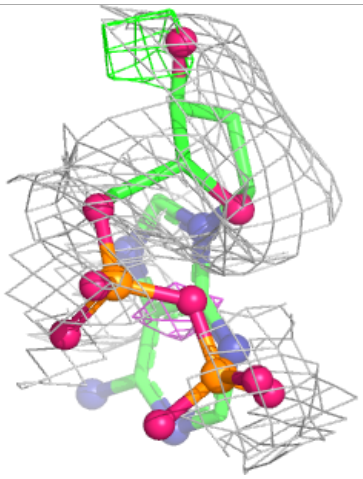


Electron density around DAT D 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

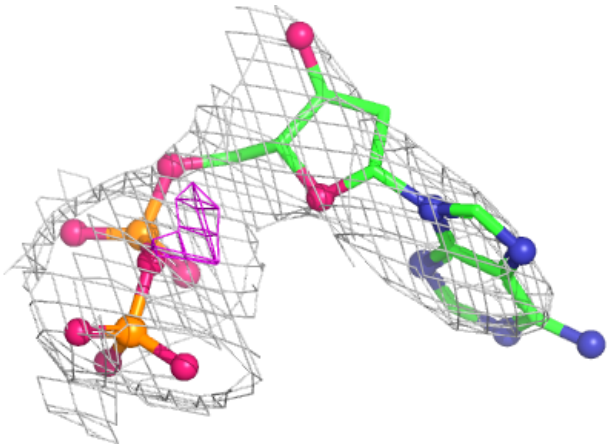


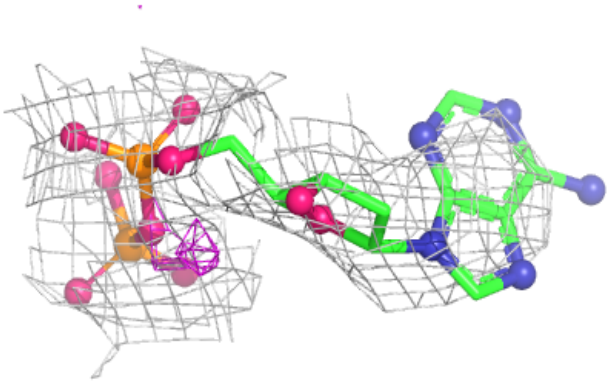


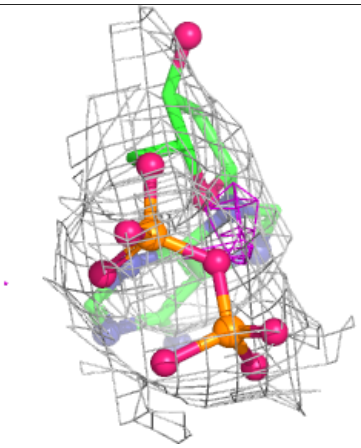


Electron density around DAT B 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

