Full wwPDB EM Validation Report (i)

Aug 27, 2026 – 12:30 am BST

PDB ID	:	7ADE / pdb_00007ade
EMDB ID	:	EMD-11725
Title	:	Transcription termination complex IVa
Authors	:	Said, N.; Hilal, T.; Loll, B.; Wahl, C.M.
Deposited on	:	2020-09-14
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

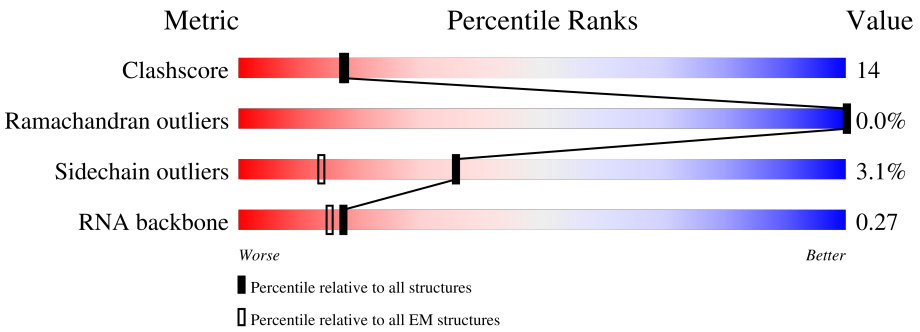
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

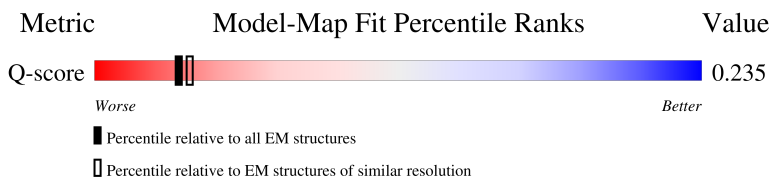
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	419	64% 32%
1	b	419	65% 32%
1	c	419	65% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	d	419	64% 33%
1	e	419	6% 66% 30%
1	f	419	9% 64% 32%
2	A	497	48% 68% 32%
3	U	329	47% 25% 29%
3	V	329	10% 71% 26%
4	W	91	78% 63% 24% 13%
5	X	1342	70% 30%
6	Y	1416	13% 66% 29% 5%
7	L	50	14% 16% 58% 26%
8	K	50	6% 10% 36% 54%
9	R	99	6% 12% 13% 7% 68%

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
12	BEF	c	1002	-	-	X	-
12	BEF	e	1002	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 51553 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	f	417	3280	2065	581	617	17	0	0
1	a	417	3280	2065	581	617	17	0	0
1	b	417	3280	2065	581	617	17	0	0
1	c	417	3280	2065	581	617	17	0	0
1	d	417	3280	2065	581	617	17	0	0
1	e	417	3280	2065	581	617	17	0	0

- Molecule 2 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	495	3852	2396	669	774	13	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C3SSN7
A	0	ALA	-	expression tag	UNP C3SSN7

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	235	1825	1135	325	359	6	0	0
3	V	321	2504	1566	441	489	8	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	W	79	627	382	118	126	1	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	X	1340	10567	6631	1841	2052	43	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Y	1343	10431	6553	1854	1974	50	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1408	LEU	-	expression tag	UNP C3SIA2
Y	1409	GLU	-	expression tag	UNP C3SIA2
Y	1410	VAL	-	expression tag	UNP C3SIA2
Y	1411	HIS	-	expression tag	UNP C3SIA2
Y	1412	HIS	-	expression tag	UNP C3SIA2
Y	1413	HIS	-	expression tag	UNP C3SIA2
Y	1414	HIS	-	expression tag	UNP C3SIA2
Y	1415	HIS	-	expression tag	UNP C3SIA2
Y	1416	HIS	-	expression tag	UNP C3SIA2

- Molecule 7 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	L	37	741	355	131	218	37	0	0

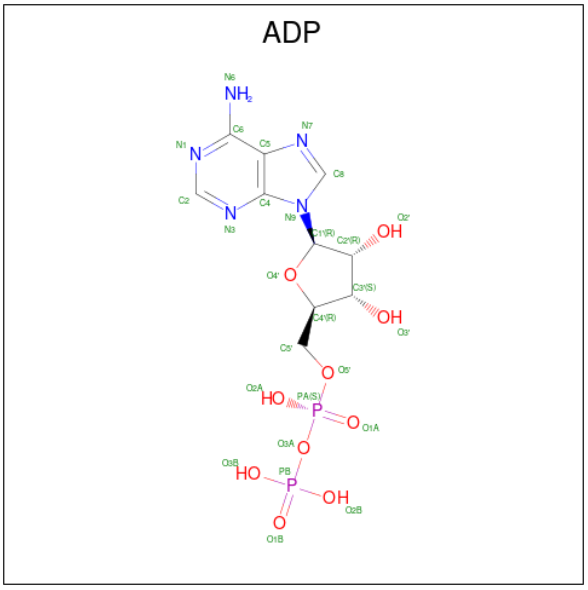
- Molecule 8 is a DNA chain called ntDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	K	23	474	225	96	130	23	0	0

- Molecule 9 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	R	32	674	302	117	223	32	0	0

- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	a	1	27	10	5	10	2	0
10	b	1	27	10	5	10	2	0
10	c	1	27	10	5	10	2	0
10	d	1	27	10	5	10	2	0
10	e	1	27	10	5	10	2	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

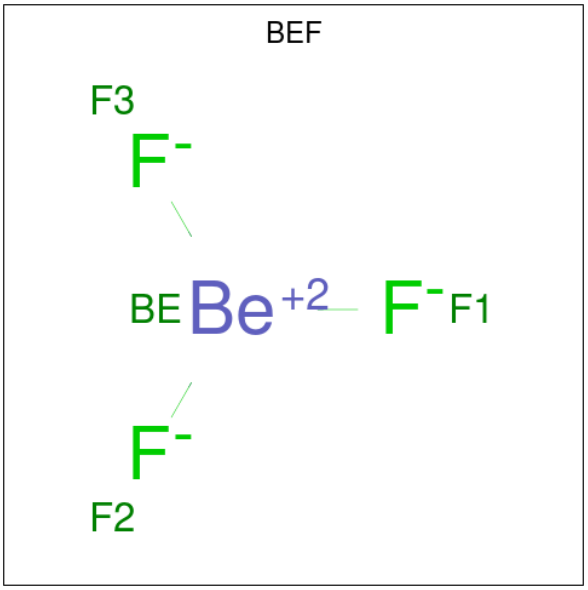
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	a	1	1	1	0
11	b	1	1	1	0
11	c	1	1	1	0
11	d	1	1	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
11	e	1	1	1	0
			Total	Mg	
11	Y	1	1	1	0

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
12	a	1	4	1	3	0
			Total	Be	F	
12	b	1	4	1	3	0
			Total	Be	F	
12	c	1	4	1	3	0
			Total	Be	F	
12	d	1	4	1	3	0
			Total	Be	F	
12	e	1	4	1	3	0

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
13	Y	2	2	2	0

- Molecule 14 is water.

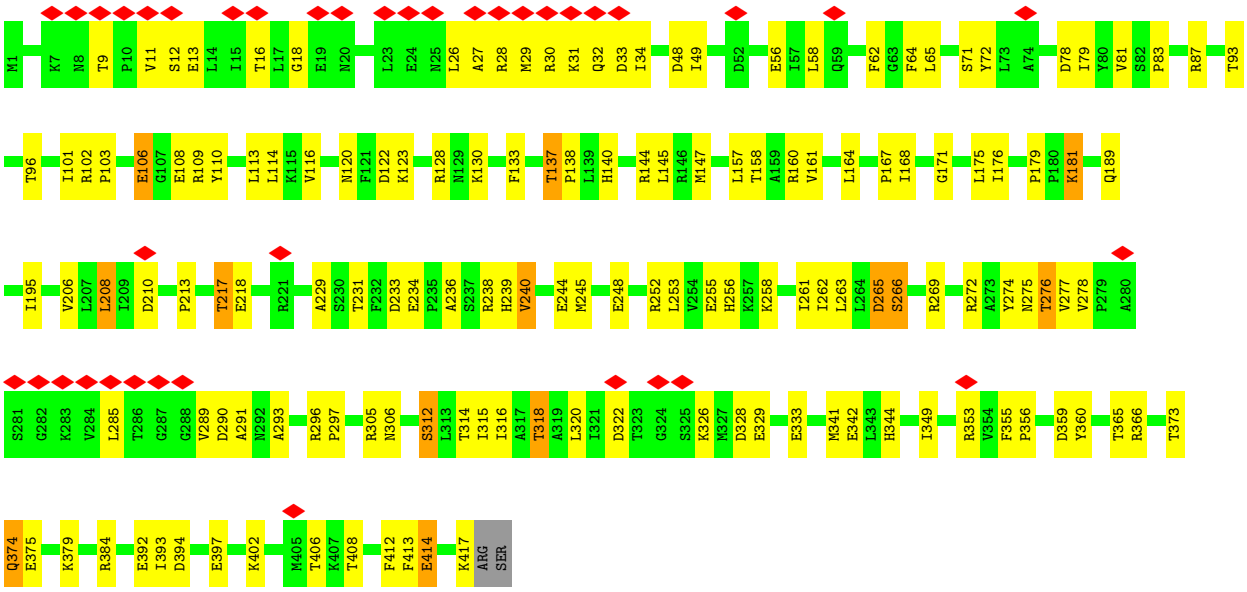
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
14	a	3	3	3	0
			Total	O	
14	b	3	3	3	0
			Total	O	
14	c	3	3	3	0
			Total	O	
14	d	3	3	3	0
			Total	O	
14	e	3	3	3	0

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

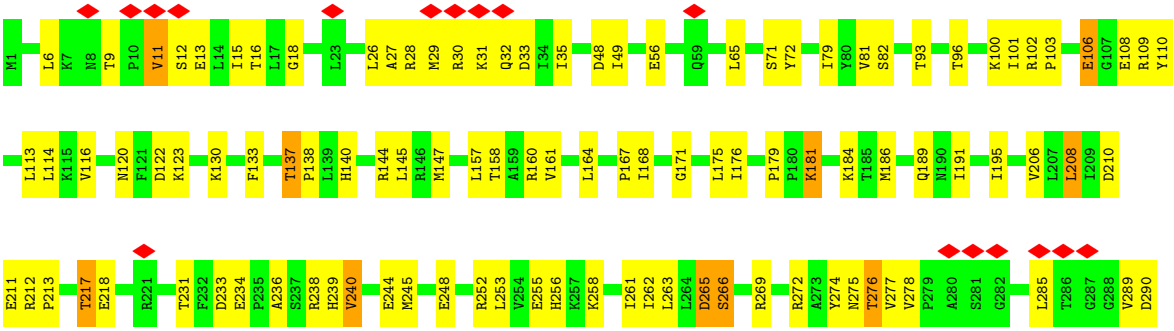
• Molecule 1: Transcription termination factor Rho

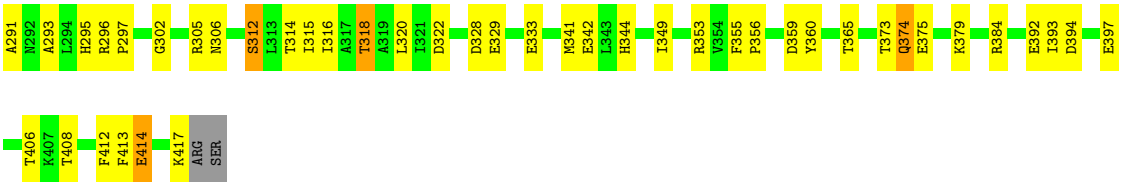
Chain f:



• Molecule 1: Transcription termination factor Rho

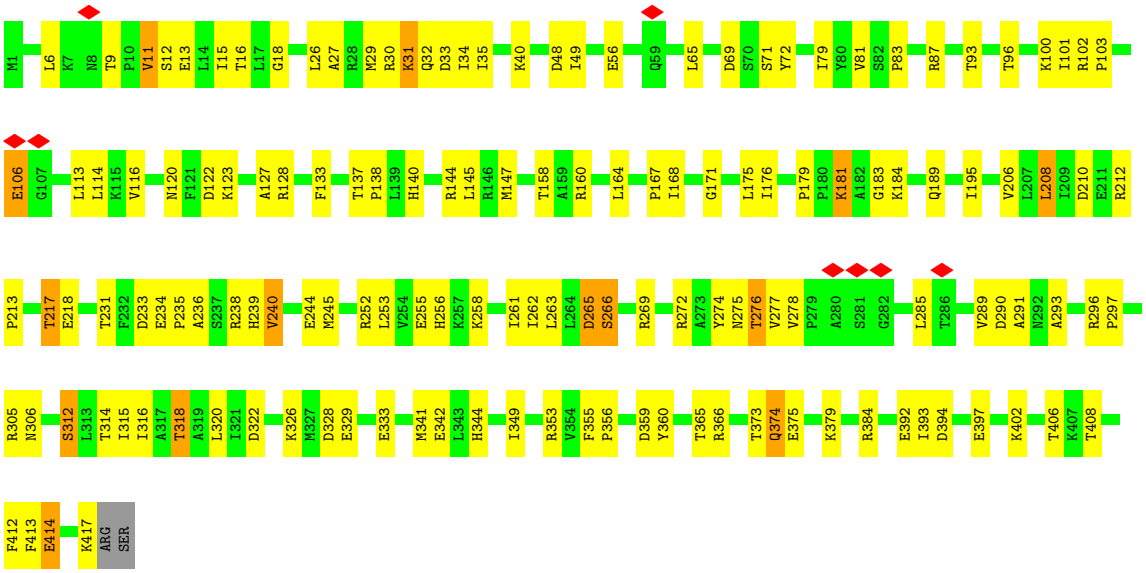
Chain a:





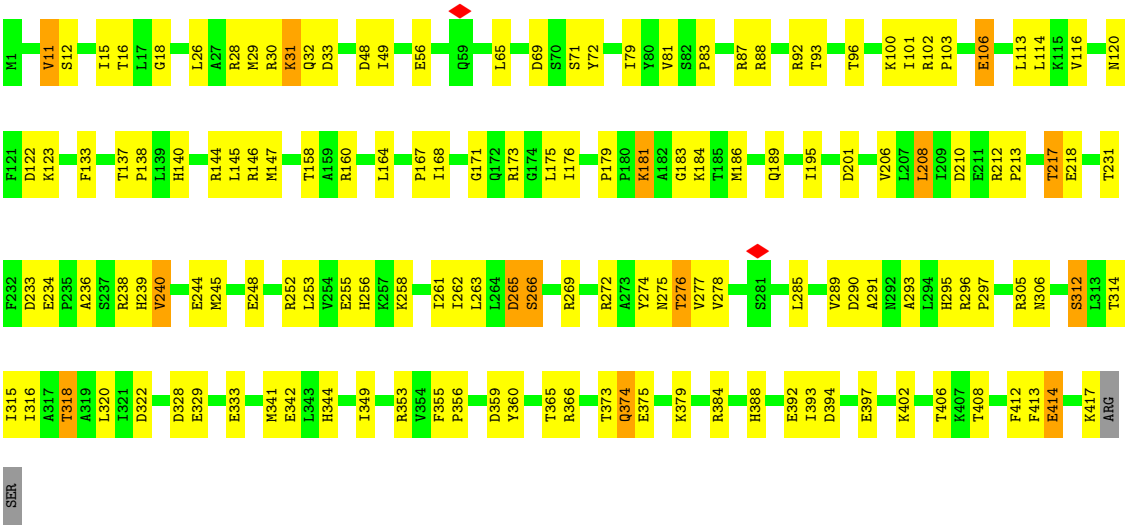
• Molecule 1: Transcription termination factor Rho

Chain b:



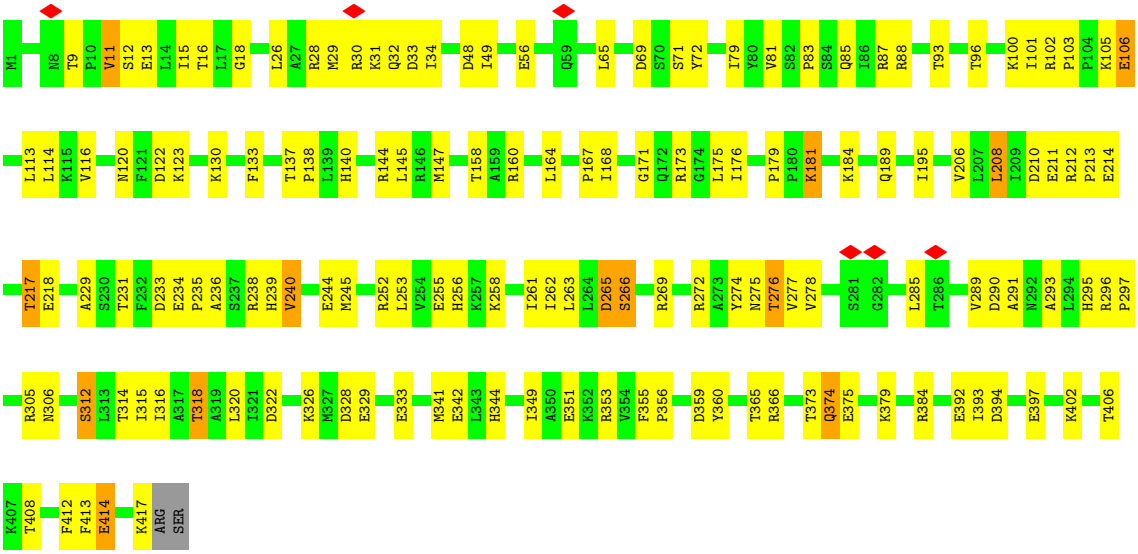
• Molecule 1: Transcription termination factor Rho

Chain c:



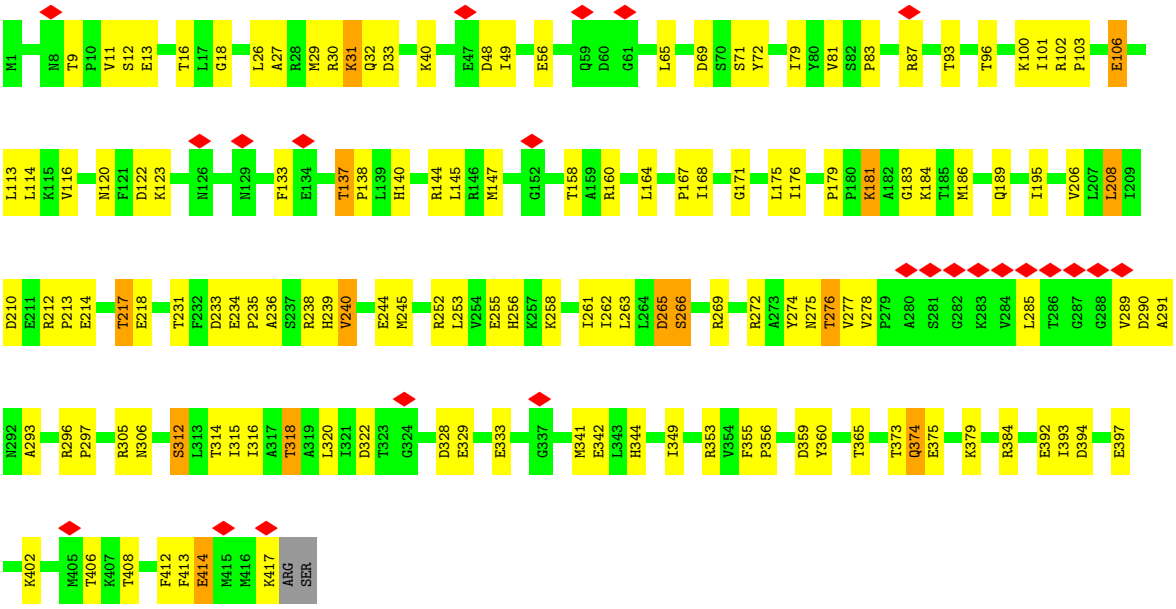
• Molecule 1: Transcription termination factor Rho

Chain d:



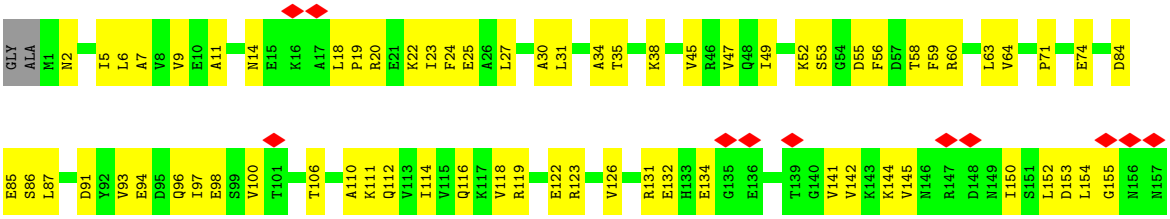
• Molecule 1: Transcription termination factor Rho

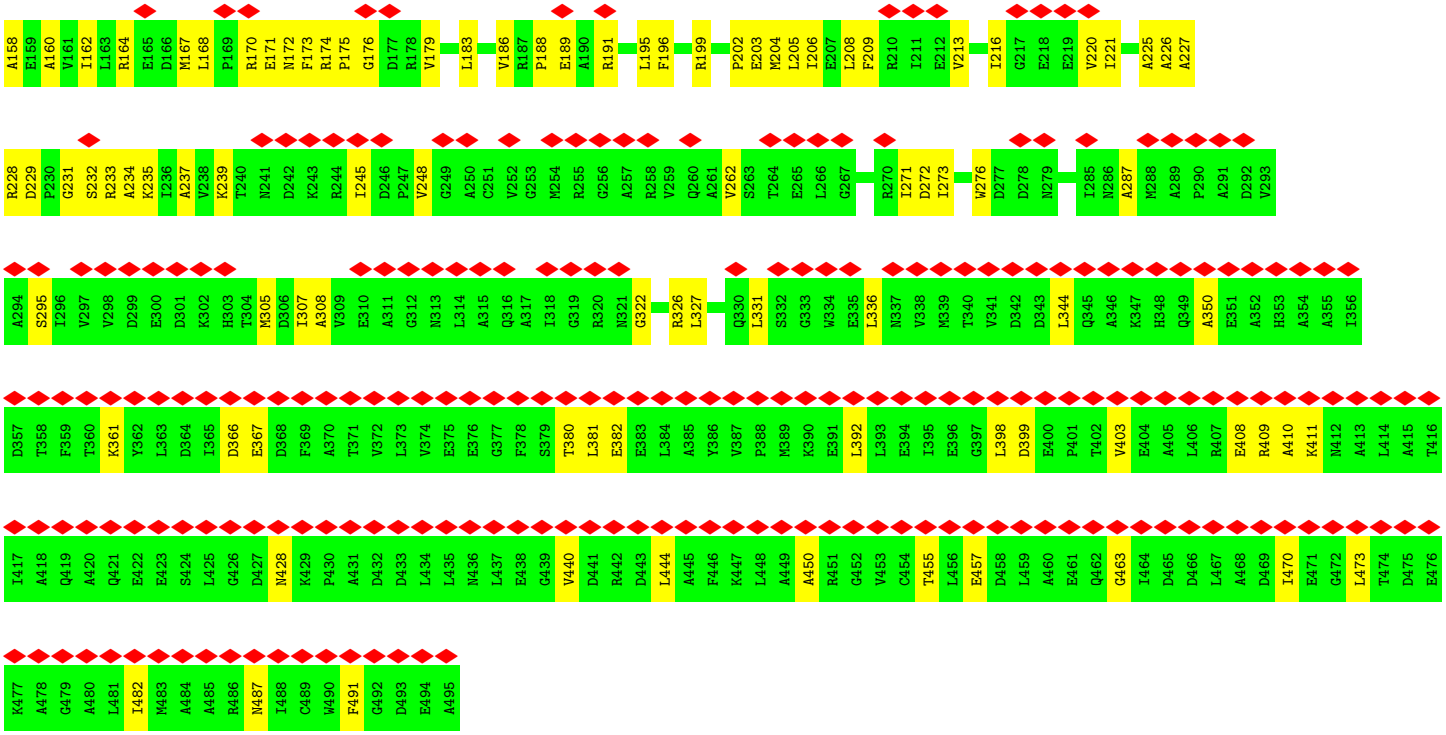
Chain e:



• Molecule 2: Transcription termination/antitermination protein NusA

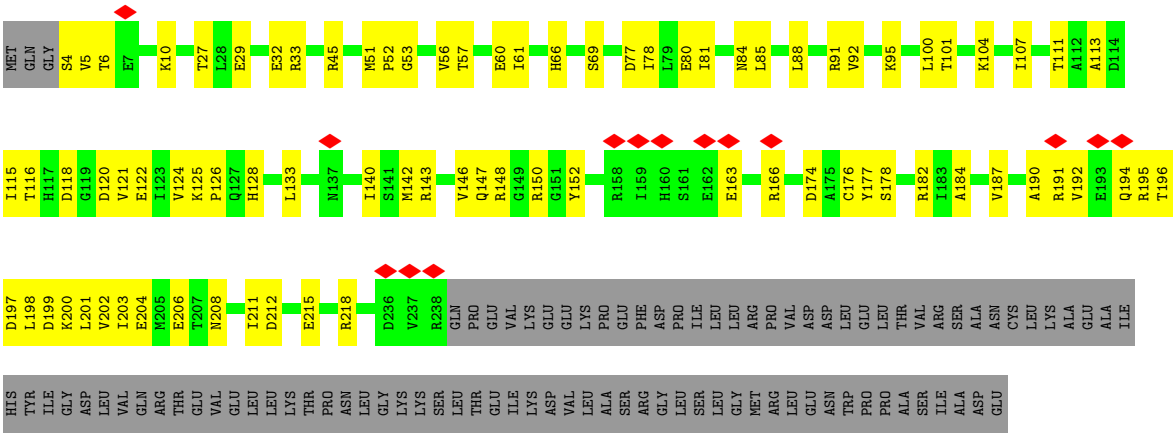
Chain A:





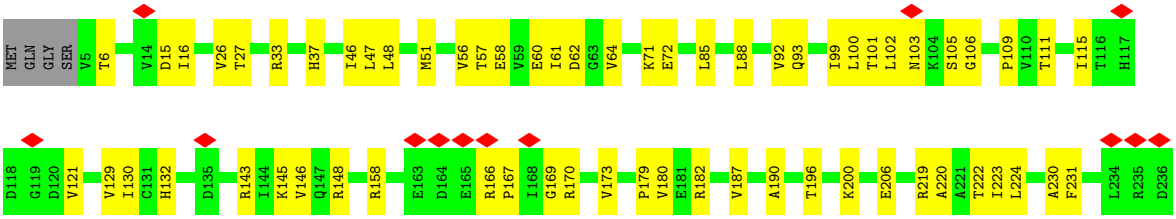
- Molecule 3: DNA-directed RNA polymerase subunit alpha

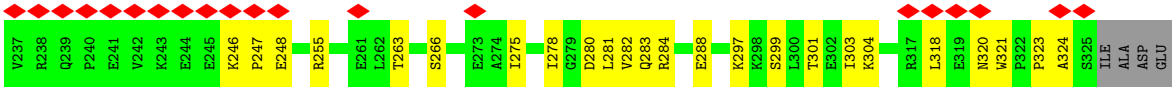
Chain U:



- Molecule 3: DNA-directed RNA polymerase subunit alpha

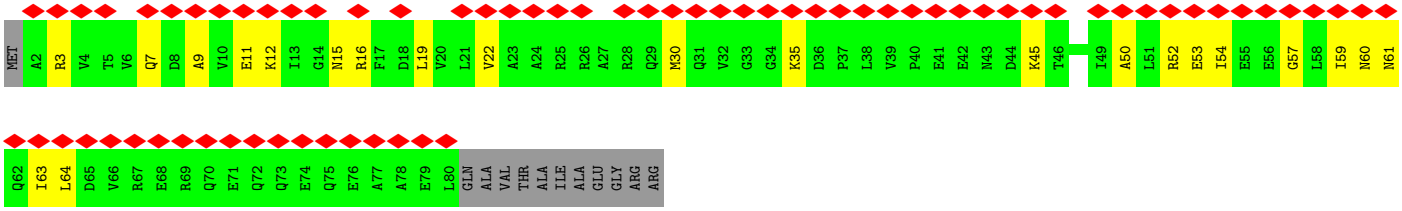
Chain V:





