Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 08:14 AM EDT

PDB ID	:	2AFI / pdb_00002afi
Title	:	Crystal Structure of MgADP bound Av2-Av1 Complex
Authors	:	Tezcan, F.A.; Kaiser, J.T.; Mustafi, D.; Walton, M.Y.; Howard, J.B.; Rees, D.C.
Deposited on	:	2005-07-25
Resolution	:	3.10 Å(reported)

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

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

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

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

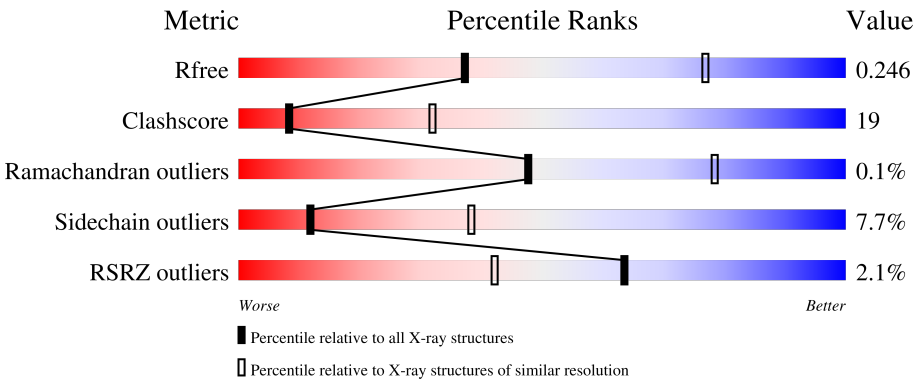
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	491	52% 37% 8% •
1	C	491	50% 38% 8% •
1	I	491	49% 40% 8% •
1	K	491	51% 38% 8% •
2	B	522	58% 35% 7% •

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Mol	Chain	Length	Quality of chain
2	D	522	56% 37% 6%
2	J	522	55% 38% 6% •
2	L	522	56% 38% 5% •
3	E	289	7% 47% 36% 9% • 6%
3	F	289	3% 39% 44% 11% • 5%
3	G	289	6% 39% 41% 11% 9%
3	H	289	3% 55% 33% 5% 7%
3	M	289	7% 43% 40% 8% • 7%
3	N	289	8% 61% 25% 7% 7%
3	O	289	7% 42% 36% 12% 9%
3	P	289	2% 54% 29% 8% • 8%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 48501 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3782	2405	645	708	24	31	0	0
1	C	476	3782	2405	645	708	24	28	0	0
1	I	476	3782	2405	645	708	24	0	0	0
1	K	476	3782	2405	645	708	24	17	0	0

- Molecule 2 is a protein called Nitrogenase molybdenum-iron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	522	4174	2666	705	775	28	39	0	0
2	D	522	4174	2666	705	775	28	10	0	0
2	J	522	4174	2666	705	775	28	5	0	0
2	L	522	4174	2666	705	775	28	5	0	0

- Molecule 3 is a protein called Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	271	2053	1283	350	400	20	453	0	0
3	F	275	2082	1301	354	406	21	242	0	0
3	G	263	1983	1236	342	386	19	280	0	0
3	H	269	2037	1271	348	398	20	1031	0	0

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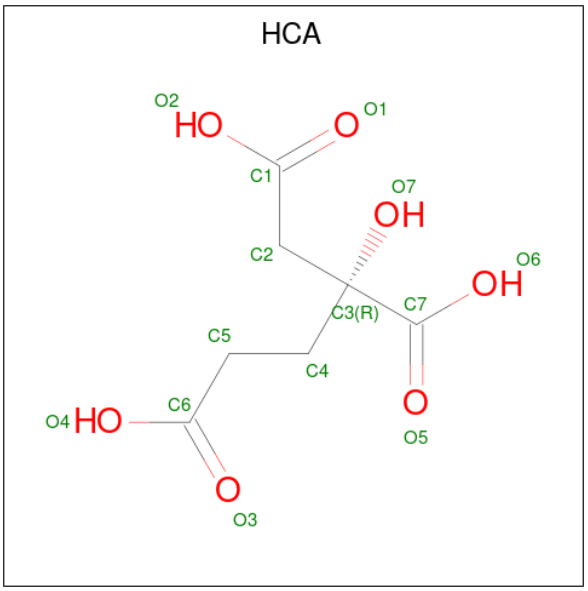
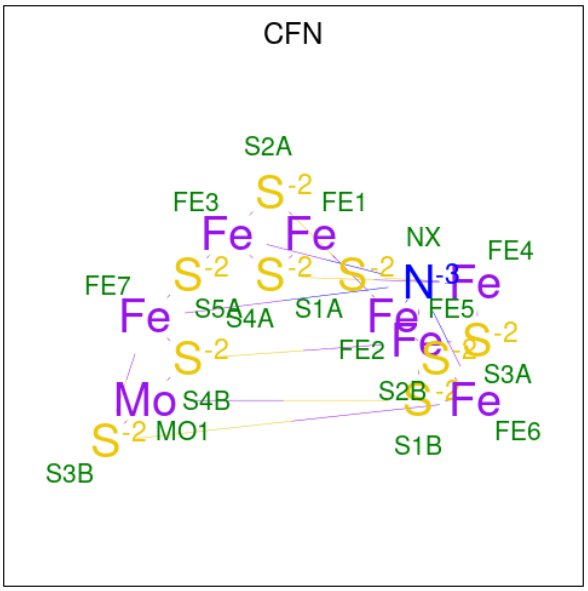
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	268	2029	1269	344	397	19	458	0	0
			Total	C	N	O	S			
3	N	270	2041	1277	346	399	19	1220	0	0
			Total	C	N	O	S			
3	O	262	1978	1233	341	385	19	302	0	0
			Total	C	N	O	S			
3	P	267	2018	1263	342	395	18	868	0	0

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	14	7	7	0	0
			Total	C	O		
4	C	1	14	7	7	0	0
			Total	C	O		
4	I	1	14	7	7	0	0
			Total	C	O		
4	K	1	14	7	7	0	0

- Molecule 5 is FE(7)-MO-S(9)-N CLUSTER (CCD ID: CFN) (formula: Fe_7MoNS_9).

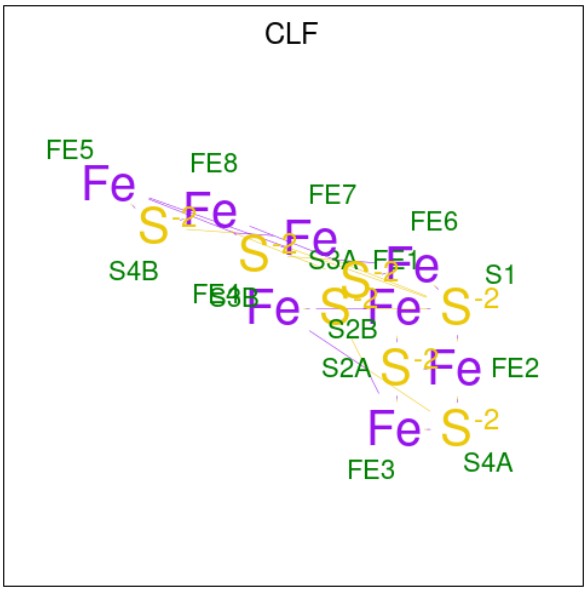


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Fe	Mo	N	S		
5	A	1	18	7	1	1	9	0	0
5	C	1	18	7	1	1	9	0	0
5	I	1	18	7	1	1	9	0	0
5	K	1	18	7	1	1	9	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B	2	2	2	0	0
6	J	1	1	1	0	0
6	L	1	1	1	0	0

- Molecule 7 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe_8S_7).

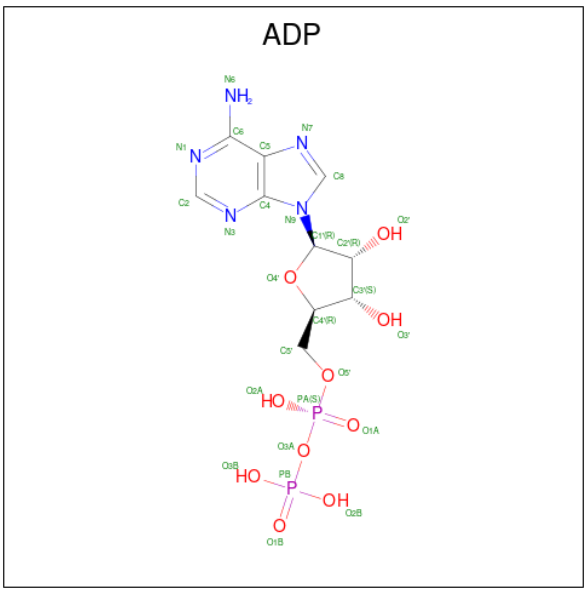


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Fe S 15 8 7	0	0
7	D	1	Total Fe S 15 8 7	0	0
7	J	1	Total Fe S 15 8 7	0	0
7	L	1	Total Fe S 15 8 7	0	0

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

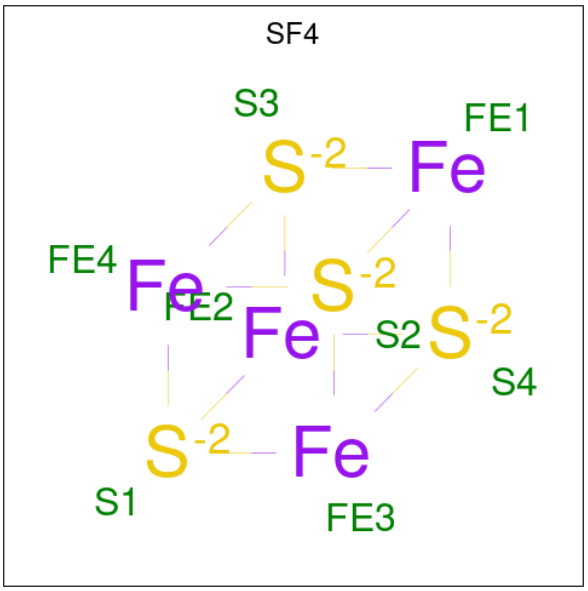
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	E	1	Total Mg 1 1	0	0
8	F	1	Total Mg 1 1	0	0
8	G	1	Total Mg 1 1	0	0
8	H	1	Total Mg 1 1	0	0
8	M	1	Total Mg 1 1	0	0
8	N	1	Total Mg 1 1	0	0
8	O	1	Total Mg 1 1	0	0
8	P	1	Total Mg 1 1	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	E	1	27	10	5	10	2	0	0
9	F	1	27	10	5	10	2	0	0
9	G	1	27	10	5	10	2	0	0
9	H	1	27	10	5	10	2	10	0
9	M	1	27	10	5	10	2	0	0
9	N	1	27	10	5	10	2	10	0
9	O	1	27	10	5	10	2	0	0
9	P	1	27	10	5	10	2	0	0

- Molecule 10 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
10	F	1	8	4	4	0	0
			Total	Fe	S		
10	G	1	8	4	4	0	0
			Total	Fe	S		
10	N	1	8	4	4	0	0
			Total	Fe	S		
10	P	1	8	4	4	0	0

- Molecule 11 is water.

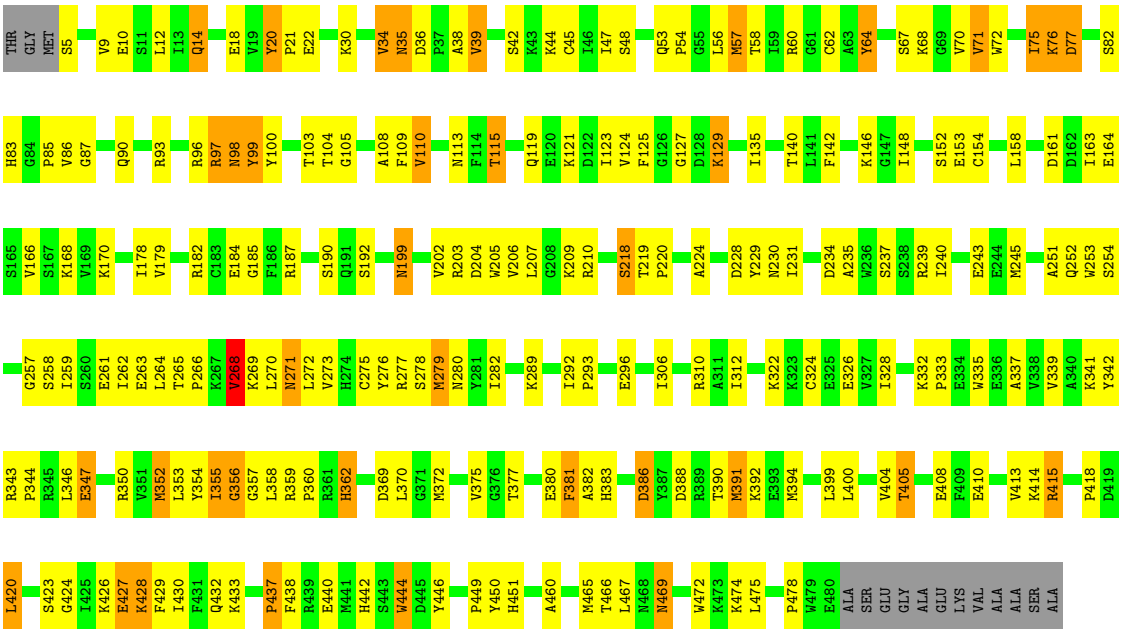
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	B	2	2	2	0	0
			Total	O		
11	D	2	2	2	0	0
			Total	O		
11	J	2	2	2	0	0
			Total	O		
11	L	2	2	2	0	0

3 Residue-property plots (i)

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

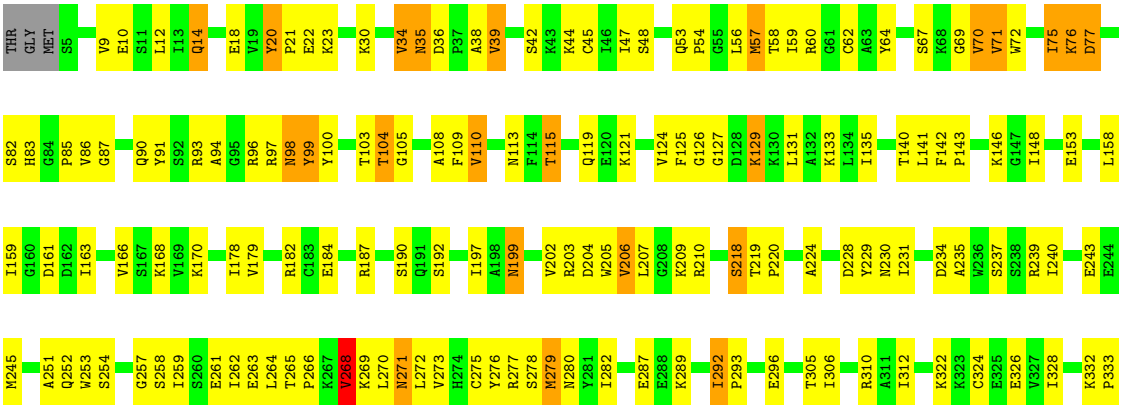
• Molecule 1: Nitrogenase molybdenum-iron protein

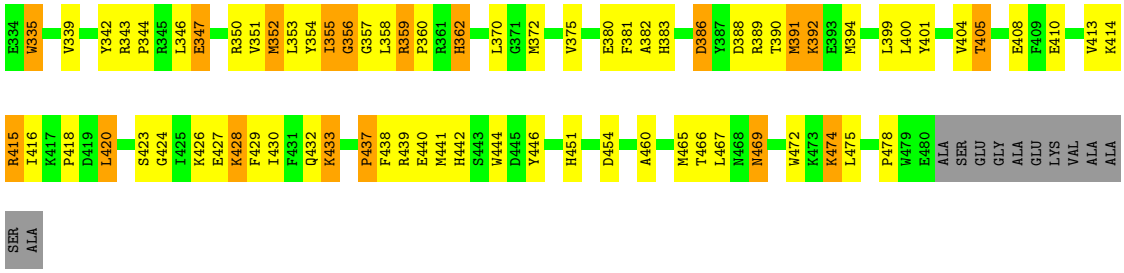
Chain A:



• Molecule 1: Nitrogenase molybdenum-iron protein

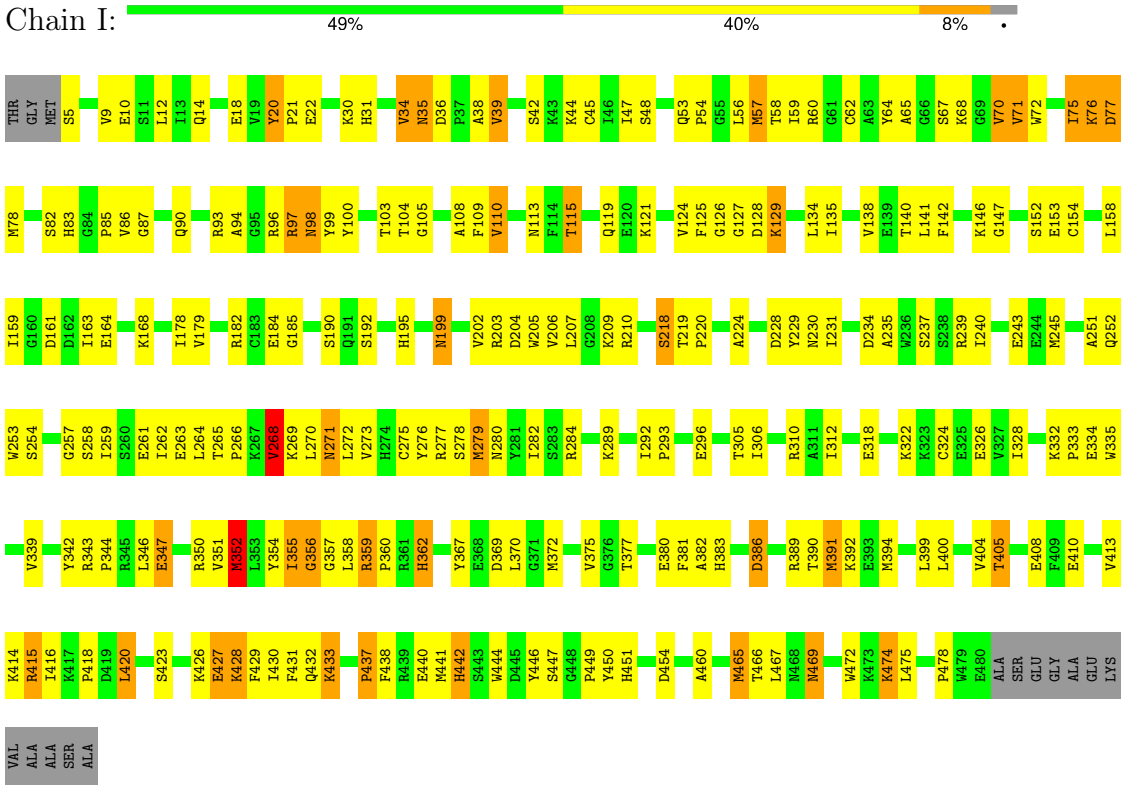
Chain C:





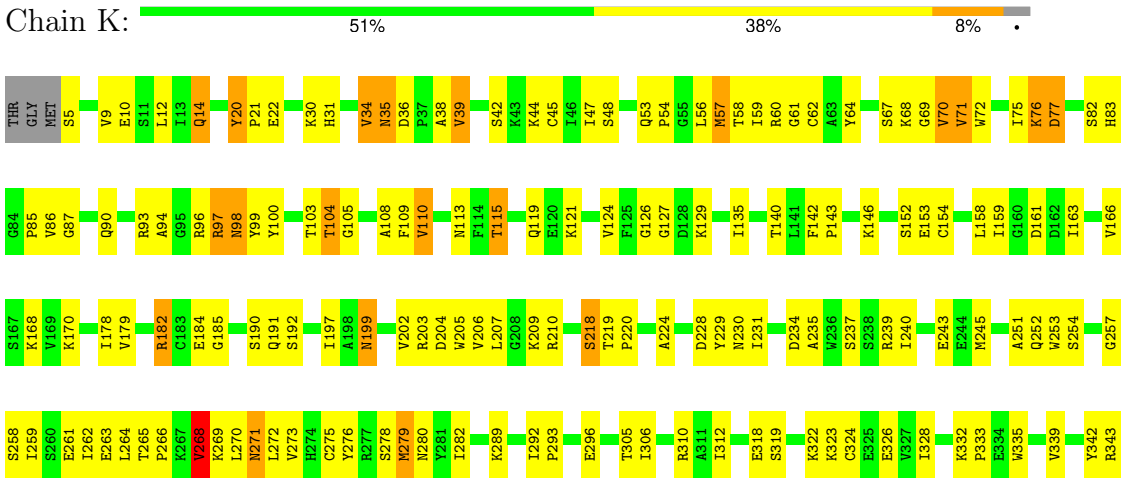
- Molecule 1: Nitrogenase molybdenum-iron protein

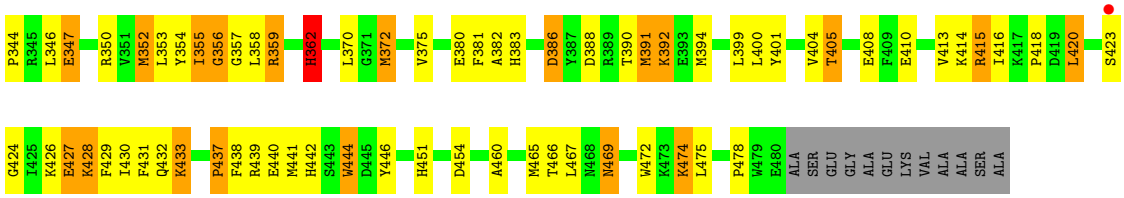
Chain I:



- Molecule 1: Nitrogenase molybdenum-iron protein

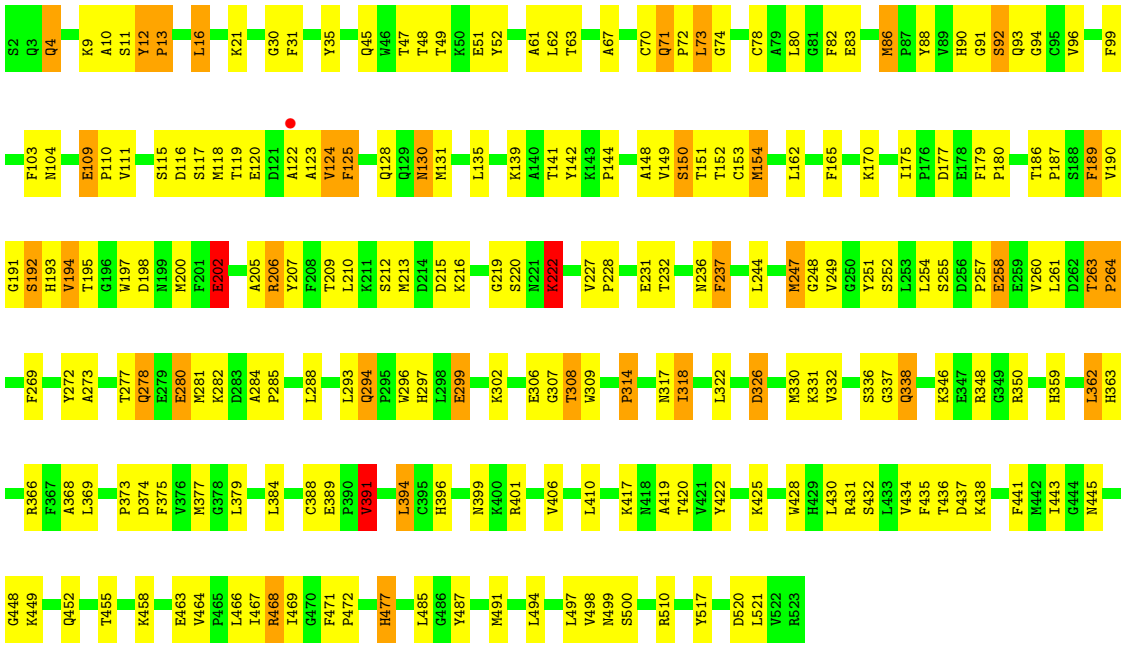
Chain K:





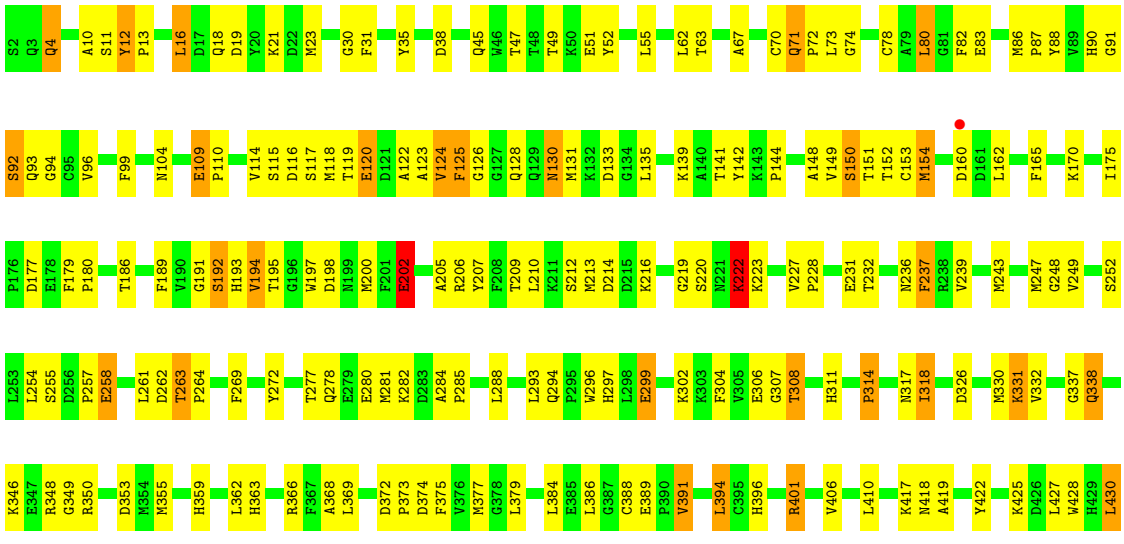
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain B:



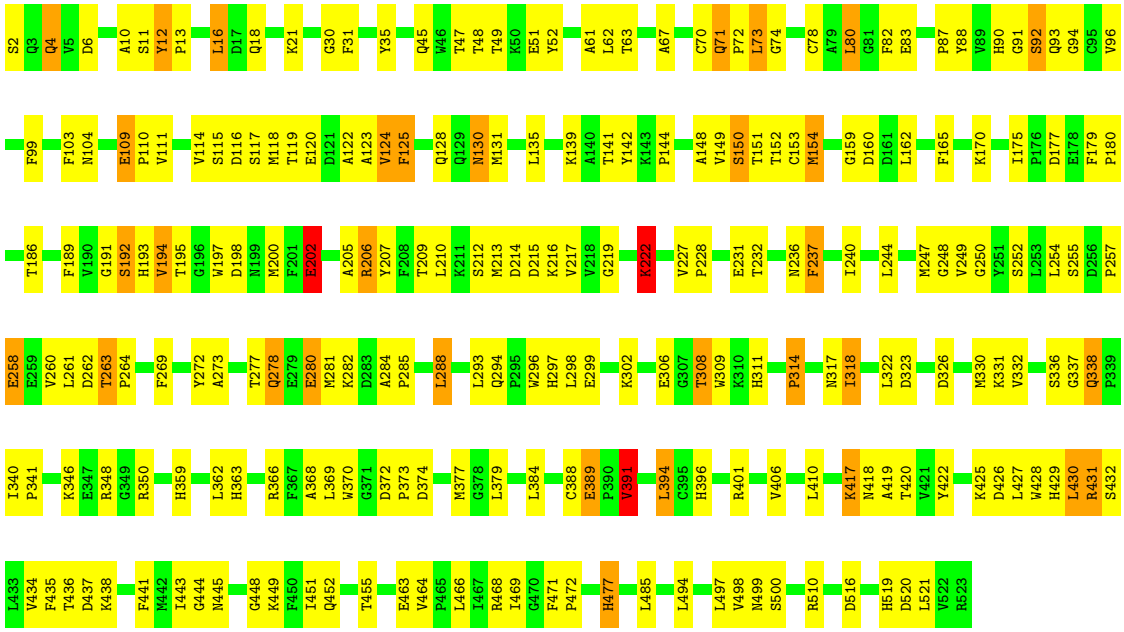
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain D:



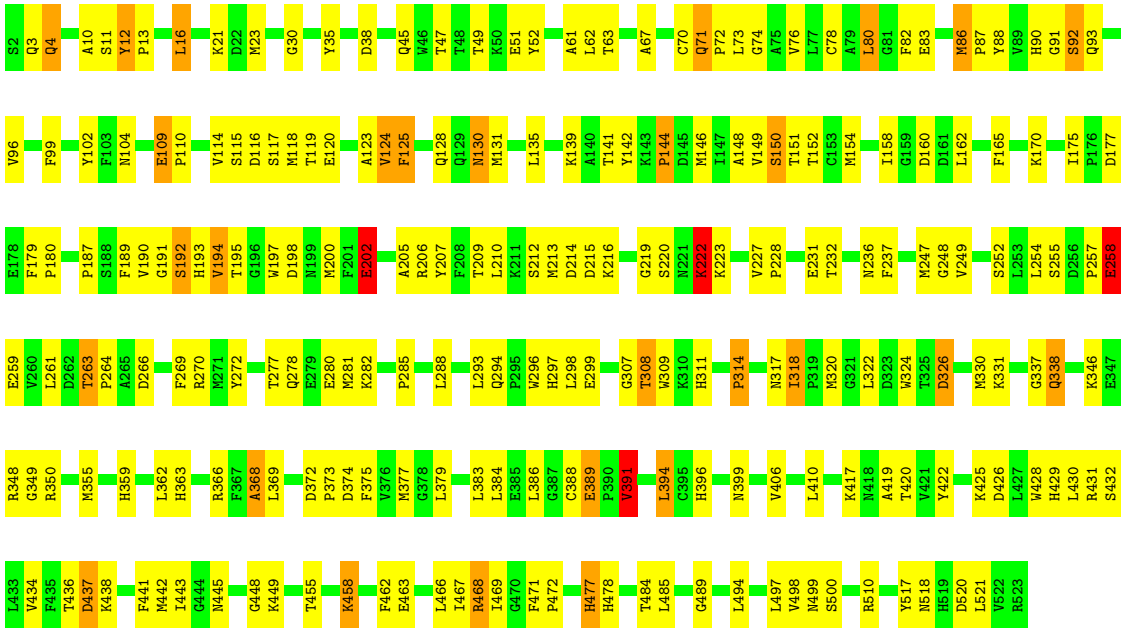
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain J:



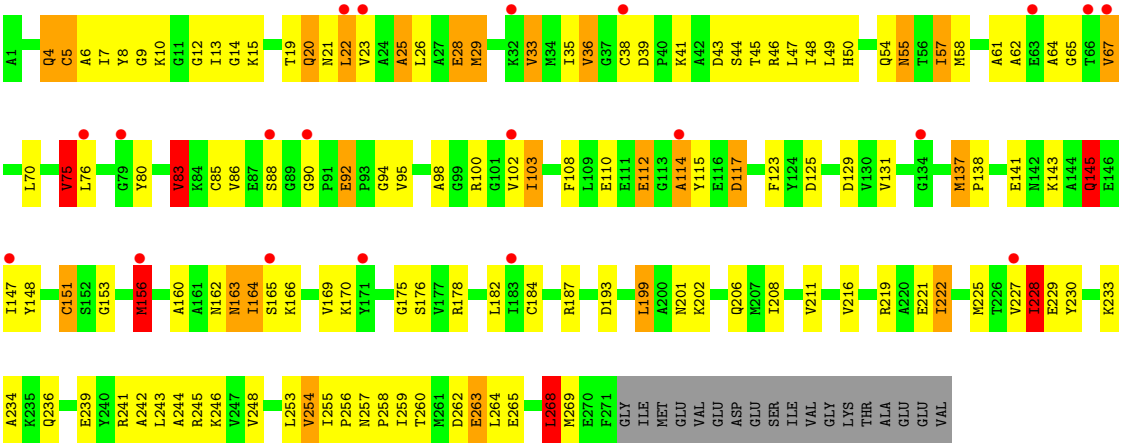
• Molecule 2: Nitrogenase molybdenum-iron protein

Chain L:



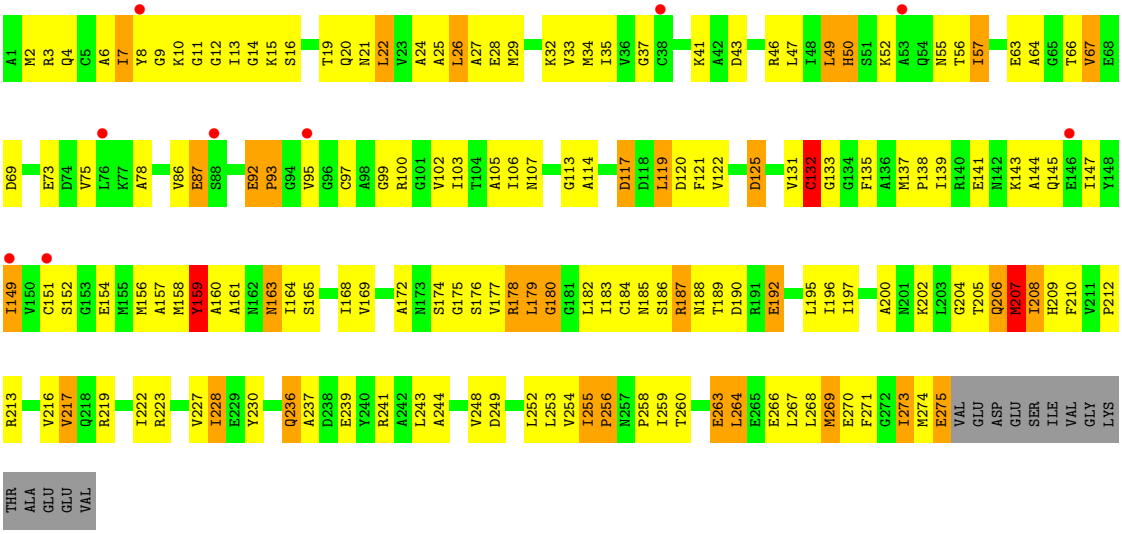
• Molecule 3: Nitrogenase iron protein 1

Chain E:



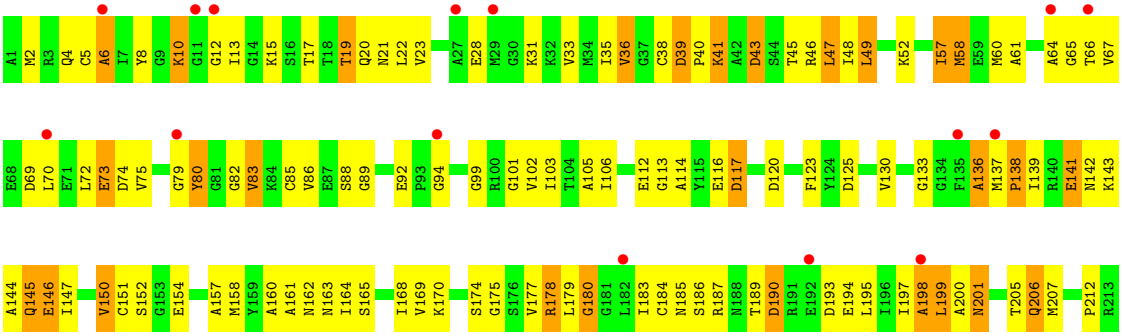
- Molecule 3: Nitrogenase iron protein 1

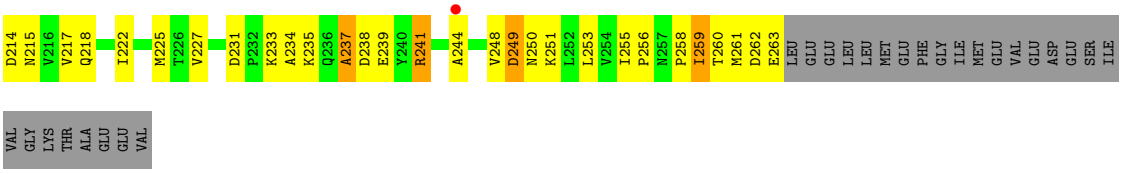
Chain F:



- Molecule 3: Nitrogenase iron protein 1

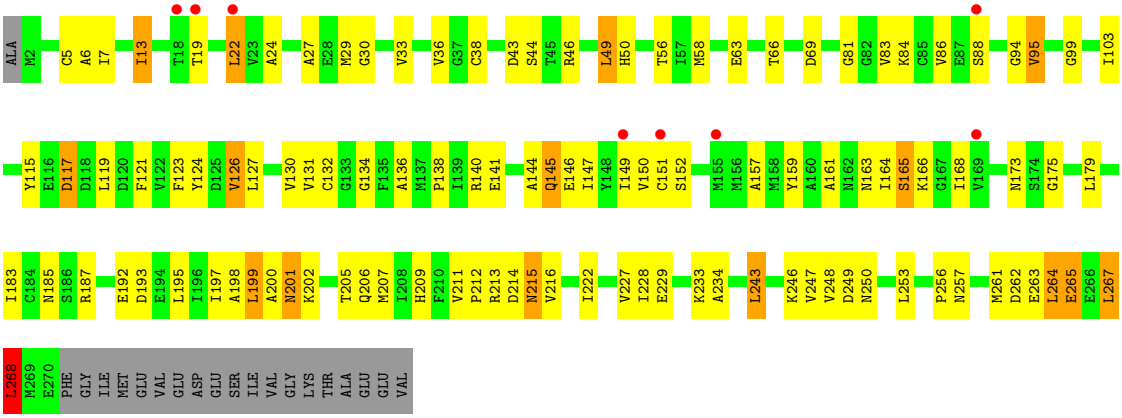
Chain G:





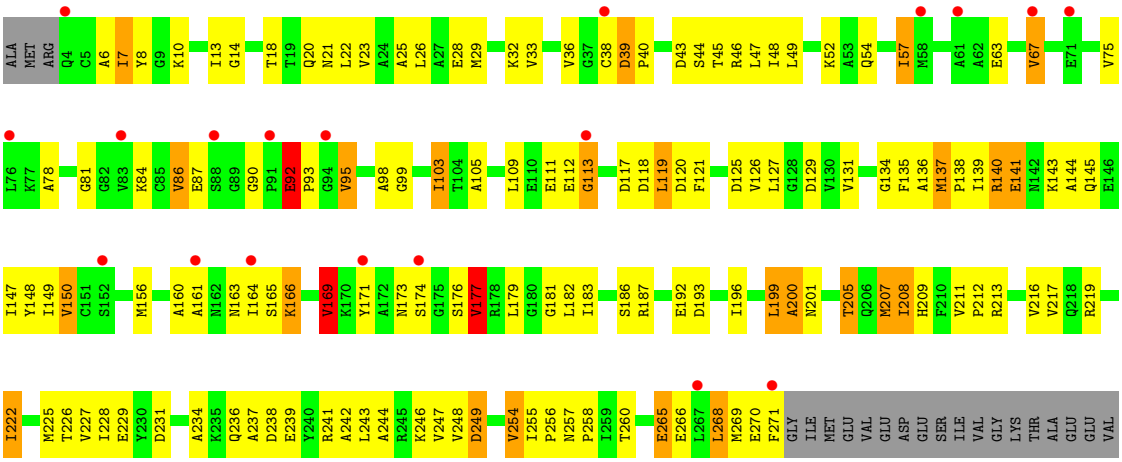
• Molecule 3: Nitrogenase iron protein 1

Chain H:



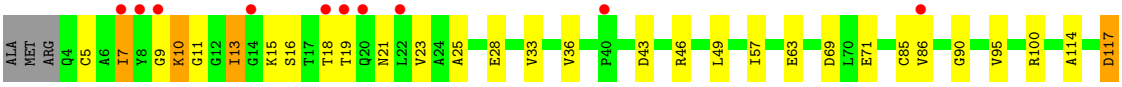
• Molecule 3: Nitrogenase iron protein 1

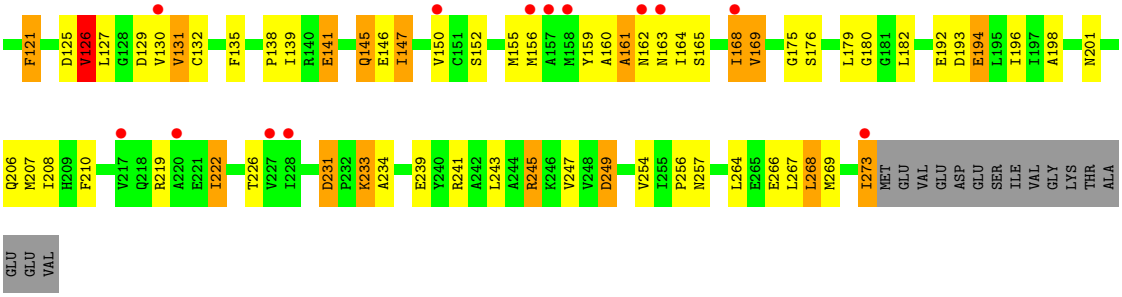
Chain M:



• Molecule 3: Nitrogenase iron protein 1

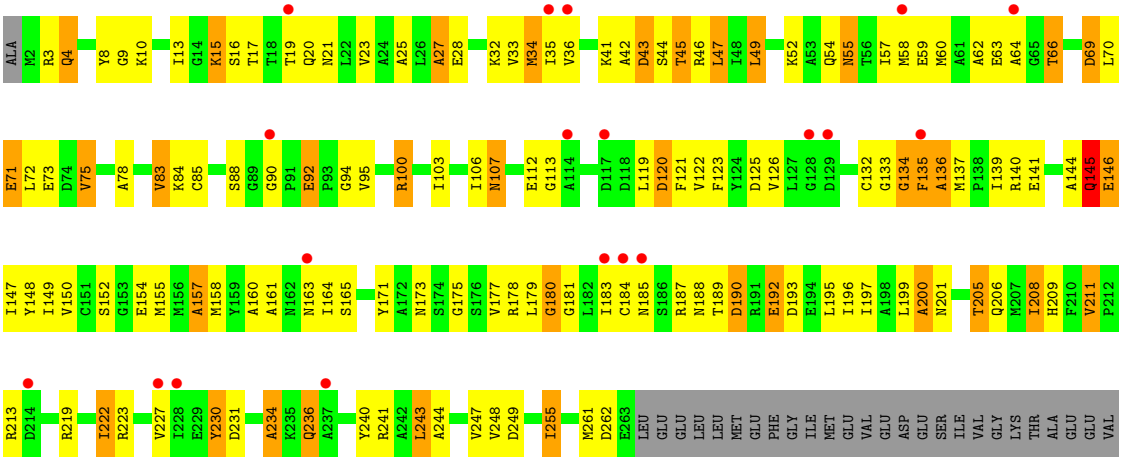
Chain N:





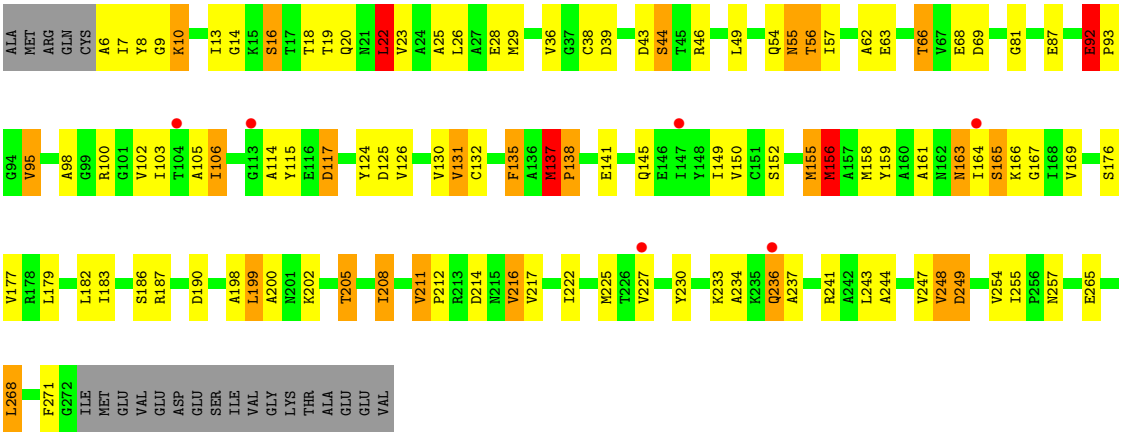
- Molecule 3: Nitrogenase iron protein 1

Chain O:



- Molecule 3: Nitrogenase iron protein 1

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.92Å 141.43Å 165.55Å 73.69° 79.37° 76.58°	Depositor
Resolution (Å)	49.43 – 3.10 49.43 – 3.10	Depositor EDS
% Data completeness (in resolution range)	87.5 (49.43-3.10) 87.5 (49.43-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.77 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.270 0.207 , 0.246	Depositor DCC
R_{free} test set	10115 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.048 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	48501	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HCA, MG, CFN, SF4, ADP, CA, CLF

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	0.89	0/3870	1.57	82/5219 (1.6%)
1	C	0.93	1/3870 (0.0%)	1.57	83/5219 (1.6%)
1	I	0.88	2/3870 (0.1%)	1.58	86/5219 (1.6%)
1	K	0.88	1/3870 (0.0%)	1.62	89/5219 (1.7%)
2	B	0.99	0/4280	1.47	88/5786 (1.5%)
2	D	0.99	1/4280 (0.0%)	1.48	88/5786 (1.5%)
2	J	0.98	2/4280 (0.0%)	1.49	95/5786 (1.6%)
2	L	0.94	0/4280	1.48	86/5786 (1.5%)
3	E	0.82	0/2077	1.72	56/2798 (2.0%)
3	F	0.83	0/2106	1.61	49/2836 (1.7%)
3	G	0.90	0/2006	1.66	58/2703 (2.1%)
3	H	0.75	0/2060	1.61	46/2775 (1.7%)
3	M	0.77	0/2053	1.66	56/2767 (2.0%)
3	N	0.76	1/2065 (0.0%)	1.71	54/2783 (1.9%)
3	O	0.84	1/2001 (0.0%)	1.74	62/2696 (2.3%)
3	P	0.76	1/2042 (0.0%)	1.70	62/2752 (2.3%)
All	All	0.90	10/49010 (0.0%)	1.58	1140/66130 (1.7%)

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
1	A	0	2
1	C	0	3
1	I	0	1
1	K	0	1
2	B	0	1
2	D	0	1
2	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
3	F	0	1
All	All	0	12

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	352	MET	SD-CE	-6.21	1.64	1.79
1	I	465	MET	SD-CE	5.96	1.94	1.79
3	P	156	MET	SD-CE	-5.85	1.65	1.79
3	N	7	ILE	CA-CB	5.83	1.61	1.54
2	J	186	THR	CA-CB	5.55	1.59	1.53
1	K	372	MET	SD-CE	5.42	1.93	1.79
2	J	217	VAL	CA-CB	-5.20	1.48	1.54
2	D	331	LYS	C-O	-5.15	1.18	1.24
3	O	34	MET	SD-CE	5.12	1.92	1.79
1	C	110	VAL	CA-CB	5.01	1.60	1.54