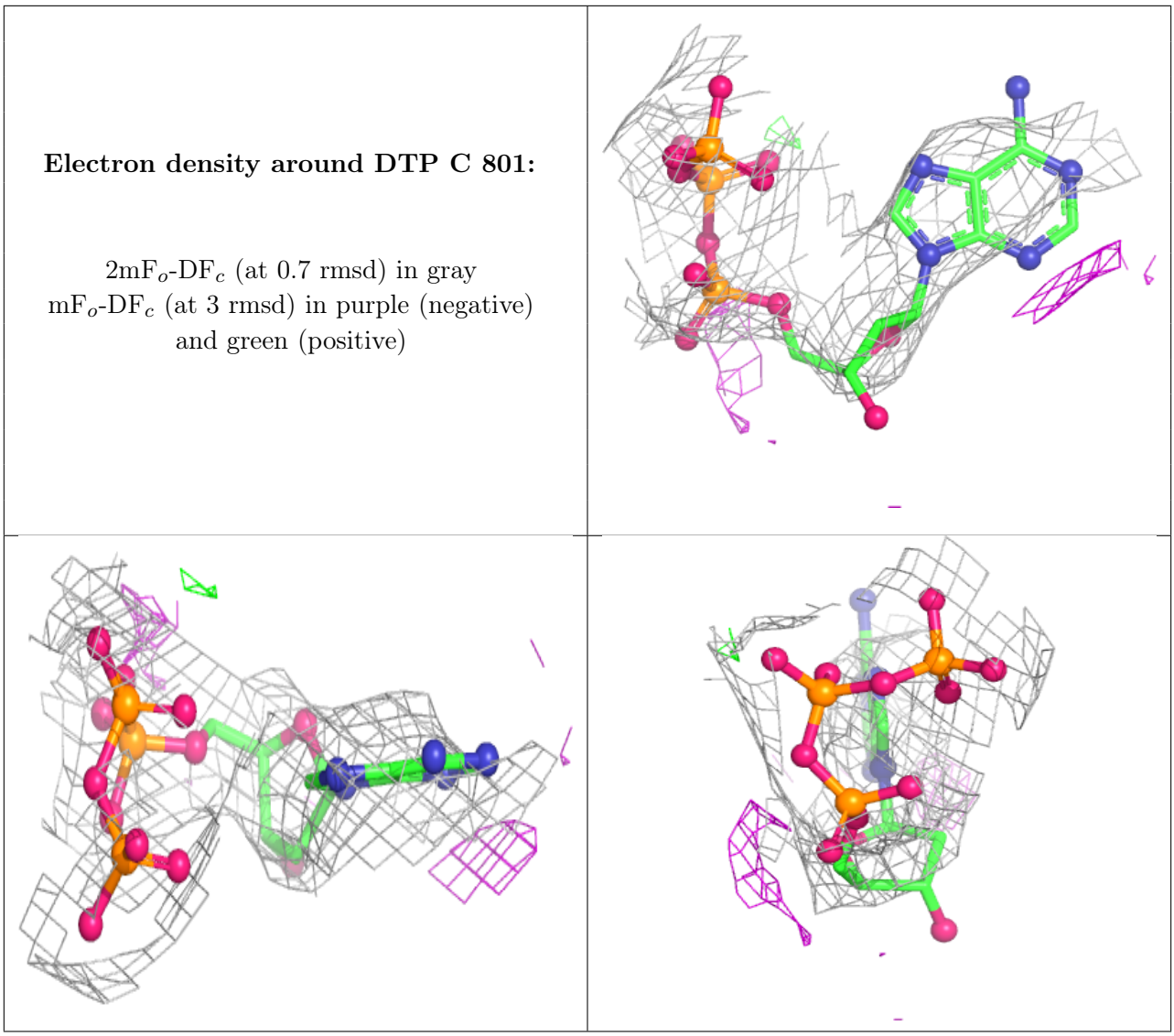






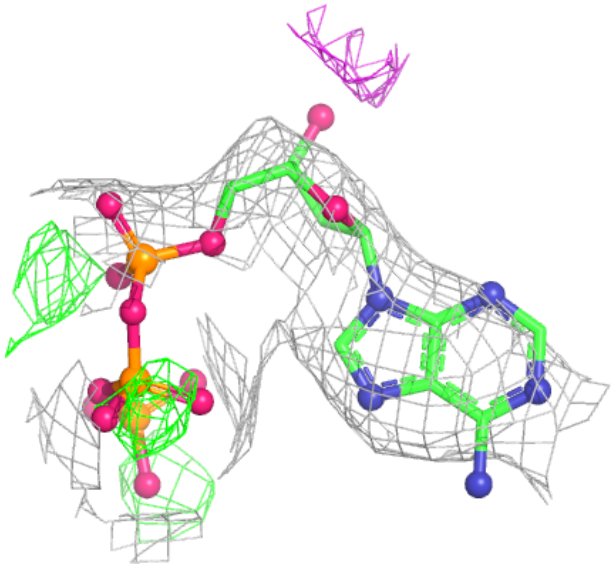
Electron density around DTP C 801:

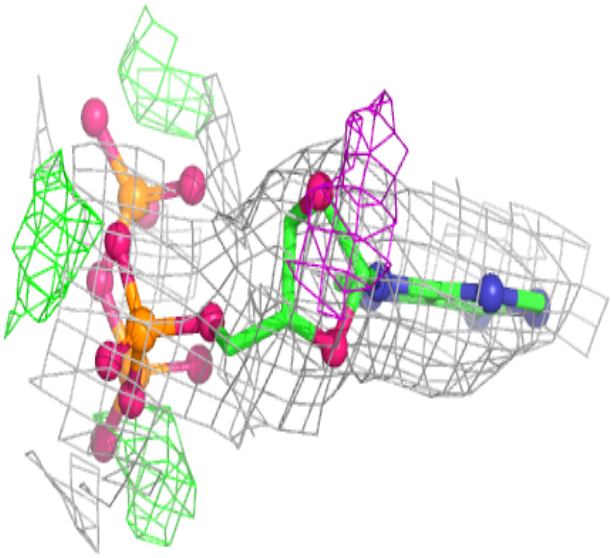
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