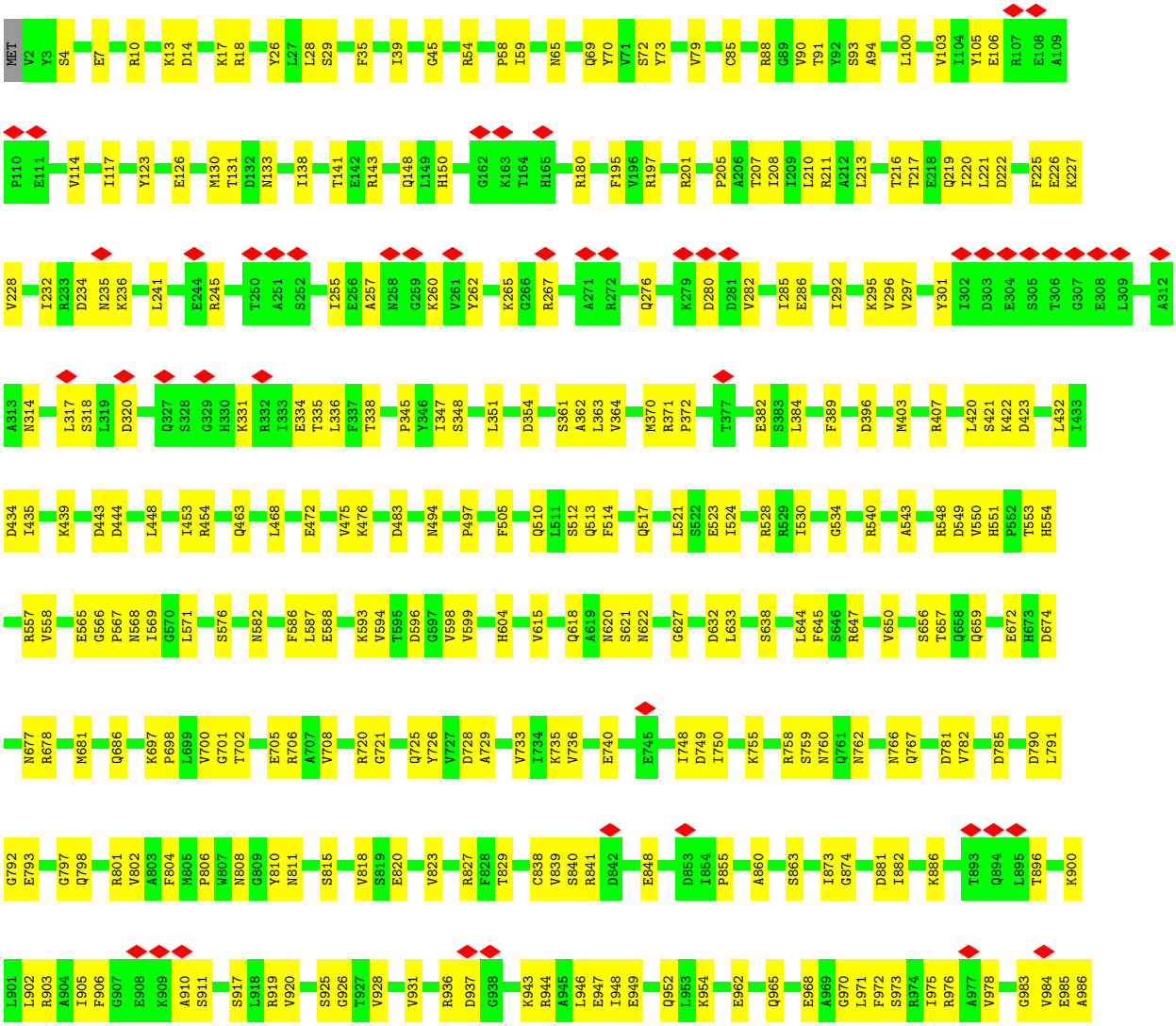
• Molecule 4: DNA-directed RNA polymerase subunit omega

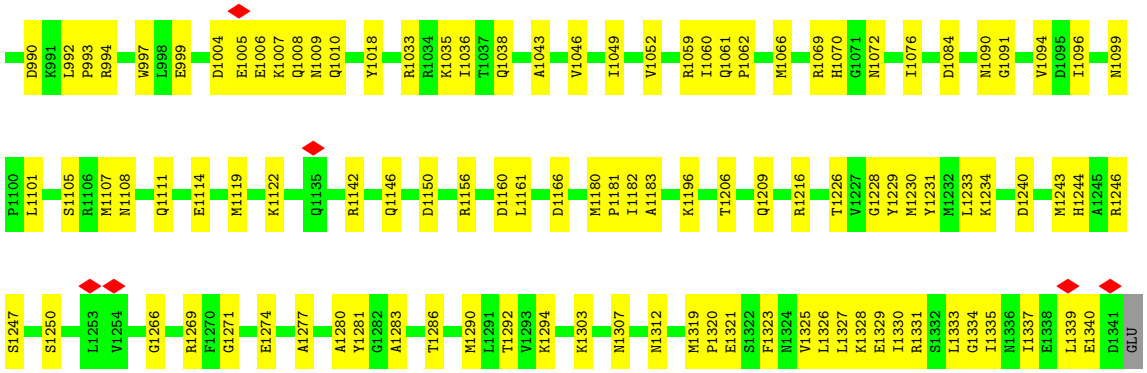
Chain W:



• Molecule 5: DNA-directed RNA polymerase subunit beta

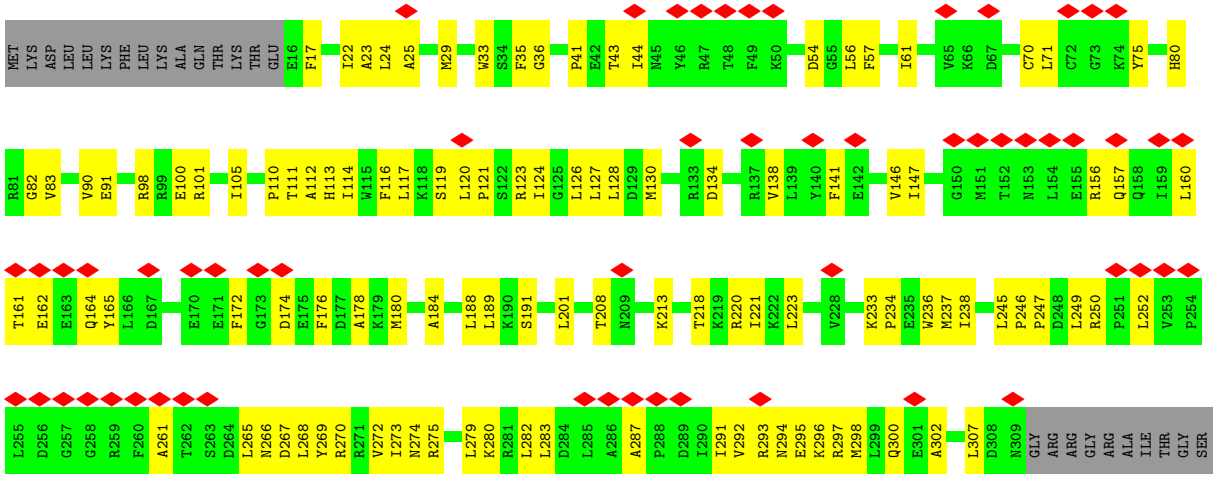
Chain X:

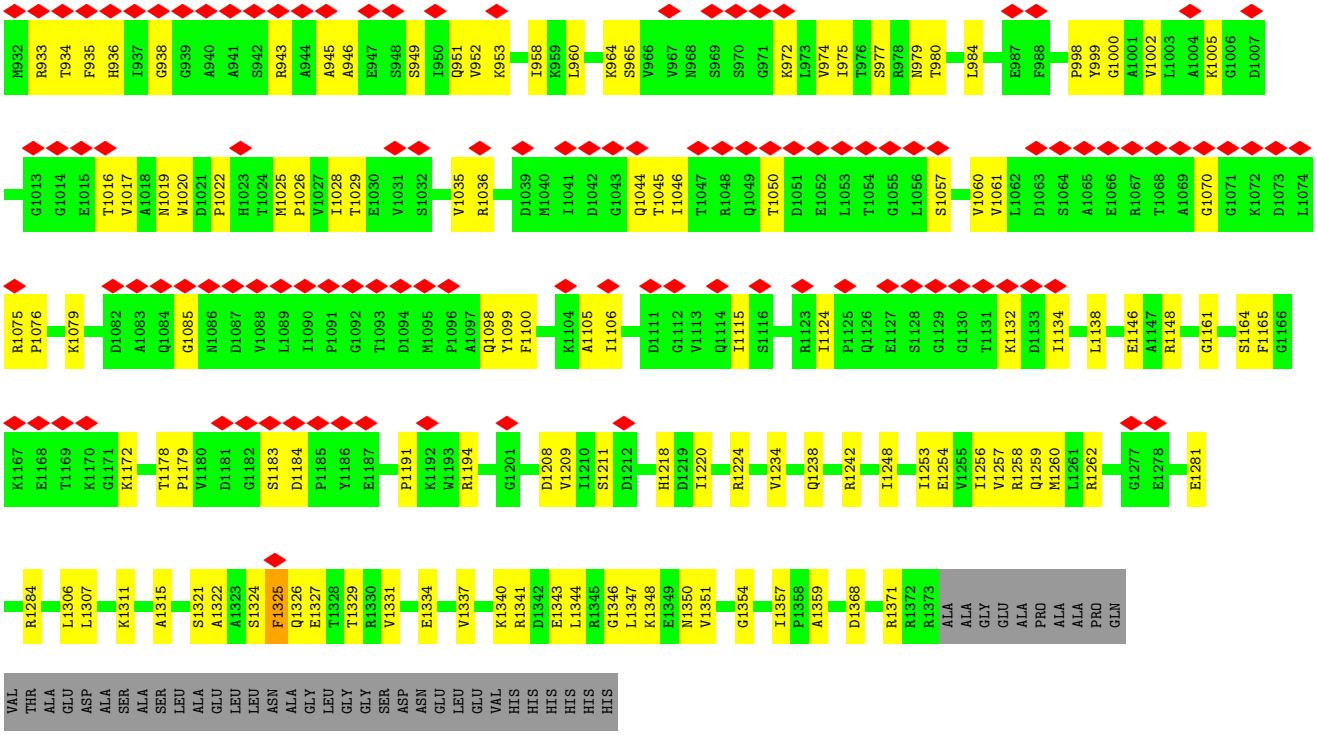




• Molecule 6: DNA-directed RNA polymerase subunit beta'

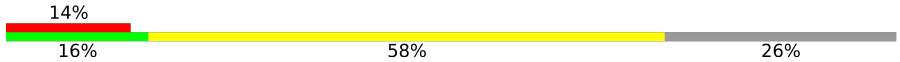
Chain Y:

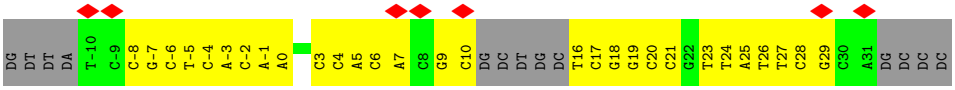




- Molecule 7: tDNA

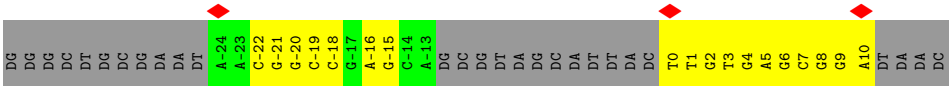
Chain L:





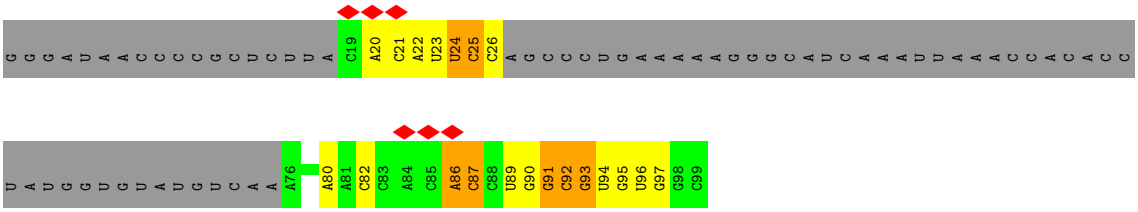
- Molecule 8: ntDNA

Chain K:



- Molecule 9: rut RNA

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	42083	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.323	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ZN, BEF

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	0.12	0/3329	0.34	0/4483
1	b	0.12	0/3329	0.33	0/4483
1	c	0.12	0/3329	0.34	0/4483
1	d	0.12	0/3329	0.34	0/4483
1	e	0.12	0/3329	0.34	0/4483
1	f	0.12	0/3329	0.34	0/4483
2	A	0.11	0/3897	0.33	0/5273
3	U	0.11	0/1847	0.29	0/2503
3	V	0.10	0/2538	0.31	0/3441
4	W	0.12	0/629	0.34	0/847
5	X	0.11	0/10736	0.30	0/14487
6	Y	0.11	0/10590	0.33	0/14301
7	L	0.24	0/827	0.50	0/1262
8	K	0.23	0/533	0.45	0/812
9	R	0.14	0/750	0.40	0/1162
All	All	0.12	0/52321	0.33	0/70986

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	Y	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Y	120	LEU	Peptide

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	3280	0	3358	108	0
1	b	3280	0	3358	90	0
1	c	3280	0	3358	91	0
1	d	3280	0	3358	100	0
1	e	3280	0	3358	87	0
1	f	3280	0	3359	102	0
2	A	3852	0	3835	115	0
3	U	1825	0	1853	58	0
3	V	2504	0	2558	58	0
4	W	627	0	634	17	0
5	X	10567	0	10585	301	0
6	Y	10431	0	10636	300	0
7	L	741	0	417	56	0
8	K	474	0	258	20	0
9	R	674	0	347	20	0
10	a	27	0	12	2	0
10	b	27	0	12	3	0
10	c	27	0	12	3	0
10	d	27	0	12	1	0
10	e	27	0	12	5	0
11	Y	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	c	1	0	0	0	0
11	d	1	0	0	0	0
11	e	1	0	0	0	0
12	a	4	0	0	1	0
12	b	4	0	0	1	0
12	c	4	0	0	2	0
12	d	4	0	0	0	0
12	e	4	0	0	2	0
13	Y	2	0	0	0	0
14	a	3	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	3	0	0	3	0
14	c	3	0	0	2	0
14	d	3	0	0	4	0
14	e	3	0	0	2	0
All	All	51553	0	51332	1410	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 14.