All (1140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	356	GLY	N-CA-C	17.02	133.09	112.49
1	A	356	GLY	N-CA-C	16.75	134.21	112.77
1	K	356	GLY	N-CA-C	16.47	133.86	112.77
1	K	182	ARG	NE-CZ-NH2	16.07	133.66	119.20
1	C	356	GLY	N-CA-C	15.53	132.65	112.77
1	K	182	ARG	NE-CZ-NH1	-15.18	106.32	121.50
1	K	182	ARG	CD-NE-CZ	13.46	143.24	124.40
3	E	90	GLY	CA-C-N	12.43	132.33	120.03
3	E	90	GLY	C-N-CA	12.43	132.33	120.03
3	E	67	VAL	N-CA-C	12.40	123.25	110.72
3	M	187	ARG	N-CA-C	12.26	124.72	111.36
3	E	141	GLU	N-CA-C	-12.20	92.46	110.52
1	C	428	LYS	N-CA-C	11.93	124.28	111.28
2	D	438	LYS	N-CA-C	11.86	125.72	109.24
3	P	46	ARG	N-CA-C	11.78	124.20	111.36
1	K	87	GLY	N-CA-C	11.73	126.81	112.73
1	I	72	TRP	N-CA-C	11.67	124.08	111.36
3	O	141	GLU	N-CA-C	-11.63	94.85	110.55
1	A	428	LYS	N-CA-C	11.61	123.94	111.28
2	L	438	LYS	N-CA-C	11.60	125.36	109.24
3	N	46	ARG	N-CA-C	11.57	123.90	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	N	234	ALA	N-CA-C	11.57	125.28	110.24
3	G	69	ASP	N-CA-C	-11.56	96.64	112.94
3	P	117	ASP	N-CA-C	-11.46	91.38	109.72
3	N	141	GLU	N-CA-C	-11.44	93.55	110.48
1	K	110	VAL	N-CA-C	11.43	121.39	110.42
1	C	45	CYS	N-CA-C	11.31	123.36	111.14
1	K	428	LYS	N-CA-C	11.28	123.57	111.28
1	I	45	CYS	N-CA-C	11.25	123.29	111.14
1	C	76	LYS	N-CA-C	11.22	123.59	111.36
1	A	87	GLY	N-CA-C	11.18	126.14	112.73
1	A	475	LEU	N-CA-C	11.18	123.46	111.28
1	A	76	LYS	N-CA-C	11.16	123.52	111.36
1	C	110	VAL	N-CA-C	11.08	121.05	110.42
3	P	222	ILE	N-CA-C	-11.05	99.55	110.72
3	M	270	GLU	N-CA-C	10.95	122.97	111.14
1	A	110	VAL	N-CA-C	10.92	120.90	110.42
1	I	475	LEU	N-CA-C	10.92	123.18	111.28
1	C	71	VAL	N-CA-C	10.79	120.67	110.53
1	I	87	GLY	N-CA-C	10.77	125.65	112.73
3	H	69	ASP	N-CA-C	-10.74	97.80	112.94
3	P	69	ASP	N-CA-C	-10.70	97.57	113.61
2	B	438	LYS	N-CA-C	10.67	124.07	109.24
1	A	71	VAL	N-CA-C	10.66	120.55	110.53
1	K	475	LEU	N-CA-C	10.64	122.88	111.28
1	K	192	SER	N-CA-C	10.64	122.95	111.36
2	L	141	THR	N-CA-C	10.57	122.56	111.14
3	F	64	ALA	N-CA-C	-10.57	99.84	111.36
1	K	45	CYS	N-CA-C	10.56	122.54	111.14
3	M	57	ILE	N-CA-C	-10.55	100.06	110.72
1	A	45	CYS	N-CA-C	10.47	122.45	111.14
2	D	141	THR	N-CA-C	10.46	122.43	111.14
2	B	141	THR	N-CA-C	10.39	122.68	111.36
1	I	76	LYS	N-CA-C	10.34	122.63	111.36
1	I	428	LYS	N-CA-C	10.28	122.49	111.28
2	J	141	THR	N-CA-C	10.27	122.55	111.36
2	B	210	LEU	N-CA-C	10.23	122.52	111.36
1	I	474	LYS	N-CA-C	10.20	125.32	113.19
3	N	43	ASP	N-CA-C	-10.19	99.73	112.88
3	G	52	LYS	N-CA-C	-10.17	100.28	111.36
3	F	208	ILE	N-CA-C	10.11	120.93	110.72
2	J	438	LYS	N-CA-C	10.08	124.36	109.04
1	K	76	LYS	N-CA-C	10.06	122.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	22	GLU	N-CA-C	10.05	122.24	111.28
1	A	192	SER	N-CA-C	9.98	122.24	111.36
1	K	72	TRP	N-CA-C	9.98	123.97	111.69
3	O	90	GLY	CA-C-N	9.95	129.90	119.85
3	O	90	GLY	C-N-CA	9.95	129.90	119.85
1	C	206	VAL	N-CA-C	9.92	123.25	113.53
1	C	87	GLY	N-CA-C	9.90	124.61	112.73
1	I	390	THR	N-CA-C	9.83	122.08	111.36
1	K	35	ASN	N-CA-C	9.79	124.65	109.96
1	A	22	GLU	N-CA-C	9.76	121.92	111.28
1	K	206	VAL	N-CA-C	9.71	123.05	113.53
1	K	22	GLU	N-CA-C	9.70	121.86	111.28
3	M	43	ASP	N-CA-C	-9.69	100.38	112.88
1	C	22	GLU	N-CA-C	9.68	121.83	111.28
1	A	474	LYS	N-CA-C	9.67	124.70	113.19
1	I	71	VAL	N-CA-C	9.66	119.61	110.53
3	P	114	ALA	N-CA-C	-9.65	100.84	111.36
2	B	30	GLY	N-CA-C	9.63	124.14	112.49
3	P	141	GLU	N-CA-C	-9.62	95.03	110.32
1	I	192	SER	N-CA-C	9.61	121.83	111.36
1	I	206	VAL	N-CA-C	9.57	122.91	113.53
1	A	206	VAL	N-CA-C	9.57	122.91	113.53
1	C	35	ASN	N-CA-C	9.57	124.31	109.96
1	I	362	HIS	N-CA-C	9.57	121.71	111.28
3	M	92	GLU	N-CA-C	-9.55	97.71	109.83
1	C	474	LYS	N-CA-C	9.51	124.70	113.20
1	K	474	LYS	N-CA-C	9.50	124.50	113.19
1	A	35	ASN	N-CA-C	9.43	124.11	109.96
1	C	67	SER	N-CA-C	9.39	121.29	111.14
1	A	72	TRP	N-CA-C	9.39	123.24	111.69
1	C	390	THR	N-CA-C	9.39	121.59	111.36
3	G	174	SER	N-CA-C	9.37	121.57	111.36
1	I	35	ASN	N-CA-C	9.33	123.96	109.96
3	E	255	ILE	N-CA-C	-9.33	98.34	107.76
3	O	69	ASP	N-CA-C	-9.31	99.64	113.61
1	K	71	VAL	N-CA-C	9.31	119.28	110.53
3	P	44	SER	N-CA-C	9.28	121.47	111.36
1	I	342	TYR	N-CA-C	9.27	124.72	113.23
1	K	362	HIS	N-CA-C	9.25	121.36	111.28
1	C	475	LEU	N-CA-C	9.23	121.42	111.36
3	O	222	ILE	N-CA-C	-9.23	101.40	110.72
2	J	191	GLY	N-CA-C	9.19	128.11	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	93	GLN	N-CA-C	9.19	122.47	111.82
2	D	30	GLY	N-CA-C	9.18	124.52	112.77
2	D	191	GLY	N-CA-C	9.13	128.01	111.02
2	L	210	LEU	N-CA-C	9.13	121.31	111.36
2	J	209	THR	N-CA-C	9.08	124.36	113.28
2	B	510	ARG	NE-CZ-NH1	-9.07	112.43	121.50
1	K	251	ALA	N-CA-C	9.06	123.28	109.23
3	O	57	ILE	N-CA-C	-9.05	101.58	110.72
2	D	210	LEU	N-CA-C	9.04	121.21	111.36
3	E	187	ARG	N-CA-C	-9.03	101.23	112.88
3	P	165	SER	N-CA-C	-9.02	101.45	111.28
3	O	52	LYS	N-CA-C	-9.01	101.54	111.36
2	B	209	THR	N-CA-C	8.96	124.21	113.28
1	C	72	TRP	N-CA-C	8.95	122.70	111.69
1	C	192	SER	N-CA-C	8.94	121.10	111.36
2	D	209	THR	N-CA-C	8.83	124.05	113.28
2	J	520	ASP	N-CA-C	8.80	123.30	110.28
1	A	390	THR	N-CA-C	8.79	120.94	111.36
3	O	46	ARG	N-CA-C	8.76	120.83	111.28
2	L	93	GLN	N-CA-C	8.76	121.98	111.82
2	B	191	GLY	N-CA-C	8.73	127.26	111.02
3	F	175	GLY	N-CA-C	8.70	126.33	112.58
3	N	207	MET	N-CA-C	-8.70	95.94	109.25
3	E	228	ILE	N-CA-C	-8.69	102.07	110.42
2	L	391	VAL	N-CA-C	8.69	118.70	110.53
2	L	191	GLY	N-CA-C	8.68	127.17	111.02
2	L	469	ILE	N-CA-C	-8.68	95.50	108.17
1	C	86	VAL	N-CA-C	8.64	121.86	111.05
1	C	292	ILE	CA-C-N	8.64	128.58	119.85
1	C	292	ILE	C-N-CA	8.64	128.58	119.85
1	K	342	TYR	N-CA-C	8.64	124.01	113.38
3	E	263	GLU	N-CA-C	-8.62	101.88	111.28
2	L	520	ASP	N-CA-C	8.62	123.04	110.28
3	N	135	PHE	N-CA-C	8.62	120.76	111.36
1	A	278	SER	N-CA-C	8.61	120.75	111.36
3	E	125	ASP	N-CA-C	-8.59	95.30	108.96
1	I	110	VAL	N-CA-C	8.58	119.39	110.72
3	F	92	GLU	N-CA-C	-8.58	98.93	109.83
1	A	206	VAL	CB-CA-C	-8.58	102.24	110.65
1	A	362	HIS	N-CA-C	8.57	120.62	111.28
3	G	237	ALA	N-CA-C	-8.57	102.02	111.36
2	L	209	THR	N-CA-C	8.55	123.89	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	251	ALA	N-CA-C	8.55	122.48	109.23
3	H	141	GLU	N-CA-C	-8.54	99.02	110.55
3	P	186	SER	N-CA-C	8.53	123.33	109.76
3	H	46	ARG	N-CA-C	8.52	120.65	111.36
2	B	469	ILE	N-CA-C	-8.51	95.74	108.17
3	E	129	ASP	N-CA-C	8.50	120.62	111.36
3	E	64	ALA	N-CA-C	-8.49	102.10	111.36
3	F	3	ARG	N-CA-C	8.49	123.26	109.59
3	F	141	GLU	N-CA-C	-8.48	99.10	110.55
2	D	469	ILE	N-CA-C	-8.47	95.80	108.17
3	E	57	ILE	N-CA-C	-8.46	101.99	110.62
2	J	30	GLY	N-CA-C	8.46	123.60	112.77
1	K	390	THR	N-CA-C	8.43	120.54	111.36
3	G	125	ASP	N-CA-C	-8.42	95.56	108.96
1	I	278	SER	N-CA-C	8.40	120.52	111.36
1	A	342	TYR	N-CA-C	8.38	123.80	113.50
3	M	117	ASP	N-CA-C	-8.38	102.37	112.59
3	G	255	ILE	CA-C-N	8.37	128.31	119.85
3	G	255	ILE	C-N-CA	8.37	128.31	119.85
2	D	391	VAL	N-CA-C	8.37	118.40	110.53
3	P	43	ASP	N-CA-C	-8.37	102.63	113.17
3	O	43	ASP	N-CA-C	-8.36	102.10	112.88
1	I	206	VAL	CB-CA-C	-8.34	102.47	110.65
3	F	43	ASP	N-CA-C	-8.31	102.70	113.17
2	D	93	GLN	N-CA-C	8.30	121.45	111.82
3	M	67	VAL	N-CA-C	8.28	119.09	110.72
1	C	279	MET	N-CA-C	8.28	123.17	112.41
2	J	93	GLN	N-CA-C	8.26	121.41	111.82
2	B	520	ASP	N-CA-C	8.24	122.48	110.28
1	K	278	SER	N-CA-C	8.24	120.34	111.36
1	C	278	SER	N-CA-C	8.22	120.32	111.36
3	H	222	ILE	N-CA-C	-8.22	102.24	110.62
3	H	49	LEU	N-CA-C	8.20	121.34	111.82
3	P	115	TYR	N-CA-C	-8.13	96.43	109.76
3	F	57	ILE	N-CA-C	-8.11	102.53	110.72
2	J	210	LEU	N-CA-C	8.11	120.20	111.36
2	D	468	ARG	N-CA-C	8.10	121.45	108.41
1	C	362	HIS	N-CA-C	8.10	120.11	111.28
2	B	391	VAL	N-CA-C	8.09	118.14	110.53
3	O	119	LEU	N-CA-C	-8.09	96.90	109.76
3	H	207	MET	N-CA-C	-8.07	96.13	108.96
3	F	67	VAL	N-CA-C	8.07	118.11	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	255	ILE	N-CA-C	-8.07	101.04	108.95
2	D	520	ASP	N-CA-C	8.06	122.21	110.28
2	L	30	GLY	N-CA-C	8.05	123.07	112.77
1	I	207	LEU	N-CA-C	8.04	120.12	111.36
1	I	292	ILE	CA-C-N	8.04	127.97	119.85
1	I	292	ILE	C-N-CA	8.04	127.97	119.85
3	N	192	GLU	N-CA-C	8.02	119.80	111.14
3	F	46	ARG	N-CA-C	8.02	120.10	111.36
1	A	86	VAL	N-CA-C	8.01	121.07	111.05
3	O	230	TYR	N-CA-C	8.01	120.09	111.36
3	E	46	ARG	N-CA-C	8.00	120.08	111.36
3	P	271	PHE	N-CA-C	7.99	120.07	111.36
2	J	468	ARG	N-CA-C	7.99	121.27	108.41
3	E	103	ILE	N-CA-C	7.97	118.77	110.72
3	E	36	VAL	CA-C-N	-7.96	114.64	122.20
3	E	36	VAL	C-N-CA	-7.96	114.64	122.20
3	N	231	ASP	N-CA-C	7.95	125.09	108.39
3	G	150	VAL	N-CA-C	-7.95	98.39	109.21
2	J	469	ILE	N-CA-C	-7.94	96.58	108.17
2	B	510	ARG	NE-CZ-NH2	7.93	126.34	119.20
3	H	159	TYR	N-CA-C	-7.92	102.64	111.28
3	G	64	ALA	N-CA-C	-7.92	102.72	111.36
1	K	206	VAL	CB-CA-C	-7.91	102.90	110.65
1	A	39	VAL	N-CA-C	7.89	119.58	108.93
1	C	342	TYR	N-CA-C	7.88	123.07	113.38
1	I	251	ALA	N-CA-C	7.86	121.41	109.23
3	M	29	MET	N-CA-C	-7.86	102.67	111.71
3	O	185	ASN	N-CA-C	-7.83	96.47	109.24
1	A	279	MET	N-CA-C	7.81	122.56	112.41
3	G	39	ASP	CA-C-N	7.81	127.44	119.56
3	G	39	ASP	C-N-CA	7.81	127.44	119.56
3	G	214	ASP	N-CA-C	7.79	121.31	109.23
1	I	205	TRP	N-CA-C	7.79	122.89	113.23
3	E	117	ASP	N-CA-C	-7.79	103.09	112.59
2	L	263	THR	CA-C-N	7.79	127.71	119.85
2	L	263	THR	C-N-CA	7.79	127.71	119.85
3	M	150	VAL	N-CA-C	-7.78	98.62	108.89
1	K	39	VAL	N-CA-C	7.78	119.43	108.93
3	M	90	GLY	CA-C-N	7.76	127.71	120.03
3	M	90	GLY	C-N-CA	7.76	127.71	120.03
3	O	75	VAL	N-CA-C	7.76	118.56	110.72
1	A	251	ALA	N-CA-C	7.75	121.25	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	205	TRP	N-CA-C	7.75	122.84	113.23
3	G	47	LEU	N-CA-C	7.75	119.81	111.36
1	K	292	ILE	CA-C-N	7.75	127.67	119.85
1	K	292	ILE	C-N-CA	7.75	127.67	119.85
3	N	222	ILE	N-CA-C	-7.75	101.41	111.09
3	G	207	MET	N-CA-C	-7.74	96.66	108.96
1	K	67	SER	N-CA-C	7.74	119.49	111.14
3	M	121	PHE	N-CA-C	7.74	121.51	108.90
3	O	155	MET	N-CA-C	7.74	119.79	111.36
3	O	134	GLY	N-CA-C	-7.73	102.88	112.77
1	C	206	VAL	CB-CA-C	-7.72	103.08	110.65
1	A	82	SER	N-CA-C	-7.71	96.71	108.96
3	O	192	GLU	N-CA-C	7.70	119.76	111.36
3	E	264	LEU	N-CA-C	-7.70	102.97	111.36
3	N	69	ASP	N-CA-C	-7.69	102.09	112.94
2	D	49	THR	N-CA-C	7.67	120.43	110.53
3	E	208	ILE	N-CA-C	7.67	118.46	110.72
1	A	205	TRP	N-CA-C	7.67	122.73	113.23
3	O	175	GLY	N-CA-C	7.66	124.69	112.58
3	O	190	ASP	N-CA-C	7.66	119.71	111.36
1	A	218	SER	N-CA-C	7.65	120.88	108.41
1	A	292	ILE	CA-C-N	7.64	127.57	119.85
1	A	292	ILE	C-N-CA	7.64	127.57	119.85
2	D	258	GLU	N-CA-C	7.63	119.60	111.28
3	M	176	SER	N-CA-C	7.62	122.78	113.17
3	H	249	ASP	N-CA-C	7.59	119.63	111.36
3	N	13	ILE	CB-CA-C	-7.59	101.49	111.88
2	L	70	CYS	N-CA-C	7.58	120.31	110.53
3	O	200	ALA	N-CA-C	-7.58	103.10	111.36
2	L	149	VAL	N-CA-C	7.58	119.49	108.58
2	J	391	VAL	N-CA-C	7.57	117.64	110.53
2	D	510	ARG	NE-CZ-NH2	7.54	125.99	119.20
1	A	21	PRO	N-CA-C	-7.53	100.11	111.41
3	N	16	SER	N-CA-C	7.53	119.27	111.14
1	C	205	TRP	N-CA-C	7.53	122.56	113.23
3	M	207	MET	N-CA-C	-7.51	98.69	109.96
3	O	135	PHE	N-CA-C	7.51	119.54	111.36
3	P	202	LYS	N-CA-C	-7.51	103.18	111.36
2	J	125	PHE	N-CA-C	7.50	119.54	111.36
3	E	153	GLY	N-CA-C	7.50	123.59	113.99
3	H	227	VAL	N-CA-C	-7.50	103.15	110.72
3	G	141	GLU	N-CA-C	-7.49	98.41	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	289	LYS	N-CA-C	7.49	119.23	111.14
3	O	49	LEU	N-CA-C	7.49	120.51	111.82
3	O	241	ARG	N-CA-C	-7.49	103.20	111.36
3	F	113	GLY	N-CA-C	7.47	127.46	114.76
1	K	228	ASP	N-CA-C	-7.47	96.23	108.41
1	I	279	MET	N-CA-C	7.47	122.12	112.41
3	H	166	LYS	N-CA-C	-7.46	103.15	111.28
3	G	117	ASP	N-CA-C	-7.44	103.77	112.92
1	C	82	SER	N-CA-C	-7.44	97.14	108.96
3	G	43	ASP	N-CA-C	-7.43	103.30	112.88
3	N	256	PRO	N-CA-C	7.41	123.16	111.38
1	K	207	LEU	N-CA-C	7.40	119.43	111.36
1	C	39	VAL	N-CA-C	7.39	118.91	108.93
3	P	36	VAL	CA-C-N	-7.38	115.18	122.20
3	P	36	VAL	C-N-CA	-7.38	115.18	122.20
3	G	180	GLY	N-CA-C	7.38	122.21	112.77
1	I	39	VAL	N-CA-C	7.37	118.88	108.93
1	K	121	LYS	N-CA-C	-7.36	103.25	111.28
1	I	67	SER	N-CA-C	7.36	119.09	111.14
1	I	218	SER	N-CA-C	7.36	120.40	108.41
3	E	28	GLU	N-CA-C	-7.34	103.30	111.82
1	K	60	ARG	N-CA-C	7.34	121.15	110.28
3	N	257	ASN	N-CA-C	-7.34	95.08	109.10
3	M	177	VAL	N-CA-C	7.33	119.27	109.37
3	H	29	MET	N-CA-C	-7.33	103.60	112.54
1	K	347	GLU	N-CA-C	7.32	121.00	110.10
1	K	21	PRO	N-CA-C	-7.31	100.45	111.41
2	D	449	LYS	N-CA-C	-7.29	103.33	111.28
1	K	218	SER	N-CA-C	7.27	120.27	108.41
2	L	449	LYS	N-CA-C	-7.27	103.35	111.28
1	C	228	ASP	N-CA-C	-7.25	96.59	108.41
1	I	119	GLN	N-CA-C	-7.24	99.26	109.69
3	O	262	ASP	N-CA-C	-7.23	103.48	111.36
2	J	419	ALA	N-CA-C	7.21	120.78	109.96
3	E	75	VAL	N-CA-C	7.19	117.99	110.72
3	F	117	ASP	N-CA-C	-7.19	103.60	112.88
3	O	234	ALA	N-CA-C	7.19	120.64	110.50
3	P	237	ALA	N-CA-C	-7.17	103.50	111.82
2	J	227	VAL	CA-C-N	7.17	127.01	119.05
2	J	227	VAL	C-N-CA	7.17	127.01	119.05
2	J	500	SER	N-CA-C	-7.17	103.55	111.36
1	I	21	PRO	N-CA-C	-7.17	100.66	111.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	21	PRO	N-CA-C	-7.16	100.66	111.41
3	M	119	LEU	N-CA-C	-7.16	98.88	110.20
3	H	43	ASP	N-CA-C	-7.15	104.16	113.17
2	D	359	HIS	N-CA-C	7.14	119.06	111.28
3	M	98	ALA	N-CA-C	-7.14	103.50	111.28
1	C	218	SER	N-CA-C	7.12	120.01	108.41
1	I	82	SER	N-CA-C	-7.11	97.66	108.96
1	A	121	LYS	N-CA-C	-7.11	103.53	111.28
2	B	308	THR	N-CA-C	7.10	120.42	111.69
3	N	57	ILE	N-CA-C	-7.10	103.55	110.72
1	A	228	ASP	N-CA-C	-7.10	96.84	108.41
2	L	195	THR	N-CA-C	-7.09	103.63	111.36
1	K	82	SER	N-CA-C	-7.08	97.70	108.96
3	F	207	MET	N-CA-C	-7.07	98.44	109.25
2	B	337	GLY	N-CA-C	-7.06	105.57	115.32
3	F	27	ALA	N-CA-C	-7.06	103.63	111.82
3	N	49	LEU	N-CA-C	7.06	120.01	111.82
3	O	133	GLY	N-CA-C	7.06	121.45	112.83
2	J	49	THR	N-CA-C	7.05	119.62	110.53
3	N	193	ASP	N-CA-C	7.04	119.04	111.36
1	C	60	ARG	N-CA-C	7.04	120.69	110.28
3	N	150	VAL	N-CA-C	-7.03	99.61	108.89
3	H	185	ASN	N-CA-C	-7.03	97.45	108.90
2	B	419	ALA	N-CA-C	7.02	120.48	109.96
3	N	168	ILE	N-CA-C	-7.02	103.63	110.72
1	I	228	ASP	N-CA-C	-7.02	96.97	108.41
1	I	86	VAL	N-CA-C	6.99	119.79	111.05
1	C	347	GLU	N-CA-C	6.99	120.52	110.10
3	F	187	ARG	N-CA-C	-6.99	103.87	112.88
3	M	166	LYS	N-CA-C	-6.98	103.75	111.36
2	L	468	ARG	N-CA-C	6.97	119.64	108.41
2	J	263	THR	CA-C-N	6.97	126.89	119.85
2	J	263	THR	C-N-CA	6.97	126.89	119.85
2	D	227	VAL	CA-C-N	6.96	126.78	119.05
2	D	227	VAL	C-N-CA	6.96	126.78	119.05
1	I	347	GLU	N-CA-C	6.96	120.48	110.10
3	P	137	MET	CA-C-N	-6.96	112.46	119.56
3	P	137	MET	C-N-CA	-6.96	112.46	119.56
1	A	207	LEU	N-CA-C	6.96	118.94	111.36
2	J	394	LEU	N-CA-C	6.96	119.75	108.41
2	L	128	GLN	N-CA-C	6.96	118.86	111.28
3	F	133	GLY	N-CA-C	6.95	121.31	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	279	MET	N-CA-C	6.94	121.44	112.41
2	B	4	GLN	N-CA-C	-6.93	98.73	109.76
2	B	227	VAL	CA-C-N	6.92	126.73	119.05
2	B	227	VAL	C-N-CA	6.92	126.73	119.05
3	H	268	LEU	N-CA-C	6.92	118.82	111.28
3	G	190	ASP	N-CA-C	6.91	118.61	111.14
1	A	127	GLY	N-CA-C	6.91	126.73	115.46
3	N	117	ASP	N-CA-C	-6.91	104.42	112.92
3	P	265	GLU	N-CA-C	-6.91	103.83	111.36
1	K	127	GLY	N-CA-C	6.90	126.87	115.34
2	B	318	ILE	N-CA-C	-6.90	101.44	108.96
1	C	469	ASN	CA-C-N	6.90	126.60	119.56
1	C	469	ASN	C-N-CA	6.90	126.60	119.56
1	A	119	GLN	N-CA-C	-6.89	99.76	109.69
2	L	510	ARG	NE-CZ-NH2	-6.89	113.00	119.20
3	E	216	VAL	N-CA-C	-6.89	103.76	110.72
2	D	510	ARG	NE-CZ-NH1	-6.88	114.62	121.50
2	D	500	SER	N-CA-C	-6.88	103.86	111.36
1	A	347	GLU	N-CA-C	6.87	120.34	110.10
3	P	131	VAL	N-CA-C	-6.86	97.73	108.23
2	D	308	THR	N-CA-C	6.86	120.13	111.69
2	B	70	CYS	N-CA-C	6.85	119.36	110.53
2	D	318	ILE	N-CA-C	-6.84	101.50	108.96
3	M	208	ILE	N-CA-C	6.84	117.63	110.72
3	G	133	GLY	N-CA-C	6.83	120.93	112.73