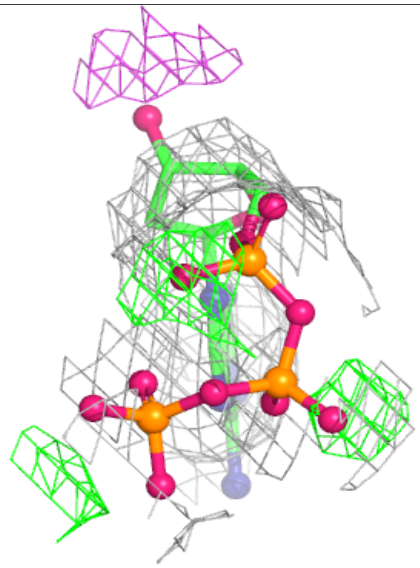


Electron density around DTP D 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

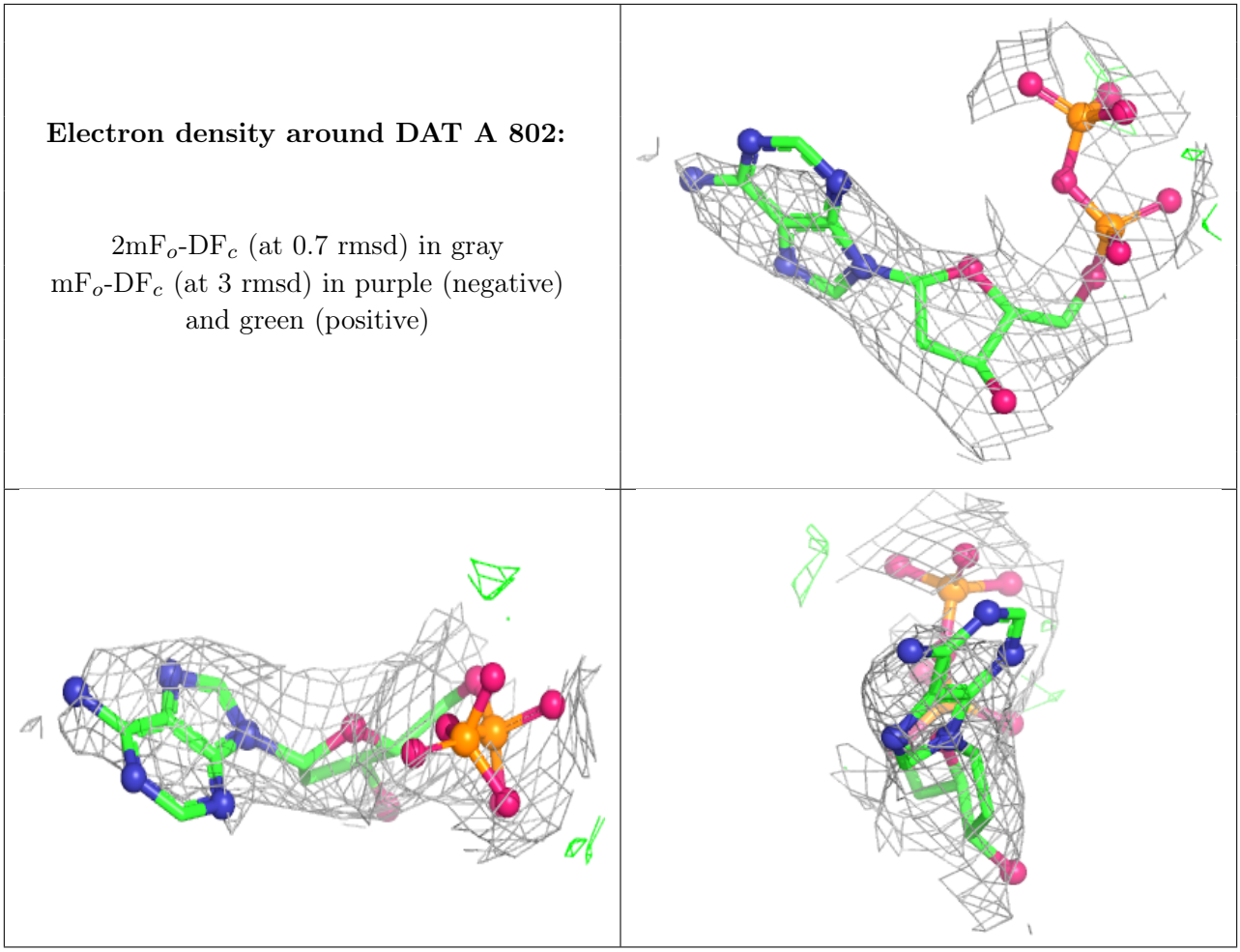