All (1410) 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:f:62:PHE:HE1	1:f:64:PHE:HE2	1.13	0.89
1:f:62:PHE:HE1	1:f:64:PHE:CE2	1.91	0.89
3:V:167:PRO:HD2	3:V:170:ARG:HG2	1.58	0.85
5:X:1327:LEU:HB3	5:X:1337:ILE:HG21	1.58	0.85
6:Y:287:ALA:HB1	6:Y:291:ILE:HG21	1.57	0.84
1:f:62:PHE:CE1	1:f:64:PHE:HE2	1.93	0.84
2:A:142:VAL:HG12	2:A:152:LEU:HG	1.60	0.83
3:U:107:ILE:HA	3:U:133:LEU:O	1.78	0.82
6:Y:886:VAL:HG12	6:Y:1258:ARG:HB2	1.62	0.81
5:X:227:LYS:HA	5:X:335:THR:O	1.79	0.81
5:X:510:GLN:HG2	5:X:534:GLY:HA2	1.62	0.81
7:L:17:DC:H2'	7:L:18:DG:C8	2.17	0.79
1:f:62:PHE:CE1	1:f:64:PHE:CE2	2.69	0.79
5:X:986:ALA:O	5:X:990:ASP:HB2	1.83	0.79
8:K:0:DT:H2'	8:K:1:DT:H71	1.62	0.79
1:a:82:SER:OG	7:L:25:DA:N6	2.16	0.78
6:Y:362:ARG:H	6:Y:365:GLN:HE21	1.29	0.78
7:L:24:DT:H2"	7:L:25:DA:C8	2.19	0.77
2:A:145:VAL:HG22	2:A:175:PRO:HD3	1.68	0.76
7:L:26:DT:H3'	7:L:27:DT:H5"	1.67	0.76
1:f:406:THR:HG21	1:f:412:PHE:HB2	1.68	0.76
1:e:406:THR:HG21	1:e:412:PHE:HB2	1.69	0.75
1:d:88:ARG:NH2	2:A:85:GLU:O	2.19	0.75
1:b:128:ARG:HA	1:c:28:ARG:HH21	1.51	0.75
1:d:406:THR:HG21	1:d:412:PHE:HB2	1.68	0.75
1:a:108:GLU:OE1	7:L:27:DT:H73	1.86	0.75
5:X:818:VAL:HB	5:X:1076:ILE:HD11	1.68	0.74
1:c:406:THR:HG21	1:c:412:PHE:HB2	1.69	0.74
1:f:64:PHE:CE1	1:f:78:ASP:OD2	2.41	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:406:THR:HG21	1:b:412:PHE:HB2	1.68	0.74
6:Y:705:THR:HG21	6:Y:718:SER:HA	1.70	0.74
1:f:176:ILE:HB	1:f:318:THR:HB	1.70	0.74
1:b:176:ILE:HB	1:b:318:THR:HB	1.70	0.74
7:L:-6:DC:H2"	7:L:-5:DT:H71	1.70	0.74
1:d:176:ILE:HB	1:d:318:THR:HB	1.70	0.73
5:X:226:GLU:HB3	5:X:245:ARG:HH21	1.53	0.73
1:a:406:THR:HG21	1:a:412:PHE:HB2	1.69	0.73
1:a:110:TYR:CD2	7:L:27:DT:O2	2.42	0.73
1:c:176:ILE:HB	1:c:318:THR:HB	1.70	0.73
1:d:138:PRO:HD2	1:e:217:THR:HG21	1.71	0.73
1:e:176:ILE:HB	1:e:318:THR:HB	1.70	0.73
1:a:176:ILE:HB	1:a:318:THR:HB	1.70	0.73
6:Y:1075:ARG:HE	6:Y:1100:PHE:HB3	1.52	0.73
3:U:32:GLU:OE1	3:U:195:ARG:NH2	2.21	0.73
5:X:448:LEU:HD21	5:X:587:LEU:HB2	1.70	0.72
5:X:1271:GLY:N	5:X:1274:GLU:OE2	2.23	0.72
6:Y:41:PRO:HG3	6:Y:274:ASN:HD22	1.53	0.72
6:Y:335:GLN:HB3	6:Y:340:GLN:HB3	1.72	0.72
5:X:448:LEU:HD23	5:X:557:ARG:HD3	1.71	0.72
1:f:138:PRO:HD2	1:a:217:THR:HG21	1.72	0.71
2:A:144:LYS:HA	2:A:175:PRO:HG3	1.70	0.71
1:c:72:TYR:HB3	1:c:245:MET:HE3	1.73	0.71
1:d:88:ARG:HH22	2:A:87:LEU:HB3	1.54	0.71
1:b:72:TYR:HB3	1:b:245:MET:HE3	1.73	0.71
1:f:64:PHE:CD1	1:f:78:ASP:OD2	2.44	0.71
6:Y:291:ILE:HG13	6:Y:292:VAL:H	1.56	0.71
7:L:4:DC:H2'	7:L:5:DA:C8	2.26	0.70
7:L:18:DG:H2'	7:L:19:DG:C8	2.25	0.70
1:a:72:TYR:HB3	1:a:245:MET:HE3	1.73	0.70
1:e:72:TYR:HB3	1:e:245:MET:HE3	1.73	0.70
5:X:1274:GLU:HB2	6:Y:434:ILE:HD11	1.72	0.70
1:d:72:TYR:HB3	1:d:245:MET:HE3	1.73	0.70
6:Y:527:LEU:HD23	6:Y:548:VAL:HG11	1.72	0.70
1:a:110:TYR:CE2	7:L:27:DT:O2	2.45	0.70
1:f:72:TYR:HB3	1:f:245:MET:HE3	1.73	0.70
7:L:6:DC:H2'	7:L:7:DA:C8	2.26	0.70
6:Y:809:VAL:HG13	6:Y:912:GLY:H	1.56	0.70
5:X:141:THR:OG1	5:X:760:ASN:ND2	2.24	0.70
1:f:138:PRO:HG3	1:f:305:ARG:HD3	1.74	0.69
1:b:138:PRO:HG3	1:b:305:ARG:HD3	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:56:LEU:HD21	6:Y:266:ASN:HB2	1.74	0.69
3:V:109:PRO:HB3	3:V:132:HIS:HA	1.74	0.69
6:Y:425:ARG:HG3	6:Y:427:PRO:HD2	1.74	0.69
1:d:236:ALA:HA	1:d:239:HIS:HD2	1.58	0.69
1:e:138:PRO:HG3	1:e:305:ARG:HD3	1.75	0.69
6:Y:43:THR:HA	6:Y:56:LEU:HB3	1.75	0.69
1:f:236:ALA:HA	1:f:239:HIS:HD2	1.58	0.68
4:W:30:MET:HA	4:W:35:LYS:HG2	1.75	0.68
5:X:838:CYS:SG	5:X:886:LYS:NZ	2.63	0.68
1:b:236:ALA:HA	1:b:239:HIS:HD2	1.58	0.68
1:d:138:PRO:HG3	1:d:305:ARG:HD3	1.74	0.68
2:A:186:VAL:HG12	2:A:188:PRO:HD3	1.75	0.68
3:U:57:THR:HG21	3:U:147:GLN:HE21	1.58	0.68
5:X:14:ASP:HA	5:X:1183:ALA:HB3	1.74	0.68
6:Y:128:LEU:HD22	6:Y:130:MET:HB2	1.74	0.68
1:a:236:ALA:HA	1:a:239:HIS:HD2	1.58	0.68
1:e:236:ALA:HA	1:e:239:HIS:HD2	1.58	0.68
1:c:138:PRO:HG3	1:c:305:ARG:HD3	1.75	0.67
1:c:236:ALA:HA	1:c:239:HIS:HD2	1.58	0.67
1:d:49:ILE:HB	1:d:101:ILE:HG13	1.77	0.67
1:a:138:PRO:HG3	1:a:305:ARG:HD3	1.75	0.67
5:X:211:ARG:HH12	5:X:217:THR:HG23	1.59	0.67
1:b:49:ILE:HB	1:b:101:ILE:HG13	1.77	0.67
2:A:97:ILE:HG22	2:A:98:GLU:H	1.59	0.67
6:Y:126:LEU:HG	6:Y:223:LEU:HD22	1.77	0.67
1:f:49:ILE:HB	1:f:101:ILE:HG13	1.77	0.67
1:a:49:ILE:HB	1:a:101:ILE:HG13	1.77	0.67
5:X:1070:HIS:NE2	5:X:1114:GLU:OE1	2.28	0.67
5:X:1340:GLU:OE2	6:Y:1341:ARG:NH2	2.27	0.67
1:b:101:ILE:HG22	1:b:113:LEU:HA	1.77	0.67
1:c:49:ILE:HB	1:c:101:ILE:HG13	1.77	0.67
5:X:241:LEU:HD11	5:X:285:ILE:HG12	1.77	0.66
3:U:182:ARG:HG2	3:U:206:GLU:HB3	1.76	0.66
6:Y:926:PRO:HG2	6:Y:1248:ILE:HD11	1.76	0.66
6:Y:418:GLU:HB3	6:Y:481:ARG:HH12	1.60	0.66
1:e:30:ARG:HG2	1:e:32:GLN:H	1.61	0.66
1:d:101:ILE:HG22	1:d:113:LEU:HA	1.77	0.66
5:X:296:VAL:HG23	5:X:336:LEU:HD13	1.77	0.66
1:f:101:ILE:HG22	1:f:113:LEU:HA	1.77	0.66
1:c:101:ILE:HG22	1:c:113:LEU:HA	1.77	0.66
5:X:726:TYR:HB3	5:X:733:VAL:HB	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:1322:ALA:HB1	6:Y:1331:VAL:HB	1.78	0.66
1:a:101:ILE:HG22	1:a:113:LEU:HA	1.77	0.66
1:e:49:ILE:HB	1:e:101:ILE:HG13	1.77	0.66
1:e:101:ILE:HG22	1:e:113:LEU:HA	1.77	0.65
5:X:1334:GLY:HA3	6:Y:25:ALA:HB2	1.77	0.65
6:Y:746:LEU:HD23	6:Y:758:PRO:HB3	1.77	0.65
2:A:31:LEU:HB3	2:A:47:VAL:HG11	1.78	0.65
3:U:118:ASP:HA	3:V:255:ARG:HH22	1.60	0.65
5:X:528:ARG:NH2	5:X:576:SER:O	2.30	0.65
5:X:700:VAL:HG21	5:X:1114:GLU:HG3	1.78	0.65
6:Y:267:ASP:HA	6:Y:270:ARG:HG2	1.79	0.65
7:L:16:DT:H2'	7:L:17:DC:C6	2.32	0.65
1:c:30:ARG:HG2	1:c:32:GLN:H	1.61	0.65
5:X:255:ILE:HD11	5:X:285:ILE:HD12	1.78	0.65
6:Y:582:ILE:HD12	6:Y:623:GLN:HB3	1.79	0.65
6:Y:824:PRO:HD3	6:Y:835:LEU:HB2	1.77	0.65
5:X:615:VAL:HG12	5:X:638:SER:HA	1.78	0.65
1:b:30:ARG:HG2	1:b:32:GLN:H	1.61	0.65
3:V:321:TRP:HA	3:V:323:PRO:HD3	1.79	0.65
6:Y:36:GLY:HA3	6:Y:61:ILE:HG12	1.78	0.65
6:Y:972:LYS:HE2	6:Y:1002:VAL:HG13	1.79	0.65
5:X:983:GLY:O	5:X:986:ALA:HB3	1.97	0.65
6:Y:452:LEU:HD21	6:Y:500:ILE:HA	1.79	0.65
1:d:30:ARG:HG2	1:d:32:GLN:H	1.61	0.64
1:d:211:GLU:OE2	14:d:1101:HOH:O	2.15	0.64
5:X:829:THR:HG22	5:X:1059:ARG:HA	1.79	0.64
1:b:212:ARG:NH2	14:b:1101:HOH:O	2.30	0.64
3:U:124:VAL:HG13	3:U:125:LYS:HG2	1.79	0.64
2:A:71:PRO:HA	2:A:74:GLU:HB2	1.79	0.64
1:f:30:ARG:HG2	1:f:32:GLN:H	1.61	0.64
5:X:1323:PHE:O	5:X:1327:LEU:HG	1.98	0.64
1:a:30:ARG:HG2	1:a:32:GLN:H	1.61	0.64
1:b:18:GLY:HA3	1:b:26:LEU:HD22	1.80	0.64
1:f:18:GLY:HA3	1:f:26:LEU:HD22	1.80	0.64
9:R:92:C:H2'	9:R:93:G:C8	2.33	0.64
1:a:212:ARG:NH2	14:a:1101:HOH:O	2.31	0.64
2:A:134:GLU:HA	2:A:183:LEU:HB3	1.80	0.64
2:A:209:PHE:HE1	2:A:262:VAL:HG21	1.63	0.63
1:a:147:MET:HE1	1:a:195:ILE:HB	1.80	0.63
1:d:85:GLN:NE2	2:A:84:ASP:OD2	2.31	0.63
5:X:217:THR:HG22	5:X:351:LEU:HD11	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:1142:ARG:NH1	5:X:1161:LEU:O	2.32	0.63
5:X:1303:LYS:O	5:X:1307:ASN:ND2	2.31	0.63
1:d:147:MET:HE1	1:d:195:ILE:HB	1.80	0.63
1:e:147:MET:HE1	1:e:195:ILE:HB	1.80	0.63
2:A:142:VAL:HG23	2:A:175:PRO:HA	1.79	0.63
1:c:147:MET:HE1	1:c:195:ILE:HB	1.81	0.62
2:A:142:VAL:HA	2:A:152:LEU:HA	1.81	0.62
5:X:88:ARG:NH1	5:X:1035:LYS:O	2.32	0.62
1:f:109:ARG:NH2	9:R:25:C:H3'	2.14	0.62
6:Y:82:GLY:HA2	6:Y:91:GLU:HG2	1.80	0.62
6:Y:945:ALA:HB3	6:Y:1022:PRO:HA	1.82	0.62
8:K:2:DG:H2'	8:K:3:DT:C6	2.34	0.62
1:d:295:HIS:CD2	1:e:235:PRO:HD3	2.34	0.62
3:U:80:GLU:O	3:U:84:ASN:ND2	2.32	0.62
5:X:720:ARG:HH21	5:X:736:VAL:HG21	1.64	0.62
1:f:147:MET:HE1	1:f:195:ILE:HB	1.81	0.62
1:b:147:MET:HE1	1:b:195:ILE:HB	1.81	0.62
1:c:18:GLY:HA3	1:c:26:LEU:HD22	1.80	0.62
2:A:123:ARG:NH2	2:A:191:ARG:O	2.32	0.62
2:A:444:LEU:HD12	2:A:473:LEU:HD11	1.82	0.62
5:X:314:ASN:HD21	5:X:348:SER:HA	1.63	0.62
6:Y:180:MET:HG3	6:Y:296:LYS:HE3	1.81	0.62
1:f:349:ILE:HD11	1:f:392:GLU:HB3	1.82	0.62
1:a:18:GLY:HA3	1:a:26:LEU:HD22	1.80	0.62
1:d:18:GLY:HA3	1:d:26:LEU:HD22	1.80	0.62
5:X:1277:ALA:HA	6:Y:921:GLN:HE22	1.65	0.62
6:Y:933:ARG:NH2	6:Y:934:THR:O	2.33	0.62
2:A:145:VAL:HG11	2:A:173:PHE:HB3	1.82	0.62
1:e:18:GLY:HA3	1:e:26:LEU:HD22	1.80	0.62
5:X:1066:MET:HE1	5:X:1076:ILE:HB	1.82	0.62
6:Y:291:ILE:HG13	6:Y:292:VAL:N	2.15	0.62
1:c:349:ILE:HD11	1:c:392:GLU:HB3	1.82	0.62
2:A:154:LEU:HD11	2:A:160:ALA:HB2	1.82	0.62
3:V:16:ILE:HG23	3:V:26:VAL:HG12	1.82	0.62
5:X:265:LYS:O	5:X:267:ARG:NH1	2.33	0.62
1:f:234:GLU:OE1	1:f:238:ARG:NH1	2.33	0.62
1:a:234:GLU:OE1	1:a:238:ARG:NH1	2.33	0.62
1:a:349:ILE:HD11	1:a:392:GLU:HB3	1.82	0.62
1:d:234:GLU:OE1	1:d:238:ARG:NH1	2.33	0.62
2:A:209:PHE:O	2:A:213:VAL:N	2.32	0.62
5:X:180:ARG:NH2	5:X:396:ASP:OD2	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:234:GLU:OE1	1:b:238:ARG:NH1	2.33	0.61
3:V:283:GLN:NE2	3:V:318:LEU:O	2.32	0.61
5:X:672:GLU:HB2	6:Y:767:LEU:HB2	1.82	0.61
1:b:349:ILE:HD11	1:b:392:GLU:HB3	1.82	0.61
1:e:234:GLU:OE1	1:e:238:ARG:NH1	2.33	0.61
6:Y:972:LYS:HZ3	6:Y:1002:VAL:HA	1.66	0.61
1:f:109:ARG:HH21	9:R:25:C:H3'	1.65	0.61
1:d:349:ILE:HD11	1:d:392:GLU:HB3	1.82	0.61
6:Y:576:ARG:HD3	6:Y:593:ASN:HA	1.82	0.61
1:c:234:GLU:OE1	1:c:238:ARG:NH1	2.33	0.61
5:X:841:ARG:HA	5:X:1046:VAL:HA	1.81	0.61
1:d:210:ASP:HB2	1:d:269:ARG:HD3	1.83	0.61
3:U:33:ARG:HH11	3:U:197:ASP:HB2	1.66	0.61
5:X:733:VAL:HG22	5:X:750:ILE:HG12	1.81	0.61
6:Y:884:SER:OG	6:Y:1254:GLU:OE2	2.18	0.61
5:X:839:VAL:O	5:X:886:LYS:NZ	2.33	0.61
7:L:17:DC:H2'	7:L:18:DG:H8	1.63	0.61
1:e:171:GLY:H	1:e:314:THR:HG1	1.49	0.61
5:X:618:GLN:HB3	5:X:621:SER:HB3	1.83	0.61
7:L:4:DC:H2'	7:L:5:DA:H8	1.65	0.61
1:b:210:ASP:HB2	1:b:269:ARG:HD3	1.83	0.60
1:e:212:ARG:NH2	14:e:1101:HOH:O	2.33	0.60
1:c:210:ASP:HB2	1:c:269:ARG:HD3	1.83	0.60
2:A:131:ARG:HG3	2:A:186:VAL:HG21	1.83	0.60
3:U:92:VAL:O	3:U:148:ARG:NH2	2.33	0.60
3:V:60:GLU:HB2	3:V:143:ARG:HB3	1.82	0.60
6:Y:117:LEU:HD23	6:Y:124:ILE:HD13	1.83	0.60
7:L:3:DC:H2'	7:L:4:DC:C6	2.36	0.60
1:f:210:ASP:HB2	1:f:269:ARG:HD3	1.83	0.60
1:e:210:ASP:HB2	1:e:269:ARG:HD3	1.83	0.60
5:X:1246:ARG:NH2	5:X:1250:SER:O	2.34	0.60
1:a:210:ASP:HB2	1:a:269:ARG:HD3	1.83	0.60
1:e:349:ILE:HD11	1:e:392:GLU:HB3	1.82	0.60
5:X:1330:ILE:O	5:X:1334:GLY:N	2.33	0.60
2:A:168:LEU:HD23	2:A:170:ARG:HG2	1.82	0.60
5:X:512:SER:N	9:R:89:U:O4	2.35	0.60
1:a:110:TYR:CD2	7:L:27:DT:C2	2.90	0.60
5:X:195:PHE:HA	5:X:205:PRO:HA	1.84	0.60
1:f:171:GLY:H	1:f:314:THR:HG1	1.48	0.60
1:a:109:ARG:HH12	7:L:27:DT:H2'	1.66	0.60
6:Y:1046:ILE:HG22	6:Y:1061:VAL:HG12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:936:ARG:NH2	5:X:1043:ALA:O	2.35	0.60
1:d:65:LEU:HB3	1:d:79:ILE:HB	1.84	0.59
5:X:1269:ARG:HH22	6:Y:340:GLN:HE22	1.48	0.59
5:X:210:LEU:HD22	5:X:220:ILE:HG12	1.84	0.59
7:L:6:DC:H2'	7:L:7:DA:H8	1.67	0.59
1:a:379:LYS:HD3	1:a:413:PHE:HB3	1.85	0.59
9:R:96:U:H2'	9:R:97:G:C8	2.38	0.59
1:c:88:ARG:NH1	5:X:999:GLU:OE2	2.36	0.59
5:X:1066:MET:HG3	5:X:1234:LYS:HA	1.83	0.59
5:X:1072:ASN:ND2	5:X:1111:GLN:OE1	2.34	0.59
6:Y:340:GLN:HA	6:Y:343:LEU:HB2	1.85	0.59
1:d:379:LYS:HD3	1:d:413:PHE:HB3	1.85	0.59
2:A:47:VAL:HG12	2:A:58:THR:HG22	1.84	0.59
2:A:305:MET:HB2	2:A:336:LEU:HD22	1.84	0.59
6:Y:141:PHE:CE2	6:Y:297:ARG:HA	2.37	0.59
1:a:138:PRO:HD2	1:b:217:THR:HG21	1.84	0.59
5:X:1005:GLU:O	5:X:1009:ASN:ND2	2.35	0.59
6:Y:105:ILE:HG12	6:Y:273:ILE:HD11	1.85	0.59
6:Y:1000:GLY:HA3	6:Y:1026:PRO:HG3	1.84	0.59
1:f:65:LEU:HB3	1:f:79:ILE:HB	1.84	0.59
1:e:65:LEU:HB3	1:e:79:ILE:HB	1.84	0.59
6:Y:747:MET:HE2	6:Y:775:SER:HA	1.83	0.59
7:L:-2:DC:H2"	7:L:-1:DA:C8	2.37	0.59
1:b:65:LEU:HB3	1:b:79:ILE:HB	1.84	0.59
7:L:3:DC:H2'	7:L:4:DC:H6	1.67	0.59
2:A:487:ASN:HA	2:A:491:PHE:HB2	1.85	0.58
1:a:12:SER:O	1:a:16:THR:HG23	2.03	0.58
1:a:65:LEU:HB3	1:a:79:ILE:HB	1.84	0.58
3:V:57:THR:O	3:V:158:ARG:NH1	2.36	0.58
1:f:12:SER:O	1:f:16:THR:HG23	2.03	0.58
1:a:108:GLU:OE1	7:L:27:DT:C7	2.51	0.58
1:b:379:LYS:HD3	1:b:413:PHE:HB3	1.84	0.58
2:A:116:GLN:OE1	2:A:119:ARG:NH1	2.33	0.58
2:A:202:PRO:HA	2:A:228:ARG:HD3	1.85	0.58
5:X:213:LEU:HD13	5:X:422:LYS:HG2	1.85	0.58
6:Y:294:ASN:HA	6:Y:297:ARG:HG2	1.84	0.58
6:Y:1029:THR:HA	6:Y:1099:TYR:HE2	1.68	0.58
2:A:205:LEU:HD23	2:A:228:ARG:HD2	1.86	0.58
1:f:379:LYS:HD3	1:f:413:PHE:HB3	1.85	0.58
1:a:211:GLU:OE2	14:a:1101:HOH:O	2.17	0.58
1:d:12:SER:O	1:d:16:THR:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:253:LEU:HD22	1:d:258:LYS:HD2	1.86	0.58
5:X:582:ASN:HB3	5:X:586:PHE:H	1.68	0.58
6:Y:337:ARG:O	6:Y:341:ASN:ND2	2.36	0.58
1:a:253:LEU:HD22	1:a:258:LYS:HD2	1.86	0.58
2:A:52:LYS:HD2	2:A:53:SER:HB3	1.85	0.58
6:Y:1218:HIS:NE2	6:Y:1306:LEU:O	2.36	0.58
6:Y:1346:GLY:O	6:Y:1350:ASN:ND2	2.37	0.58
6:Y:201:LEU:HD21	6:Y:220:ARG:HB2	1.84	0.58
1:e:379:LYS:HD3	1:e:413:PHE:HB3	1.84	0.58
5:X:720:ARG:NH2	5:X:749:ASP:OD1	2.37	0.58
6:Y:279:LEU:HD12	6:Y:295:GLU:HA	1.85	0.58
1:a:272:ARG:O	1:a:276:THR:HG22	2.04	0.58
1:b:12:SER:O	1:b:16:THR:HG23	2.03	0.58
5:X:633:LEU:HD21	5:X:644:LEU:HD23	1.85	0.58
5:X:1339:LEU:HB3	6:Y:17:PHE:HB3	1.86	0.58
6:Y:161:THR:H	6:Y:164:GLN:HB2	1.68	0.58
1:b:253:LEU:HD22	1:b:258:LYS:HD2	1.86	0.58
1:d:272:ARG:O	1:d:276:THR:HG22	2.04	0.58
5:X:633:LEU:HA	5:X:645:PHE:O	2.03	0.58
5:X:971:LEU:O	5:X:975:ILE:HG23	2.03	0.58
5:X:222:ASP:HA	5:X:227:LYS:HD3	1.86	0.57
6:Y:43:THR:HB	6:Y:56:LEU:HD23	1.85	0.57
1:e:272:ARG:O	1:e:276:THR:HG22	2.04	0.57
3:V:56:VAL:HA	3:V:146:VAL:HG12	1.86	0.57
1:a:109:ARG:HD2	7:L:29:DG:C5	2.37	0.57
1:b:127:ALA:O	1:c:28:ARG:NH2	2.38	0.57
1:c:65:LEU:HB3	1:c:79:ILE:HB	1.84	0.57
1:c:144:ARG:HE	1:c:167:PRO:HB3	1.69	0.57
2:A:199:ARG:HD2	2:A:228:ARG:HH22	1.70	0.57
5:X:524:ILE:HD13	5:X:708:VAL:HG23	1.86	0.57
5:X:952:GLN:HG3	5:X:1036:ILE:HD12	1.85	0.57
1:e:262:ILE:HB	1:e:315:ILE:HG13	1.87	0.57
5:X:1283:ALA:HB1	5:X:1286:THR:HB	1.87	0.57
1:a:144:ARG:HE	1:a:167:PRO:HB3	1.70	0.57
1:c:262:ILE:HB	1:c:315:ILE:HG13	1.87	0.57
1:b:262:ILE:HB	1:b:315:ILE:HG13	1.87	0.57
2:A:131:ARG:NH2	2:A:132:GLU:OE2	2.35	0.57
1:f:144:ARG:HE	1:f:167:PRO:HB3	1.69	0.57
1:c:360:TYR:O	1:c:384:ARG:NH2	2.38	0.57
3:V:102:LEU:HD13	3:V:115:ILE:HD13	1.87	0.57
5:X:197:ARG:NH1	5:X:201:ARG:O	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:1119:MET:HB2	5:X:1228:GLY:HA2	1.86	0.57
6:Y:124:ILE:HA	6:Y:127:LEU:HD12	1.87	0.57
6:Y:1178:THR:HA	6:Y:1184:ASP:HB3	1.86	0.57
1:c:12:SER:O	1:c:16:THR:HG23	2.04	0.57
1:c:179:PRO:HB3	1:c:322:ASP:HB3	1.87	0.57
1:c:212:ARG:NH2	14:c:1101:HOH:O	2.38	0.57
1:c:253:LEU:HD22	1:c:258:LYS:HD2	1.86	0.57
1:c:379:LYS:HD3	1:c:413:PHE:HB3	1.85	0.57
5:X:700:VAL:HG23	5:X:1069:ARG:HH22	1.70	0.57
1:f:253:LEU:HD22	1:f:258:LYS:HD2	1.86	0.57
1:a:360:TYR:O	1:a:384:ARG:NH2	2.38	0.57
2:A:34:ALA:HB1	2:A:106:THR:HG22	1.87	0.57
3:V:248:GLU:OE2	3:V:320:ASN:ND2	2.37	0.57
5:X:972:PHE:HA	5:X:975:ILE:HG12	1.86	0.57
1:d:360:TYR:O	1:d:384:ARG:NH2	2.38	0.56
1:e:12:SER:O	1:e:16:THR:HG23	2.03	0.56
1:b:272:ARG:O	1:b:276:THR:HG22	2.04	0.56
1:e:253:LEU:HD22	1:e:258:LYS:HD2	1.86	0.56
3:V:51:MET:HG3	3:V:179:PRO:HD2	1.86	0.56
1:f:27:ALA:HB3	2:A:172:ASN:HD22	1.69	0.56
1:f:272:ARG:O	1:f:276:THR:HG22	2.04	0.56
1:f:360:TYR:O	1:f:384:ARG:NH2	2.38	0.56
3:V:100:LEU:HD21	3:V:121:VAL:HG21	1.87	0.56
3:V:196:THR:HG21	6:Y:370:LYS:HD2	1.86	0.56
6:Y:172:PHE:HB2	6:Y:176:PHE:HB2	1.87	0.56
9:R:87:C:O2'	9:R:91:G:N7	2.33	0.56
1:a:179:PRO:HB3	1:a:322:ASP:HB3	1.87	0.56
1:b:144:ARG:HE	1:b:167:PRO:HB3	1.69	0.56
2:A:38:LYS:HE3	2:A:100:VAL:H	1.70	0.56
6:Y:576:ARG:NH1	6:Y:593:ASN:OD1	2.39	0.56
1:b:360:TYR:O	1:b:384:ARG:NH2	2.38	0.56
1:e:360:TYR:O	1:e:384:ARG:NH2	2.38	0.56
1:f:179:PRO:HB3	1:f:322:ASP:HB3	1.87	0.56
1:c:272:ARG:O	1:c:276:THR:HG22	2.04	0.56
1:e:179:PRO:HB3	1:e:322:ASP:HB3	1.87	0.56
3:U:212:ASP:HB3	3:U:215:GLU:HB3	1.87	0.56
1:f:306:ASN:HA	1:f:312:SER:HB3	1.88	0.56
5:X:656:SER:HB3	5:X:659:GLN:HE21	1.70	0.56
1:d:144:ARG:HE	1:d:167:PRO:HB3	1.70	0.56
2:A:30:ALA:HB1	2:A:110:ALA:HA	1.87	0.56
1:f:262:ILE:HB	1:f:315:ILE:HG13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:306:ASN:HA	1:b:312:SER:HB3	1.88	0.56
1:e:144:ARG:HE	1:e:167:PRO:HB3	1.70	0.56
5:X:1329:GLU:HG2	6:Y:331:ILE:HD11	1.88	0.56
1:c:306:ASN:HA	1:c:312:SER:HB3	1.88	0.56
2:A:216:ILE:HB	2:A:221:ILE:HD11	1.86	0.56
5:X:1307:ASN:OD1	5:X:1312:ASN:ND2	2.38	0.56
5:X:1326:LEU:HB3	6:Y:337:ARG:HH21	1.70	0.56
1:c:102:ARG:NH1	1:c:103:PRO:O	2.40	0.55
5:X:598:VAL:HG23	5:X:627:GLY:HA3	1.88	0.55
5:X:808:ASN:H	6:Y:633:ALA:HB2	1.71	0.55
1:a:102:ARG:NH1	1:a:103:PRO:O	2.40	0.55
1:b:184:LYS:NZ	14:b:1102:HOH:O	2.39	0.55
1:d:179:PRO:HB3	1:d:322:ASP:HB3	1.87	0.55
4:W:22:VAL:HG13	4:W:64:LEU:HD23	1.88	0.55
5:X:1290:MET:HA	5:X:1294:LYS:HD3	1.88	0.55
6:Y:960:LEU:HD11	6:Y:980:THR:HB	1.87	0.55
1:f:28:ARG:HA	2:A:172:ASN:HB3	1.88	0.55
1:f:28:ARG:O	2:A:174:ARG:HB2	2.05	0.55
5:X:260:LYS:NZ	5:X:280:ASP:OD2	2.39	0.55
6:Y:1002:VAL:HB	6:Y:1019:ASN:HB3	1.87	0.55
1:f:102:ARG:NH1	1:f:103:PRO:O	2.40	0.55
1:a:262:ILE:HB	1:a:315:ILE:HG13	1.87	0.55
5:X:45:GLY:HA3	5:X:54:ARG:HD2	1.88	0.55
6:Y:952:VAL:HG11	6:Y:984:LEU:HD13	1.89	0.55
7:L:29:DG:H2'	7:L:29:DG:N3	2.20	0.55
1:d:102:ARG:NH1	1:d:103:PRO:O	2.40	0.55
1:e:102:ARG:NH1	1:e:103:PRO:O	2.40	0.55
6:Y:372:MET:HE1	6:Y:447:ILE:HD11	1.88	0.55
6:Y:1045:THR:HG21	6:Y:1076:PRO:HD3	1.89	0.55
1:b:102:ARG:NH1	1:b:103:PRO:O	2.39	0.55
1:d:262:ILE:HB	1:d:315:ILE:HG13	1.87	0.55
2:A:225:ALA:HB1	2:A:331:LEU:HD11	1.88	0.55
2:A:344:LEU:HD23	2:A:350:ALA:HA	1.88	0.55
2:A:60:ARG:N	2:A:93:VAL:O	2.31	0.55
3:V:190:ALA:HB2	3:V:200:LYS:HB2	1.89	0.55
5:X:798:GLN:HG2	5:X:827:ARG:HG2	1.88	0.55
9:R:94:U:H2'	9:R:95:G:H8	1.72	0.55
5:X:873:ILE:HG13	5:X:944:ARG:HH21	1.70	0.55
1:f:108:GLU:HB3	9:R:24:U:C4	2.42	0.55
6:Y:709:ARG:NH1	6:Y:710:ASP:OD2	2.40	0.55
6:Y:1044:GLN:NE2	6:Y:1070:GLY:O	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:1280:ALA:HB1	6:Y:918:ILE:HG22	1.90	0.54
6:Y:437:PHE:HZ	6:Y:453:VAL:HG21	1.72	0.54
2:A:145:VAL:HG12	2:A:150:ILE:HB	1.88	0.54
5:X:1006:GLU:O	5:X:1010:GLN:NE2	2.39	0.54
6:Y:393:THR:HG23	6:Y:396:ALA:H	1.72	0.54
9:R:94:U:H2'	9:R:95:G:C8	2.43	0.54
3:U:81:ILE:O	3:U:85:LEU:HG	2.07	0.54
5:X:632:ASP:HA	5:X:647:ARG:HB3	1.89	0.54
6:Y:269:TYR:O	6:Y:272:VAL:HG12	2.07	0.54
6:Y:1146:GLU:HB3	6:Y:1148:ARG:HG3	1.90	0.54
1:b:179:PRO:HB3	1:b:322:ASP:HB3	1.87	0.54
2:A:233:ARG:HB3	2:A:327:LEU:HD11	1.88	0.54
6:Y:250:ARG:NE	6:Y:269:TYR:OH	2.40	0.54
1:d:213:PRO:O	1:d:217:THR:HG23	2.08	0.54
1:e:306:ASN:HA	1:e:312:SER:HB3	1.88	0.54
1:a:184:LYS:NZ	14:a:1102:HOH:O	2.41	0.54
1:c:213:PRO:O	1:c:217:THR:HG23	2.08	0.54
1:f:213:PRO:O	1:f:217:THR:HG23	2.08	0.54
1:a:213:PRO:O	1:a:217:THR:HG23	2.08	0.54
5:X:811:ASN:O	5:X:1099:ASN:ND2	2.41	0.54
2:A:141:VAL:O	2:A:153:ASP:N	2.40	0.54
6:Y:958:ILE:HG13	6:Y:1005:LYS:HE2	1.90	0.54
3:U:201:LEU:HD21	3:U:203:ILE:HG13	1.88	0.54
5:X:785:ASP:OD2	5:X:791:LEU:N	2.40	0.54
1:d:306:ASN:HA	1:d:312:SER:HB3	1.88	0.53
1:e:374:GLN:OE1	1:e:374:GLN:HA	2.08	0.53
5:X:855:PRO:HG3	5:X:910:ALA:HB3	1.88	0.53
1:f:374:GLN:OE1	1:f:374:GLN:HA	2.08	0.53
1:a:306:ASN:HA	1:a:312:SER:HB3	1.88	0.53
1:c:374:GLN:OE1	1:c:374:GLN:HA	2.08	0.53
1:d:212:ARG:NH2	14:d:1101:HOH:O	2.41	0.53
1:e:213:PRO:O	1:e:217:THR:HG23	2.08	0.53
2:A:63:LEU:N	2:A:91:ASP:OD1	2.41	0.53
6:Y:491:LEU:HB2	6:Y:904:ALA:HA	1.89	0.53
5:X:513:GLN:HB3	9:R:89:U:C4	2.44	0.53
1:b:213:PRO:O	1:b:217:THR:HG23	2.08	0.53
1:b:374:GLN:HA	1:b:374:GLN:OE1	2.08	0.53
2:A:18:LEU:HD12	2:A:22:LYS:HB3	1.90	0.53
6:Y:201:LEU:HD21	6:Y:220:ARG:CB	2.38	0.53
1:a:374:GLN:OE1	1:a:374:GLN:HA	2.08	0.53
2:A:19:PRO:HG2	2:A:22:LYS:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:140:HIS:O	1:c:306:ASN:ND2	2.34	0.53
1:e:140:HIS:O	1:e:306:ASN:ND2	2.34	0.53
2:A:470:ILE:HB	2:A:473:LEU:HD13	1.90	0.53
5:X:1146:GLN:NE2	5:X:1150:ASP:OD2	2.40	0.53
5:X:1323:PHE:O	5:X:1326:LEU:HG	2.08	0.53
5:X:1331:ARG:HH21	6:Y:29:MET:HB2	1.73	0.53
5:X:1105:SER:HB3	6:Y:731:ARG:HG3	1.90	0.53
6:Y:848:VAL:HG22	6:Y:858:VAL:HB	1.91	0.53
7:L:5:DA:H2'	7:L:6:DC:C6	2.43	0.53
2:A:381:LEU:HD13	2:A:410:ALA:HA	1.90	0.53
3:V:158:ARG:NH1	3:V:173:VAL:O	2.41	0.53
7:L:-8:DC:H2"	7:L:-7:DG:C8	2.44	0.53
8:K:7:DC:H2"	8:K:8:DG:C8	2.44	0.53
1:b:341:MET:HB2	1:b:365:THR:HG23	1.91	0.53
6:Y:110:PRO:HB2	6:Y:238:ILE:HG22	1.89	0.53
6:Y:218:THR:HA	6:Y:221:ILE:HG22	1.91	0.53
5:X:594:VAL:HG11	5:X:650:VAL:HG23	1.91	0.52
3:U:95:LYS:NZ	3:U:120:ASP:OD2	2.34	0.52
3:V:85:LEU:HA	3:V:88:LEU:HG	1.91	0.52
5:X:123:TYR:OH	5:X:126:GLU:OE1	2.28	0.52
1:a:110:TYR:CB	7:L:27:DT:H3	2.22	0.52
6:Y:949:SER:HB3	6:Y:1020:TRP:CD1	2.44	0.52
1:d:341:MET:HB2	1:d:365:THR:HG23	1.91	0.52
10:e:1000:ADP:O2B	12:e:1002:BEF:F3	2.18	0.52
1:f:290:ASP:OD1	1:f:291:ALA:N	2.43	0.52
5:X:26:TYR:HB3	5:X:29:SER:HB3	1.90	0.52
5:X:1196:LYS:HD2	5:X:1206:THR:HG22	1.90	0.52
6:Y:174:ASP:OD1	6:Y:174:ASP:N	2.42	0.52
6:Y:658:GLU:O	6:Y:659:ALA:C	2.52	0.52
7:L:-2:DC:H2"	7:L:-1:DA:H8	1.73	0.52
1:a:96:THR:N	1:a:120:ASN:OD1	2.43	0.52