2	D	294	GLN	CA-C-N	6.83	126.79	119.28
2	D	294	GLN	C-N-CA	6.83	126.79	119.28
3	E	25	ALA	N-CA-C	-6.83	103.92	111.36
1	K	86	VAL	N-CA-C	6.83	119.58	111.05
2	B	49	THR	N-CA-C	6.82	119.75	110.55
3	F	26	LEU	N-CA-C	-6.81	103.93	111.36
2	L	389	GLU	CA-C-N	-6.81	111.32	119.84
2	L	389	GLU	C-N-CA	-6.81	111.32	119.84
2	J	4	GLN	N-CA-C	-6.81	98.93	109.76
2	J	308	THR	N-CA-C	6.81	120.06	111.69
1	C	207	LEU	N-CA-C	6.80	118.78	111.36
1	K	469	ASN	CA-C-N	6.80	126.50	119.56
1	K	469	ASN	C-N-CA	6.80	126.50	119.56
1	C	179	VAL	N-CA-C	6.80	114.88	107.60
2	J	363	HIS	N-CA-C	6.80	120.23	110.10
3	G	231	ASP	N-CA-C	6.79	120.30	108.75
2	J	70	CYS	N-CA-C	6.79	119.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	261	MET	N-CA-C	-6.79	103.94	111.82
3	M	141	GLU	N-CA-C	-6.79	100.43	110.48
2	D	363	HIS	N-CA-C	6.78	120.20	110.10
3	M	265	GLU	N-CA-C	6.78	118.75	111.36
3	M	25	ALA	N-CA-C	-6.77	103.90	111.28
3	P	167	GLY	N-CA-C	-6.77	104.61	112.73
2	J	154	MET	N-CA-C	-6.77	103.99	111.36
3	E	199	LEU	N-CA-C	-6.76	103.99	111.36
2	B	222	LYS	N-CA-C	6.76	120.73	111.54
2	D	117	SER	N-CA-C	6.76	120.98	111.52
3	N	194	GLU	N-CA-C	-6.76	103.92	111.28
3	O	4	GLN	N-CA-C	-6.75	97.89	108.90
1	I	57	MET	N-CA-C	6.75	120.96	111.52
1	C	121	LYS	N-CA-C	-6.74	103.94	111.28
2	J	391	VAL	CB-CA-C	-6.73	103.20	112.02
2	D	125	PHE	N-CA-C	6.73	118.69	111.36
2	L	86	MET	CA-C-N	-6.72	113.04	119.76
2	L	86	MET	C-N-CA	-6.72	113.04	119.76
2	L	394	LEU	N-CA-C	6.72	119.36	108.34
2	J	441	PHE	N-CA-C	6.71	119.38	109.24
3	O	187	ARG	N-CA-C	-6.71	104.72	113.17
3	H	30	GLY	N-CA-C	6.70	124.72	115.27
2	J	149	VAL	N-CA-C	6.70	119.06	108.87
2	J	417	LYS	N-CA-C	6.70	118.66	111.36
2	D	31	PHE	N-CA-C	6.70	122.95	114.31
3	M	113	GLY	N-CA-C	6.70	126.32	115.67
1	A	60	ARG	N-CA-C	6.69	120.19	110.28
2	B	128	GLN	N-CA-C	6.69	118.57	111.28
2	D	149	VAL	N-CA-C	6.68	118.30	109.21
2	L	337	GLY	N-CA-C	-6.68	106.52	115.21
1	K	119	GLN	N-CA-C	-6.68	100.07	109.69
3	O	136	ALA	N-CA-C	-6.67	105.46	112.93
3	P	198	ALA	N-CA-C	-6.67	104.09	111.36
2	B	468	ARG	N-CA-C	6.66	119.56	108.96
3	O	15	LYS	N-CA-C	-6.66	104.10	111.36
2	B	195	THR	N-CA-C	-6.66	104.11	111.36
3	P	20	GLN	N-CA-C	6.65	118.61	111.36
2	L	308	THR	N-CA-C	6.65	119.86	111.69
3	F	132	CYS	N-CA-C	-6.63	98.92	108.60
3	M	249	ASP	N-CA-C	6.63	118.59	111.36
3	F	230	TYR	N-CA-C	6.63	118.30	111.14
2	B	73	LEU	N-CA-C	-6.62	104.14	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	28	GLU	N-CA-C	-6.62	104.06	111.28
1	A	115	THR	N-CA-C	6.62	119.49	109.23
2	L	363	HIS	N-CA-C	6.60	119.94	110.10
3	O	208	ILE	N-CA-C	6.60	117.39	110.72
3	H	202	LYS	N-CA-C	-6.60	104.16	111.36
2	B	149	VAL	N-CA-C	6.60	118.90	108.87
3	N	90	GLY	CA-C-N	6.60	126.56	120.03
3	N	90	GLY	C-N-CA	6.60	126.56	120.03
3	P	187	ARG	N-CA-C	-6.60	104.37	112.88
2	J	82	PHE	N-CA-C	6.59	120.61	110.20
2	L	368	ALA	N-CA-C	-6.59	97.67	108.41
3	F	119	LEU	N-CA-C	-6.59	99.28	109.76
3	N	175	GLY	N-CA-C	6.58	122.67	112.60
2	J	128	GLN	N-CA-C	6.58	118.45	111.28
2	L	117	SER	N-CA-C	6.57	120.72	111.52
1	I	115	THR	N-CA-C	6.57	119.42	109.23
1	K	359	ARG	N-CA-C	6.57	124.33	109.81
3	O	62	ALA	N-CA-C	6.57	118.23	111.14
3	P	22	LEU	N-CA-C	-6.57	104.20	111.36
1	C	48	SER	N-CA-C	6.56	118.74	108.96
2	D	73	LEU	N-CA-C	-6.56	104.21	111.36
2	L	419	ALA	N-CA-C	6.56	119.80	109.96
2	J	31	PHE	N-CA-C	6.56	122.77	114.31
3	H	151	CYS	N-CA-C	6.55	118.82	108.79
3	H	213	ARG	N-CA-C	-6.55	99.23	109.25
2	J	258	GLU	N-CA-C	6.55	118.50	111.36
3	O	92	GLU	N-CA-C	-6.54	101.05	110.08
1	K	90	GLN	N-CA-C	6.54	118.49	111.36
3	P	16	SER	N-CA-C	6.53	118.48	111.36
2	J	359	HIS	N-CA-C	6.53	118.40	111.28
1	A	98	ASN	N-CA-C	-6.52	96.51	107.99
2	B	359	HIS	N-CA-C	6.52	118.39	111.28
1	K	289	LYS	N-CA-C	6.52	118.18	111.14
3	M	118	ASP	N-CA-C	6.52	120.40	111.54
1	C	359	ARG	N-CA-C	6.51	124.19	109.81
1	K	346	LEU	N-CA-C	6.50	121.37	113.17
2	B	12	TYR	N-CA-C	-6.50	99.50	109.64
1	C	115	THR	N-CA-C	6.50	119.30	109.23
2	D	372	ASP	N-CA-C	-6.49	100.66	110.39
1	C	20	TYR	CA-C-N	6.48	126.45	120.03
1	C	20	TYR	C-N-CA	6.48	126.45	120.03
2	D	263	THR	CA-C-N	6.48	126.40	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	263	THR	C-N-CA	6.48	126.40	119.85
1	I	142	PHE	CA-C-N	6.48	126.10	119.56
1	I	142	PHE	C-N-CA	6.48	126.10	119.56
3	O	180	GLY	N-CA-C	6.48	121.06	112.77
2	B	154	MET	N-CA-C	-6.47	104.31	111.36
1	K	179	VAL	N-CA-C	6.47	114.52	107.60
2	J	314	PRO	CA-C-N	-6.46	113.82	122.42
2	J	314	PRO	C-N-CA	-6.46	113.82	122.42
3	E	202	LYS	N-CA-C	-6.46	104.24	111.28
3	P	211	VAL	N-CA-C	6.45	115.09	107.73
2	L	373	PRO	N-CA-C	6.45	122.50	113.53
1	I	60	ARG	N-CA-C	6.44	119.81	110.28
2	L	49	THR	N-CA-C	6.44	119.25	110.55
1	A	469	ASN	CA-C-N	6.44	126.13	119.56
1	A	469	ASN	C-N-CA	6.44	126.13	119.56
1	I	44	LYS	N-CA-C	-6.44	104.18	111.14
2	L	510	ARG	CD-NE-CZ	6.44	133.42	124.40
3	O	125	ASP	N-CA-C	-6.44	98.23	108.73
2	D	70	CYS	N-CA-C	6.44	118.84	110.53
2	B	373	PRO	N-CA-C	6.43	122.47	113.53
3	G	75	VAL	N-CA-C	6.43	117.21	110.72
3	H	257	ASN	N-CA-C	-6.42	97.14	108.69
1	I	179	VAL	N-CA-C	6.42	114.47	107.60
3	M	111	GLU	N-CA-C	-6.42	104.36	111.36
1	A	289	LYS	N-CA-C	6.41	118.06	111.14
2	D	419	ALA	N-CA-C	6.41	119.76	110.28
2	D	368	ALA	N-CA-C	-6.40	97.97	108.41
3	O	25	ALA	N-CA-C	-6.39	104.31	111.28
1	I	70	VAL	CB-CA-C	-6.39	106.28	111.71
3	F	243	LEU	N-CA-C	-6.39	104.40	111.36
3	M	257	ASN	N-CA-C	-6.39	98.48	109.15
2	L	359	HIS	N-CA-C	6.38	118.23	111.28
2	J	280	GLU	N-CA-C	-6.38	104.33	111.28
3	P	177	VAL	N-CA-C	6.38	117.27	109.30
1	C	98	ASN	N-CA-C	-6.36	96.79	107.99
3	P	249	ASP	N-CA-C	6.36	118.30	111.36
1	I	391	MET	N-CA-C	6.36	119.02	111.71
2	L	125	PHE	N-CA-C	6.35	118.29	111.36
2	L	417	LYS	N-CA-C	6.35	118.28	111.36
1	I	48	SER	N-CA-C	6.35	118.42	108.96
1	I	103	THR	N-CA-C	-6.35	96.76	107.99
3	G	215	ASN	N-CA-C	6.34	118.28	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	46	ARG	N-CA-C	6.34	118.27	111.36
1	C	119	GLN	N-CA-C	-6.34	100.56	109.69
2	J	338	GLN	CA-C-N	6.34	126.52	120.31
2	J	338	GLN	C-N-CA	6.34	126.52	120.31
2	J	373	PRO	N-CA-C	6.34	122.34	113.53
2	B	117	SER	N-CA-C	6.34	120.39	111.52
2	L	227	VAL	CA-C-N	6.34	126.08	119.05
2	L	227	VAL	C-N-CA	6.34	126.08	119.05
1	A	386	ASP	N-CA-C	-6.33	104.46	111.36
2	B	215	ASP	N-CA-C	-6.33	104.46	111.36
2	L	71	GLN	N-CA-C	6.33	122.14	113.16
1	I	121	LYS	N-CA-C	-6.32	104.39	111.28
3	G	113	GLY	N-CA-C	6.32	125.50	114.76
2	B	391	VAL	CB-CA-C	-6.31	103.75	112.02
3	E	257	ASN	N-CA-C	-6.30	97.07	109.10
3	G	198	ALA	N-CA-C	-6.29	104.34	111.14
3	H	248	VAL	N-CA-C	-6.28	104.38	110.72
3	F	255	ILE	CA-C-N	6.27	126.03	119.76
3	F	255	ILE	C-N-CA	6.27	126.03	119.76
3	G	194	GLU	N-CA-C	-6.27	104.55	111.82
3	M	216	VAL	N-CA-C	-6.26	103.26	111.09
3	M	200	ALA	N-CA-C	-6.26	104.46	111.28
3	N	180	GLY	N-CA-C	6.25	120.78	112.77
2	B	35	TYR	N-CA-C	-6.25	101.45	110.08
1	A	103	THR	N-CA-C	-6.25	96.92	107.99
1	I	98	ASN	N-CA-C	-6.25	96.99	107.99
2	J	368	ALA	N-CA-C	-6.24	98.23	108.41
3	N	239	GLU	N-CA-C	-6.24	104.56	111.36
2	L	391	VAL	CB-CA-C	-6.24	103.84	112.02
2	D	195	THR	N-CA-C	-6.24	104.56	111.36
2	D	391	VAL	CB-CA-C	-6.23	103.86	112.02
1	A	359	ARG	N-CA-C	6.23	123.58	109.81
2	L	318	ILE	N-CA-C	-6.23	102.17	108.96
1	I	415	ARG	N-CA-C	6.22	117.86	111.14
3	P	125	ASP	N-CA-C	-6.22	99.08	108.96
3	H	234	ALA	N-CA-C	6.21	118.94	110.55
1	I	127	GLY	N-CA-C	6.21	125.71	115.34
2	J	12	TYR	N-CA-C	-6.21	99.95	109.64
2	B	314	PRO	CA-C-N	-6.21	114.17	122.42
2	B	314	PRO	C-N-CA	-6.21	114.17	122.42
2	D	314	PRO	CA-C-N	-6.21	114.17	122.42
2	D	314	PRO	C-N-CA	-6.21	114.17	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	258	GLU	N-CA-C	6.20	118.12	111.36
3	F	49	LEU	N-CA-C	6.20	118.12	111.36
2	J	318	ILE	N-CA-C	-6.20	102.20	108.96
2	D	128	GLN	N-CA-C	6.20	118.03	111.28
3	E	145	GLN	N-CA-C	6.20	117.83	111.14
3	E	255	ILE	CA-C-N	6.19	126.11	119.85
3	E	255	ILE	C-N-CA	6.19	126.11	119.85
1	I	70	VAL	N-CA-C	6.19	117.30	111.48
3	O	157	ALA	N-CA-C	-6.19	104.61	111.36
2	D	154	MET	N-CA-C	-6.19	104.62	111.36
3	O	141	GLU	CA-C-N	-6.19	113.05	122.21
3	O	141	GLU	C-N-CA	-6.19	113.05	122.21
1	K	109	PHE	N-CA-C	6.19	120.59	111.87
3	O	33	VAL	N-CA-C	6.18	119.16	108.90
3	F	159	TYR	N-CA-C	-6.18	104.62	111.36
3	H	206	GLN	N-CA-C	6.17	119.20	110.50
3	F	263	GLU	N-CA-C	-6.17	104.63	111.36
1	I	346	LEU	N-CA-C	6.17	120.95	113.17
2	D	473	ILE	N-CA-C	-6.17	98.74	107.75
2	L	258	GLU	N-CA-C	6.16	118.08	111.36
1	A	105	GLY	N-CA-C	-6.16	107.27	115.40
3	M	186	SER	N-CA-C	6.16	119.55	109.76
3	H	119	LEU	N-CA-C	-6.16	99.83	109.25
3	M	199	LEU	N-CA-C	-6.15	104.65	111.36
3	N	131	VAL	N-CA-C	-6.15	99.01	107.99
3	P	234	ALA	N-CA-C	6.15	118.24	110.24
2	B	31	PHE	N-CA-C	6.15	122.24	114.31
2	B	368	ALA	N-CA-C	-6.15	98.39	108.41
3	F	273	ILE	N-CA-C	-6.15	104.51	110.72
2	J	311	HIS	CA-C-N	-6.14	114.86	122.84
2	J	311	HIS	C-N-CA	-6.14	114.86	122.84
1	I	359	ARG	N-CA-C	6.14	123.37	109.81
2	L	467	ILE	N-CA-C	-6.14	98.79	107.75
3	N	121	PHE	N-CA-C	6.12	119.47	109.06
2	L	311	HIS	CA-C-N	-6.12	114.88	122.84
2	L	311	HIS	C-N-CA	-6.12	114.88	122.84
3	N	126	VAL	N-CA-C	6.12	117.58	108.46
2	J	49	THR	CA-C-N	6.12	128.98	120.29
2	J	49	THR	C-N-CA	6.12	128.98	120.29
2	L	500	SER	N-CA-C	-6.12	104.69	111.36
2	J	35	TYR	N-CA-C	-6.11	101.64	110.08
3	G	261	MET	N-CA-C	-6.11	104.70	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	PHE	CA-C-N	6.11	125.73	119.56
1	A	142	PHE	C-N-CA	6.11	125.73	119.56
2	D	4	GLN	N-CA-C	-6.11	100.05	109.76
2	D	332	VAL	N-CA-C	-6.10	104.40	110.62
2	B	202	GLU	N-CA-C	-6.10	104.63	111.28
2	J	117	SER	N-CA-C	6.09	120.05	111.52
1	I	105	GLY	N-CA-C	-6.08	107.37	115.40
3	M	254	VAL	N-CA-C	6.08	118.22	108.85
3	N	71	GLU	N-CA-C	6.08	119.48	110.48
1	I	392	LYS	N-CA-C	-6.07	104.75	111.36
3	M	228	ILE	N-CA-C	-6.06	104.60	110.42
3	F	93	PRO	N-CA-C	6.06	120.72	111.15
2	J	237	PHE	N-CA-C	-6.05	104.76	111.36
3	P	208	ILE	N-CA-C	6.05	116.22	110.53
2	D	82	PHE	N-CA-C	6.05	120.12	109.96
1	A	124	VAL	N-CA-C	6.04	116.21	110.53
2	D	373	PRO	N-CA-C	6.04	121.92	113.53
1	A	67	SER	N-CA-C	6.04	117.66	111.14
3	E	14	GLY	N-CA-C	6.04	124.45	115.64
3	M	222	ILE	N-CA-C	-6.04	104.62	110.72
1	C	142	PHE	CA-C-N	6.03	125.92	119.28
1	C	142	PHE	C-N-CA	6.03	125.92	119.28
3	H	173	ASN	N-CA-C	6.03	117.65	111.14
3	M	156	MET	N-CA-C	-6.02	104.72	111.28
1	K	98	ASN	N-CA-C	-6.02	97.40	107.99
2	J	202	GLU	N-CA-C	-6.00	104.73	111.28
2	L	83	GLU	N-CA-C	6.00	119.04	110.10
1	C	127	GLY	N-CA-C	6.00	125.88	115.62
3	G	92	GLU	N-CA-C	-5.99	101.81	110.08
2	D	337	GLY	N-CA-C	-5.99	107.06	115.32
3	E	268	LEU	N-CA-C	-5.99	104.83	111.36
1	A	179	VAL	N-CA-C	5.99	114.01	107.60
3	F	78	ALA	N-CA-C	5.98	119.27	109.76
1	K	115	THR	N-CA-C	5.98	118.50	109.23
1	A	109	PHE	N-CA-C	5.97	120.30	111.87
2	J	449	LYS	N-CA-C	-5.97	104.77	111.28
2	L	82	PHE	N-CA-C	5.97	119.63	110.20
1	K	433	LYS	N-CA-C	-5.96	104.78	111.28
3	M	21	ASN	N-CA-C	-5.96	104.87	111.36
3	N	161	ALA	N-CA-C	-5.96	104.79	111.28
3	H	117	ASP	N-CA-C	-5.95	105.60	112.92
3	F	223	ARG	N-CA-C	-5.95	105.98	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	57	ILE	N-CA-C	-5.95	104.71	110.72
2	J	244	LEU	N-CA-C	-5.94	104.80	111.28
2	J	332	VAL	N-CA-C	-5.94	104.56	110.62
2	L	314	PRO	CA-C-N	-5.94	114.52	122.42
2	L	314	PRO	C-N-CA	-5.94	114.52	122.42
2	L	215	ASP	N-CA-C	-5.94	104.89	111.36
3	O	145	GLN	N-CA-C	5.93	117.83	111.36
2	D	436	THR	N-CA-C	5.93	117.83	111.36
3	H	136	ALA	N-CA-C	-5.93	106.28	112.93
1	C	103	THR	N-CA-C	-5.93	97.50	107.99
1	K	70	VAL	N-CA-C	5.93	117.05	111.48
1	K	142	PHE	CA-C-N	5.92	125.60	119.56
1	K	142	PHE	C-N-CA	5.92	125.60	119.56
1	A	382	ALA	N-CA-C	5.91	119.03	110.28
3	P	268	LEU	N-CA-C	-5.91	104.92	111.36
2	L	73	LEU	N-CA-C	-5.91	104.92	111.36
1	K	268	VAL	N-CA-C	5.90	117.20	109.58
1	K	392	LYS	N-CA-C	-5.90	104.93	111.36
3	M	211	VAL	CA-C-N	5.90	125.81	119.85
3	M	211	VAL	C-N-CA	5.90	125.81	119.85
2	B	477	HIS	N-CA-C	5.89	119.43	109.76
3	E	236	GLN	N-CA-C	-5.89	104.94	111.36
1	I	431	PHE	N-CA-C	5.88	117.77	111.36
2	B	394	LEU	N-CA-C	5.88	117.98	108.34
2	J	222	LYS	N-CA-C	5.87	119.53	111.54
2	D	109	GLU	CA-C-N	-5.87	113.92	119.85
2	D	109	GLU	C-N-CA	-5.87	113.92	119.85
2	L	4	GLN	N-CA-C	-5.86	100.44	109.76
3	F	149	ILE	N-CA-C	5.86	116.54	107.99
2	J	215	ASP	N-CA-C	-5.85	104.98	111.36
1	I	469	ASN	CA-C-N	5.85	125.53	119.56
1	I	469	ASN	C-N-CA	5.85	125.53	119.56
1	K	57	MET	N-CA-C	5.85	119.70	111.52
3	P	49	LEU	N-CA-C	5.84	118.60	111.82
1	I	289	LYS	N-CA-C	5.84	117.45	111.14
3	N	155	MET	N-CA-C	5.84	117.73	111.36
2	D	122	ALA	N-CA-C	-5.84	105.41	112.54
1	I	65	ALA	CA-C-N	-5.84	113.58	120.00
1	I	65	ALA	C-N-CA	-5.84	113.58	120.00
3	G	49	LEU	N-CA-C	5.82	120.22	113.18
3	P	106	ILE	N-CA-C	5.81	116.59	110.72
3	O	107	ASN	N-CA-C	-5.81	104.94	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	50	HIS	N-CA-C	-5.81	105.49	112.58
1	K	105	GLY	N-CA-C	-5.81	107.73	115.40
2	D	153	CYS	N-CA-C	5.80	119.17	111.75
1	K	20	TYR	CA-C-N	5.80	125.77	120.03
1	K	20	TYR	C-N-CA	5.80	125.77	120.03
1	A	346	LEU	N-CA-C	5.80	120.47	113.17
1	A	48	SER	N-CA-C	5.79	117.59	108.96
2	B	109	GLU	CA-C-N	-5.79	114.00	119.85
2	B	109	GLU	C-N-CA	-5.79	114.00	119.85
1	A	381	PHE	N-CA-C	5.79	119.47	111.71
3	M	255	ILE	N-CA-C	-5.79	96.38	108.88
3	N	176	SER	N-CA-C	-5.78	105.55	113.30
3	F	141	GLU	CA-C-N	-5.78	113.50	122.05
3	F	141	GLU	C-N-CA	-5.78	113.50	122.05
3	N	5	CYS	N-CA-C	5.77	118.18	109.23
1	A	64	TYR	N-CA-C	-5.77	105.07	111.36
3	P	10	LYS	N-CA-C	-5.77	101.74	110.28
2	B	399	ASN	N-CA-C	5.76	116.98	108.86
1	A	18	GLU	N-CA-C	5.76	118.33	111.71
1	I	433	LYS	N-CA-C	-5.76	105.08	111.36
3	G	138	PRO	N-CA-C	-5.75	105.88	113.65
3	P	81	GLY	N-CA-C	-5.75	107.71	115.36
1	K	48	SER	N-CA-C	5.75	117.52	108.96
2	B	49	THR	CA-C-N	5.74	128.45	120.29
2	B	49	THR	C-N-CA	5.74	128.45	120.29
1	C	105	GLY	N-CA-C	-5.74	107.82	115.40
1	C	382	ALA	N-CA-C	5.74	118.77	110.28
1	K	44	LYS	N-CA-C	-5.74	104.94	111.14
2	D	12	TYR	N-CA-C	-5.73	100.70	109.64
3	M	28	GLU	N-CA-C	-5.73	105.11	111.36
1	C	90	GLN	N-CA-C	5.72	117.60	111.36
3	E	166	LYS	CA-C-N	5.72	126.33	119.98
3	E	166	LYS	C-N-CA	5.72	126.33	119.98
1	A	57	MET	N-CA-C	5.72	119.53	111.52
3	G	73	GLU	N-CA-C	-5.72	105.05	111.28
3	O	236	GLN	N-CA-C	-5.71	105.13	111.36
2	L	307	GLY	N-CA-C	5.71	119.40	112.49
3	H	229	GLU	N-CA-C	5.71	117.30	111.14
2	B	71	GLN	N-CA-C	5.70	121.26	113.16
3	G	17	THR	N-CA-C	-5.70	105.14	111.36
3	M	81	GLY	N-CA-C	-5.70	107.78	115.36
2	L	35	TYR	N-CA-C	-5.70	102.22	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	156	MET	N-CA-C	5.70	117.49	111.28
3	F	87	GLU	N-CA-C	5.69	117.69	108.41
2	D	222	LYS	N-CA-C	5.69	119.28	111.54
2	L	294	GLN	CA-C-N	5.69	125.22	119.19
2	L	294	GLN	C-N-CA	5.69	125.22	119.19
3	H	209	HIS	N-CA-C	5.69	117.72	109.07
3	F	210	PHE	N-CA-C	-5.69	99.25	108.52
3	E	160	ALA	N-CA-C	-5.68	105.17	111.36
1	I	90	GLN	N-CA-C	5.67	117.55	111.36
2	B	83	GLU	N-CA-C	5.67	118.55	110.10
3	N	210	PHE	CA-C-N	-5.67	118.40	123.33
3	N	210	PHE	C-N-CA	-5.67	118.40	123.33
3	E	83	VAL	CB-CA-C	-5.66	102.65	111.26
2	D	458	LYS	N-CA-C	-5.66	105.01	111.07
2	D	510	ARG	CD-NE-CZ	5.66	132.32	124.40
3	E	114	ALA	N-CA-C	-5.66	105.19	111.36
3	E	245	ARG	N-CA-C	-5.66	105.19	111.36
3	M	103	ILE	CB-CA-C	-5.66	104.50	112.14
2	D	299	GLU	N-CA-C	5.66	117.45	111.28
2	L	326	ASP	N-CA-C	-5.66	105.20	111.36
1	A	369	ASP	N-CA-C	-5.65	105.65	112.54
2	J	294	GLN	CA-C-N	5.65	125.49	119.28
2	J	294	GLN	C-N-CA	5.65	125.49	119.28
2	B	263	THR	CA-C-N	5.65	125.55	119.85
2	B	263	THR	C-N-CA	5.65	125.55	119.85
2	B	125	PHE	N-CA-C	5.64	117.23	111.14
1	I	442	HIS	N-CA-C	5.64	117.23	111.14
1	C	346	LEU	N-CA-C	5.64	120.28	113.17
2	B	417	LYS	N-CA-C	5.63	117.50	111.36
2	J	122	ALA	N-CA-C	-5.63	105.29	111.82
1	C	392	LYS	N-CA-C	-5.63	105.22	111.36