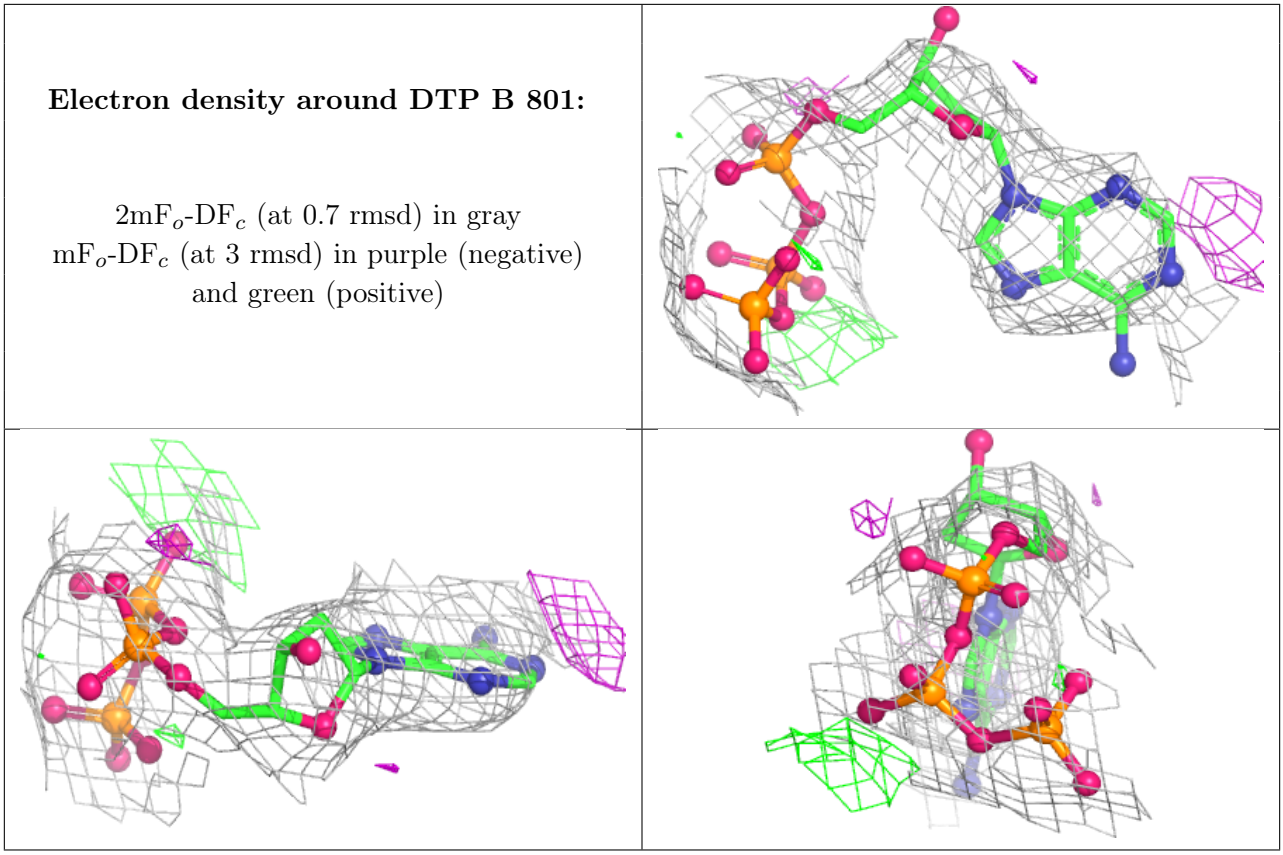
Electron density around DAT A 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