3:U:174:ASP:OD1	3:U:174:ASP:N	2.40	0.52
3:V:301:THR:HA	3:V:304:LYS:HG2	1.92	0.52
5:X:148:GLN:HB3	5:X:454:ARG:HG2	1.92	0.52
5:X:1243:MET:HE3	6:Y:372:MET:HG3	1.91	0.52
1:d:374:GLN:HA	1:d:374:GLN:OE1	2.08	0.52
2:A:27:LEU:HD22	2:A:114:ILE:HD11	1.90	0.52
2:A:322:GLY:O	2:A:326:ARG:N	2.40	0.52
2:A:463:GLY:HA2	2:A:482:ILE:HG12	1.91	0.52
5:X:1119:MET:HE2	5:X:1228:GLY:HA2	1.91	0.52
1:b:290:ASP:OD1	1:b:291:ALA:N	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:366:ARG:HH12	1:e:212:ARG:CZ	2.23	0.52
3:U:27:THR:HG22	3:U:202:VAL:HG22	1.91	0.52
1:a:236:ALA:HA	1:a:239:HIS:CD2	2.43	0.52
1:e:290:ASP:OD1	1:e:291:ALA:N	2.43	0.52
2:A:168:LEU:HB3	2:A:171:GLU:H	1.74	0.52
3:U:91:ARG:NH1	3:U:122:GLU:OE1	2.43	0.52
3:V:93:GLN:O	3:V:148:ARG:NH2	2.43	0.52
5:X:236:LYS:HE3	5:X:286:GLU:HG2	1.91	0.52
6:Y:130:MET:HG3	6:Y:157:GLN:HB2	1.92	0.52
6:Y:245:LEU:HD11	6:Y:249:LEU:HD22	1.91	0.52
6:Y:329:ASP:HA	6:Y:332:LYS:HB2	1.92	0.52
1:e:158:THR:HA	1:e:356:PRO:HG3	1.92	0.52
1:e:393:ILE:O	1:e:397:GLU:HG2	2.11	0.52
5:X:59:ILE:HD11	5:X:476:LYS:HD2	1.91	0.52
6:Y:741:ALA:O	6:Y:762:ASN:ND2	2.43	0.52
6:Y:804:ALA:O	6:Y:805:GLN:HG2	2.10	0.52
7:L:27:DT:O3'	7:L:28:DC:H3'	2.10	0.52
1:f:341:MET:HB2	1:f:365:THR:HG23	1.91	0.51
1:b:353:ARG:HD2	1:b:355:PHE:HE2	1.76	0.51
7:L:-6:DC:H2"	7:L:-5:DT:C7	2.39	0.51
1:a:290:ASP:OD1	1:a:291:ALA:N	2.43	0.51
1:b:393:ILE:O	1:b:397:GLU:HG2	2.11	0.51
5:X:232:ILE:HG12	5:X:331:LYS:HG3	1.91	0.51
8:K:1:DT:C2	8:K:2:DG:C8	2.98	0.51
1:d:393:ILE:O	1:d:397:GLU:HG2	2.10	0.51
3:V:246:LYS:NZ	3:V:247:PRO:O	2.35	0.51
5:X:801:ARG:HD3	5:X:1094:VAL:HA	1.93	0.51
6:Y:330:MET:HG2	6:Y:337:ARG:HB2	1.92	0.51
6:Y:421:VAL:HG22	6:Y:439:PRO:HG3	1.91	0.51
1:f:263:LEU:HD13	1:f:316:ILE:HB	1.93	0.51
1:a:158:THR:HA	1:a:356:PRO:HG3	1.92	0.51
1:a:393:ILE:O	1:a:397:GLU:HG2	2.10	0.51
1:b:158:THR:HA	1:b:356:PRO:HG3	1.92	0.51
1:b:160:ARG:HH22	1:b:406:THR:HG23	1.76	0.51
1:c:158:THR:HA	1:c:356:PRO:HG3	1.92	0.51
1:c:341:MET:HB2	1:c:365:THR:HG23	1.91	0.51
1:d:88:ARG:NH1	2:A:86:SER:O	2.44	0.51
1:e:96:THR:N	1:e:120:ASN:OD1	2.43	0.51
1:e:184:LYS:N	10:e:1000:ADP:O1B	2.44	0.51
2:A:173:PHE:HE1	2:A:179:VAL:HG11	1.74	0.51
5:X:721:GLY:N	5:X:740:GLU:OE1	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:726:TYR:OH	5:X:728:ASP:OD2	2.26	0.51
1:f:140:HIS:O	1:f:306:ASN:ND2	2.34	0.51
1:f:353:ARG:HD2	1:f:355:PHE:HE2	1.76	0.51
1:d:160:ARG:HH22	1:d:406:THR:HG23	1.76	0.51
1:e:341:MET:HB2	1:e:365:THR:HG23	1.91	0.51
2:A:18:LEU:HD22	2:A:118:VAL:HG12	1.93	0.51
2:A:49:ILE:HA	2:A:56:PHE:HA	1.92	0.51
3:U:5:VAL:HG23	3:U:6:THR:HG23	1.93	0.51
3:V:61:ILE:HG21	3:V:64:VAL:HB	1.93	0.51
5:X:88:ARG:HH22	5:X:1038:GLN:HG3	1.75	0.51
5:X:1321:GLU:O	5:X:1325:VAL:HG23	2.11	0.51
1:b:96:THR:N	1:b:120:ASN:OD1	2.43	0.51
1:d:184:LYS:NZ	14:d:1103:HOH:O	2.43	0.51
1:d:263:LEU:HD13	1:d:316:ILE:HB	1.93	0.51
5:X:79:VAL:O	5:X:1035:LYS:NZ	2.40	0.51
5:X:1244:HIS:NE2	5:X:1266:GLY:O	2.44	0.51
6:Y:116:PHE:HB2	6:Y:237:MET:SD	2.51	0.51
6:Y:1258:ARG:NH2	6:Y:1259:GLN:OE1	2.43	0.51
7:L:26:DT:H3'	7:L:27:DT:C5'	2.38	0.51
1:f:28:ARG:HD3	2:A:172:ASN:HB3	1.93	0.51
1:a:274:TYR:O	1:a:278:VAL:HG12	2.11	0.51
1:b:263:LEU:HD13	1:b:316:ILE:HB	1.93	0.51
1:c:160:ARG:HH22	1:c:406:THR:HG23	1.76	0.51
1:c:353:ARG:HD2	1:c:355:PHE:HE2	1.76	0.51
1:d:206:VAL:HG12	1:d:263:LEU:HB2	1.93	0.51
2:A:235:LYS:NZ	2:A:287:ALA:O	2.43	0.51
5:X:292:ILE:HD12	5:X:295:LYS:HD2	1.90	0.51
6:Y:660:GLU:O	6:Y:663:GLU:HG3	2.10	0.51
1:b:236:ALA:HA	1:b:239:HIS:CD2	2.43	0.51
1:c:96:THR:N	1:c:120:ASN:OD1	2.43	0.51
1:d:158:THR:HA	1:d:356:PRO:HG3	1.92	0.51
1:e:184:LYS:NZ	14:e:1102:HOH:O	2.43	0.51
2:A:227:ALA:HB2	2:A:331:LEU:HD22	1.93	0.51
5:X:403:MET:HE3	5:X:407:ARG:HE	1.75	0.51
5:X:806:PRO:HA	5:X:811:ASN:HD21	1.76	0.51
6:Y:473:THR:HG22	6:Y:476:ALA:H	1.75	0.51
6:Y:836:ARG:NE	6:Y:869:CYS:SG	2.84	0.51
6:Y:1281:GLU:OE1	6:Y:1284:ARG:N	2.43	0.51
1:d:236:ALA:HA	1:d:239:HIS:CD2	2.43	0.51
6:Y:1002:VAL:N	6:Y:1019:ASN:O	2.39	0.51
6:Y:1321:SER:O	6:Y:1324:SER:OG	2.26	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:-21:DG:H2"	8:K:-20:DG:H8	1.76	0.51
1:f:160:ARG:HH22	1:f:406:THR:HG23	1.76	0.51
1:f:274:TYR:O	1:f:278:VAL:HG12	2.11	0.51
1:a:263:LEU:HD13	1:a:316:ILE:HB	1.93	0.51
1:a:341:MET:HB2	1:a:365:THR:HG23	1.91	0.51
1:c:92:ARG:NH1	1:d:28:ARG:HH11	2.09	0.51
1:c:206:VAL:HG12	1:c:263:LEU:HB2	1.93	0.51
2:A:440:VAL:HG13	2:A:444:LEU:HD22	1.92	0.51
3:U:100:LEU:HD23	3:U:115:ILE:HD12	1.93	0.51
3:U:133:LEU:HD11	3:U:140:ILE:HG12	1.93	0.51
5:X:448:LEU:H	5:X:553:THR:HG21	1.76	0.51
5:X:781:ASP:OD1	5:X:782:VAL:N	2.44	0.51
5:X:965:GLN:HA	5:X:968:GLU:HG3	1.93	0.51
1:f:393:ILE:O	1:f:397:GLU:HG2	2.10	0.50
1:a:206:VAL:HG12	1:a:263:LEU:HB2	1.93	0.50
1:c:393:ILE:O	1:c:397:GLU:HG2	2.11	0.50
1:e:329:GLU:O	1:e:333:GLU:HG2	2.11	0.50
2:A:220:VAL:HG23	2:A:221:ILE:HG23	1.92	0.50
6:Y:80:HIS:HB3	6:Y:83:VAL:HB	1.93	0.50
6:Y:141:PHE:HB3	6:Y:293:ARG:HD2	1.91	0.50
1:a:120:ASN:HB2	1:a:256:HIS:CE1	2.46	0.50
1:d:96:THR:N	1:d:120:ASN:OD1	2.43	0.50
1:e:206:VAL:HG12	1:e:263:LEU:HB2	1.93	0.50
1:e:353:ARG:HD2	1:e:355:PHE:HE2	1.76	0.50
2:A:20:ARG:HD3	2:A:23:ILE:HD12	1.93	0.50
3:U:88:LEU:HB3	3:U:128:HIS:HD2	1.76	0.50
5:X:211:ARG:NH2	5:X:354:ASP:OD2	2.44	0.50
6:Y:1262:ARG:NH2	6:Y:1315:ALA:O	2.44	0.50
10:b:1000:ADP:O2B	12:b:1002:BEF:F3	2.20	0.50
2:A:160:ALA:HA	2:A:195:LEU:HB3	1.93	0.50
6:Y:1025:MET:HB2	6:Y:1124:ILE:HB	1.93	0.50
6:Y:1321:SER:HA	6:Y:1348:LYS:HZ1	1.76	0.50
8:K:-21:DG:H2"	8:K:-20:DG:C8	2.46	0.50
1:f:96:THR:N	1:f:120:ASN:OD1	2.43	0.50
1:b:171:GLY:H	1:b:314:THR:HG1	1.53	0.50
1:b:274:TYR:O	1:b:278:VAL:HG12	2.11	0.50
1:c:120:ASN:HB2	1:c:256:HIS:CE1	2.47	0.50
1:e:274:TYR:O	1:e:278:VAL:HG12	2.11	0.50
1:d:290:ASP:OD1	1:d:291:ALA:N	2.43	0.50
1:e:263:LEU:HD13	1:e:316:ILE:HB	1.93	0.50
3:U:192:VAL:HB	3:U:198:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:290:ASP:OD1	1:c:291:ALA:N	2.43	0.50
1:c:329:GLU:O	1:c:333:GLU:HG2	2.11	0.50
1:c:375:GLU:OE1	1:c:375:GLU:N	2.34	0.50
1:d:274:TYR:O	1:d:278:VAL:HG12	2.11	0.50
1:e:160:ARG:HH22	1:e:406:THR:HG23	1.76	0.50
3:V:92:VAL:HG13	3:V:121:VAL:HG12	1.92	0.50
5:X:58:PRO:HB3	5:X:69:GLN:HA	1.92	0.50
5:X:297:VAL:HB	5:X:317:LEU:HD21	1.92	0.50
1:a:375:GLU:OE1	1:a:375:GLU:N	2.34	0.50
1:c:274:TYR:O	1:c:278:VAL:HG12	2.11	0.50
3:V:101:THR:OG1	3:V:103:ASN:OD1	2.30	0.50
5:X:235:ASN:O	5:X:236:LYS:HG2	2.11	0.50
6:Y:640:GLY:N	6:Y:643:ASP:OD2	2.45	0.50
6:Y:1164:SER:OG	6:Y:1165:PHE:N	2.45	0.50
1:f:120:ASN:HB2	1:f:256:HIS:CE1	2.47	0.50
1:d:171:GLY:H	1:d:314:THR:HG1	1.55	0.50
6:Y:280:LYS:HG2	6:Y:283:LEU:HD12	1.94	0.50
6:Y:797:THR:HG22	6:Y:924:GLY:HA3	1.93	0.50
6:Y:975:ILE:HG22	6:Y:977:SER:H	1.76	0.50
6:Y:1026:PRO:HB2	6:Y:1028:ILE:HG23	1.94	0.50
1:f:158:THR:HA	1:f:356:PRO:HG3	1.92	0.50
1:f:236:ALA:HA	1:f:239:HIS:CD2	2.43	0.50
1:f:329:GLU:O	1:f:333:GLU:HG2	2.11	0.50
1:a:160:ARG:HH22	1:a:406:THR:HG23	1.76	0.50
1:a:329:GLU:O	1:a:333:GLU:HG2	2.11	0.50
1:a:353:ARG:HD2	1:a:355:PHE:HE2	1.76	0.50
1:c:388:HIS:NE2	1:d:351:GLU:OE1	2.44	0.50
1:d:353:ARG:HD2	1:d:355:PHE:HE2	1.76	0.50
3:U:45:ARG:NH1	5:X:1084:ASP:OD1	2.45	0.50
5:X:823:VAL:HG12	5:X:1060:ILE:HG23	1.94	0.50
6:Y:147:ILE:HD13	6:Y:188:LEU:HD23	1.94	0.50
1:b:329:GLU:O	1:b:333:GLU:HG2	2.11	0.49
1:e:120:ASN:HB2	1:e:256:HIS:CE1	2.46	0.49
2:A:35:THR:HA	2:A:38:LYS:HD2	1.93	0.49
6:Y:1061:VAL:HG22	6:Y:1105:ALA:H	1.77	0.49
1:f:30:ARG:HH11	2:A:176:GLY:CA	2.25	0.49
1:f:130:LYS:O	1:a:27:ALA:HB1	2.12	0.49
1:f:206:VAL:HG12	1:f:263:LEU:HB2	1.93	0.49
1:b:206:VAL:HG12	1:b:263:LEU:HB2	1.93	0.49
1:c:171:GLY:N	1:c:314:THR:OG1	2.28	0.49
1:d:120:ASN:HB2	1:d:256:HIS:CE1	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:428:ASN:HD21	2:A:450:ALA:N	2.10	0.49
5:X:105:TYR:HB2	5:X:114:VAL:HG13	1.94	0.49
5:X:925:SER:OG	5:X:926:GLY:N	2.45	0.49
1:b:184:LYS:N	10:b:1000:ADP:O3B	2.45	0.49
2:A:164:ARG:HG3	2:A:167:MET:HE2	1.95	0.49
3:V:299:SER:O	3:V:303:ILE:HG12	2.13	0.49
5:X:216:THR:O	5:X:220:ILE:HG13	2.13	0.49
5:X:1061:GLN:NE2	5:X:1240:ASP:OD1	2.46	0.49
5:X:1335:ILE:HG12	6:Y:22:ILE:HA	1.95	0.49
6:Y:516:ASP:HA	6:Y:545:HIS:HB2	1.95	0.49
6:Y:883:ARG:NH1	6:Y:898:CYS:SG	2.85	0.49
1:f:96:THR:HB	1:f:120:ASN:HA	1.95	0.49
1:a:96:THR:HB	1:a:120:ASN:HA	1.95	0.49
1:b:120:ASN:HB2	1:b:256:HIS:CE1	2.46	0.49
2:A:229:ASP:HB3	2:A:232:SER:HB2	1.94	0.49
4:W:16:ARG:HD2	6:Y:483:LEU:HG	1.94	0.49
5:X:841:ARG:HB3	5:X:1046:VAL:HG12	1.93	0.49
5:X:881:ASP:H	5:X:920:VAL:HG12	1.77	0.49
6:Y:1060:VAL:HG12	6:Y:1106:ILE:HG12	1.93	0.49
6:Y:1183:SER:OG	6:Y:1184:ASP:N	2.46	0.49
1:f:58:LEU:HD21	9:R:25:C:N4	2.27	0.49
2:A:455:THR:HG23	2:A:457:GLU:H	1.77	0.49
5:X:65:ASN:ND2	5:X:106:GLU:O	2.45	0.49
5:X:975:ILE:HA	5:X:978:VAL:HG12	1.94	0.49
6:Y:70:CYS:SG	6:Y:71:LEU:N	2.84	0.49
6:Y:1321:SER:HA	6:Y:1348:LYS:NZ	2.27	0.49
7:L:-4:DC:C2	7:L:-3:DA:N7	2.80	0.49
1:a:274:TYR:HA	1:a:277:VAL:HG12	1.95	0.49
1:c:263:LEU:HD13	1:c:316:ILE:HB	1.93	0.49
5:X:656:SER:OG	5:X:657:THR:N	2.44	0.49
5:X:903:ARG:NH1	5:X:911:SER:OG	2.45	0.49
6:Y:117:LEU:HD23	6:Y:124:ILE:HG21	1.92	0.49
6:Y:279:LEU:HD21	6:Y:298:MET:HG3	1.94	0.49
6:Y:287:ALA:HB1	6:Y:291:ILE:HD13	1.93	0.49
6:Y:527:LEU:HB2	6:Y:550:VAL:HG12	1.93	0.49
1:d:173:ARG:HH12	1:e:213:PRO:HD2	1.77	0.49
3:U:101:THR:OG1	3:U:116:THR:OG1	2.29	0.49
5:X:201:ARG:NE	5:X:370:MET:SD	2.86	0.49
6:Y:272:VAL:HG23	6:Y:302:ALA:HB1	1.93	0.49
8:K:5:DA:H4'	8:K:6:DG:OP1	2.12	0.49
1:c:96:THR:HB	1:c:120:ASN:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:274:TYR:HA	1:d:277:VAL:HG12	1.95	0.49
1:d:329:GLU:O	1:d:333:GLU:HG2	2.12	0.49
3:U:53:GLY:HA3	3:U:177:TYR:HB2	1.94	0.49
1:f:108:GLU:HB3	9:R:24:U:N3	2.28	0.49
1:c:366:ARG:HH12	1:d:212:ARG:CZ	2.26	0.49
1:e:274:TYR:HA	1:e:277:VAL:HG12	1.95	0.49
5:X:962:GLU:O	5:X:965:GLN:HG2	2.13	0.49
6:Y:613:GLY:O	6:Y:617:THR:OG1	2.30	0.49
6:Y:1253:ILE:HA	6:Y:1256:ILE:HG22	1.95	0.49
6:Y:1326:GLN:HE22	7:L:0:DA:H4'	1.78	0.49
1:d:212:ARG:NH2	14:d:1102:HOH:O	2.46	0.49
5:X:882:ILE:HA	5:X:919:ARG:HG3	1.95	0.49
5:X:1160:ASP:OD1	5:X:1160:ASP:N	2.44	0.49
5:X:1331:ARG:HD2	5:X:1334:GLY:HA2	1.95	0.49
6:Y:1172:LYS:HD2	6:Y:1191:PRO:HA	1.95	0.49
7:L:25:DA:H1'	7:L:26:DT:O4'	2.13	0.49
1:e:96:THR:HB	1:e:120:ASN:HA	1.95	0.48
5:X:1331:ARG:NH2	6:Y:29:MET:HB2	2.27	0.48
6:Y:111:THR:HG22	6:Y:300:GLN:HE22	1.78	0.48
6:Y:156:ARG:NH2	6:Y:191:SER:OG	2.44	0.48
6:Y:265:LEU:HD13	6:Y:268:LEU:HD12	1.94	0.48
7:L:24:DT:H2"	7:L:25:DA:N9	2.27	0.48
2:A:111:LYS:HG3	5:X:905:ILE:HG23	1.96	0.48
5:X:1062:PRO:HA	5:X:1076:ILE:HG23	1.95	0.48
5:X:1331:ARG:HG2	6:Y:33:TRP:CZ3	2.48	0.48
6:Y:280:LYS:HA	6:Y:283:LEU:HD12	1.95	0.48
6:Y:503:SER:OG	6:Y:504:GLN:N	2.45	0.48
1:a:189:GLN:NE2	1:a:218:GLU:OE2	2.46	0.48
1:b:96:THR:HB	1:b:120:ASN:HA	1.95	0.48
2:A:126:VAL:HG21	2:A:158:ALA:HA	1.94	0.48
5:X:361:SER:HA	5:X:364:VAL:HG22	1.95	0.48
1:f:128:ARG:HA	1:a:28:ARG:HH21	1.77	0.48
10:a:1000:ADP:O1B	12:a:1002:BEF:F2	2.21	0.48
1:b:189:GLN:NE2	1:b:218:GLU:OE2	2.46	0.48
8:K:-22:DC:H2"	8:K:-21:DG:O4'	2.13	0.48
3:V:180:VAL:O	6:Y:535:ARG:NH1	2.45	0.48
5:X:551:HIS:HB3	5:X:553:THR:HG22	1.96	0.48
6:Y:1347:LEU:HD22	6:Y:1357:ILE:HG23	1.94	0.48
4:W:9:ALA:HB1	4:W:19:LEU:HD11	1.94	0.48
5:X:363:LEU:HD22	5:X:382:GLU:HA	1.96	0.48
7:L:-2:DC:H2"	7:L:-1:DA:H5'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:276:GLN:NE2	5:X:280:ASP:OD2	2.46	0.48
1:b:171:GLY:N	1:b:314:THR:OG1	2.28	0.48
1:c:236:ALA:HA	1:c:239:HIS:CD2	2.43	0.48
10:c:1000:ADP:O2B	12:c:1002:BEF:F3	2.21	0.48
3:V:33:ARG:NH1	5:X:820:GLU:OE1	2.45	0.48
3:V:278:ILE:O	3:V:282:VAL:HG23	2.13	0.48
5:X:1107:MET:HE2	6:Y:736:GLN:HG2	1.95	0.48
6:Y:510:LEU:HD12	6:Y:601:ILE:HD12	1.96	0.48
1:c:189:GLN:NE2	1:c:218:GLU:OE2	2.46	0.48
3:V:71:LYS:NZ	3:V:72:GLU:O	2.41	0.48
6:Y:298:MET:HE2	8:K:-20:DG:H5”	1.96	0.48
6:Y:885:VAL:HG12	6:Y:1258:ARG:HD2	1.95	0.48
1:f:30:ARG:HH11	2:A:176:GLY:HA2	1.79	0.48
1:e:145:LEU:HB2	1:e:168:ILE:HG23	1.96	0.48
2:A:96:GLN:NE2	2:A:97:ILE:O	2.47	0.48
5:X:886:LYS:HB3	5:X:917:SER:HA	1.96	0.48
6:Y:1326:GLN:HG3	6:Y:1327:GLU:HG2	1.96	0.48
1:f:189:GLN:NE2	1:f:218:GLU:OE2	2.46	0.47
1:c:274:TYR:HA	1:c:277:VAL:HG12	1.95	0.47
1:d:145:LEU:HB2	1:d:168:ILE:HG23	1.96	0.47
1:e:189:GLN:NE2	1:e:218:GLU:OE2	2.46	0.47
1:e:236:ALA:HA	1:e:239:HIS:CD2	2.43	0.47
1:e:265:ASP:HA	1:e:266:SER:HA	1.54	0.47
2:A:168:LEU:HD21	2:A:231:GLY:HA3	1.96	0.47
3:U:92:VAL:HG12	3:U:121:VAL:HG22	1.96	0.47
3:V:182:ARG:HB3	6:Y:531:LYS:HB3	1.96	0.47
6:Y:112:ALA:HB1	6:Y:237:MET:HE3	1.95	0.47
6:Y:123:ARG:HG2	6:Y:1337:VAL:HG21	1.95	0.47
6:Y:377:PHE:HD1	6:Y:380:PHE:HD2	1.60	0.47
1:f:274:TYR:HA	1:f:277:VAL:HG12	1.95	0.47
1:b:56:GLU:HA	1:b:93:THR:HG23	1.97	0.47
1:c:184:LYS:NZ	14:c:1102:HOH:O	2.46	0.47
3:U:152:TYR:HD1	3:U:176:CYS:HA	1.79	0.47
5:X:517:GLN:HB3	5:X:760:ASN:H	1.77	0.47
5:X:1320:PRO:HG2	6:Y:1354:GLY:HA3	1.95	0.47
1:d:189:GLN:NE2	1:d:218:GLU:OE2	2.46	0.47
5:X:13:LYS:HB2	5:X:1180:MET:HE2	1.95	0.47
5:X:483:ASP:OD1	5:X:483:ASP:N	2.46	0.47
5:X:984:VAL:HG13	5:X:985:GLU:H	1.80	0.47
6:Y:972:LYS:NZ	6:Y:1002:VAL:HA	2.28	0.47
1:d:56:GLU:HA	1:d:93:THR:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:453:ILE:HD11	5:X:530:ILE:HD12	1.96	0.47
5:X:594:VAL:HG22	5:X:599:VAL:HG22	1.94	0.47
5:X:946:LEU:O	5:X:949:GLU:HG3	2.14	0.47
6:Y:161:THR:HG22	6:Y:162:GLU:H	1.79	0.47
6:Y:405:GLU:HG3	6:Y:407:VAL:HG12	1.97	0.47
1:f:145:LEU:HB2	1:f:168:ILE:HG23	1.96	0.47
6:Y:116:PHE:CE2	6:Y:1337:VAL:HG23	2.50	0.47
6:Y:1324:SER:HB3	6:Y:1348:LYS:HZ1	1.79	0.47
1:f:9:THR:OG1	1:f:13:GLU:OE1	2.31	0.47
1:a:145:LEU:HB2	1:a:168:ILE:HG23	1.96	0.47
1:b:274:TYR:HA	1:b:277:VAL:HG12	1.95	0.47
1:c:56:GLU:HA	1:c:93:THR:HG23	1.97	0.47
1:e:171:GLY:N	1:e:314:THR:OG1	2.28	0.47
6:Y:1079:LYS:HD2	6:Y:1098:GLN:HB3	1.96	0.47
1:f:56:GLU:HA	1:f:93:THR:HG23	1.97	0.47
1:b:145:LEU:HB2	1:b:168:ILE:HG23	1.96	0.47
1:d:96:THR:HB	1:d:120:ASN:HA	1.95	0.47
1:d:184:LYS:N	10:d:1000:ADP:O1B	2.47	0.47
2:A:19:PRO:O	2:A:23:ILE:HG13	2.14	0.47
2:A:380:THR:HG22	2:A:382:GLU:H	1.79	0.47
5:X:943:LYS:NZ	5:X:947:GLU:OE1	2.43	0.47
5:X:1070:HIS:CG	5:X:1111:GLN:HB3	2.49	0.47
6:Y:482:ALA:O	6:Y:488:ASN:ND2	2.47	0.47
6:Y:517:CYS:H	6:Y:545:HIS:HD2	1.62	0.47
1:a:109:ARG:HD2	7:L:29:DG:C4	2.49	0.47
1:d:265:ASP:HA	1:d:266:SER:HA	1.54	0.47
2:A:221:ILE:HG22	2:A:245:ILE:HD12	1.96	0.47
5:X:735:LYS:HA	5:X:748:ILE:HG22	1.97	0.47
6:Y:419:HIS:CE1	6:Y:471:PRO:HD2	2.49	0.47
6:Y:494:ALA:HB2	6:Y:922:SER:HB2	1.97	0.47
6:Y:620:PHE:CZ	6:Y:624:ILE:HD11	2.50	0.47
1:a:171:GLY:H	1:a:314:THR:HG1	1.55	0.47
1:b:69:ASP:OD1	1:b:69:ASP:N	2.48	0.47
6:Y:803:VAL:HG13	6:Y:1256:ILE:HD11	1.97	0.47
3:U:163:GLU:HA	3:U:166:ARG:HG2	1.97	0.47
3:V:47:LEU:HB3	3:V:180:VAL:HG11	1.97	0.47
5:X:338:THR:HG23	5:X:345:PRO:HG3	1.96	0.47
5:X:568:ASN:HB2	5:X:571:LEU:HB2	1.97	0.47
5:X:1246:ARG:HH11	5:X:1266:GLY:HA2	1.80	0.47
6:Y:334:LYS:HD3	6:Y:335:GLN:N	2.30	0.47
8:K:9:DG:H2"	8:K:10:DA:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:366:ARG:HD2	1:a:181:LYS:NZ	2.30	0.46
1:b:212:ARG:NH2	14:b:1103:HOH:O	2.47	0.46
1:c:145:LEU:HB2	1:c:168:ILE:HG23	1.96	0.46
1:c:295:HIS:CD2	1:d:235:PRO:HD3	2.49	0.46
2:A:203:GLU:O	2:A:206:ILE:HB	2.15	0.46
2:A:408:GLU:HA	2:A:411:LYS:HE3	1.97	0.46
4:W:50:ALA:O	4:W:54:ILE:HG13	2.14	0.46
5:X:874:GLY:H	5:X:928:VAL:HG13	1.80	0.46
6:Y:327:LEU:HA	6:Y:330:MET:HE2	1.96	0.46
9:R:89:U:H2'	9:R:89:U:O2	2.15	0.46
3:U:218:ARG:HH12	3:V:231:PHE:HA	1.79	0.46
5:X:226:GLU:OE1	5:X:245:ARG:NE	2.47	0.46
5:X:521:LEU:HA	5:X:524:ILE:HG22	1.97	0.46
5:X:1004:ASP:HA	5:X:1008:GLN:HG2	1.98	0.46
1:a:140:HIS:O	1:a:306:ASN:ND2	2.34	0.46
1:c:106:GLU:OE1	1:c:106:GLU:N	2.49	0.46
1:d:106:GLU:N	1:d:106:GLU:OE1	2.49	0.46
3:U:88:LEU:HB3	3:U:128:HIS:CD2	2.50	0.46
1:a:106:GLU:OE1	1:a:106:GLU:N	2.49	0.46
1:e:56:GLU:HA	1:e:93:THR:HG23	1.97	0.46
1:e:106:GLU:N	1:e:106:GLU:OE1	2.49	0.46
1:e:394:ASP:OD1	1:e:394:ASP:N	2.48	0.46
2:A:234:ALA:HB3	2:A:271:ILE:HG12	1.98	0.46
3:V:62:ASP:OD1	3:V:62:ASP:N	2.48	0.46
5:X:549:ASP:OD1	5:X:550:VAL:N	2.48	0.46
6:Y:287:ALA:CB	6:Y:291:ILE:HD13	2.46	0.46
6:Y:684:ASP:OD1	6:Y:684:ASP:N	2.48	0.46
1:f:394:ASP:OD1	1:f:394:ASP:N	2.48	0.46
1:a:110:TYR:HB2	7:L:27:DT:H3	1.81	0.46
1:b:231:THR:HG23	1:b:233:ASP:HB2	1.98	0.46
1:c:69:ASP:OD1	1:c:69:ASP:N	2.48	0.46
3:U:182:ARG:NH1	5:X:1090:ASN:O	2.48	0.46
3:V:323:PRO:HA	3:V:324:ALA:HA	1.52	0.46
5:X:216:THR:N	5:X:219:GLN:OE1	2.38	0.46
5:X:1331:ARG:HA	5:X:1335:ILE:H	1.81	0.46
6:Y:886:VAL:HA	6:Y:1258:ARG:HG3	1.98	0.46
6:Y:999:TYR:HD1	6:Y:1026:PRO:HG2	1.79	0.46
1:b:183:GLY:N	10:b:1000:ADP:O1B	2.47	0.46
3:V:58:GLU:HB3	3:V:145:LYS:HB3	1.96	0.46
1:f:106:GLU:OE1	1:f:106:GLU:N	2.49	0.46
1:b:140:HIS:O	1:b:306:ASN:ND2	2.34	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:366:ARG:HH12	1:c:212:ARG:CZ	2.29	0.46
1:d:69:ASP:OD1	1:d:69:ASP:N	2.48	0.46
2:A:59:PHE:HA	2:A:94:GLU:HA	1.97	0.46
6:Y:753:SER:OG	6:Y:754:ILE:N	2.45	0.46
6:Y:951:GLN:HG3	6:Y:1016:THR:HA	1.97	0.46
6:Y:1194:ARG:NH1	6:Y:1211:SER:OG	2.49	0.46
1:f:231:THR:HG23	1:f:233:ASP:HB2	1.98	0.46
1:a:394:ASP:OD1	1:a:394:ASP:N	2.48	0.46
1:d:105:LYS:HD2	3:V:297:LYS:NZ	2.31	0.46
1:d:231:THR:HG23	1:d:233:ASP:HB2	1.98	0.46
1:d:244:GLU:OE2	1:d:274:TYR:OH	2.34	0.46
1:e:375:GLU:OE1	1:e:375:GLU:N	2.33	0.46
2:A:225:ALA:HB3	2:A:237:ALA:HB3	1.98	0.46
2:A:361:LYS:HE2	2:A:409:ARG:HH12	1.81	0.46
3:U:78:ILE:HD13	3:U:81:ILE:HD12	1.98	0.46
5:X:143:ARG:HA	5:X:514:PHE:HA	1.98	0.46
5:X:370:MET:HG2	5:X:384:LEU:HD21	1.97	0.46
5:X:566:GLY:H	5:X:569:ILE:HD11	1.80	0.46
6:Y:410:ASP:OD1	6:Y:410:ASP:N	2.46	0.46
8:K:8:DG:H2"	8:K:9:DG:C8	2.50	0.46
1:f:102:ARG:HB3	1:f:114:LEU:HD11	1.98	0.46
1:f:181:LYS:HA	1:f:181:LYS:HD3	1.71	0.46
1:b:106:GLU:N	1:b:106:GLU:OE1	2.49	0.46
2:A:205:LEU:HA	2:A:208:LEU:HD12	1.97	0.46
2:A:233:ARG:NH1	2:A:272:ASP:OD2	2.49	0.46
5:X:208:ILE:HD11	5:X:362:ALA:HA	1.98	0.46
5:X:1328:LYS:NZ	6:Y:100:GLU:O	2.37	0.46
6:Y:189:LEU:HB3	6:Y:234:PRO:HB2	1.98	0.46
6:Y:339:ARG:NH1	6:Y:1325:PHE:O	2.31	0.46
6:Y:436:ALA:HB3	6:Y:485:MET:HA	1.97	0.46
6:Y:868:TRP:O	6:Y:872:LEU:HD23	2.16	0.46
9:R:96:U:H2'	9:R:97:G:H8	1.79	0.46
1:a:56:GLU:HA	1:a:93:THR:HG23	1.97	0.46
1:c:231:THR:HG23	1:c:233:ASP:HB2	1.98	0.46
2:A:45:VAL:HG22	2:A:60:ARG:HA	1.97	0.46
2:A:295:SER:HB3	2:A:308:ALA:HB3	1.98	0.46
3:U:66:HIS:CE1	3:U:69:SER:HB3	2.51	0.46
3:U:120:ASP:OD1	3:U:120:ASP:N	2.44	0.46
3:U:178:SER:O	3:U:208:ASN:ND2	2.49	0.46
3:V:15:ASP:H	3:V:27:THR:HG22	1.81	0.46
5:X:758:ARG:NE	5:X:762:ASN:OD1	2.44	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:128:LEU:HD11	6:Y:188:LEU:HD22	1.98	0.46
6:Y:450:HIS:HB3	6:Y:453:VAL:HG12	1.98	0.46
1:c:183:GLY:N	10:c:1000:ADP:O1B	2.45	0.45
3:U:4:SER:OG	3:U:5:VAL:N	2.46	0.45
3:V:37:HIS:CE1	5:X:1216:ARG:HD2	2.51	0.45
5:X:494:ASN:O	5:X:497:PRO:HD2	2.16	0.45
5:X:701:GLY:N	5:X:1182:ILE:O	2.42	0.45
5:X:808:ASN:HD21	5:X:1216:ARG:HH22	1.64	0.45
5:X:949:GLU:HA	5:X:952:GLN:HG2	1.97	0.45
5:X:985:GLU:HG2	5:X:986:ALA:N	2.30	0.45
5:X:1281:TYR:CE1	6:Y:431:ARG:HD2	2.50	0.45
2:A:64:VAL:HG23	2:A:91:ASP:CG	2.42	0.45
2:A:150:ILE:HG12	2:A:162:ILE:HB	1.98	0.45
2:A:307:ILE:HD13	2:A:336:LEU:HD13	1.98	0.45
3:U:191:ARG:HD3	3:U:192:VAL:H	1.81	0.45
5:X:881:ASP:OD1	5:X:882:ILE:N	2.45	0.45
5:X:1333:LEU:HD23	6:Y:113:HIS:HE2	1.80	0.45
6:Y:43:THR:HG23	6:Y:44:ILE:H	1.80	0.45
6:Y:265:LEU:HD11	6:Y:327:LEU:H	1.80	0.45
1:f:133:PHE:N	1:f:255:GLU:OE2	2.50	0.45
1:a:231:THR:HG23	1:a:233:ASP:HB2	1.98	0.45
2:A:112:GLN:O	2:A:116:GLN:HG2	2.17	0.45
4:W:12:LYS:HE2	4:W:57:GLY:HA2	1.98	0.45
5:X:444:ASP:OD1	5:X:444:ASP:N	2.49	0.45
5:X:596:ASP:OD1	5:X:596:ASP:N	2.47	0.45
6:Y:141:PHE:HE1	6:Y:296:LYS:HE2	1.82	0.45
1:a:102:ARG:HB3	1:a:114:LEU:HD11	1.98	0.45
1:a:171:GLY:N	1:a:314:THR:OG1	2.28	0.45
1:c:133:PHE:N	1:c:255:GLU:OE2	2.50	0.45
3:U:56:VAL:HA	3:U:146:VAL:HG22	1.97	0.45
5:X:674:ASP:OD2	5:X:1070:HIS:ND1	2.50	0.45
5:X:993:PRO:HB2	5:X:997:TRP:HD1	1.82	0.45
5:X:1069:ARG:NH2	5:X:1114:GLU:OE2	2.47	0.45
6:Y:1256:ILE:O	6:Y:1260:MET:HG2	2.16	0.45
1:f:64:PHE:HE1	1:f:78:ASP:OD2	1.95	0.45
1:c:344:HIS:HB2	1:c:359:ASP:HB3	1.99	0.45
1:d:140:HIS:O	1:d:306:ASN:ND2	2.34	0.45
1:e:133:PHE:N	1:e:255:GLU:OE2	2.50	0.45
1:e:181:LYS:HD3	1:e:181:LYS:HA	1.71	0.45
2:A:22:LYS:O	2:A:25:GLU:HG2	2.17	0.45
3:V:170:ARG:HD3	3:V:170:ARG:HA	1.71	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:182:ARG:HG2	3:V:206:GLU:HB3	1.98	0.45
4:W:60:ASN:H	4:W:63:ILE:HB	1.82	0.45
5:X:886:LYS:N	5:X:917:SER:OG	2.49	0.45
6:Y:146:VAL:HG12	6:Y:178:ALA:HB2	1.99	0.45
6:Y:998:PRO:HD3	6:Y:1020:TRP:CE2	2.52	0.45
6:Y:1050:THR:HG23	6:Y:1057:SER:HA	1.98	0.45
6:Y:1368:ASP:OD1	6:Y:1371:ARG:NH2	2.49	0.45
1:f:244:GLU:OE2	1:f:274:TYR:OH	2.34	0.45