3	O	36	VAL	CA-C-N	-5.63	117.28	122.29
3	O	36	VAL	C-N-CA	-5.63	117.28	122.29
1	C	433	LYS	N-CA-C	-5.62	105.23	111.36
1	C	353	LEU	N-CA-C	5.62	118.63	109.24
1	K	382	ALA	N-CA-C	5.62	118.60	110.28
2	B	86	MET	CA-C-N	-5.62	114.14	119.76
2	B	86	MET	C-N-CA	-5.62	114.14	119.76
1	I	427	GLU	N-CA-C	5.62	118.34	111.82
1	A	388	ASP	N-CA-C	-5.62	105.24	111.36
3	G	249	ASP	N-CA-C	5.62	117.48	111.36
2	J	83	GLU	N-CA-C	5.62	118.47	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	153	CYS	N-CA-C	5.62	118.94	111.75
2	L	109	GLU	CA-C-N	-5.61	114.18	119.85
2	L	109	GLU	C-N-CA	-5.61	114.18	119.85
3	O	42	ALA	N-CA-C	5.61	119.42	112.24
2	J	431	ARG	N-CA-C	-5.61	105.16	111.28
2	L	458	LYS	N-CA-C	-5.61	105.17	111.28
2	B	362	LEU	N-CA-C	5.61	118.33	111.82
3	P	241	ARG	CA-C-N	5.61	128.25	120.29
3	P	241	ARG	C-N-CA	5.61	128.25	120.29
1	A	34	VAL	N-CA-C	-5.60	99.66	108.23
1	C	454	ASP	N-CA-C	-5.60	105.26	111.36
1	A	392	LYS	N-CA-C	-5.60	105.26	111.36
3	F	125	ASP	N-CA-C	-5.59	99.61	108.73
3	N	28	GLU	N-CA-C	-5.59	105.19	111.28
3	H	175	GLY	N-CA-C	5.59	121.41	112.58
1	C	405	THR	N-CA-C	-5.58	103.01	110.55
1	K	444	TRP	N-CA-C	-5.58	105.09	112.24
3	G	185	ASN	N-CA-C	-5.58	99.63	108.73
2	L	510	ARG	NE-CZ-NH1	5.58	127.08	121.50
3	F	176	SER	N-CA-C	-5.58	105.83	113.30
2	L	436	THR	N-CA-C	5.58	117.16	111.14
3	O	243	LEU	N-CA-C	-5.57	105.29	111.36
1	K	431	PHE	N-CA-C	5.57	118.28	111.82
1	C	110	VAL	CB-CA-C	-5.56	104.85	111.97
3	F	50	HIS	CB-CA-C	-5.56	104.07	111.63
3	F	52	LYS	N-CA-C	-5.56	105.30	111.36
3	F	107	ASN	N-CA-C	-5.55	105.31	111.36
2	B	517	TYR	N-CA-C	-5.55	105.38	111.82
1	C	70	VAL	CB-CA-C	-5.55	107.00	111.71
2	J	150	SER	N-CA-C	-5.55	100.98	109.41
3	G	10	LYS	N-CA-C	-5.54	102.28	110.48
2	L	222	LYS	N-CA-C	5.54	119.08	111.54
2	B	500	SER	N-CA-C	-5.54	105.32	111.36
1	C	109	PHE	N-CA-C	5.54	119.68	111.87
3	M	33	VAL	N-CA-C	5.54	117.78	108.81
3	E	98	ALA	N-CA-C	-5.54	105.33	111.36
2	J	428	TRP	N-CA-C	-5.54	105.33	111.36
2	D	437	ASP	N-CA-C	-5.53	99.39	108.41
3	F	183	ILE	N-CA-C	-5.53	101.76	109.45
1	C	277	ARG	N-CA-C	5.53	116.99	111.07
3	N	196	ILE	CB-CA-C	-5.53	104.59	112.22
1	I	34	VAL	N-CA-C	-5.53	99.78	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	250	GLY	N-CA-C	-5.53	104.63	112.37
2	D	49	THR	CA-C-N	5.52	128.13	120.29
2	D	49	THR	C-N-CA	5.52	128.13	120.29
2	J	70	CYS	CA-CB-SG	5.52	127.10	114.40
3	M	137	MET	CA-C-N	-5.52	113.21	119.28
3	M	137	MET	C-N-CA	-5.52	113.21	119.28
3	N	145	GLN	N-CA-C	5.52	117.38	111.36
1	I	382	ALA	N-CA-C	5.52	118.45	110.28
1	C	44	LYS	N-CA-C	-5.52	105.18	111.14
3	M	52	LYS	N-CA-C	-5.51	105.35	111.36
3	F	7	ILE	N-CA-C	-5.51	99.81	107.80
1	K	110	VAL	CB-CA-C	-5.51	104.92	111.97
2	B	326	ASP	N-CA-C	-5.51	105.36	111.36
2	B	278	GLN	N-CA-C	-5.51	105.36	111.36
1	I	20	TYR	N-CA-C	5.51	117.68	110.08
1	K	388	ASP	N-CA-C	-5.51	105.36	111.36
3	N	25	ALA	N-CA-C	-5.51	105.28	111.28
3	F	217	VAL	N-CA-C	-5.50	105.16	110.72
1	I	405	THR	N-CA-C	-5.50	103.12	110.55
2	J	278	GLN	N-CA-C	-5.50	105.36	111.36
1	I	369	ASP	N-CA-C	-5.50	105.83	112.54
1	A	202	VAL	CB-CA-C	-5.50	104.72	112.14
2	B	338	GLN	CA-C-N	5.50	125.70	120.31
2	B	338	GLN	C-N-CA	5.50	125.70	120.31
2	D	262	ASP	N-CA-C	5.50	119.62	111.87
3	H	95	VAL	N-CA-C	5.50	116.65	108.46
2	B	363	HIS	N-CA-C	5.50	118.29	110.10
3	O	165	SER	N-CA-C	-5.50	105.39	111.71
2	J	262	ASP	N-CA-C	5.49	119.61	111.87
2	B	70	CYS	CA-CB-SG	5.49	127.02	114.40
1	C	124	VAL	N-CA-C	5.48	115.69	110.53
2	D	18	GLN	N-CA-C	5.48	117.26	111.28
1	A	415	ARG	N-CA-C	5.48	117.06	111.14
3	E	92	GLU	CA-C-N	-5.48	114.31	119.90
3	E	92	GLU	C-N-CA	-5.48	114.31	119.90
1	C	18	GLU	N-CA-C	5.48	118.01	111.71
3	P	138	PRO	N-CA-C	-5.48	106.72	113.84
1	I	110	VAL	CB-CA-C	-5.48	104.66	112.22
2	J	340	ILE	CA-C-N	5.47	125.45	120.03
2	J	340	ILE	C-N-CA	5.47	125.45	120.03
3	N	245	ARG	N-CA-C	-5.47	105.32	111.28
3	O	47	LEU	N-CA-C	5.47	117.32	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	VAL	CB-CA-C	-5.47	104.97	111.97
3	N	147	ILE	N-CA-C	5.46	115.82	108.17
2	B	458	LYS	N-CA-C	-5.46	105.24	111.14
3	P	92	GLU	N-CA-C	-5.46	102.54	110.08
1	C	57	MET	N-CA-C	5.46	119.16	111.52
3	G	36	VAL	CA-C-N	-5.46	117.02	122.20
3	G	36	VAL	C-N-CA	-5.46	117.02	122.20
1	I	277	ARG	N-CA-C	5.46	116.91	111.07
1	A	405	THR	N-CA-C	-5.45	103.19	110.55
2	B	237	PHE	N-CA-C	-5.45	105.42	111.36
2	B	437	ASP	N-CA-C	-5.45	99.52	108.41
3	P	155	MET	N-CA-C	5.45	117.22	111.28
3	H	121	PHE	N-CA-C	5.45	117.97	108.76
1	I	97	ARG	N-CA-C	5.45	118.06	109.39
3	O	173	ASN	N-CA-C	5.45	116.90	111.07
1	A	359	ARG	CA-C-N	-5.45	113.00	119.05
1	A	359	ARG	C-N-CA	-5.45	113.00	119.05
1	K	103	THR	N-CA-C	-5.45	98.35	107.99
3	P	56	THR	N-CA-C	5.44	117.90	110.55
2	L	517	TYR	N-CA-C	-5.44	105.51	111.82
3	G	175	GLY	N-CA-C	5.44	118.76	111.20
1	I	386	ASP	N-CA-C	-5.44	105.43	111.36
1	K	20	TYR	N-CA-C	5.43	117.58	110.08
2	J	372	ASP	N-CA-C	-5.43	102.25	110.39
1	K	202	VAL	CB-CA-C	-5.43	104.81	112.14
2	L	202	GLU	N-CA-C	-5.42	105.37	111.28
2	D	441	PHE	N-CA-C	5.42	117.43	109.24
2	J	109	GLU	CA-C-N	-5.42	114.37	119.85
2	J	109	GLU	C-N-CA	-5.42	114.37	119.85
2	B	153	CYS	N-CA-C	5.42	118.69	111.75
3	G	136	ALA	N-CA-C	-5.42	106.25	112.92
3	H	228	ILE	N-CA-C	-5.42	105.25	110.72
2	J	437	ASP	N-CA-C	-5.41	99.58	108.41
1	A	427	GLU	N-CA-C	5.41	118.10	111.82
3	H	43	ASP	CA-C-N	5.41	127.53	120.28
3	H	43	ASP	C-N-CA	5.41	127.53	120.28
1	K	69	GLY	CA-C-N	-5.41	117.67	122.97
1	K	69	GLY	C-N-CA	-5.41	117.67	122.97
2	B	441	PHE	N-CA-C	5.41	117.40	109.24
2	D	38	ASP	N-CA-C	-5.41	105.47	111.36
2	D	83	GLU	N-CA-C	5.40	118.15	110.10
1	C	69	GLY	N-CA-C	5.40	119.68	112.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	61	ALA	N-CA-C	5.40	121.28	114.31
1	K	391	MET	N-CA-C	5.40	117.92	111.71
3	E	176	SER	N-CA-C	-5.39	105.92	112.88
3	G	186	SER	N-CA-C	5.39	118.26	110.28
1	A	97	ARG	N-CA-C	5.39	117.70	109.62
2	B	428	TRP	N-CA-C	-5.39	105.49	111.36
2	D	35	TYR	N-CA-C	-5.38	102.65	110.08
2	L	70	CYS	CA-CB-SG	5.38	126.78	114.40
2	D	237	PHE	N-CA-C	-5.38	105.50	111.36
2	D	55	LEU	N-CA-C	-5.38	105.50	111.36
3	H	13	ILE	N-CA-C	5.38	117.28	112.17
2	D	70	CYS	CA-CB-SG	5.38	126.77	114.40
1	K	97	ARG	N-CA-C	5.38	117.94	109.39
1	K	405	THR	N-CA-C	-5.38	103.29	110.55
3	N	152	SER	N-CA-C	5.37	117.58	109.41
2	D	478	HIS	N-CA-C	5.37	119.11	112.24
3	E	234	ALA	N-CA-C	5.37	118.08	110.50
1	C	34	VAL	N-CA-C	-5.37	100.02	108.23
2	L	428	TRP	N-CA-C	-5.37	105.51	111.36
3	E	102	VAL	CB-CA-C	-5.37	104.81	112.22
1	A	44	LYS	N-CA-C	-5.36	105.35	111.14
2	B	436	THR	N-CA-C	5.36	117.21	111.36
3	H	138	PRO	N-CA-C	-5.36	106.08	113.53
2	L	223	LYS	N-CA-C	-5.36	101.22	109.52
3	G	82	GLY	CA-C-N	-5.35	116.18	122.93
3	G	82	GLY	C-N-CA	-5.35	116.18	122.93
3	H	263	GLU	N-CA-C	-5.35	105.61	111.82
2	L	12	TYR	N-CA-C	-5.35	101.29	109.64
1	I	318	GLU	N-CA-C	5.35	118.60	111.75
2	B	449	LYS	N-CA-C	-5.35	105.45	111.28
3	G	46	ARG	N-CA-C	5.35	117.11	111.28
3	G	28	GLU	N-CA-C	-5.34	105.53	111.36
1	I	454	ASP	N-CA-C	-5.34	105.54	111.36
1	K	427	GLU	N-CA-C	5.34	118.02	111.82
3	E	39	ASP	CA-C-N	5.34	125.01	119.56
3	E	39	ASP	C-N-CA	5.34	125.01	119.56
3	P	159	TYR	N-CA-C	-5.34	105.54	111.36
2	L	299	GLU	N-CA-C	5.34	117.10	111.28
3	P	257	ASN	N-CA-C	-5.34	98.91	109.10
2	D	202	GLU	N-CA-C	-5.33	105.63	111.82
3	E	193	ASP	N-CA-C	5.33	117.17	111.36
3	H	198	ALA	CA-C-N	5.33	127.85	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	198	ALA	C-N-CA	5.33	127.85	120.29
2	B	122	ALA	N-CA-C	-5.31	106.06	112.54
3	F	73	GLU	N-CA-C	-5.31	105.49	111.28
3	N	10	LYS	N-CA-C	-5.31	102.42	110.28
2	J	18	GLN	N-CA-C	5.31	117.07	111.28
3	O	73	GLU	N-CA-C	-5.31	105.57	111.36
3	F	75	VAL	N-CA-C	5.31	116.08	110.72
2	D	307	GLY	N-CA-C	5.30	118.91	112.49
2	B	82	PHE	N-CA-C	5.30	118.87	109.96
1	C	391	MET	N-CA-C	5.30	117.81	111.71
3	P	66	THR	N-CA-C	5.30	118.13	110.28
1	C	202	VAL	CB-CA-C	-5.30	104.99	112.14
1	C	335	TRP	N-CA-C	5.30	117.14	111.36
1	K	386	ASP	N-CA-C	-5.30	105.58	111.36
3	E	137	MET	CA-C-N	-5.30	113.45	119.28
3	E	137	MET	C-N-CA	-5.30	113.45	119.28
2	L	49	THR	CA-C-N	5.30	127.81	120.29
2	L	49	THR	C-N-CA	5.30	127.81	120.29
2	J	73	LEU	N-CA-C	-5.29	105.51	111.28
2	D	126	GLY	N-CA-C	-5.29	106.24	111.85
1	C	268	VAL	N-CA-C	5.29	116.83	109.80
1	K	318	GLU	N-CA-C	5.29	118.52	111.75
1	K	353	LEU	N-CA-C	5.29	118.07	109.24
3	F	256	PRO	N-CA-C	5.29	119.49	111.19
2	D	317	ASN	N-CA-C	-5.29	103.41	110.55
3	G	222	ILE	N-CA-C	-5.29	105.23	110.62
3	G	179	LEU	CA-C-N	5.28	125.81	120.00
3	G	179	LEU	C-N-CA	5.28	125.81	120.00
2	D	428	TRP	N-CA-C	-5.28	105.61	111.36
2	J	477	HIS	N-CA-C	5.28	118.42	109.76
2	D	223	LYS	N-CA-C	-5.28	101.34	109.52
1	I	268	VAL	N-CA-C	5.28	116.39	109.58
3	E	164	ILE	N-CA-C	-5.28	105.39	110.72
3	G	241	ARG	N-CA-C	-5.28	105.61	111.36
3	O	63	GLU	N-CA-C	-5.27	105.61	111.36
1	I	20	TYR	CA-C-N	5.27	125.25	120.03
1	I	20	TYR	C-N-CA	5.27	125.25	120.03
1	I	124	VAL	N-CA-C	5.27	115.48	110.53
3	P	130	VAL	CA-C-N	-5.27	115.78	122.37
3	P	130	VAL	C-N-CA	-5.27	115.78	122.37
3	O	71	GLU	N-CA-C	5.27	118.08	110.28
1	C	197	ILE	N-CA-C	-5.27	105.25	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	255	ILE	CA-C-N	5.26	125.02	119.76
3	M	255	ILE	C-N-CA	5.26	125.02	119.76
3	M	241	ARG	N-CA-C	-5.26	105.72	111.82
1	A	86	VAL	CB-CA-C	-5.26	104.01	112.16
2	L	478	HIS	N-CA-C	5.26	119.28	112.86
2	D	394	LEU	N-CA-C	5.25	116.96	108.34
2	D	150	SER	N-CA-C	-5.25	101.31	109.14
1	C	287	GLU	N-CA-C	-5.25	105.64	111.36
3	O	255	ILE	N-CA-C	-5.25	97.54	108.88
3	N	139	ILE	CB-CA-C	-5.25	104.98	112.22
3	P	236	GLN	N-CA-C	-5.25	105.74	111.82
2	L	38	ASP	N-CA-C	-5.24	105.64	111.36
3	G	41	LYS	N-CA-C	-5.24	105.57	111.28
1	K	70	VAL	CB-CA-C	-5.24	107.26	111.71
2	B	150	SER	N-CA-C	-5.24	101.45	109.41
3	E	175	GLY	N-CA-C	5.24	120.86	112.58
3	O	27	ALA	CA-C-N	5.24	127.30	120.28
3	O	27	ALA	C-N-CA	5.24	127.30	120.28
1	C	351	VAL	N-CA-C	5.24	116.02	108.48
2	D	467	ILE	N-CA-C	-5.24	100.11	107.75
3	M	135	PHE	N-CA-C	5.23	117.06	111.36
2	B	332	VAL	N-CA-C	-5.23	105.28	110.62
2	J	71	GLN	N-CA-C	5.23	121.37	109.81
2	J	394	LEU	CA-C-N	-5.23	115.62	123.00
2	J	394	LEU	C-N-CA	-5.23	115.62	123.00
3	M	54	GLN	N-CA-C	-5.23	100.87	109.40
1	A	20	TYR	N-CA-C	5.22	117.29	110.08
3	M	238	ASP	N-CA-C	-5.22	105.67	111.36
3	G	141	GLU	CA-C-N	-5.22	114.49	122.21
3	G	141	GLU	C-N-CA	-5.22	114.49	122.21
3	P	190	ASP	N-CA-C	5.22	116.78	111.14
1	I	18	GLU	N-CA-C	5.22	117.71	111.71
3	N	156	MET	N-CA-C	5.22	116.97	111.28
3	N	266	GLU	N-CA-C	-5.21	105.68	111.36
1	I	351	VAL	N-CA-C	5.21	115.99	108.48
2	B	307	GLY	N-CA-C	5.21	118.80	112.49
3	O	64	ALA	N-CA-C	-5.21	105.68	111.36
1	C	70	VAL	CA-C-O	-5.21	116.28	120.70
3	H	192	GLU	N-CA-C	5.21	117.03	111.36
2	J	73	LEU	CA-C-N	5.21	125.76	119.98
2	J	73	LEU	C-N-CA	5.21	125.76	119.98
3	M	169	VAL	CB-CA-C	-5.20	105.11	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	280	GLU	N-CA-C	-5.20	105.61	111.28
3	P	216	VAL	N-CA-C	-5.20	104.59	111.09
2	B	467	ILE	N-CA-C	-5.20	100.26	107.80
3	F	24	ALA	N-CA-C	-5.20	105.69	111.36
2	L	437	ASP	N-CA-C	-5.20	99.94	108.41
3	G	6	ALA	CA-C-N	-5.20	115.88	122.37
3	G	6	ALA	C-N-CA	-5.20	115.88	122.37
1	K	197	ILE	N-CA-C	-5.20	105.32	110.62
1	I	109	PHE	N-CA-C	5.19	119.19	111.87
3	H	227	VAL	CB-CA-C	-5.19	105.05	112.22
3	N	241	ARG	N-CA-C	-5.19	105.70	111.36
3	F	180	GLY	N-CA-C	5.19	118.77	112.49
3	N	233	LYS	CA-C-N	5.19	128.45	120.82
3	N	233	LYS	C-N-CA	5.19	128.45	120.82
1	C	388	ASP	N-CA-C	-5.19	105.70	111.36
1	I	367	TYR	N-CA-C	-5.19	105.62	111.28
2	J	299	GLU	N-CA-C	5.19	116.94	111.28
2	L	150	SER	N-CA-C	-5.18	101.53	109.41
3	H	243	LEU	N-CA-C	-5.18	105.63	111.28
1	I	202	VAL	CB-CA-C	-5.18	105.14	112.14
3	P	254	VAL	N-CA-C	5.18	116.12	108.45
1	C	386	ASP	N-CA-C	-5.18	105.71	111.36
2	D	338	GLN	CA-C-N	5.18	125.39	120.31
2	D	338	GLN	C-N-CA	5.18	125.39	120.31
3	H	253	LEU	N-CA-C	-5.18	100.01	108.76
3	P	198	ALA	CA-C-N	5.18	128.18	120.31
3	P	198	ALA	C-N-CA	5.18	128.18	120.31
3	P	176	SER	N-CA-C	-5.18	106.20	112.88
2	B	251	TYR	N-CA-C	5.17	116.71	108.79
3	G	161	ALA	N-CA-C	-5.17	105.65	111.28
3	P	135	PHE	N-CA-C	5.16	116.98	111.36
1	A	391	MET	N-CA-C	5.16	117.64	111.71
2	L	477	HIS	N-CA-C	5.15	118.21	109.76
3	O	100	ARG	N-CA-C	-5.15	106.83	113.01
3	G	38	CYS	N-CA-C	-5.15	106.40	113.30
2	J	436	THR	N-CA-C	5.15	116.97	111.36
3	O	113	GLY	N-CA-C	5.15	123.51	114.76
2	D	71	GLN	N-CA-C	5.15	121.18	109.81
2	D	120	GLU	N-CA-C	-5.14	105.67	111.28
2	D	517	TYR	N-CA-C	-5.14	105.85	111.82
1	K	39	VAL	CB-CA-C	-5.14	103.67	111.69
2	L	372	ASP	N-CA-C	-5.14	102.68	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	75	VAL	N-CA-C	5.14	115.91	110.72
2	D	353	ASP	N-CA-C	-5.13	105.68	111.28
1	K	143	PRO	N-CA-C	5.13	120.51	113.84
3	N	125	ASP	N-CA-C	-5.13	100.80	108.96
3	H	103	ILE	CB-CA-C	-5.13	105.14	112.22
3	P	62	ALA	N-CA-C	5.13	116.87	111.28
2	L	399	ASN	N-CA-C	5.12	116.08	108.86
2	B	299	GLU	N-CA-C	5.12	116.86	111.28
1	C	415	ARG	N-CA-C	5.12	116.67	111.14
2	J	317	ASN	N-CA-C	-5.12	103.64	110.55
3	P	39	ASP	CA-C-N	5.11	124.78	119.56
3	P	39	ASP	C-N-CA	5.11	124.78	119.56
1	A	444	TRP	N-CA-C	-5.11	104.59	111.54
2	J	195	THR	N-CA-C	-5.11	105.79	111.36
2	L	102	TYR	N-CA-C	-5.11	105.71	111.28
2	B	317	ASN	N-CA-C	-5.11	103.66	110.55
2	L	338	GLN	CA-C-N	5.10	125.31	120.31
2	L	338	GLN	C-N-CA	5.10	125.31	120.31
3	E	143	LYS	N-CA-C	-5.10	105.80	111.36
3	N	208	ILE	N-CA-C	5.10	115.87	110.72
3	P	68	GLU	N-CA-C	-5.09	107.42	113.38
2	B	510	ARG	CD-NE-CZ	5.09	131.53	124.40
2	L	61	ALA	N-CA-C	5.09	120.88	114.31
1	I	31	HIS	N-CA-C	5.09	119.47	113.16
1	K	34	VAL	N-CA-C	-5.08	100.45	108.23
1	C	359	ARG	CA-C-N	-5.08	113.41	119.05
1	C	359	ARG	C-N-CA	-5.08	113.41	119.05
3	N	169	VAL	N-CA-C	5.08	115.80	110.62
2	J	159	GLY	N-CA-C	5.08	123.39	114.76
2	J	323	ASP	N-CA-C	5.08	116.89	111.36
2	B	244	LEU	N-CA-C	-5.07	105.75	111.28
1	C	143	PRO	N-CA-C	5.07	120.49	113.65
2	J	451	ILE	N-CA-C	-5.07	105.60	110.72
1	K	359	ARG	CA-C-N	-5.07	113.42	119.05
1	K	359	ARG	C-N-CA	-5.07	113.42	119.05
1	A	341	LYS	N-CA-C	5.07	116.88	111.36
1	A	129	LYS	N-CA-C	-5.06	105.76	111.28
3	F	270	GLU	N-CA-C	-5.06	105.89	111.71
2	J	337	GLY	N-CA-C	-5.06	108.34	115.32
2	L	317	ASN	N-CA-C	-5.06	103.72	110.55
3	N	198	ALA	N-CA-C	-5.06	105.85	111.36
3	G	89	GLY	N-CA-C	-5.06	103.16	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ARG	N-CA-C	5.05	116.48	111.07
1	K	31	HIS	N-CA-C	5.05	119.42	113.16
3	G	67	VAL	N-CA-C	-5.05	104.55	110.05
3	E	50	HIS	CB-CA-C	-5.05	104.77	111.63
1	I	195	HIS	N-CA-C	-5.04	105.86	111.36
3	O	43	ASP	CA-C-N	5.04	127.45	120.29
3	O	43	ASP	C-N-CA	5.04	127.45	120.29
3	P	248	VAL	CB-CA-C	-5.04	105.27	112.22
2	J	510	ARG	CD-NE-CZ	5.04	131.45	124.40
1	K	415	ARG	N-CA-C	5.04	116.58	111.14
1	K	124	VAL	N-CA-C	5.04	115.26	110.53
1	A	268	VAL	N-CA-C	5.03	116.07	109.58
2	B	61	ALA	N-CA-C	5.03	120.80	114.31
3	E	43	ASP	N-CA-C	-5.03	106.83	113.17
2	L	441	PHE	N-CA-C	5.03	116.84	109.24
1	A	337	ALA	N-CA-C	-5.03	105.88	111.36
2	B	294	GLN	CA-C-N	5.02	124.81	119.28
2	B	294	GLN	C-N-CA	5.02	124.81	119.28
2	D	311	HIS	CA-C-N	-5.02	115.87	122.85
2	D	311	HIS	C-N-CA	-5.02	115.87	122.85
1	A	353	LEU	N-CA-C	5.01	117.61	109.24
2	J	389	GLU	CA-C-N	-5.01	113.58	119.84
2	J	389	GLU	C-N-CA	-5.01	113.58	119.84
1	A	90	GLN	N-CA-C	5.01	116.82	111.36
3	H	103	ILE	N-CA-C	5.01	115.78	110.72
3	M	86	VAL	N-CA-C	5.00	116.92	108.81
2	J	288	LEU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	446	TYR	Sidechain
1	A	99	TYR	Sidechain
2	B	12	TYR	Sidechain
1	C	446	TYR	Sidechain
1	C	91	TYR	Sidechain
1	C	99	TYR	Sidechain
2	D	12	TYR	Sidechain
3	F	159	TYR	Sidechain
1	I	446	TYR	Sidechain
2	J	12	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	K	446	TYR	Sidechain
2	L	12	TYR	Sidechain