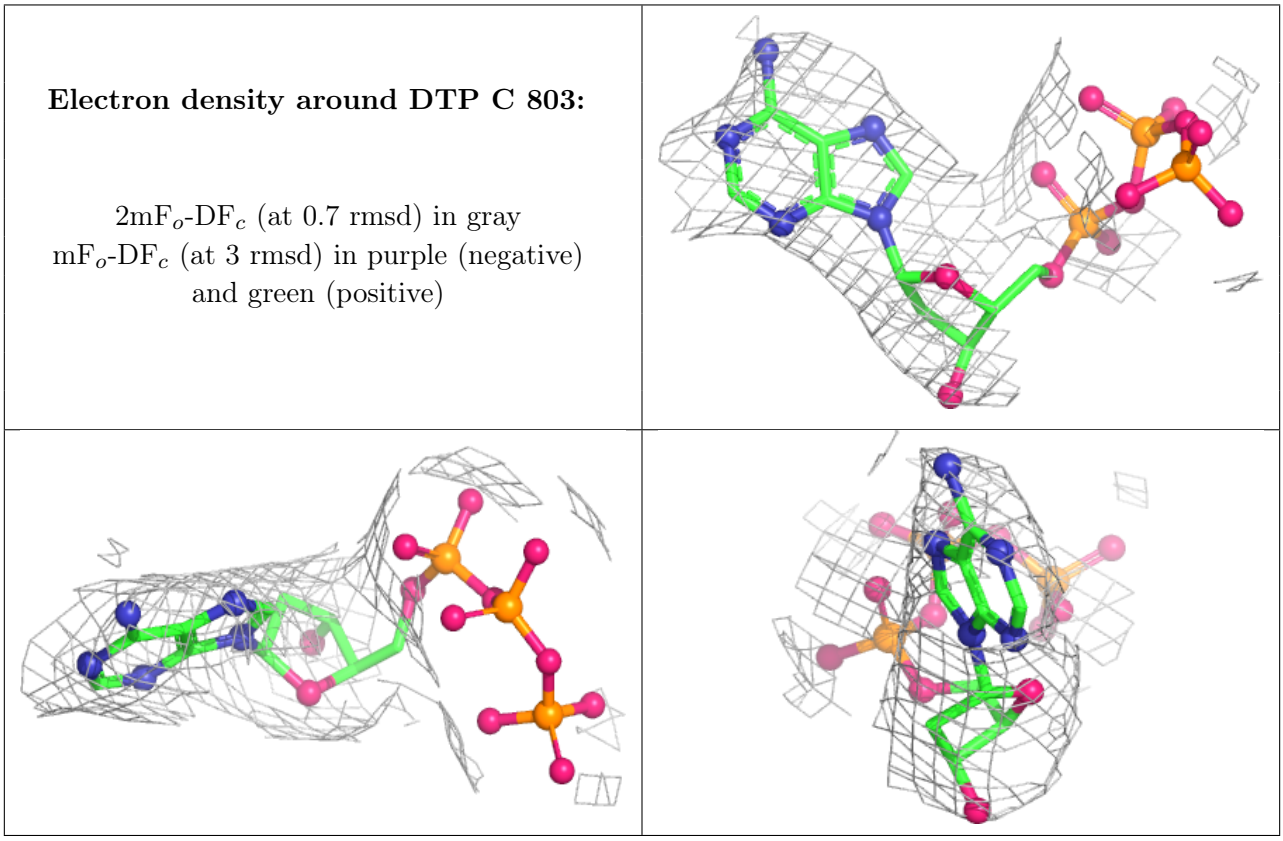
Electron density around DTP B 801:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