1:f:326:LYS:HA	1:f:326:LYS:HD2	1.83	0.45
1:a:265:ASP:HA	1:a:266:SER:HA	1.54	0.45
1:b:102:ARG:HB3	1:b:114:LEU:HD11	1.98	0.45
1:b:133:PHE:N	1:b:255:GLU:OE2	2.50	0.45
3:V:60:GLU:OE1	3:V:169:GLY:HA2	2.16	0.45
5:X:472:GLU:HA	5:X:475:VAL:HG12	1.98	0.45
5:X:540:ARG:NH2	7:L:3:DC:O3'	2.50	0.45
6:Y:43:THR:O	6:Y:57:PHE:HB2	2.17	0.45
7:L:19:DG:C2	7:L:20:DC:C2	3.05	0.45
1:f:344:HIS:HB2	1:f:359:ASP:HB3	1.99	0.45
1:a:344:HIS:HB2	1:a:359:ASP:HB3	1.99	0.45
1:e:102:ARG:HB3	1:e:114:LEU:HD11	1.98	0.45
2:A:119:ARG:O	2:A:122:GLU:HG3	2.15	0.45
3:U:150:ARG:HB2	3:V:6:THR:H	1.81	0.45
4:W:7:GLN:O	4:W:11:GLU:HG3	2.17	0.45
5:X:1269:ARG:NH2	6:Y:340:GLN:HE22	2.15	0.45
7:L:-4:DC:H2"	7:L:-3:DA:H8	1.82	0.45
1:c:171:GLY:H	1:c:314:THR:HG1	1.54	0.45
1:c:394:ASP:OD1	1:c:394:ASP:N	2.48	0.45
1:d:394:ASP:OD1	1:d:394:ASP:N	2.48	0.45
3:U:196:THR:O	3:U:198:LEU:HD12	2.16	0.45
5:X:39:ILE:HG13	5:X:39:ILE:O	2.17	0.45
6:Y:740:LEU:HA	6:Y:763:PHE:HD2	1.82	0.45
8:K:-20:DG:C4	8:K:-19:DC:C5	3.05	0.45
1:a:133:PHE:N	1:a:255:GLU:OE2	2.50	0.45
1:b:344:HIS:HB2	1:b:359:ASP:HB3	1.99	0.45
2:A:7:ALA:O	2:A:11:ALA:HB3	2.17	0.45
3:V:105:SER:OG	3:V:106:GLY:N	2.50	0.45
5:X:257:ALA:HB2	5:X:285:ILE:HA	1.98	0.45
6:Y:274:ASN:ND2	8:K:-22:DC:H4'	2.31	0.45
6:Y:979:ASN:ND2	6:Y:1208:ASP:OD2	2.50	0.45
9:R:20:A:H2'	9:R:21:C:C6	2.52	0.45
1:e:231:THR:HG23	1:e:233:ASP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:228:VAL:HB	5:X:335:THR:HG23	1.98	0.45
5:X:839:VAL:HG12	5:X:1049:ILE:HG12	1.98	0.45
5:X:978:VAL:O	5:X:1007:LYS:NZ	2.49	0.45
5:X:1006:GLU:OE1	5:X:1010:GLN:NE2	2.50	0.45
6:Y:180:MET:N	6:Y:184:ALA:HB2	2.32	0.45
1:a:110:TYR:HB2	7:L:27:DT:N3	2.31	0.44
1:d:375:GLU:OE1	1:d:375:GLU:N	2.34	0.44
5:X:804:PHE:O	6:Y:638:SER:HB2	2.16	0.44
1:b:265:ASP:HA	1:b:266:SER:HA	1.54	0.44
1:e:344:HIS:HB2	1:e:359:ASP:HB3	1.99	0.44
2:A:20:ARG:HG3	2:A:24:PHE:CZ	2.52	0.44
3:U:184:ALA:HB2	5:X:1091:GLY:HA3	1.98	0.44
5:X:818:VAL:HG23	5:X:1096:ILE:HG12	1.99	0.44
6:Y:130:MET:HE2	6:Y:157:GLN:HA	1.99	0.44
6:Y:848:VAL:HG21	6:Y:872:LEU:HD11	1.99	0.44
6:Y:965:SER:OG	6:Y:974:VAL:O	2.32	0.44
7:L:19:DG:H2"	7:L:20:DC:H6	1.82	0.44
1:a:236:ALA:O	1:a:240:VAL:HG12	2.18	0.44
3:V:111:THR:HA	3:V:129:VAL:HA	1.99	0.44
5:X:517:GLN:HA	5:X:523:GLU:OE2	2.16	0.44
5:X:931:VAL:HG12	5:X:1052:VAL:HG22	1.98	0.44
5:X:1331:ARG:HD3	5:X:1335:ILE:C	2.43	0.44
6:Y:934:THR:OG1	6:Y:935:PHE:N	2.51	0.44
1:f:64:PHE:HE1	1:f:110:TYR:CE2	2.36	0.44
1:a:9:THR:OG1	1:a:13:GLU:OE1	2.31	0.44
1:b:9:THR:OG1	1:b:13:GLU:OE1	2.31	0.44
1:b:236:ALA:O	1:b:240:VAL:HG12	2.18	0.44
1:b:375:GLU:OE1	1:b:375:GLU:N	2.34	0.44
2:A:47:VAL:HA	2:A:58:THR:HG22	1.99	0.44
3:U:192:VAL:HG21	3:U:195:ARG:HB2	1.99	0.44
3:V:46:ILE:HD11	3:V:224:LEU:HD13	1.99	0.44
5:X:949:GLU:OE1	5:X:1033:ARG:NH1	2.50	0.44
6:Y:336:GLY:C	6:Y:341:ASN:HB3	2.42	0.44
6:Y:1238:GLN:NE2	6:Y:1248:ILE:O	2.40	0.44
1:d:102:ARG:HB3	1:d:114:LEU:HD11	1.98	0.44
1:d:133:PHE:N	1:d:255:GLU:OE2	2.50	0.44
1:d:181:LYS:HA	1:d:181:LYS:HD3	1.71	0.44
5:X:93:SER:OG	5:X:94:ALA:N	2.50	0.44
5:X:931:VAL:HG21	5:X:944:ARG:HE	1.81	0.44
5:X:1101:LEU:HD13	6:Y:504:GLN:HB2	1.99	0.44
6:Y:114:ILE:HA	6:Y:117:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Y:530:PRO:HB3	6:Y:577:ALA:O	2.18	0.44
6:Y:823:THR:HA	6:Y:835:LEU:HD12	1.99	0.44
6:Y:844:THR:HA	6:Y:882:VAL:HG23	2.00	0.44
6:Y:1322:ALA:C	6:Y:1331:VAL:HG21	2.42	0.44
1:b:275:ASN:HA	1:b:293:ALA:HB1	2.00	0.44
3:U:113:ALA:HB2	3:U:126:PRO:HB2	1.98	0.44
3:V:99:ILE:HG22	3:V:145:LYS:HG3	1.99	0.44
5:X:860:ALA:O	5:X:863:SER:OG	2.33	0.44
5:X:1108:ASN:O	5:X:1111:GLN:HG2	2.18	0.44
6:Y:886:VAL:HG13	6:Y:1254:GLU:OE2	2.17	0.44
1:c:275:ASN:HA	1:c:293:ALA:HB1	2.00	0.44
1:e:69:ASP:OD1	1:e:69:ASP:N	2.48	0.44
1:e:122:ASP:OD1	1:e:123:LYS:N	2.51	0.44
2:A:204:MET:HE3	2:A:208:LEU:HD21	2.00	0.44
2:A:399:ASP:O	2:A:403:VAL:HG23	2.18	0.44
5:X:35:PHE:CD2	5:X:130:MET:HG2	2.53	0.44
5:X:733:VAL:HG13	5:X:748:ILE:HD12	1.99	0.44
6:Y:537:TYR:OH	6:Y:634:ARG:NH2	2.51	0.44
6:Y:1161:GLY:HA3	6:Y:1179:PRO:HA	1.99	0.44
1:e:244:GLU:OE2	1:e:274:TYR:OH	2.34	0.44
3:V:61:ILE:HD13	3:V:64:VAL:HB	2.00	0.44
8:K:-19:DC:H1'	8:K:-18:DC:H5'	1.99	0.44
1:a:295:HIS:CD2	1:b:235:PRO:HD3	2.53	0.44
1:e:9:THR:OG1	1:e:13:GLU:OE1	2.31	0.44
5:X:103:VAL:HG12	5:X:117:ILE:HA	1.98	0.44
5:X:150:HIS:CE1	5:X:454:ARG:HE	2.35	0.44
5:X:697:LYS:HD2	5:X:1181:PRO:HG3	2.00	0.44
6:Y:298:MET:HE1	8:K:-20:DG:OP1	2.18	0.44
1:a:275:ASN:HA	1:a:293:ALA:HB1	2.00	0.43
1:c:102:ARG:HB3	1:c:114:LEU:HD11	1.98	0.43
1:c:236:ALA:O	1:c:240:VAL:HG12	2.18	0.43
1:d:344:HIS:HB2	1:d:359:ASP:HB3	1.99	0.43
5:X:221:LEU:HD22	5:X:336:LEU:HD21	2.00	0.43
6:Y:119:SER:OG	6:Y:121:PRO:HD2	2.18	0.43
6:Y:332:LYS:O	6:Y:339:ARG:HD2	2.18	0.43
6:Y:513:MET:HE2	6:Y:631:TYR:CG	2.52	0.43
6:Y:934:THR:HG23	6:Y:936:HIS:H	1.82	0.43
1:b:122:ASP:OD1	1:b:123:LYS:N	2.51	0.43
1:d:122:ASP:OD1	1:d:123:LYS:N	2.51	0.43
1:d:236:ALA:O	1:d:240:VAL:HG12	2.18	0.43
3:U:100:LEU:HD11	3:U:121:VAL:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:100:LEU:O	3:V:143:ARG:HG3	2.18	0.43
6:Y:743:MET:HE2	6:Y:745:GLY:HA2	2.00	0.43
7:L:-3:DA:H2"	7:L:-2:DC:O5'	2.18	0.43
8:K:2:DG:H2'	8:K:3:DT:H71	1.99	0.43
8:K:3:DT:H2"	8:K:4:DG:H8	1.83	0.43
6:Y:71:LEU:H	6:Y:90:VAL:HG21	1.83	0.43
6:Y:796:LEU:HD22	6:Y:1138:LEU:HD11	2.00	0.43
1:e:236:ALA:O	1:e:240:VAL:HG12	2.18	0.43
2:A:202:PRO:HB2	2:A:226:ALA:HB3	1.99	0.43
3:V:284:ARG:NH2	3:V:288:GLU:HB3	2.33	0.43
5:X:463:GLN:HG3	5:X:505:PHE:CG	2.53	0.43
5:X:582:ASN:HB2	5:X:588:GLU:HG3	1.99	0.43
5:X:992:LEU:HG	5:X:993:PRO:HD3	2.00	0.43
1:f:275:ASN:HA	1:f:293:ALA:HB1	2.00	0.43
3:U:60:GLU:HB3	3:U:143:ARG:HB2	2.00	0.43
3:U:77:ASP:O	3:U:81:ILE:HG13	2.18	0.43
6:Y:123:ARG:HH12	6:Y:1334:GLU:HG2	1.84	0.43
6:Y:332:LYS:HE3	6:Y:1329:THR:HA	2.01	0.43
6:Y:833:GLU:OE2	6:Y:1242:ARG:NH2	2.42	0.43
6:Y:946:ALA:HB2	6:Y:1022:PRO:HB3	2.00	0.43
6:Y:964:LYS:HD3	6:Y:964:LYS:HA	1.82	0.43
1:c:208:LEU:HD23	1:c:265:ASP:OD1	2.19	0.43
1:d:275:ASN:HA	1:d:293:ALA:HB1	2.00	0.43
2:A:2:ASN:HA	2:A:5:ILE:HD12	2.00	0.43
3:V:275:ILE:HD13	3:V:281:LEU:HD13	2.01	0.43
5:X:225:PHE:HE2	5:X:347:ILE:HB	1.83	0.43
5:X:678:ARG:HG3	5:X:1108:ASN:HB3	2.01	0.43
5:X:936:ARG:HH21	5:X:1043:ALA:H	1.67	0.43
5:X:1330:ILE:HG22	5:X:1335:ILE:HG22	2.01	0.43
6:Y:245:LEU:O	6:Y:250:ARG:NH2	2.42	0.43
1:d:208:LEU:HD23	1:d:265:ASP:OD1	2.19	0.43
1:d:366:ARG:HG2	10:e:1000:ADP:O2A	2.19	0.43
1:e:275:ASN:HA	1:e:293:ALA:HB1	2.00	0.43
3:V:111:THR:C	3:V:130:ILE:HG12	2.44	0.43
3:V:263:THR:OG1	3:V:266:SER:OG	2.32	0.43
5:X:70:TYR:HA	5:X:100:LEU:HD23	2.00	0.43
5:X:421:SER:OG	5:X:423:ASP:OD1	2.26	0.43
5:X:766:ASN:OD1	5:X:767:GLN:N	2.52	0.43
5:X:1247:SER:HB2	6:Y:375:GLU:O	2.18	0.43
6:Y:492:SER:OG	6:Y:495:ASN:O	2.29	0.43
1:a:108:GLU:OE1	7:L:27:DT:C5	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:208:LEU:HD23	1:e:265:ASP:OD1	2.19	0.43
5:X:18:ARG:NH2	5:X:620:ASN:O	2.34	0.43
5:X:468:LEU:HD23	5:X:468:LEU:HA	1.91	0.43
5:X:593:LYS:HB2	5:X:604:HIS:HD2	1.83	0.43
5:X:720:ARG:HE	5:X:736:VAL:HG11	1.82	0.43
6:Y:287:ALA:CB	6:Y:291:ILE:HG21	2.38	0.43
6:Y:674:THR:O	6:Y:678:ARG:HB2	2.19	0.43
6:Y:1036:ARG:HH22	6:Y:1085:GLY:HA2	1.84	0.43
8:K:-16:DA:H1'	8:K:-15:DG:H5'	2.01	0.43
1:a:108:GLU:CD	7:L:27:DT:H73	2.43	0.43
1:c:265:ASP:HA	1:c:266:SER:HA	1.54	0.43
1:d:326:LYS:HD2	1:d:326:LYS:HA	1.83	0.43
10:e:1000:ADP:O2B	12:e:1002:BEF:F2	2.27	0.43
3:U:10:LYS:HD2	3:V:230:ALA:HB2	2.00	0.43
3:U:187:VAL:HB	3:U:199:ASP:OD1	2.19	0.43
5:X:10:ARG:NH2	5:X:790:ASP:OD2	2.37	0.43
6:Y:54:ASP:OD1	6:Y:54:ASP:N	2.52	0.43
6:Y:938:GLY:O	6:Y:943:ARG:NH1	2.52	0.43
1:f:236:ALA:O	1:f:240:VAL:HG12	2.18	0.43
1:f:265:ASP:HA	1:f:266:SER:HA	1.54	0.43
1:a:208:LEU:HD23	1:a:265:ASP:OD1	2.19	0.43
1:a:244:GLU:OE2	1:a:274:TYR:OH	2.34	0.43
1:b:208:LEU:HD23	1:b:265:ASP:OD1	2.19	0.43
1:b:394:ASP:N	1:b:394:ASP:OD1	2.48	0.43
2:A:6:LEU:HA	2:A:9:VAL:HG12	2.01	0.43
2:A:49:ILE:HG13	2:A:55:ASP:C	2.44	0.43
2:A:392:LEU:HD13	2:A:398:LEU:HD11	2.01	0.43
5:X:802:VAL:HG21	5:X:1230:MET:HB3	2.00	0.43
5:X:840:SER:HB2	5:X:848:GLU:HG3	2.01	0.43
5:X:1247:SER:N	6:Y:375:GLU:OE1	2.51	0.43
1:a:109:ARG:NH1	7:L:28:DC:O3'	2.51	0.42
1:a:122:ASP:OD1	1:a:123:LYS:N	2.51	0.42
3:V:280:ASP:OD1	3:V:321:TRP:NE1	2.35	0.42
5:X:236:LYS:HD2	5:X:286:GLU:HA	2.01	0.42
5:X:896:THR:O	5:X:900:LYS:HG2	2.19	0.42
5:X:954:LYS:HE3	5:X:954:LYS:HB3	1.90	0.42
5:X:1335:ILE:HD13	6:Y:23:ALA:HB3	2.01	0.42
6:Y:252:LEU:HD13	6:Y:261:ALA:O	2.19	0.42
6:Y:331:ILE:HG23	6:Y:338:PHE:HB2	2.01	0.42
6:Y:587:LEU:HD21	6:Y:608:CYS:HB2	2.01	0.42
6:Y:1132:LYS:HE2	6:Y:1132:LYS:HB3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:122:ASP:OD1	1:f:123:LYS:N	2.51	0.42
1:f:208:LEU:HD23	1:f:265:ASP:OD1	2.19	0.42
1:d:173:ARG:HH22	1:e:213:PRO:CG	2.33	0.42
2:A:209:PHE:CE1	2:A:262:VAL:HG21	2.47	0.42
3:V:220:ALA:O	3:V:223:ILE:HG22	2.19	0.42
4:W:50:ALA:HA	4:W:53:GLU:HG2	2.00	0.42
5:X:4:SER:HB3	5:X:7:GLU:HG3	2.01	0.42
5:X:14:ASP:OD2	5:X:1156:ARG:NH1	2.52	0.42
5:X:725:GLN:HB3	5:X:733:VAL:HG12	2.00	0.42
6:Y:659:ALA:O	6:Y:662:ALA:HB3	2.19	0.42
6:Y:1234:VAL:HG23	6:Y:1253:ILE:HG21	2.01	0.42
6:Y:1348:LYS:HA	6:Y:1351:VAL:HG12	2.01	0.42
1:f:137:THR:O	1:f:137:THR:OG1	2.37	0.42
1:a:328:ASP:N	1:a:328:ASP:OD1	2.52	0.42
1:b:48:ASP:OD1	1:b:48:ASP:N	2.52	0.42
1:b:326:LYS:HD2	1:b:326:LYS:HA	1.83	0.42
1:c:92:ARG:HH12	1:d:28:ARG:HH11	1.68	0.42
3:U:166:ARG:NH1	5:X:863:SER:OG	2.49	0.42
6:Y:307:LEU:O	6:Y:328:ALA:HB3	2.19	0.42
1:c:244:GLU:OE2	1:c:274:TYR:OH	2.34	0.42
1:d:173:ARG:NH1	1:e:214:GLU:OE2	2.52	0.42
2:A:142:VAL:HG23	2:A:176:GLY:H	1.84	0.42
4:W:3:ARG:HH22	4:W:52:ARG:HB2	1.84	0.42
5:X:262:TYR:CE2	5:X:282:VAL:HG21	2.55	0.42
5:X:698:PRO:HG3	5:X:1231:TYR:CZ	2.54	0.42
5:X:1331:ARG:HD3	5:X:1335:ILE:O	2.20	0.42
6:Y:35:PHE:CG	6:Y:101:ARG:HD2	2.54	0.42
6:Y:160:LEU:HD22	6:Y:164:GLN:HB3	2.02	0.42
6:Y:735:ALA:HB1	6:Y:738:ARG:HH21	1.84	0.42
8:K:-21:DG:C2'	8:K:-20:DG:C8	3.03	0.42
1:e:40:LYS:HE2	1:e:40:LYS:HB3	1.86	0.42
1:e:195:ILE:HD11	1:e:261:ILE:HD13	2.02	0.42
3:U:190:ALA:HB3	3:U:198:LEU:HB3	2.01	0.42
5:X:1122:LYS:HG2	5:X:1229:TYR:CE1	2.54	0.42
6:Y:884:SER:OG	6:Y:886:VAL:HG22	2.19	0.42
6:Y:1220:ILE:HG23	6:Y:1224:ARG:HD2	2.00	0.42
1:a:108:GLU:HB3	7:L:27:DT:C4	2.55	0.42
1:e:186:MET:SD	1:e:186:MET:N	2.92	0.42
3:U:29:GLU:HB3	3:U:200:LYS:HG3	2.02	0.42
3:V:37:HIS:NE2	3:V:187:VAL:HG21	2.34	0.42
1:f:145:LEU:HD13	1:f:195:ILE:HD11	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:108:GLU:HB3	7:L:27:DT:C5	2.55	0.42
1:c:122:ASP:OD1	1:c:123:LYS:N	2.51	0.42
1:d:328:ASP:OD1	1:d:328:ASP:N	2.52	0.42
3:U:184:ALA:HB3	3:U:204:GLU:HG2	2.01	0.42
5:X:225:PHE:CG	5:X:336:LEU:HD23	2.55	0.42
5:X:554:HIS:HB3	5:X:558:VAL:HB	2.02	0.42
5:X:970:GLY:O	5:X:973:SER:OG	2.33	0.42
6:Y:272:VAL:HG23	6:Y:302:ALA:CB	2.49	0.42
1:f:62:PHE:CE2	9:R:24:U:H5"	2.55	0.42
1:b:145:LEU:HD13	1:b:195:ILE:HD11	2.02	0.42
1:e:48:ASP:OD1	1:e:48:ASP:N	2.52	0.42
2:A:155:GLY:N	2:A:158:ALA:HB3	2.34	0.42
5:X:434:ASP:HB3	5:X:439:LYS:HG3	2.01	0.42
5:X:443:ASP:OD1	5:X:443:ASP:N	2.45	0.42
5:X:566:GLY:HA3	5:X:567:PRO:HD3	1.95	0.42
5:X:622:ASN:OD1	5:X:622:ASN:N	2.50	0.42
5:X:677:ASN:O	5:X:681:MET:HG2	2.19	0.42
6:Y:134:ASP:O	6:Y:138:VAL:HG23	2.20	0.42
1:a:110:TYR:H	7:L:27:DT:H3	1.67	0.42
1:a:181:LYS:HD3	1:a:181:LYS:HA	1.71	0.42
1:a:186:MET:SD	1:a:186:MET:N	2.92	0.42
1:d:9:THR:OG1	1:d:13:GLU:OE1	2.31	0.42
1:e:328:ASP:OD1	1:e:328:ASP:N	2.52	0.42
5:X:221:LEU:HD21	5:X:314:ASN:HD22	1.83	0.42
5:X:971:LEU:HD21	5:X:1018:TYR:HB2	2.01	0.42
6:Y:279:LEU:HD13	6:Y:282:LEU:HD12	2.02	0.42
1:c:145:LEU:HD13	1:c:195:ILE:HD11	2.02	0.42
1:e:137:THR:O	1:e:137:THR:OG1	2.37	0.42
3:V:219:ARG:HA	3:V:222:THR:HG22	2.02	0.42
5:X:517:GLN:HB3	5:X:759:SER:HB2	2.02	0.42
5:X:1243:MET:HE1	6:Y:371:LYS:HB3	2.00	0.42
6:Y:269:TYR:HA	6:Y:272:VAL:HG12	2.01	0.42
1:a:184:LYS:N	10:a:1000:ADP:O2B	2.53	0.41
1:a:302:GLY:O	1:a:305:ARG:NH2	2.40	0.41
1:b:414:GLU:HA	1:b:417:LYS:HE2	2.02	0.41
5:X:976:ARG:HB2	5:X:994:ARG:HH22	1.84	0.41
5:X:1072:ASN:OD1	5:X:1072:ASN:N	2.51	0.41
5:X:1142:ARG:NH2	5:X:1166:ASP:OD1	2.52	0.41
5:X:1331:ARG:HA	5:X:1334:GLY:HA2	2.02	0.41
6:Y:1307:LEU:HD13	6:Y:1311:LYS:HB2	2.01	0.41
1:f:48:ASP:OD1	1:f:48:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:93:THR:O	1:b:252:ARG:NH1	2.53	0.41
1:c:181:LYS:HA	1:c:181:LYS:HD3	1.71	0.41
1:d:145:LEU:HD13	1:d:195:ILE:HD11	2.02	0.41
2:A:14:ASN:O	2:A:18:LEU:HB3	2.20	0.41
2:A:111:LYS:HE2	2:A:111:LYS:HB3	1.86	0.41
2:A:183:LEU:HD12	2:A:196:PHE:O	2.20	0.41
4:W:45:LYS:HE3	6:Y:419:HIS:HB2	2.03	0.41
5:X:28:LEU:HD21	5:X:524:ILE:HG13	2.01	0.41
5:X:686:GLN:HG3	5:X:1233:LEU:HD11	2.02	0.41
5:X:902:LEU:O	5:X:906:PHE:N	2.37	0.41
6:Y:412:LEU:HA	6:Y:415:VAL:HG22	2.02	0.41
6:Y:605:LEU:HD23	6:Y:605:LEU:HA	1.94	0.41
6:Y:1134:ILE:HG13	6:Y:1134:ILE:O	2.21	0.41
6:Y:1357:ILE:HG22	6:Y:1359:ALA:H	1.85	0.41
7:L:28:DC:H4'	7:L:29:DG:OP1	2.20	0.41
1:c:93:THR:O	1:c:252:ARG:NH1	2.53	0.41
1:d:195:ILE:HD11	1:d:261:ILE:HD13	2.02	0.41
3:U:111:THR:HG23	3:U:113:ALA:H	1.85	0.41
5:X:17:LYS:HE2	5:X:17:LYS:HB2	1.95	0.41
5:X:234:ASP:N	5:X:234:ASP:OD1	2.53	0.41
6:Y:111:THR:HG22	6:Y:300:GLN:NE2	2.35	0.41
6:Y:326:SER:O	6:Y:330:MET:N	2.54	0.41
6:Y:952:VAL:HG23	6:Y:1017:VAL:HG11	2.03	0.41
6:Y:1257:VAL:HA	6:Y:1260:MET:HG2	2.01	0.41
1:f:83:PRO:O	1:f:87:ARG:HG2	2.21	0.41
1:f:110:TYR:OH	9:R:25:C:O2'	2.32	0.41
1:f:414:GLU:HA	1:f:417:LYS:HE2	2.02	0.41
1:a:11:VAL:O	1:a:15:ILE:HG13	2.21	0.41
1:b:11:VAL:O	1:b:15:ILE:HG13	2.21	0.41
1:b:328:ASP:OD1	1:b:328:ASP:N	2.52	0.41
1:d:130:LYS:O	1:e:27:ALA:HB1	2.20	0.41
1:e:83:PRO:O	1:e:87:ARG:HG2	2.21	0.41
5:X:180:ARG:HG3	5:X:396:ASP:HB2	2.01	0.41
5:X:706:ARG:NE	5:X:792:GLY:O	2.52	0.41
5:X:841:ARG:HH12	9:R:86:A:H61	1.67	0.41
6:Y:24:LEU:HD23	6:Y:24:LEU:HA	1.88	0.41
6:Y:233:LYS:HB2	6:Y:236:TRP:CD2	2.56	0.41
6:Y:650:LYS:O	6:Y:651:HIS:C	2.62	0.41
1:f:328:ASP:OD1	1:f:328:ASP:N	2.52	0.41
1:a:195:ILE:HD11	1:a:261:ILE:HD13	2.02	0.41
1:a:296:ARG:HB2	1:a:297:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:83:PRO:O	1:b:87:ARG:HG2	2.21	0.41
1:b:181:LYS:HA	1:b:181:LYS:HD3	1.71	0.41
1:c:48:ASP:OD1	1:c:48:ASP:N	2.52	0.41
1:c:328:ASP:OD1	1:c:328:ASP:N	2.52	0.41
1:c:414:GLU:HA	1:c:417:LYS:HE2	2.03	0.41
1:d:402:LYS:HA	1:d:402:LYS:HD3	1.84	0.41
5:X:131:THR:HG23	5:X:133:ASN:H	1.85	0.41
6:Y:460:ASP:OD1	6:Y:460:ASP:N	2.53	0.41
6:Y:814:CYS:HB3	6:Y:895:CYS:SG	2.60	0.41
6:Y:1340:LYS:HB2	6:Y:1340:LYS:HE3	1.85	0.41
1:f:93:THR:O	1:f:252:ARG:NH1	2.53	0.41
1:f:402:LYS:HD3	1:f:402:LYS:HA	1.83	0.41
1:a:414:GLU:HA	1:a:417:LYS:HE2	2.03	0.41
1:c:31:LYS:HB2	1:c:31:LYS:HE2	1.76	0.41
1:d:93:THR:O	1:d:252:ARG:NH1	2.53	0.41
1:e:93:THR:O	1:e:252:ARG:NH1	2.53	0.41
2:A:366:ASP:CG	2:A:367:GLU:H	2.28	0.41
4:W:61:ASN:O	4:W:64:LEU:HG	2.20	0.41
5:X:85:CYS:HB3	5:X:90:VAL:O	2.21	0.41
5:X:389:PHE:HB3	5:X:420:LEU:HD12	2.03	0.41
5:X:755:LYS:HA	5:X:755:LYS:HD3	1.69	0.41
6:Y:272:VAL:HA	6:Y:275:ARG:HE	1.85	0.41
6:Y:953:LYS:HE2	6:Y:953:LYS:HB3	1.93	0.41
1:f:195:ILE:HD11	1:f:261:ILE:HD13	2.02	0.41
1:c:11:VAL:O	1:c:15:ILE:HG13	2.21	0.41
1:c:173:ARG:NH1	1:d:214:GLU:OE2	2.54	0.41
1:e:183:GLY:N	10:e:1000:ADP:O3B	2.53	0.41
5:X:207:THR:HG21	5:X:354:ASP:HB2	2.01	0.41
5:X:371:ARG:HA	5:X:372:PRO:HD3	1.94	0.41
5:X:565:GLU:HA	5:X:569:ILE:HG13	2.00	0.41
5:X:797:GLY:HA3	5:X:1233:LEU:HD23	2.03	0.41
5:X:976:ARG:HB2	5:X:994:ARG:NH2	2.35	0.41
5:X:1323:PHE:CZ	5:X:1327:LEU:HD21	2.56	0.41
1:a:93:THR:O	1:a:252:ARG:NH1	2.53	0.41
1:a:137:THR:O	1:a:137:THR:OG1	2.37	0.41
1:a:145:LEU:HD13	1:a:195:ILE:HD11	2.02	0.41
1:b:296:ARG:HB2	1:b:297:PRO:HD3	2.03	0.41
1:b:402:LYS:HA	1:b:402:LYS:HD3	1.84	0.41
1:d:11:VAL:O	1:d:15:ILE:HG13	2.21	0.41
1:d:414:GLU:HA	1:d:417:LYS:HE2	2.02	0.41
1:e:31:LYS:HB2	1:e:31:LYS:HE2	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:100:LYS:HG2	1:e:114:LEU:HB2	2.03	0.41
3:U:104:LYS:HA	3:U:104:LYS:HD2	1.87	0.41
3:U:211:ILE:HD12	3:U:211:ILE:HA	1.91	0.41
5:X:91:THR:OG1	5:X:138:ILE:O	2.29	0.41
5:X:728:ASP:OD1	5:X:729:ALA:N	2.53	0.41
5:X:936:ARG:HD3	5:X:937:ASP:H	1.86	0.41
6:Y:98:ARG:O	6:Y:246:PRO:HB3	2.20	0.41
6:Y:279:LEU:HD13	6:Y:279:LEU:HA	1.83	0.41
7:L:-1:DA:H1'	7:L:0:DA:H5'	2.02	0.41
1:f:296:ARG:HB2	1:f:297:PRO:HD3	2.03	0.41
1:a:6:LEU:HB3	1:a:35:ILE:HD11	2.03	0.41
1:a:48:ASP:OD1	1:a:48:ASP:N	2.53	0.41
1:a:109:ARG:NH1	7:L:27:DT:H2'	2.32	0.41
1:a:130:LYS:O	1:b:27:ALA:HB1	2.21	0.41
1:b:195:ILE:HD11	1:b:261:ILE:HD13	2.02	0.41
1:c:83:PRO:O	1:c:87:ARG:HG2	2.21	0.41
1:c:146:ARG:HD3	1:c:146:ARG:HA	1.91	0.41
1:c:186:MET:SD	1:c:186:MET:N	2.92	0.41
10:c:1000:ADP:O2B	12:c:1002:BEF:F2	2.29	0.41
1:d:83:PRO:O	1:d:87:ARG:HG2	2.21	0.41
1:d:100:LYS:HG2	1:d:114:LEU:HB2	2.03	0.41
4:W:15:ASN:OD1	4:W:15:ASN:N	2.54	0.41
5:X:432:LEU:O	5:X:435:ILE:HG22	2.21	0.41
5:X:702:THR:H	5:X:705:GLU:CD	2.29	0.41
5:X:705:GLU:O	5:X:706:ARG:C	2.64	0.41
5:X:810:TYR:O	5:X:815:SER:OG	2.34	0.41
5:X:1209:GLN:HA	5:X:1226:THR:HA	2.02	0.41
6:Y:658:GLU:O	6:Y:661:VAL:HG12	2.21	0.41
6:Y:1368:ASP:HA	6:Y:1371:ARG:HG2	2.02	0.41
9:R:21:C:H2'	9:R:22:A:O4'	2.21	0.41
1:f:157:LEU:O	1:f:161:VAL:HG23	2.21	0.41
1:f:208:LEU:HD12	1:f:229:ALA:HB2	2.03	0.41
1:b:31:LYS:HE2	1:b:31:LYS:HB2	1.76	0.41
1:b:100:LYS:HG2	1:b:114:LEU:HB2	2.03	0.41
1:d:48:ASP:OD1	1:d:48:ASP:N	2.52	0.41
1:e:296:ARG:HB2	1:e:297:PRO:HD3	2.03	0.41
1:e:402:LYS:HA	1:e:402:LYS:HD3	1.84	0.41
2:A:52:LYS:HE3	2:A:52:LYS:HB3	1.91	0.41
2:A:171:GLU:OE1	2:A:199:ARG:NH2	2.39	0.41
3:U:85:LEU:O	3:U:88:LEU:HG	2.21	0.41
5:X:1122:LYS:HG2	5:X:1229:TYR:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:1292:THR:HB	5:X:1320:PRO:HG3	2.03	0.41
6:Y:511:TYR:HE2	6:Y:724:MET:HG2	1.86	0.41
6:Y:586:GLY:HA3	6:Y:612:LEU:HD11	2.02	0.41
6:Y:759:ILE:HG23	6:Y:771:GLN:HB3	2.02	0.41
6:Y:857:LEU:HG	6:Y:858:VAL:HG23	2.02	0.41
6:Y:923:ILE:HD13	6:Y:923:ILE:HA	1.96	0.41
1:a:100:LYS:HG2	1:a:114:LEU:HB2	2.03	0.40
1:a:157:LEU:O	1:a:161:VAL:HG23	2.21	0.40
1:a:191:ILE:HD13	1:a:191:ILE:HA	1.89	0.40
1:c:195:ILE:HD11	1:c:261:ILE:HD13	2.02	0.40
1:c:402:LYS:HA	1:c:402:LYS:HD3	1.84	0.40
3:U:51:MET:HE3	3:U:52:PRO:HD2	2.04	0.40
3:U:194:GLN:O	3:U:195:ARG:HG3	2.20	0.40
4:W:22:VAL:HG13	4:W:64:LEU:CD2	2.51	0.40
5:X:318:SER:OG	5:X:320:ASP:OD1	2.34	0.40
5:X:543:ALA:HB3	5:X:548:ARG:HE	1.85	0.40
5:X:1283:ALA:HA	6:Y:479:GLU:HG2	2.02	0.40
6:Y:1035:VAL:HB	6:Y:1115:ILE:HD13	2.02	0.40
6:Y:1343:GLU:C	6:Y:1344:LEU:HD23	2.45	0.40
7:L:-7:DG:H2"	7:L:-6:DC:C6	2.56	0.40
1:d:26:LEU:HG	1:d:34:ILE:HG12	2.04	0.40
3:U:61:ILE:HG23	3:U:142:MET:HB3	2.03	0.40
5:X:72:SER:OG	5:X:73:TYR:N	2.54	0.40
5:X:948:ILE:HG13	5:X:949:GLU:N	2.35	0.40
6:Y:208:THR:HG21	6:Y:213:LYS:HD2	2.03	0.40
6:Y:674:THR:H	6:Y:677:GLU:CD	2.28	0.40
6:Y:885:VAL:N	6:Y:1254:GLU:OE2	2.55	0.40
6:Y:1208:ASP:OD1	6:Y:1209:VAL:N	2.55	0.40
7:L:20:DC:C2	7:L:21:DC:C4	3.09	0.40
9:R:92:C:H2'	9:R:93:G:H8	1.82	0.40
1:f:248:GLU:O	1:f:252:ARG:HG2	2.22	0.40
1:b:244:GLU:OE2	1:b:274:TYR:OH	2.34	0.40
1:c:201:ASP:OD1	1:c:201:ASP:N	2.55	0.40
1:c:296:ARG:HB2	1:c:297:PRO:HD3	2.03	0.40
2:A:239:LYS:NZ	2:A:276:TRP:O	2.42	0.40
4:W:16:ARG:HB3	6:Y:483:LEU:HD11	2.03	0.40
5:X:1319:MET:HG2	6:Y:17:PHE:HE2	1.87	0.40
6:Y:165:TYR:CE1	6:Y:178:ALA:HB3	2.57	0.40
6:Y:518:VAL:HG12	6:Y:547:ARG:HH12	1.85	0.40
6:Y:925:GLU:HB3	6:Y:926:PRO:HD3	2.03	0.40
7:L:23:DT:C4	7:L:24:DT:C4	3.10	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:5:DA:H2"	8:K:6:DG:C8	2.57	0.40
1:f:171:GLY:N	1:f:314:THR:OG1	2.28	0.40
1:b:6:LEU:HB3	1:b:35:ILE:HD11	2.03	0.40
1:b:26:LEU:HG	1:b:34:ILE:HG12	2.04	0.40
1:c:248:GLU:O	1:c:252:ARG:HG2	2.22	0.40
1:d:208:LEU:HD12	1:d:229:ALA:HB2	2.04	0.40
1:e:414:GLU:HA	1:e:417:LYS:HE2	2.03	0.40
3:V:48:LEU:HD22	6:Y:535:ARG:HG3	2.03	0.40
4:W:16:ARG:NH2	6:Y:910:ASN:OD1	2.54	0.40
5:X:10:ARG:NH1	5:X:793:GLU:OE1	2.54	0.40
5:X:301:TYR:OH	5:X:334:GLU:N	2.52	0.40
5:X:886:LYS:HB2	5:X:886:LYS:HE3	1.85	0.40
6:Y:808:VAL:HG12	6:Y:914:ALA:HB2	2.03	0.40
1:f:26:LEU:HG	1:f:34:ILE:HG12	2.04	0.40
1:f:375:GLU:OE1	1:f:375:GLU:N	2.34	0.40
1:a:248:GLU:O	1:a:252:ARG:HG2	2.22	0.40
1:b:40:LYS:HE2	1:b:40:LYS:HB3	1.86	0.40
1:c:100:LYS:HG2	1:c:114:LEU:HB2	2.03	0.40
1:d:296:ARG:HB2	1:d:297:PRO:HD3	2.03	0.40
2:A:189:GLU:H	2:A:189:GLU:CD	2.30	0.40
2:A:248:VAL:HG13	2:A:273:ILE:HB	2.04	0.40
3:V:166:ARG:O	3:V:166:ARG:HD3	2.22	0.40
4:W:53:GLU:HG3	4:W:59:ILE:HG21	2.03	0.40
5:X:150:HIS:CD2	5:X:454:ARG:HH21	2.39	0.40
6:Y:70:CYS:HB2	6:Y:75:TYR:HB2	2.03	0.40
6:Y:247:PRO:HA	6:Y:250:ARG:CZ	2.51	0.40
6:Y:430:HIS:NE2	6:Y:432:LEU:HB2	2.37	0.40
7:L:9:DG:H2"	7:L:10:DC:H5"	2.02	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 PDB entries followed by that with respect to all EM entries.