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	3782	0	3720	144	0
1	C	3782	0	3720	157	0
1	I	3782	0	3720	167	0
1	K	3782	0	3720	155	0
2	B	4174	0	4088	135	0
2	D	4174	0	4088	124	0
2	J	4174	0	4088	134	0
2	L	4174	0	4088	141	0
3	E	2053	0	2069	88	0
3	F	2082	0	2097	122	0
3	G	1983	0	2000	82	0
3	H	2037	0	2052	46	0
3	M	2029	0	2039	88	0
3	N	2041	0	2053	26	0
3	O	1978	0	1991	101	0
3	P	2018	0	2029	52	0
4	A	14	0	6	1	0
4	C	14	0	6	1	0
4	I	14	0	6	1	0
4	K	14	0	6	1	0
5	A	18	0	0	2	0
5	C	18	0	0	3	0
5	I	18	0	0	2	0
5	K	18	0	0	3	0
6	B	2	0	0	0	0
6	J	1	0	0	0	0
6	L	1	0	0	0	0
7	B	15	0	0	2	0
7	D	15	0	0	2	0
7	J	15	0	0	2	0
7	L	15	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	1	0	0	0	0
8	F	1	0	0	0	0
8	G	1	0	0	0	0
8	H	1	0	0	0	0
8	M	1	0	0	0	0
8	N	1	0	0	0	0
8	O	1	0	0	0	0
8	P	1	0	0	0	0
9	E	27	0	12	0	0
9	F	27	0	12	4	0
9	G	27	0	12	1	0
9	H	27	0	12	0	0
9	M	27	0	12	2	0
9	N	27	0	12	0	0
9	O	27	0	12	0	0
9	P	27	0	12	1	0
10	F	8	0	0	1	0
10	G	8	0	0	0	0
10	N	8	0	0	0	0
10	P	8	0	0	0	0
11	B	2	0	0	0	0
11	D	2	0	0	0	0
11	J	2	0	0	0	0
11	L	2	0	0	0	0
All	All	48501	0	47682	1629	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 19.