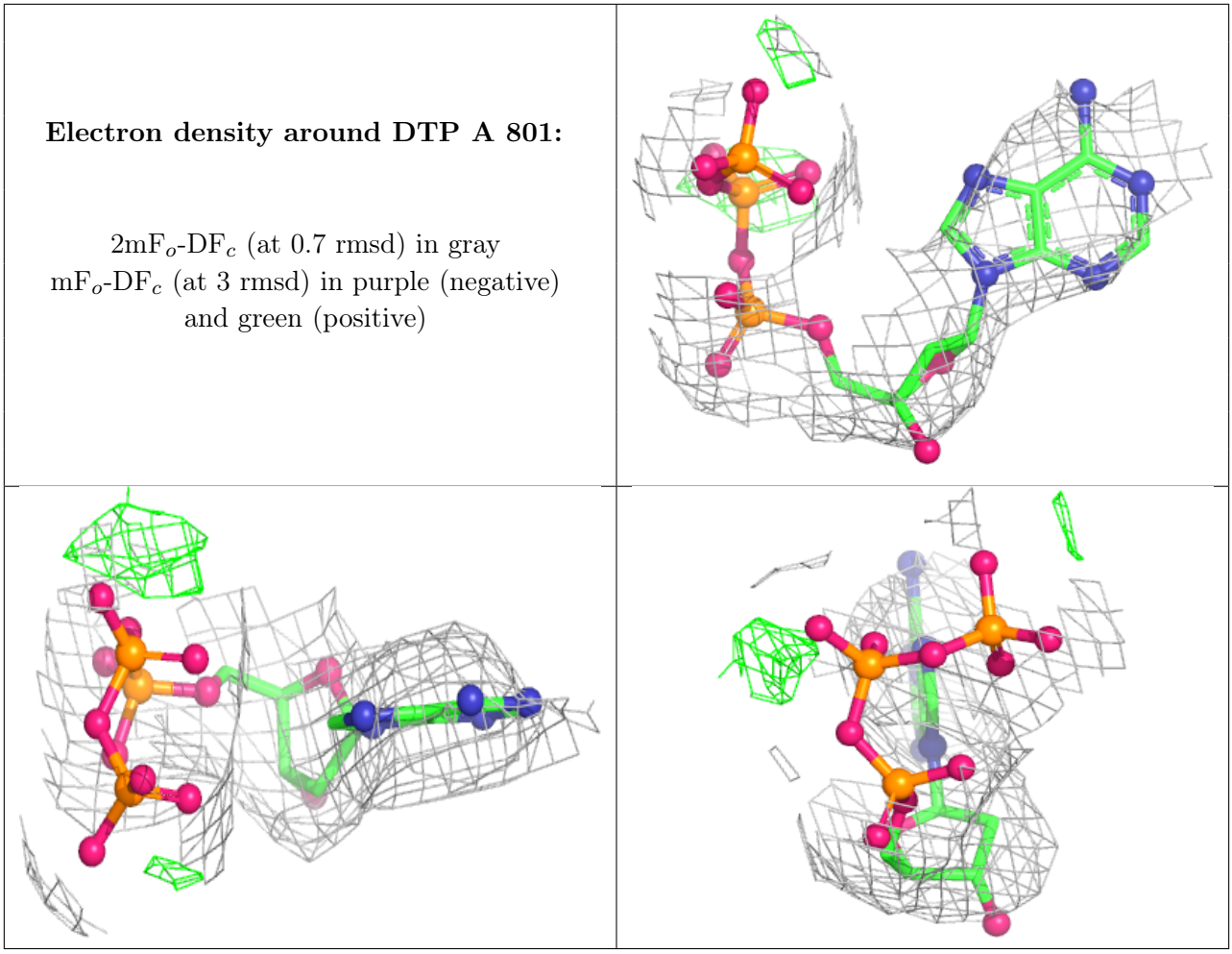
Electron density around DTP C 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



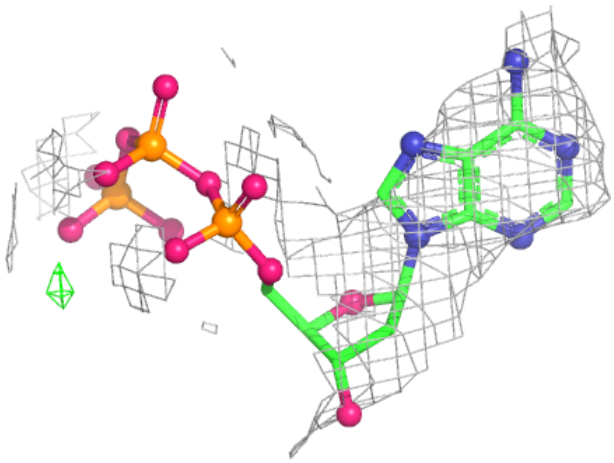
Electron density around DTP A 801:

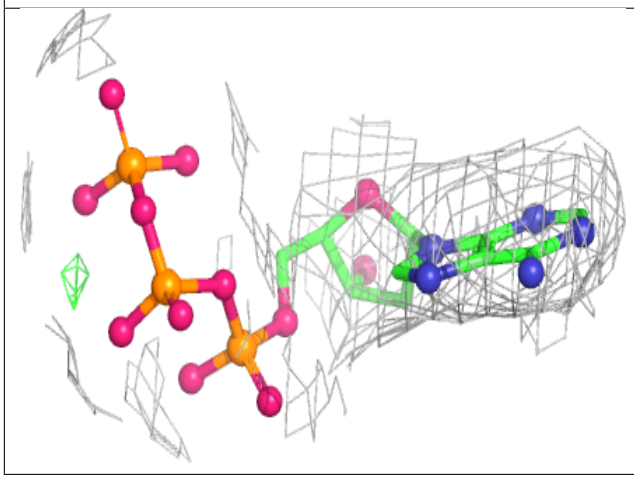
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

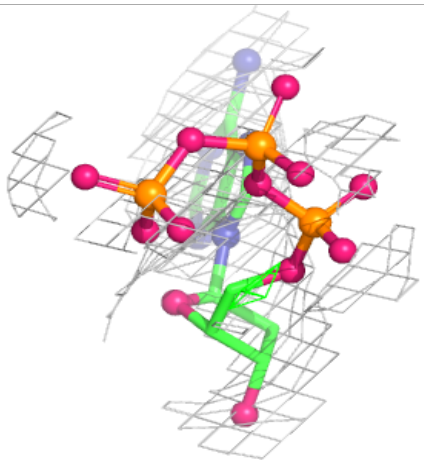


Electron density around DTP D 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