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	415/419 (99%)	406 (98%)	9 (2%)	0	100	100
1	b	415/419 (99%)	405 (98%)	10 (2%)	0	100	100
1	c	415/419 (99%)	406 (98%)	9 (2%)	0	100	100
1	d	415/419 (99%)	406 (98%)	9 (2%)	0	100	100
1	e	415/419 (99%)	406 (98%)	9 (2%)	0	100	100
1	f	415/419 (99%)	406 (98%)	9 (2%)	0	100	100
2	A	493/497 (99%)	450 (91%)	43 (9%)	0	100	100
3	U	233/329 (71%)	227 (97%)	6 (3%)	0	100	100
3	V	319/329 (97%)	292 (92%)	27 (8%)	0	100	100
4	W	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	X	1338/1342 (100%)	1252 (94%)	86 (6%)	0	100	100
6	Y	1339/1416 (95%)	1266 (94%)	72 (5%)	1 (0%)	48	82
All	All	6289/6518 (96%)	5996 (95%)	292 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	Y	1325	PHE

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 PDB entries followed by that with respect to all EM entries.

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	357/359 (99%)	329 (92%)	28 (8%)	11	33
1	b	357/359 (99%)	329 (92%)	28 (8%)	11	33
1	c	357/359 (99%)	329 (92%)	28 (8%)	11	33
1	d	357/359 (99%)	329 (92%)	28 (8%)	11	33
1	e	357/359 (99%)	329 (92%)	28 (8%)	11	33
1	f	357/359 (99%)	329 (92%)	28 (8%)	11	33
2	A	409/409 (100%)	409 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	U	203/286 (71%)	203 (100%)	0	100	100
3	V	280/286 (98%)	280 (100%)	0	100	100
4	W	67/75 (89%)	67 (100%)	0	100	100
5	X	1155/1157 (100%)	1155 (100%)	0	100	100
6	Y	1123/1177 (95%)	1123 (100%)	0	100	100
All	All	5379/5544 (97%)	5211 (97%)	168 (3%)	36	56

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	11	VAL
1	f	29	MET
1	f	31	LYS
1	f	33	ASP
1	f	71	SER
1	f	81	VAL
1	f	106	GLU
1	f	116	VAL
1	f	137	THR
1	f	164	LEU
1	f	175	LEU
1	f	181	LYS
1	f	208	LEU
1	f	217	THR
1	f	240	VAL
1	f	265	ASP
1	f	266	SER
1	f	276	THR
1	f	285	LEU
1	f	289	VAL
1	f	312	SER
1	f	318	THR
1	f	320	LEU
1	f	342	GLU
1	f	373	THR
1	f	374	GLN
1	f	408	THR
1	f	414	GLU
1	a	11	VAL
1	a	29	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	a	31	LYS
1	a	33	ASP
1	a	71	SER
1	a	81	VAL
1	a	106	GLU
1	a	116	VAL
1	a	137	THR
1	a	164	LEU
1	a	175	LEU
1	a	181	LYS
1	a	208	LEU
1	a	217	THR
1	a	240	VAL
1	a	265	ASP
1	a	266	SER
1	a	276	THR
1	a	285	LEU
1	a	289	VAL
1	a	312	SER
1	a	318	THR
1	a	320	LEU
1	a	342	GLU
1	a	373	THR
1	a	374	GLN
1	a	408	THR
1	a	414	GLU
1	b	11	VAL
1	b	29	MET
1	b	31	LYS
1	b	33	ASP
1	b	71	SER
1	b	81	VAL
1	b	106	GLU
1	b	116	VAL
1	b	137	THR
1	b	164	LEU
1	b	175	LEU
1	b	181	LYS
1	b	208	LEU
1	b	217	THR
1	b	240	VAL
1	b	265	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	b	266	SER
1	b	276	THR
1	b	285	LEU
1	b	289	VAL
1	b	312	SER
1	b	318	THR
1	b	320	LEU
1	b	342	GLU
1	b	373	THR
1	b	374	GLN
1	b	408	THR
1	b	414	GLU
1	c	11	VAL
1	c	29	MET
1	c	31	LYS
1	c	33	ASP
1	c	71	SER
1	c	81	VAL
1	c	106	GLU
1	c	116	VAL
1	c	137	THR
1	c	164	LEU
1	c	175	LEU
1	c	181	LYS
1	c	208	LEU
1	c	217	THR
1	c	240	VAL
1	c	265	ASP
1	c	266	SER
1	c	276	THR
1	c	285	LEU
1	c	289	VAL
1	c	312	SER
1	c	318	THR
1	c	320	LEU
1	c	342	GLU
1	c	373	THR
1	c	374	GLN
1	c	408	THR
1	c	414	GLU
1	d	11	VAL
1	d	29	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	d	31	LYS
1	d	33	ASP
1	d	71	SER
1	d	81	VAL
1	d	106	GLU
1	d	116	VAL
1	d	137	THR
1	d	164	LEU
1	d	175	LEU
1	d	181	LYS
1	d	208	LEU
1	d	217	THR
1	d	240	VAL
1	d	265	ASP
1	d	266	SER
1	d	276	THR
1	d	285	LEU
1	d	289	VAL
1	d	312	SER
1	d	318	THR
1	d	320	LEU
1	d	342	GLU
1	d	373	THR
1	d	374	GLN
1	d	408	THR
1	d	414	GLU
1	e	11	VAL
1	e	29	MET
1	e	31	LYS
1	e	33	ASP
1	e	71	SER
1	e	81	VAL
1	e	106	GLU
1	e	116	VAL
1	e	137	THR
1	e	164	LEU
1	e	175	LEU
1	e	181	LYS
1	e	208	LEU
1	e	217	THR
1	e	240	VAL
1	e	265	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	266	SER
1	e	276	THR
1	e	285	LEU
1	e	289	VAL
1	e	312	SER
1	e	318	THR
1	e	320	LEU
1	e	342	GLU
1	e	373	THR
1	e	374	GLN
1	e	408	THR
1	e	414	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	f	8	ASN
1	f	142	ASN
1	f	239	HIS
1	f	256	HIS
1	f	401	ASN
1	a	8	ASN
1	a	239	HIS
1	a	256	HIS
1	a	401	ASN
1	b	8	ASN
1	b	142	ASN
1	b	239	HIS
1	b	256	HIS
1	b	401	ASN
1	c	8	ASN
1	c	142	ASN
1	c	239	HIS
1	c	256	HIS
1	c	401	ASN
1	d	8	ASN
1	d	239	HIS
1	d	256	HIS
1	d	401	ASN
1	e	8	ASN
1	e	25	ASN
1	e	239	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	e	256	HIS
1	e	401	ASN
2	A	14	ASN
2	A	70	GLN
2	A	88	ASN
2	A	172	ASN
2	A	286	ASN
2	A	313	ASN
2	A	330	GLN
2	A	349	GLN
2	A	412	ASN
2	A	428	ASN
3	U	37	HIS
3	U	147	GLN
3	V	93	GLN
3	V	268	ASN
4	W	29	GLN
4	W	43	ASN
5	X	41	GLN
5	X	46	GLN
5	X	150	HIS
5	X	193	ASN
5	X	214	ASN
5	X	387	ASN
5	X	604	HIS
5	X	613	ASN
5	X	618	GLN
5	X	659	GLN
5	X	737	ASN
5	X	760	ASN
5	X	832	HIS
5	X	856	ASN
5	X	932	GLN
5	X	1008	GLN
5	X	1010	GLN
5	X	1013	GLN
5	X	1017	GLN
5	X	1061	GLN
5	X	1116	HIS
5	X	1237	HIS
5	X	1256	GLN
5	X	1288	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	X	1324	ASN
6	Y	229	GLN
6	Y	274	ASN
6	Y	300	GLN
6	Y	335	GLN
6	Y	340	GLN
6	Y	365	GLN
6	Y	435	GLN
6	Y	488	ASN
6	Y	545	HIS
6	Y	739	GLN
6	Y	865	HIS
6	Y	897	HIS
6	Y	921	GLN
6	Y	954	ASN
6	Y	968	ASN
6	Y	1197	ASN
6	Y	1227	HIS
6	Y	1268	ASN
6	Y	1326	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	30/99 (30%)	12 (40%)	1 (3%)