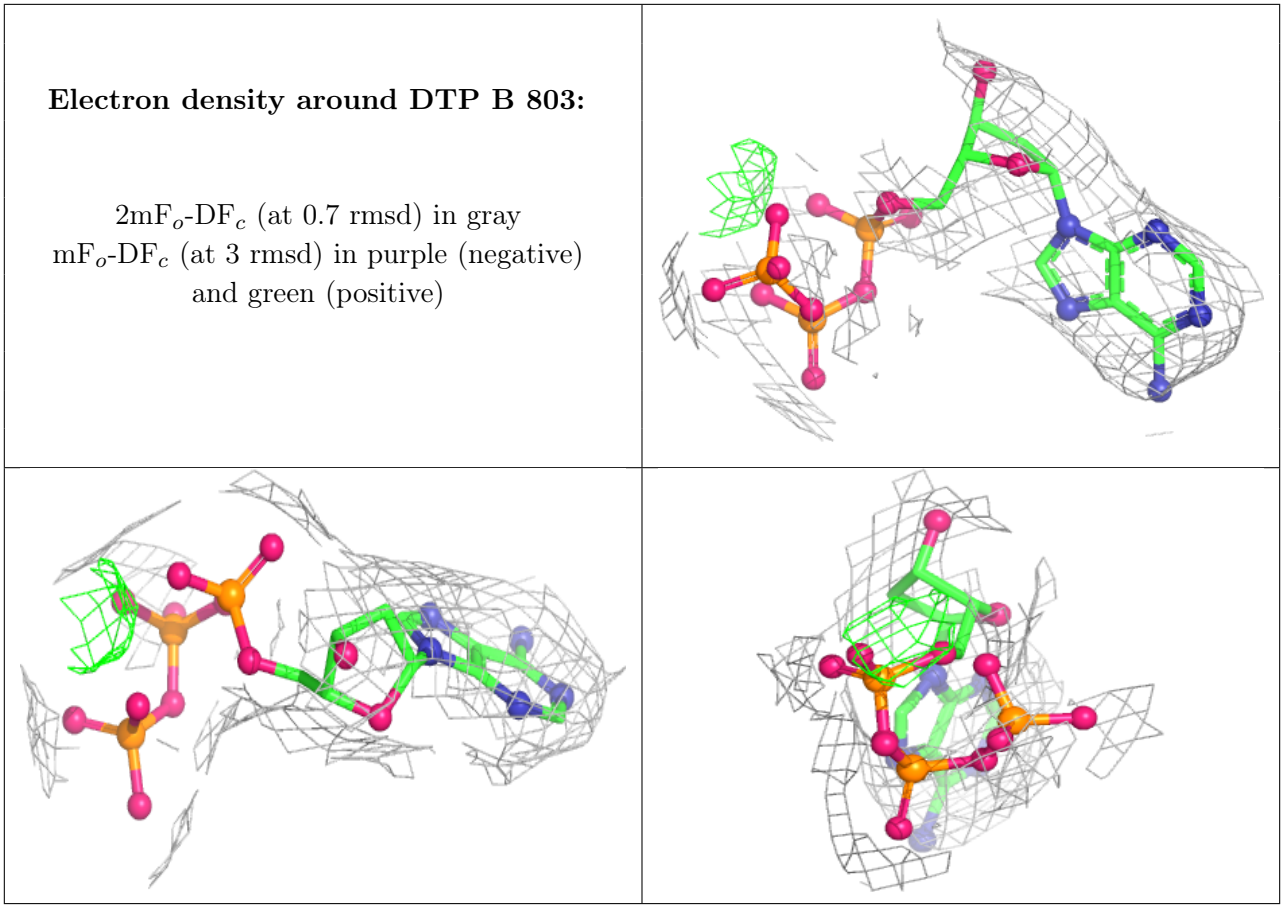






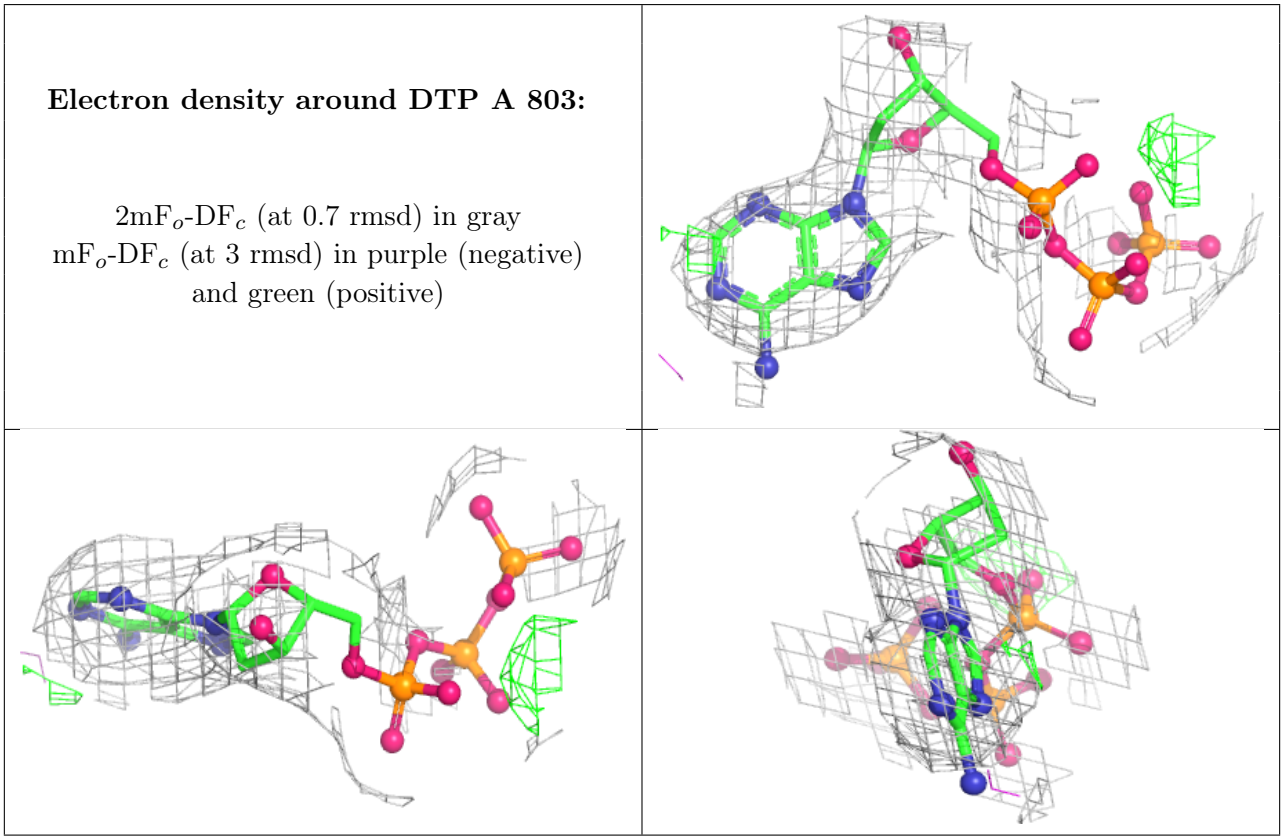
Electron density around DTP B 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DTP A 803:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.