All (12) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	24	U
9	R	25	C
9	R	26	C
9	R	80	A
9	R	82	C
9	R	86	A
9	R	87	C
9	R	90	G
9	R	91	G
9	R	92	C
9	R	93	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
10	ADP	d	1000	11	27,29,29	1.37	4 (14%)	42,45,45	1.94	10 (23%)
12	BEF	b	1002	-	0,3,3	-	-	-		
10	ADP	a	1000	11	27,29,29	1.37	4 (14%)	42,45,45	1.96	10 (23%)
10	ADP	c	1000	11	27,29,29	1.36	4 (14%)	42,45,45	1.97	11 (26%)
10	ADP	e	1000	11	27,29,29	1.37	4 (14%)	42,45,45	1.96	10 (23%)
12	BEF	a	1002	-	0,3,3	-	-	-		
12	BEF	c	1002	-	0,3,3	-	-	-		
12	BEF	e	1002	-	0,3,3	-	-	-		
10	ADP	b	1000	11	27,29,29	1.36	4 (14%)	42,45,45	1.96	11 (26%)
12	BEF	d	1002	-	0,3,3	-	-	-		

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
10	ADP	d	1000	11	-	2/16/32/32	0/3/3/3
10	ADP	a	1000	11	-	3/16/32/32	0/3/3/3
10	ADP	c	1000	11	-	4/16/32/32	0/3/3/3
10	ADP	e	1000	11	-	3/16/32/32	0/3/3/3
10	ADP	b	1000	11	-	3/16/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	a	1000	ADP	C5-C4	4.60	1.47	1.39
10	d	1000	ADP	C5-C4	4.57	1.47	1.39
10	b	1000	ADP	C5-C4	4.54	1.47	1.39
10	c	1000	ADP	C5-C4	4.54	1.47	1.39
10	e	1000	ADP	C5-C4	4.53	1.47	1.39
10	e	1000	ADP	C5-C6	2.72	1.48	1.41
10	b	1000	ADP	C5-C6	2.67	1.48	1.41
10	c	1000	ADP	C5-C6	2.67	1.48	1.41
10	a	1000	ADP	C5-C6	2.67	1.48	1.41
10	d	1000	ADP	C5-C6	2.66	1.48	1.41
10	e	1000	ADP	C8-N7	2.46	1.36	1.31
10	b	1000	ADP	C8-N7	2.41	1.36	1.31
10	a	1000	ADP	C8-N7	2.39	1.36	1.31
10	d	1000	ADP	C8-N7	2.38	1.36	1.31
10	c	1000	ADP	C8-N7	2.36	1.36	1.31
10	a	1000	ADP	C5-N7	-2.20	1.34	1.39
10	d	1000	ADP	C5-N7	-2.19	1.34	1.39
10	b	1000	ADP	C5-N7	-2.17	1.34	1.39
10	e	1000	ADP	C5-N7	-2.17	1.34	1.39
10	c	1000	ADP	C5-N7	-2.16	1.34	1.39

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	a	1000	ADP	C5-C4-N3	-6.27	118.57	126.75
10	e	1000	ADP	C5-C4-N3	-6.23	118.63	126.75
10	b	1000	ADP	C5-C4-N3	-6.20	118.67	126.75
10	d	1000	ADP	C5-C4-N3	-6.16	118.72	126.75
10	c	1000	ADP	C5-C4-N3	-6.11	118.78	126.75
10	a	1000	ADP	N3-C4-N9	4.93	135.20	127.08
10	d	1000	ADP	N3-C4-N9	4.86	135.08	127.08
10	c	1000	ADP	N3-C4-N9	4.83	135.03	127.08
10	b	1000	ADP	N3-C4-N9	4.82	135.03	127.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	e	1000	ADP	N3-C4-N9	4.80	134.98	127.08
10	e	1000	ADP	C2-N3-C4	3.86	120.87	111.75
10	a	1000	ADP	C2-N3-C4	3.86	120.87	111.75
10	b	1000	ADP	C2-N3-C4	3.86	120.87	111.75
10	d	1000	ADP	C2-N3-C4	3.83	120.80	111.75
10	c	1000	ADP	C2-N3-C4	3.81	120.75	111.75
10	e	1000	ADP	C4-C5-N7	-3.29	106.61	110.62
10	b	1000	ADP	C4-C5-N7	-3.29	106.61	110.62
10	e	1000	ADP	PA-O3A-PB	-3.25	121.67	132.83
10	c	1000	ADP	C4-C5-N7	-3.23	106.69	110.62
10	c	1000	ADP	PA-O3A-PB	-3.22	121.78	132.83
10	d	1000	ADP	C4-C5-N7	-3.22	106.70	110.62
10	a	1000	ADP	C4-C5-N7	-3.21	106.70	110.62
10	b	1000	ADP	N3-C2-N1	-3.12	123.72	128.60
10	a	1000	ADP	N3-C2-N1	-3.12	123.73	128.60
10	d	1000	ADP	N3-C2-N1	-3.11	123.74	128.60
10	e	1000	ADP	N3-C2-N1	-3.11	123.74	128.60
10	c	1000	ADP	N3-C2-N1	-3.10	123.76	128.60
10	a	1000	ADP	PA-O3A-PB	-3.01	122.48	132.83
10	b	1000	ADP	PA-O3A-PB	-2.99	122.56	132.83
10	d	1000	ADP	PA-O3A-PB	-2.86	123.01	132.83
10	b	1000	ADP	C5-N7-C8	2.77	107.44	103.51
10	c	1000	ADP	C5-N7-C8	2.73	107.39	103.51
10	e	1000	ADP	C5-N7-C8	2.71	107.36	103.51
10	d	1000	ADP	C5-N7-C8	2.68	107.32	103.51
10	a	1000	ADP	C5-N7-C8	2.67	107.30	103.51
10	c	1000	ADP	C4-N9-C8	2.63	108.58	105.73
10	d	1000	ADP	C4-N9-C8	2.58	108.52	105.73
10	d	1000	ADP	C3'-C2'-C1'	2.57	106.31	101.43
10	c	1000	ADP	C3'-C2'-C1'	2.55	106.28	101.43
10	b	1000	ADP	C4-N9-C8	2.53	108.47	105.73
10	b	1000	ADP	C3'-C2'-C1'	2.52	106.21	101.43
10	a	1000	ADP	C4-N9-C8	2.51	108.45	105.73
10	a	1000	ADP	C3'-C2'-C1'	2.50	106.18	101.43
10	e	1000	ADP	C3'-C2'-C1'	2.48	106.15	101.43
10	e	1000	ADP	C4-N9-C8	2.43	108.36	105.73
10	b	1000	ADP	C6-C5-N7	2.18	136.07	132.02
10	e	1000	ADP	C6-C5-N7	2.15	136.03	132.02
10	c	1000	ADP	C6-C5-N7	2.15	136.02	132.02
10	d	1000	ADP	C6-C5-N7	2.13	135.99	132.02
10	a	1000	ADP	C6-C5-N7	2.07	135.88	132.02
10	c	1000	ADP	N9-C8-N7	-2.01	111.16	113.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	b	1000	ADP	N9-C8-N7	-2.00	111.17	113.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	b	1000	ADP	C5'-O5'-PA-O3A
10	c	1000	ADP	C5'-O5'-PA-O1A
10	c	1000	ADP	C5'-O5'-PA-O3A
10	e	1000	ADP	C5'-O5'-PA-O1A
10	a	1000	ADP	C5'-O5'-PA-O3A
10	c	1000	ADP	C5'-O5'-PA-O2A
10	e	1000	ADP	C5'-O5'-PA-O3A
10	a	1000	ADP	O4'-C4'-C5'-O5'
10	a	1000	ADP	C5'-O5'-PA-O1A
10	b	1000	ADP	C5'-O5'-PA-O1A
10	d	1000	ADP	C5'-O5'-PA-O1A
10	b	1000	ADP	O4'-C4'-C5'-O5'
10	c	1000	ADP	O4'-C4'-C5'-O5'
10	d	1000	ADP	O4'-C4'-C5'-O5'
10	e	1000	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

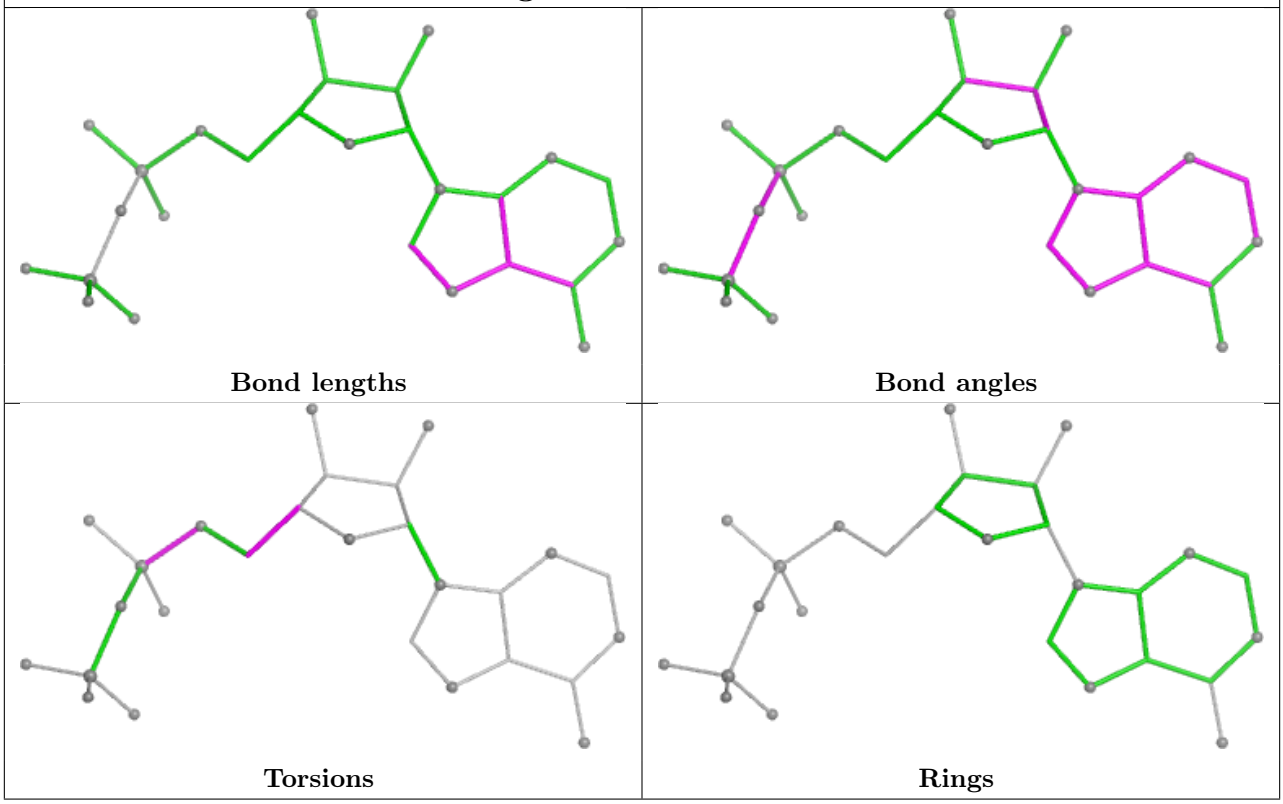
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	d	1000	ADP	1	0
12	b	1002	BEF	1	0
10	a	1000	ADP	2	0
10	c	1000	ADP	3	0
10	e	1000	ADP	5	0
12	a	1002	BEF	1	0
12	c	1002	BEF	2	0
12	e	1002	BEF	2	0
10	b	1000	ADP	3	0

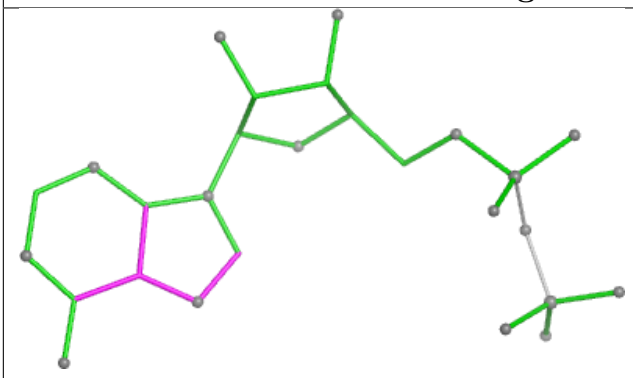
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

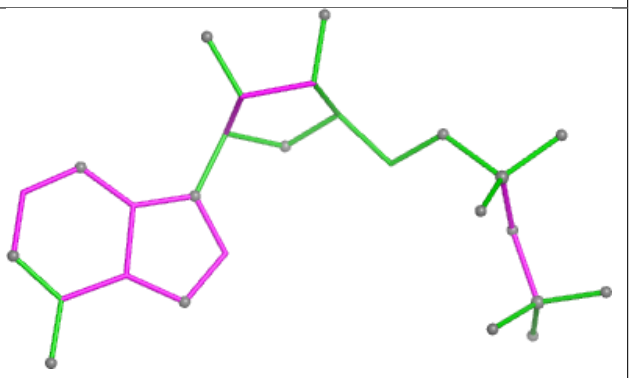
Ligand ADP d 1000



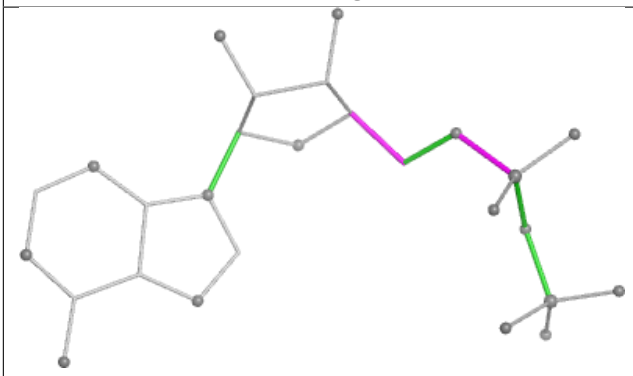
Ligand ADP a 1000



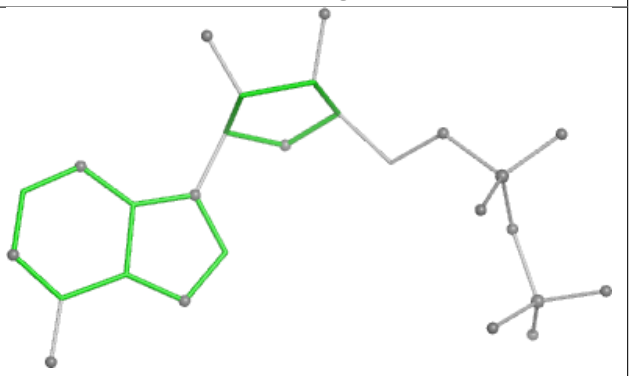
Bond lengths



Bond angles

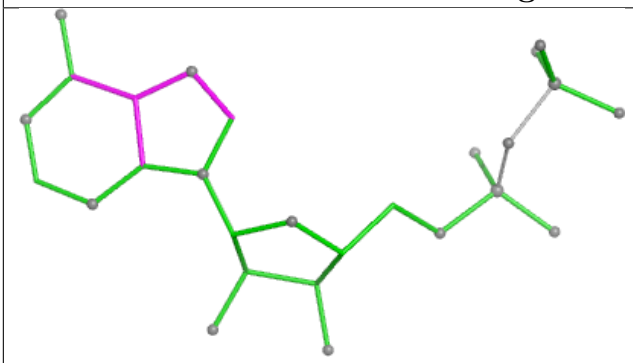


Torsions

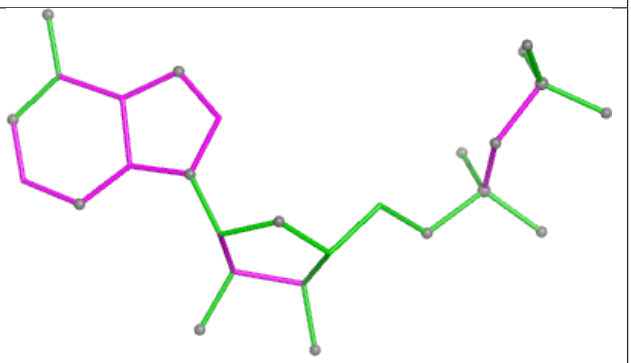


Rings

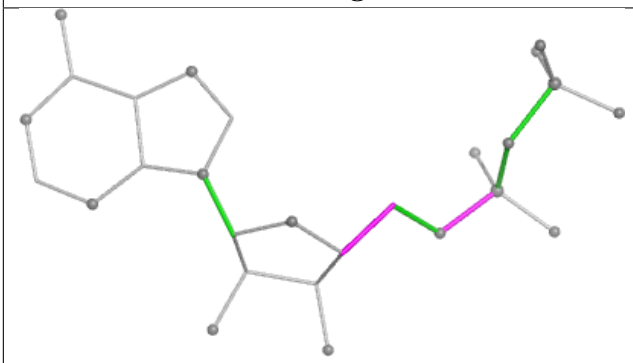
Ligand ADP c 1000



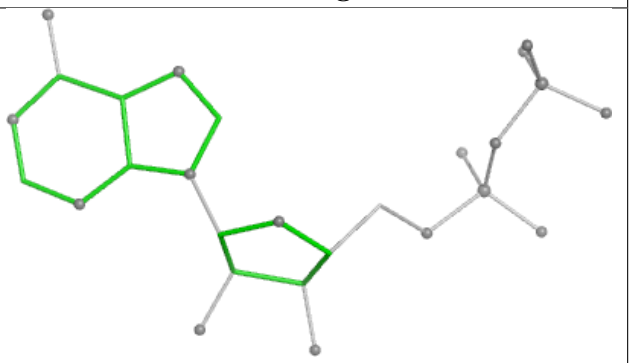
Bond lengths



Bond angles

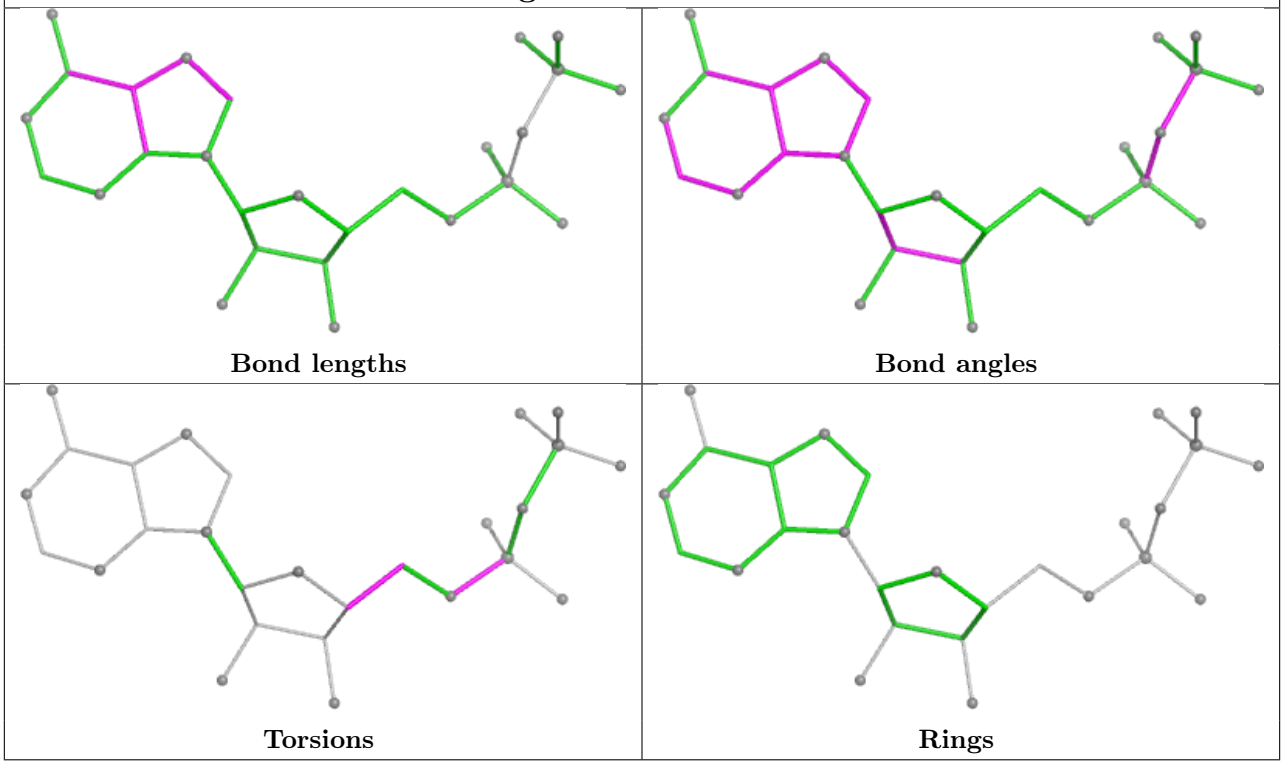


Torsions

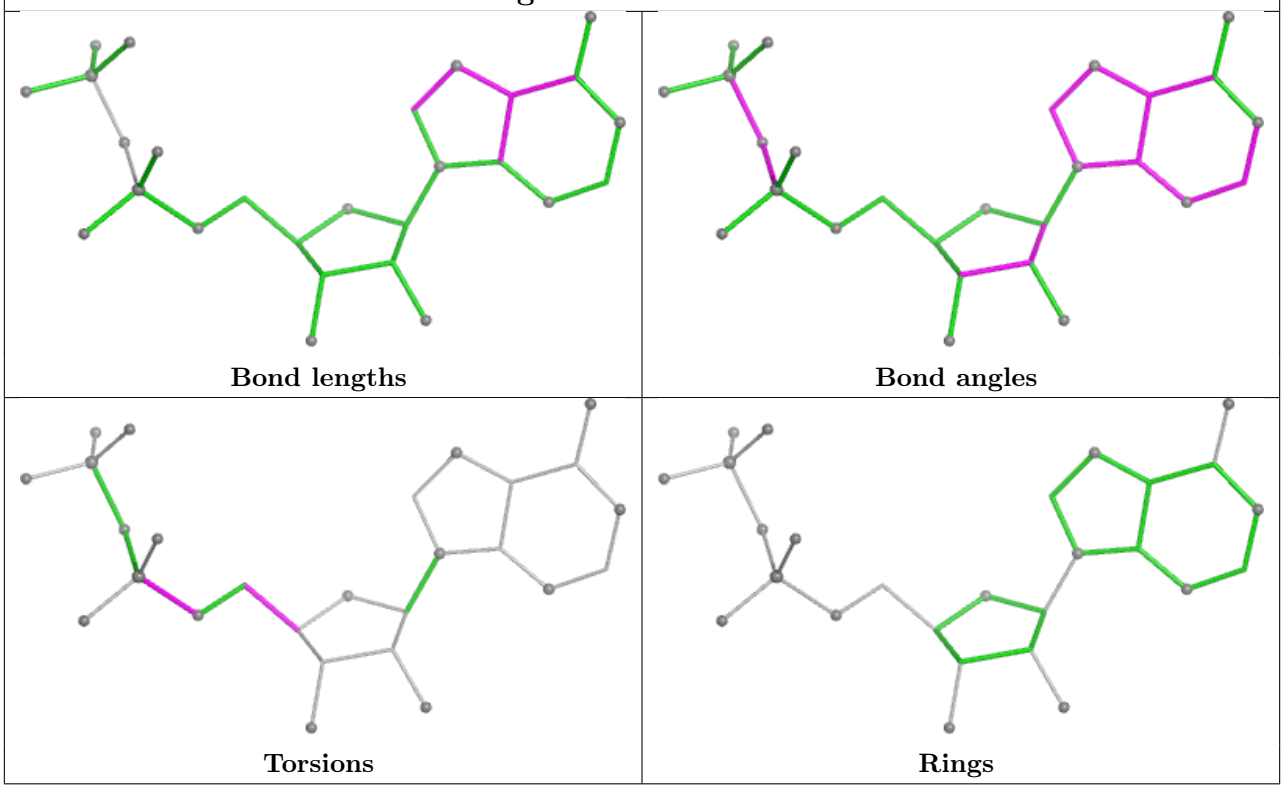


Rings

Ligand ADP e 1000



Ligand ADP b 1000



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.

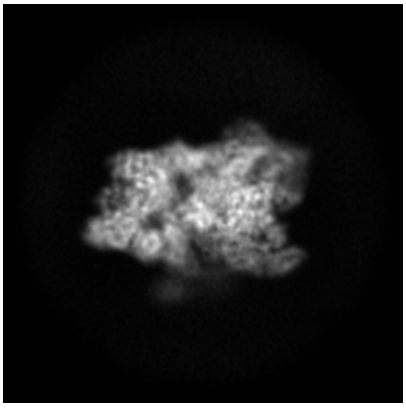
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11725. These allow visual inspection of the internal detail of the map and identification of artifacts.

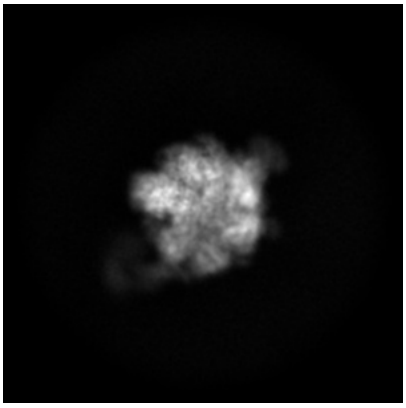
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

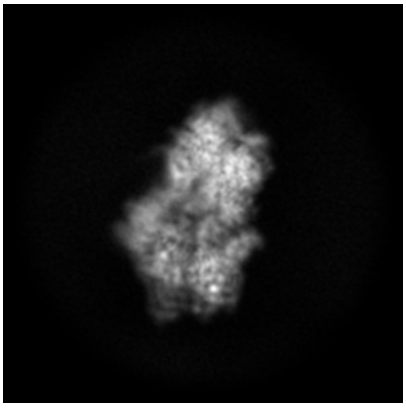
6.1.1 Primary map



X



Y

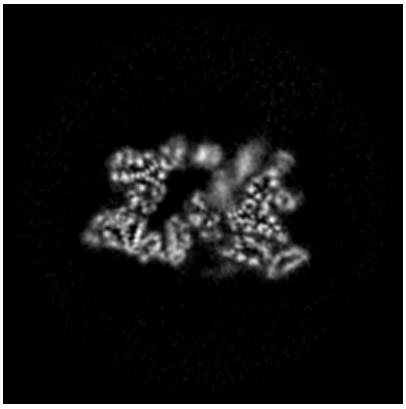


Z

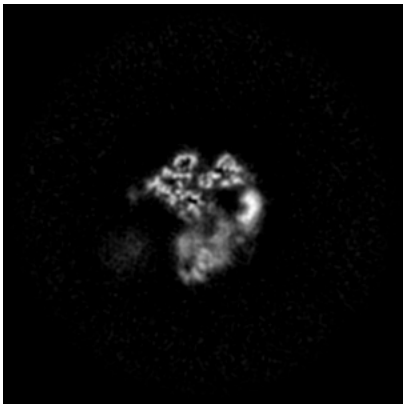
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

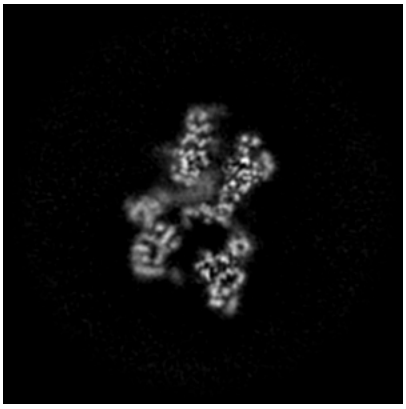
6.2.1 Primary map



X Index: 150



Y Index: 150

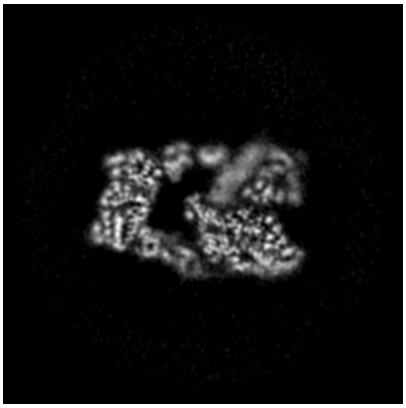


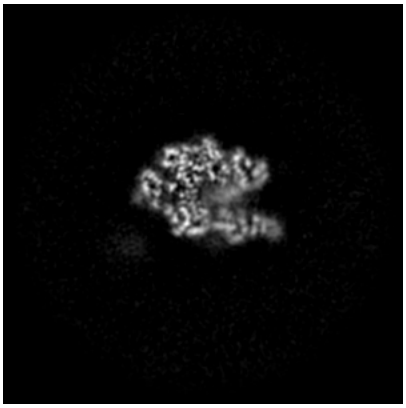
Z Index: 150

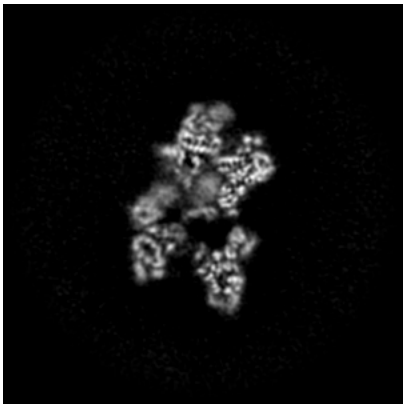
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 157

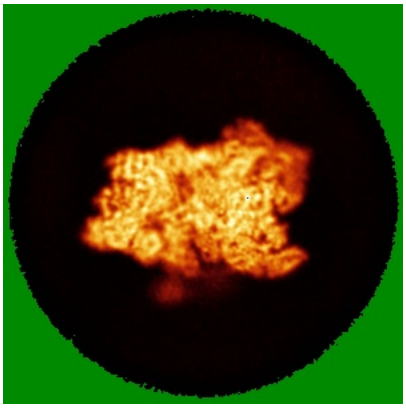

Y Index: 171

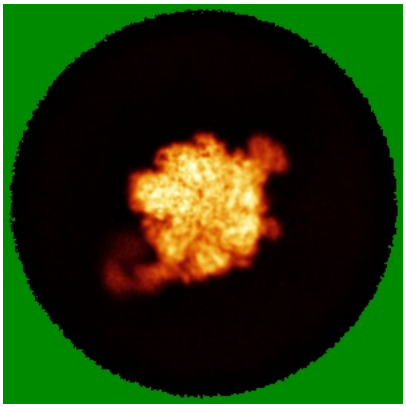

Z Index: 155

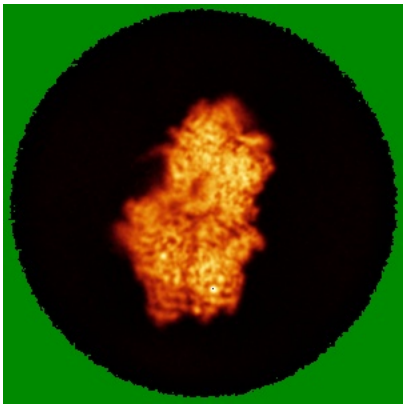
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

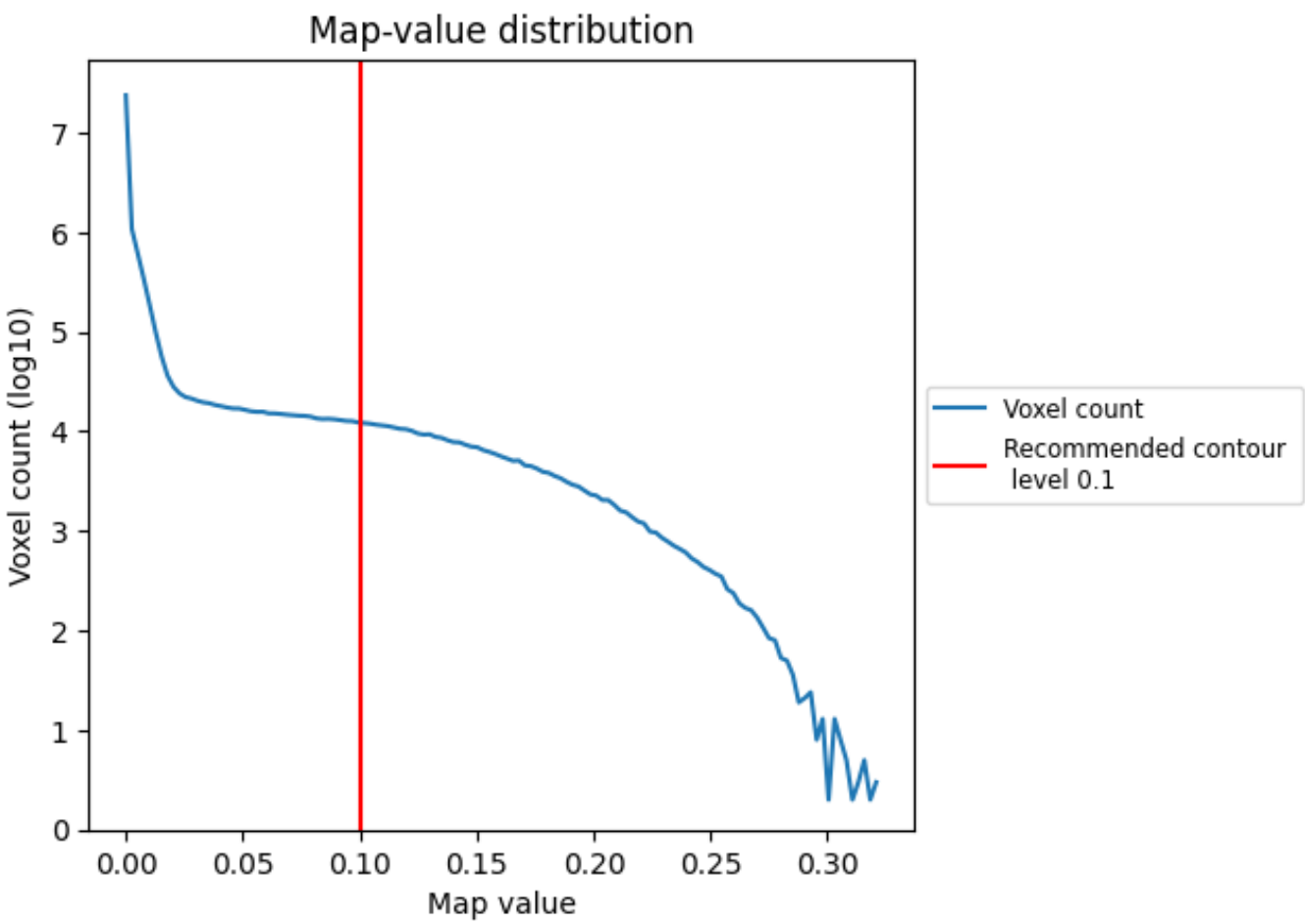
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

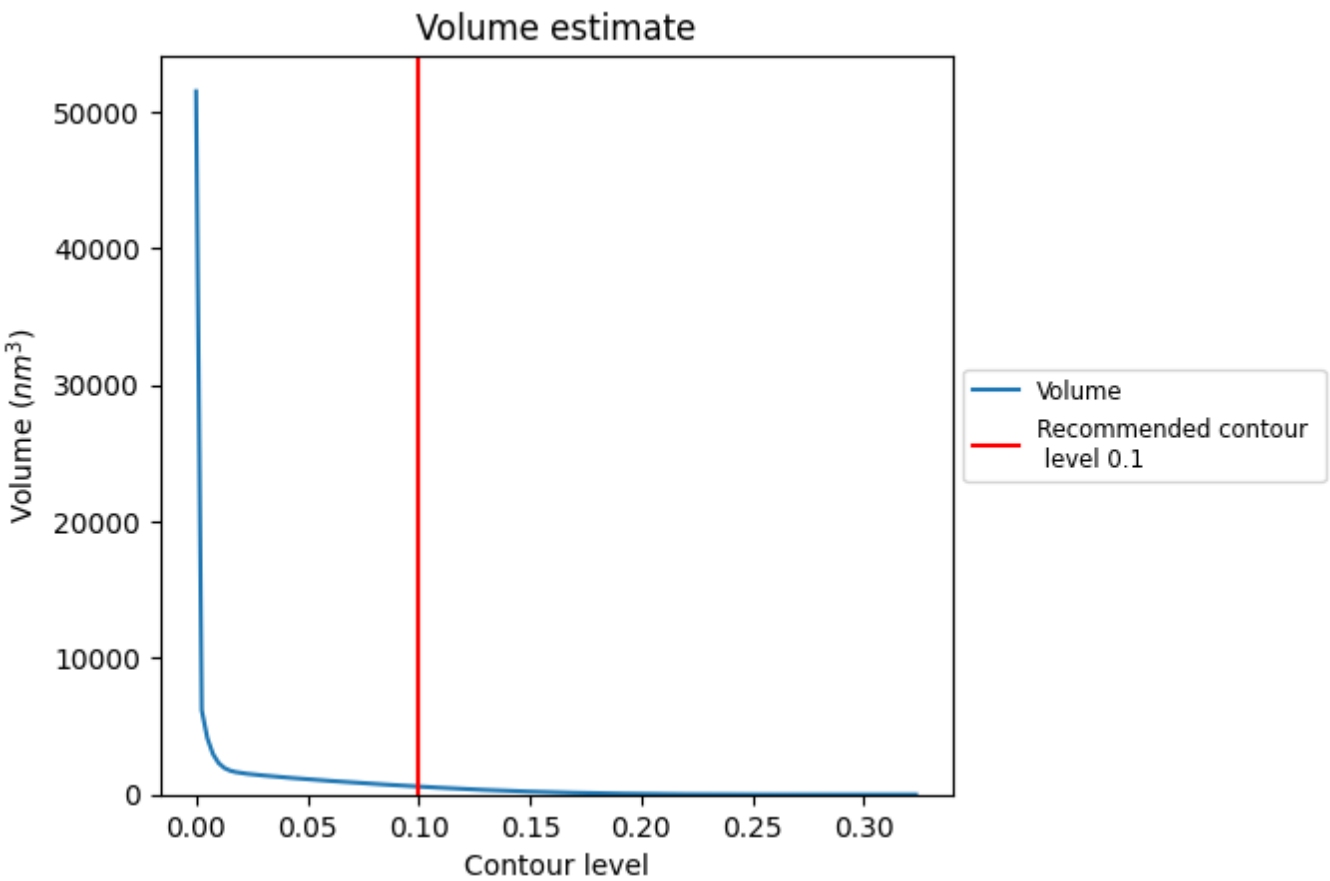
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

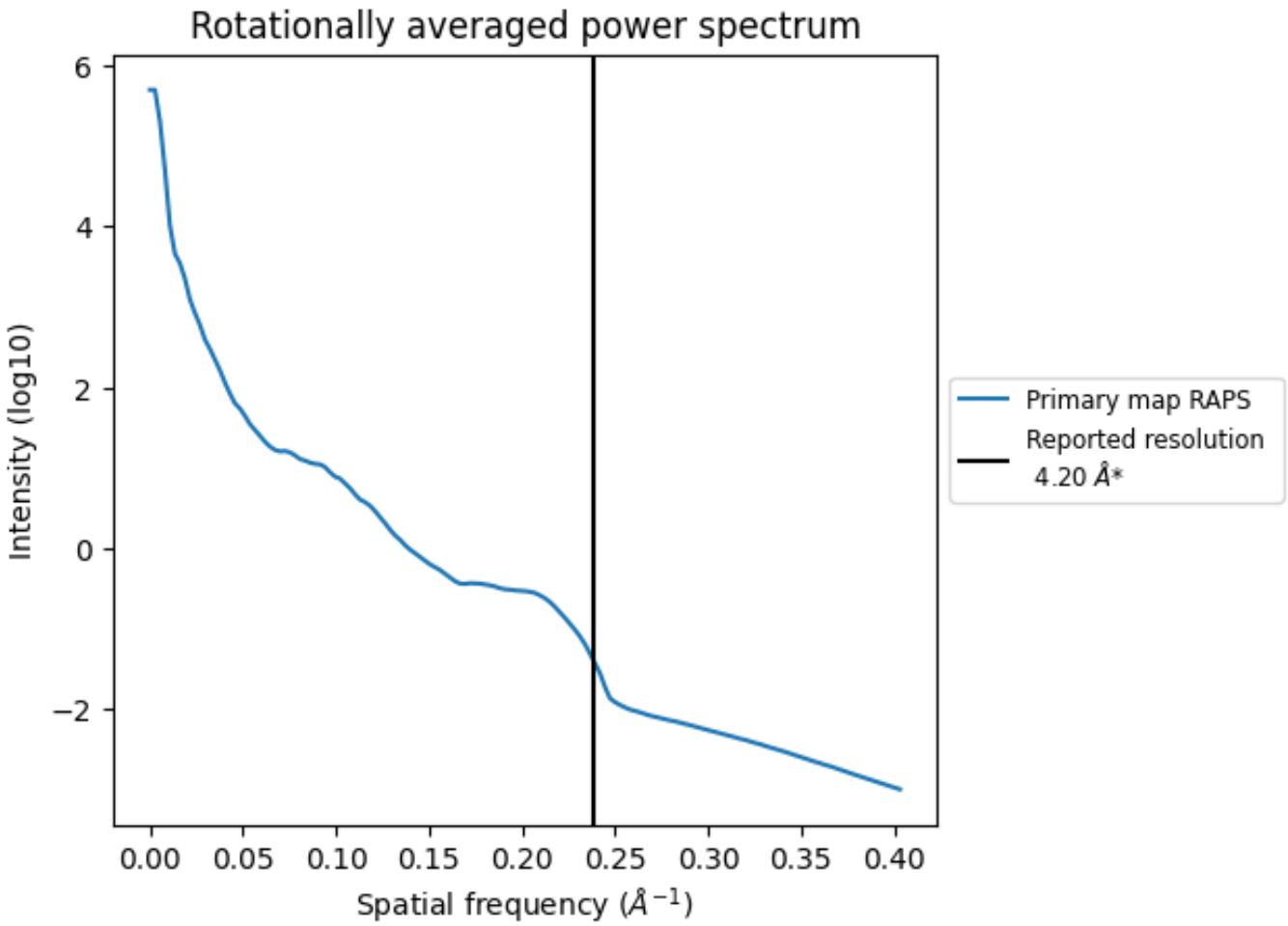
7.2 Volume estimate (i)



The volume at the recommended contour level is 585 nm^3; this corresponds to an approximate mass of 529 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

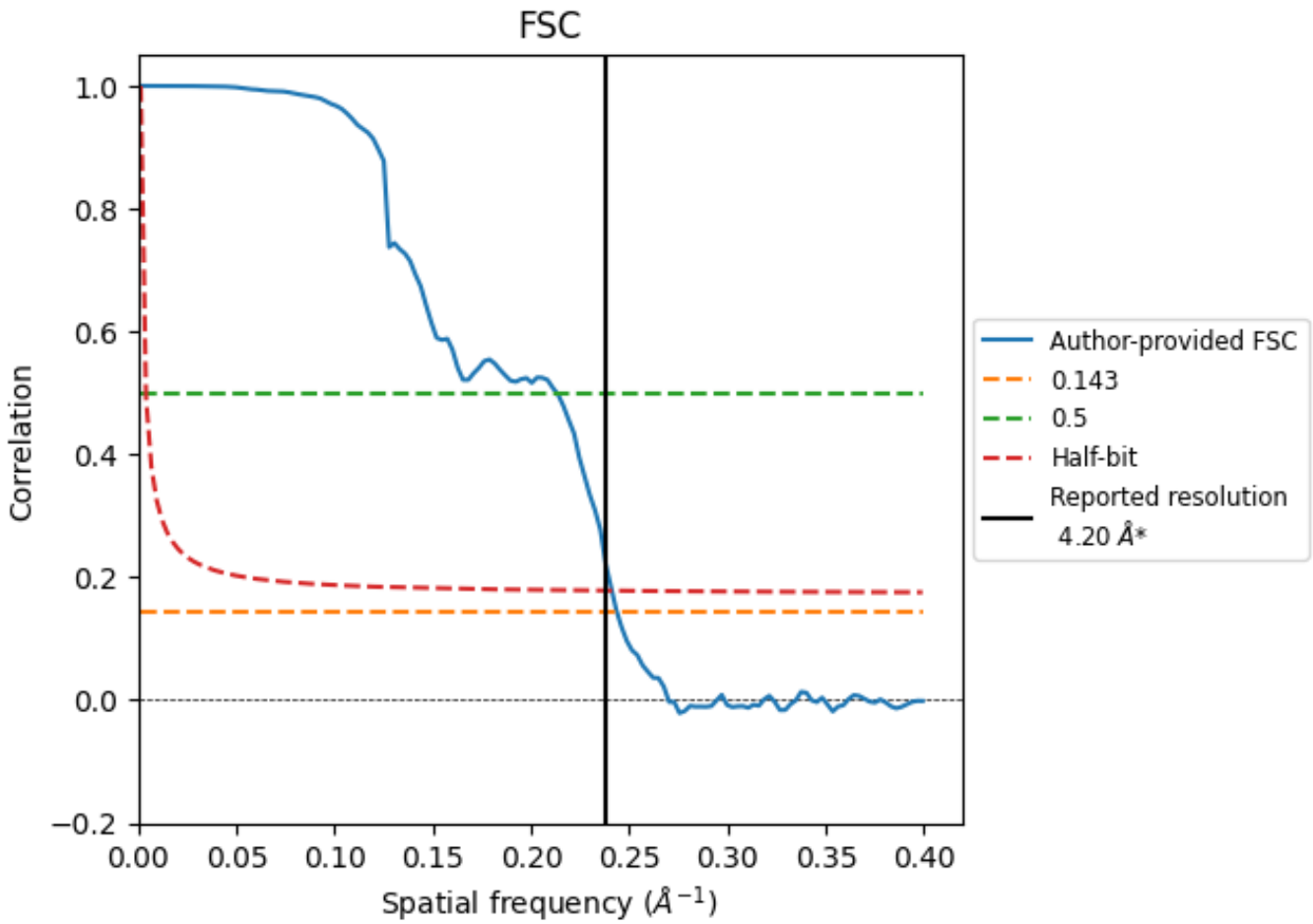


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

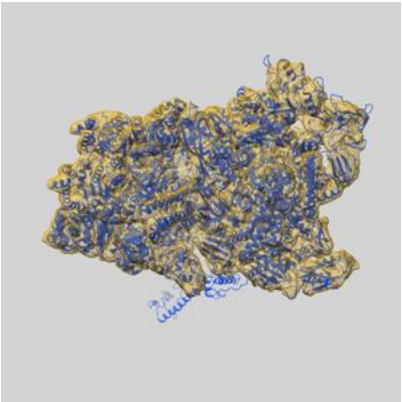
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.11	4.69	4.15
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

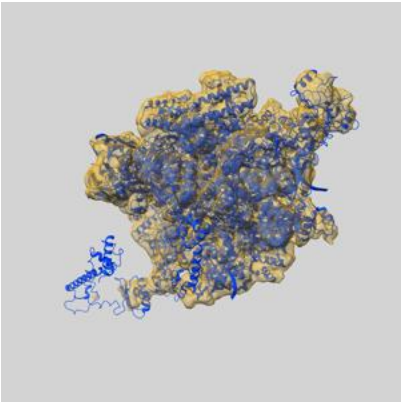
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11725 and PDB model 7ADE. Per-residue inclusion information can be found in section 3 on page 9.

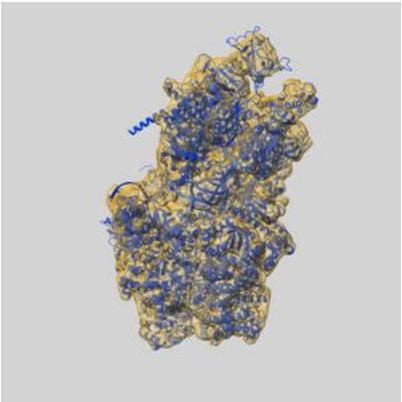
9.1 Map-model overlay (i)



X



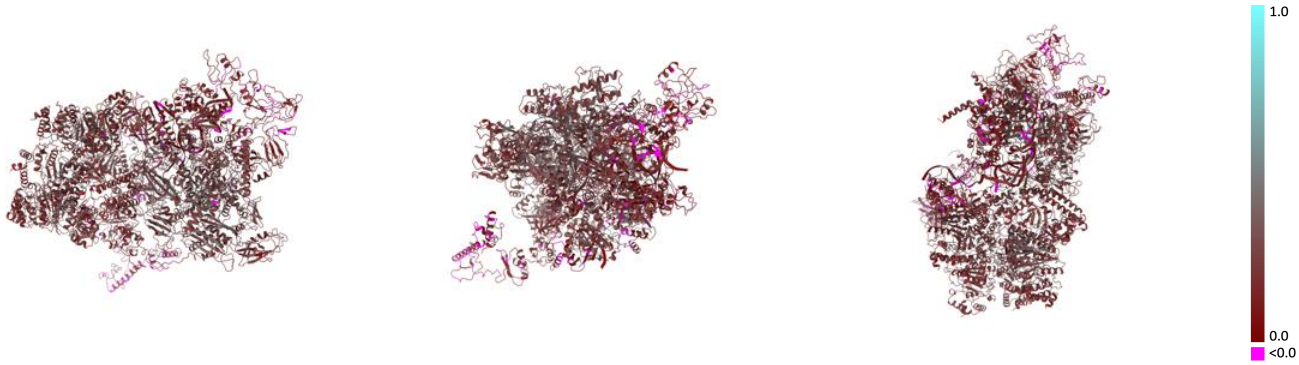
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

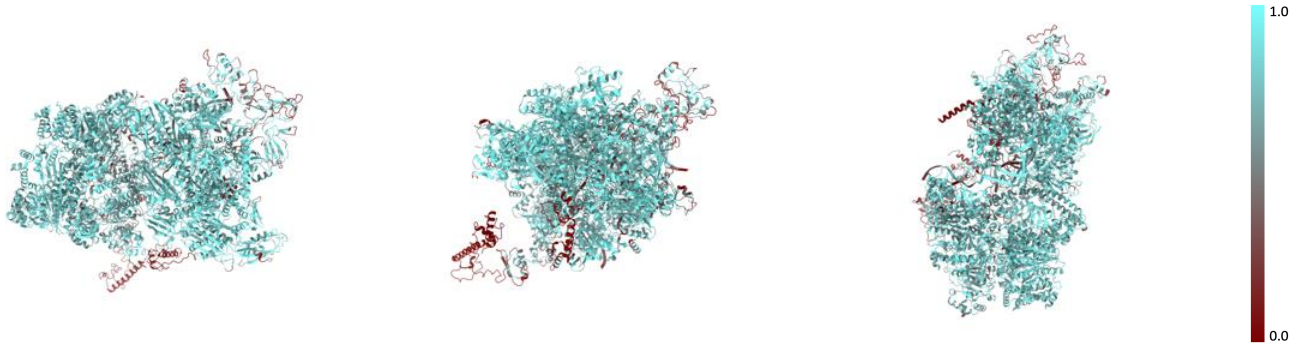
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

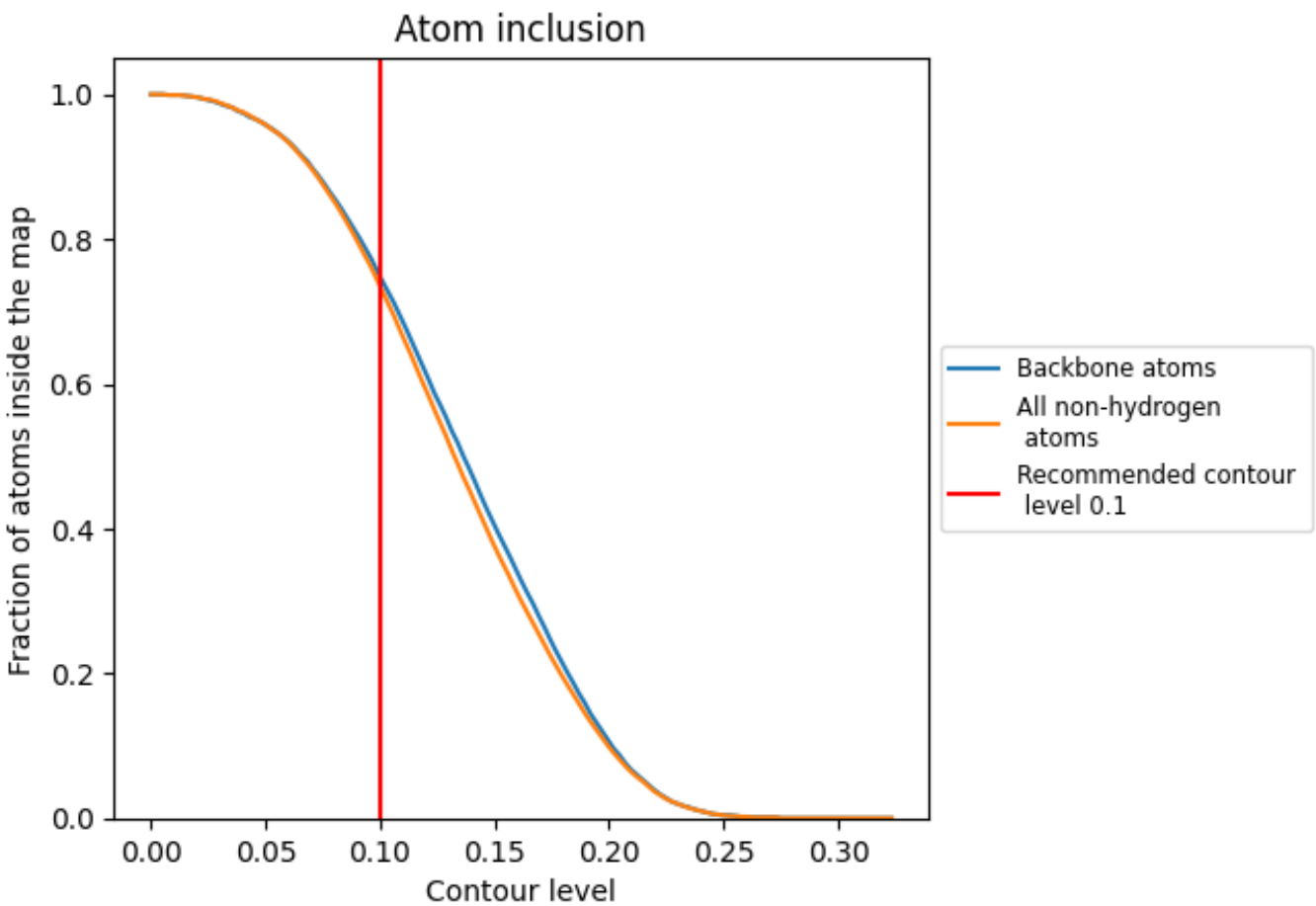
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7350	0.2350
A	0.4220	0.1450
K	0.7810	0.1130
L	0.7140	0.0770
R	0.7510	0.1610
U	0.8020	0.3050
V	0.7540	0.2480
W	0.1390	0.2090
X	0.8060	0.2790
Y	0.7280	0.2230
a	0.7920	0.2420
b	0.8260	0.2670
c	0.8230	0.2620
d	0.8100	0.2550
e	0.7520	0.2120
f	0.7360	0.2000