All (1629) 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:I:356:GLY:HA2	1:I:380:GLU:HB2	1.42	1.02
1:C:356:GLY:HA2	1:C:380:GLU:HB2	1.36	1.00
1:K:356:GLY:HA2	1:K:380:GLU:HB2	1.40	1.00
1:I:129:LYS:H	1:I:129:LYS:HD2	1.27	0.97
2:B:499:ASN:HD21	2:D:477:HIS:H	1.09	0.95
1:C:129:LYS:H	1:C:129:LYS:HD2	1.29	0.95
2:B:477:HIS:H	2:D:499:ASN:HD21	1.09	0.94
2:J:477:HIS:H	2:L:499:ASN:HD21	1.15	0.93
1:A:356:GLY:HA2	1:A:380:GLU:HB2	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:499:ASN:HD21	2:L:477:HIS:H	1.16	0.91
3:H:33:VAL:HB	3:H:83:VAL:HG12	1.51	0.90
3:O:10:LYS:O	3:O:13:ILE:HG12	1.73	0.88
2:B:346:LYS:HE3	2:B:350:ARG:NH2	1.90	0.86
2:J:346:LYS:HE3	2:J:350:ARG:NH2	1.91	0.86
3:G:8:TYR:HB3	3:G:164:ILE:HD13	1.58	0.86
3:O:8:TYR:HB3	3:O:164:ILE:HD13	1.54	0.85
1:I:275:CYS:HA	1:I:358:LEU:HD22	1.57	0.84
3:E:225:MET:HE3	3:E:229:GLU:HG2	1.58	0.84
2:B:88:TYR:OH	2:B:116:ASP:HB3	1.78	0.83
1:I:429:PHE:HB3	2:J:110:PRO:HD3	1.60	0.83
3:M:8:TYR:HB3	3:M:164:ILE:HD13	1.60	0.83
3:G:48:ILE:HG21	3:G:83:VAL:HG22	1.60	0.83
3:E:92:GLU:O	3:E:95:VAL:HG22	1.80	0.82
3:F:92:GLU:O	3:F:95:VAL:HG22	1.79	0.82
3:E:70:LEU:HD11	3:E:75:VAL:HG23	1.63	0.81
1:K:275:CYS:HA	1:K:358:LEU:HD22	1.64	0.80
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.62	0.80
3:E:80:TYR:O	3:E:83:VAL:HG23	1.82	0.80
2:B:125:PHE:CD1	3:E:62:ALA:HB2	2.18	0.79
3:O:103:ILE:HG12	3:O:137:MET:HG3	1.64	0.79
2:B:521:LEU:HD22	1:C:94:ALA:HB3	1.65	0.79
2:D:130:ASN:H	2:D:130:ASN:ND2	1.80	0.79
1:C:275:CYS:HA	1:C:358:LEU:HD22	1.65	0.79
1:I:239:ARG:HD2	1:I:252:GLN:NE2	1.98	0.79
3:H:215:ASN:N	3:H:215:ASN:HD22	1.80	0.78
3:N:160:ALA:O	3:N:164:ILE:HG13	1.82	0.78
2:L:346:LYS:HE3	2:L:350:ARG:NH2	1.98	0.78
3:E:222:ILE:HD11	3:F:275:GLU:O	1.83	0.78
2:J:90:HIS:HB3	2:J:151:THR:HG22	1.66	0.78
3:F:56:THR:HG22	3:F:87:GLU:HB3	1.66	0.77
3:O:20:GLN:HE22	3:O:47:LEU:H	1.32	0.77
3:O:45:THR:CG2	3:O:85:CYS:HB3	2.14	0.77
3:H:265:GLU:HA	3:H:268:LEU:HD22	1.65	0.76
1:C:429:PHE:HB3	2:D:110:PRO:HD3	1.67	0.76
2:L:96:VAL:HG21	2:L:115:SER:HB2	1.66	0.76
3:O:106:ILE:HD12	3:O:137:MET:HE1	1.67	0.76
3:F:202:LYS:HB3	3:F:259:ILE:HG21	1.67	0.76
1:C:115:THR:HG23	2:D:63:THR:HB	1.67	0.76
3:E:5:CYS:O	3:E:123:PHE:HA	1.86	0.76
3:P:8:TYR:HB3	3:P:164:ILE:HD13	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.67	0.76
3:P:100:ARG:HA	3:P:103:ILE:HD12	1.66	0.76
2:D:346:LYS:HE3	2:D:350:ARG:NH2	2.01	0.75
1:A:239:ARG:HD2	1:A:252:GLN:NE2	2.01	0.75
2:B:477:HIS:H	2:D:499:ASN:ND2	1.85	0.75
3:O:3:ARG:NH2	3:O:248:VAL:HA	2.00	0.75
3:E:23:VAL:HG11	3:E:35:ILE:HD11	1.69	0.75
2:L:91:GLY:HA3	2:L:152:THR:OG1	1.87	0.75
3:E:170:LYS:HE2	3:F:95:VAL:HG11	1.68	0.75
3:M:209:HIS:ND1	3:M:246:LYS:HE3	2.02	0.75
2:B:130:ASN:ND2	2:B:130:ASN:H	1.81	0.75
2:L:90:HIS:HB3	2:L:151:THR:HG22	1.69	0.74
2:B:90:HIS:HB3	2:B:151:THR:HG22	1.70	0.74
3:M:23:VAL:HA	3:M:26:LEU:HD12	1.69	0.74
3:P:6:ALA:HB2	3:P:124:TYR:HB2	1.69	0.74
2:J:91:GLY:HA3	2:J:152:THR:OG1	1.87	0.74
2:L:130:ASN:ND2	2:L:130:ASN:H	1.85	0.74
3:P:106:ILE:HD12	3:P:137:MET:HE1	1.69	0.73
1:K:429:PHE:HB3	2:L:110:PRO:HD3	1.70	0.73
3:G:48:ILE:HG21	3:G:83:VAL:CG2	2.18	0.73
2:J:205:ALA:HA	2:J:281:MET:HE2	1.69	0.73
3:E:244:ALA:O	3:E:248:VAL:HG23	1.89	0.73
1:I:428:LYS:HB2	1:I:438:PHE:CE1	2.24	0.73
2:L:422:TYR:HB3	2:L:425:LYS:HG3	1.70	0.73
1:K:239:ARG:HD2	1:K:252:GLN:NE2	2.03	0.72
1:K:410:GLU:O	1:K:414:LYS:HG3	1.89	0.72
3:M:7:ILE:HD12	3:M:148:TYR:HB2	1.72	0.72
3:F:7:ILE:HG13	3:F:19:THR:OG1	1.90	0.72
2:B:205:ALA:HA	2:B:281:MET:HE2	1.71	0.72
2:B:205:ALA:HA	2:B:281:MET:CE	2.20	0.72
1:C:71:VAL:HG13	1:C:279:MET:HE2	1.71	0.72
2:D:422:TYR:HB3	2:D:425:LYS:HG3	1.71	0.72
2:D:130:ASN:H	2:D:130:ASN:HD22	1.35	0.72
2:D:205:ALA:HA	2:D:281:MET:CE	2.20	0.71
1:K:115:THR:HG23	2:L:63:THR:HB	1.72	0.71
2:J:205:ALA:HA	2:J:281:MET:CE	2.20	0.71
1:K:428:LYS:HB2	1:K:438:PHE:CE1	2.25	0.71
3:E:55:ASN:N	3:E:55:ASN:HD22	1.86	0.71
2:L:74:GLY:HA3	2:L:193:HIS:O	1.91	0.71
3:F:268:LEU:HD12	3:F:273:ILE:HG13	1.73	0.71
3:F:269:MET:HB3	3:F:274:MET:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:21:ASN:HD21	3:G:227:VAL:H	1.37	0.71
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.71	0.71
3:E:55:ASN:HD22	3:E:55:ASN:H	1.37	0.71
1:I:258:SER:OG	1:I:261:GLU:HG3	1.90	0.71
1:K:71:VAL:HG13	1:K:279:MET:HE2	1.71	0.71
3:F:100:ARG:HD3	3:F:103:ILE:HD12	1.73	0.71
3:F:207:MET:O	2:L:222:LYS:HE2	1.89	0.71
1:K:93:ARG:HD2	1:K:113:ASN:HB2	1.72	0.71
2:B:477:HIS:N	2:D:499:ASN:HD21	1.89	0.71
3:E:21:ASN:HD21	3:E:227:VAL:H	1.38	0.71
3:P:25:ALA:O	3:P:29:MET:HG3	1.91	0.71
1:K:258:SER:OG	1:K:261:GLU:HG3	1.91	0.70
2:B:91:GLY:HA3	2:B:152:THR:OG1	1.91	0.70
3:E:76:LEU:CD1	3:E:86:VAL:HB	2.21	0.70
2:J:96:VAL:HG21	2:J:115:SER:HB2	1.73	0.70
3:H:179:LEU:HD23	3:H:256:PRO:HB3	1.72	0.70
2:L:130:ASN:H	2:L:130:ASN:HD22	1.39	0.70
2:D:90:HIS:HB3	2:D:151:THR:HG22	1.71	0.70
3:H:22:LEU:HD13	3:H:243:LEU:HG	1.72	0.70
1:I:115:THR:HG23	2:J:63:THR:HB	1.72	0.70
1:K:83:HIS:O	1:K:153:GLU:HB2	1.92	0.70
3:O:45:THR:HG22	3:O:85:CYS:HB3	1.74	0.70
2:D:205:ALA:HA	2:D:281:MET:HE2	1.73	0.70
3:O:147:ILE:O	3:O:179:LEU:HD12	1.92	0.70
3:G:193:ASP:O	3:G:197:ILE:HG13	1.92	0.70
3:F:160:ALA:O	3:F:164:ILE:HG13	1.92	0.69
1:I:93:ARG:HD2	1:I:113:ASN:HB2	1.74	0.69
1:A:104:THR:HA	1:A:108:ALA:O	1.92	0.69
3:M:44:SER:HB2	3:M:87:GLU:OE2	1.92	0.69
3:O:103:ILE:HD11	3:O:134:GLY:HA2	1.73	0.69
1:C:104:THR:HA	1:C:108:ALA:O	1.93	0.69
1:C:410:GLU:O	1:C:414:LYS:HG3	1.92	0.69
3:O:23:VAL:HG11	3:O:35:ILE:HD11	1.74	0.69
2:J:130:ASN:ND2	2:J:130:ASN:H	1.88	0.69
1:K:276:TYR:O	1:K:280:ASN:HB3	1.92	0.69
1:A:54:PRO:HB3	2:B:116:ASP:O	1.92	0.69
1:A:71:VAL:HG13	1:A:279:MET:HE2	1.73	0.69
1:I:104:THR:HA	1:I:108:ALA:O	1.92	0.69
3:F:200:ALA:HB1	3:F:205:THR:O	1.93	0.69
1:I:71:VAL:HG13	1:I:279:MET:HE2	1.73	0.69
2:B:422:TYR:HB3	2:B:425:LYS:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:41:LYS:HE2	3:O:43:ASP:OD2	1.92	0.69
1:C:239:ARG:HD2	1:C:252:GLN:NE2	2.07	0.69
3:N:161:ALA:HA	3:N:164:ILE:HD12	1.76	0.69
1:K:54:PRO:HB3	2:L:116:ASP:O	1.92	0.68
3:E:70:LEU:HD21	3:E:75:VAL:HG21	1.74	0.68
3:G:162:ASN:OD1	3:G:259:ILE:HG13	1.94	0.68
1:K:53:GLN:HB2	1:K:56:LEU:HD12	1.75	0.68
1:I:410:GLU:O	1:I:414:LYS:HG3	1.94	0.68
1:C:53:GLN:HB2	1:C:56:LEU:HD12	1.75	0.68
1:C:258:SER:OG	1:C:261:GLU:HG3	1.94	0.68
1:C:356:GLY:CA	1:C:380:GLU:HB2	2.20	0.68
1:K:135:ILE:HD13	1:K:178:ILE:HD13	1.75	0.68
1:A:115:THR:HG23	2:B:63:THR:HB	1.76	0.68
1:A:410:GLU:O	1:A:414:LYS:HG3	1.93	0.68
2:B:130:ASN:H	2:B:130:ASN:HD22	1.37	0.68
3:O:193:ASP:O	3:O:197:ILE:HG13	1.93	0.68
2:D:91:GLY:HA3	2:D:152:THR:OG1	1.94	0.68
3:G:141:GLU:HB2	3:G:143:LYS:HD3	1.75	0.68
3:G:178:ARG:HB3	3:G:253:LEU:HB3	1.76	0.68
1:I:276:TYR:O	1:I:280:ASN:HB3	1.94	0.68
1:I:12:LEU:HD13	1:I:415:ARG:HG2	1.76	0.68
2:J:118:MET:HB2	2:J:154:MET:HE1	1.75	0.68
3:M:10:LYS:O	3:M:13:ILE:HG12	1.93	0.68
3:E:225:MET:CE	3:E:229:GLU:HG2	2.23	0.67
1:I:54:PRO:HB3	2:J:116:ASP:O	1.93	0.67
3:G:2:MET:HE1	3:G:116:GLU:H	1.59	0.67
1:A:429:PHE:HB3	2:B:110:PRO:HD3	1.74	0.67
3:F:22:LEU:CD1	3:F:244:ALA:HA	2.24	0.67
1:K:10:GLU:HG3	1:K:34:VAL:HG21	1.76	0.67
3:M:8:TYR:OH	3:M:138:PRO:HG2	1.95	0.67
3:O:66:THR:HB	3:O:69:ASP:HB2	1.75	0.67
3:F:33:VAL:HG22	3:F:121:PHE:HB2	1.76	0.67
2:J:278:GLN:O	2:J:282:LYS:HG3	1.94	0.67
1:C:93:ARG:HD2	1:C:113:ASN:HB2	1.77	0.67
3:E:225:MET:HE2	3:E:230:TYR:HA	1.76	0.67
3:F:25:ALA:HB2	3:F:228:ILE:HD13	1.77	0.67
3:F:26:LEU:HD23	3:F:29:MET:HE3	1.76	0.67
3:M:268:LEU:HG	3:M:269:MET:N	2.10	0.67
3:O:152:SER:OG	3:O:154:GLU:HG2	1.95	0.67
1:I:420:LEU:HB2	1:I:467:LEU:HD12	1.76	0.67
2:J:422:TYR:HB3	2:J:425:LYS:HG3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:88:TYR:OH	2:L:116:ASP:HB3	1.95	0.66
2:J:51:GLU:CD	2:J:51:GLU:H	2.04	0.66
1:A:53:GLN:HB2	1:A:56:LEU:HD12	1.75	0.66
1:C:276:TYR:O	1:C:280:ASN:HB3	1.94	0.66
1:I:77:ASP:HB2	1:I:146:LYS:HB2	1.78	0.66
3:O:72:LEU:HD12	3:O:72:LEU:O	1.94	0.66
1:C:428:LYS:HB2	1:C:438:PHE:CE1	2.30	0.66
3:F:2:MET:HG3	3:F:119:LEU:O	1.94	0.66
2:B:278:GLN:O	2:B:282:LYS:HG3	1.94	0.66
1:C:209:LYS:HD3	1:C:263:GLU:OE2	1.95	0.66
1:I:372:MET:HE1	1:I:420:LEU:HD13	1.78	0.66
2:J:377:MET:HE3	2:J:406:VAL:HG22	1.78	0.66
3:P:200:ALA:HB1	3:P:205:THR:O	1.96	0.66
3:P:22:LEU:O	3:P:26:LEU:HG	1.96	0.66
1:C:335:TRP:O	1:C:339:VAL:HG23	1.95	0.66
3:F:206:GLN:HB2	2:L:222:LYS:HG2	1.77	0.66
1:A:209:LYS:HD3	1:A:263:GLU:OE2	1.97	0.65
1:C:465:MET:HG3	1:C:466:THR:N	2.11	0.65
3:H:265:GLU:O	3:H:268:LEU:HB2	1.96	0.65
3:M:14:GLY:HA2	9:M:5292:ADP:O2A	1.95	0.65
3:G:158:MET:HE3	3:G:199:LEU:HD12	1.78	0.65
1:I:210:ARG:HH11	1:I:264:LEU:HD21	1.61	0.65
3:H:152:SER:H	3:H:157:ALA:CB	2.08	0.65
1:I:465:MET:HG3	1:I:466:THR:N	2.09	0.65
3:P:92:GLU:O	3:P:95:VAL:HG13	1.96	0.65
1:I:209:LYS:HD3	1:I:263:GLU:OE2	1.97	0.65
3:P:6:ALA:CB	3:P:124:TYR:HB2	2.26	0.65
2:D:88:TYR:OH	2:D:116:ASP:HB3	1.96	0.65
2:J:521:LEU:HD22	1:K:94:ALA:HB3	1.79	0.65
3:F:206:GLN:CB	2:L:222:LYS:HG2	2.27	0.65
1:I:335:TRP:O	1:I:339:VAL:HG23	1.95	0.65
2:J:88:TYR:OH	2:J:116:ASP:HB3	1.97	0.65
1:K:104:THR:HA	1:K:108:ALA:O	1.97	0.65
1:A:442:HIS:HB3	4:A:494:HCA:O5	1.96	0.65
2:D:74:GLY:HA3	2:D:193:HIS:O	1.97	0.65
3:E:94:GLY:H	3:F:131:VAL:HG12	1.60	0.65
1:A:276:TYR:O	1:A:280:ASN:HB3	1.97	0.65
1:A:258:SER:OG	1:A:261:GLU:HG3	1.97	0.64
1:C:42:SER:HA	1:C:391:MET:HE1	1.79	0.64
3:G:57:ILE:HD12	3:G:105:ALA:HB1	1.79	0.64
1:K:42:SER:HA	1:K:391:MET:HE1	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:183:ILE:HG12	3:M:208:ILE:CG2	2.27	0.64
2:J:499:ASN:ND2	2:L:477:HIS:H	1.92	0.64
2:L:247:MET:HB3	2:L:249:VAL:HG23	1.79	0.64
1:I:306:ILE:HG23	1:I:328:ILE:HD13	1.79	0.64
1:K:356:GLY:CA	1:K:380:GLU:HB2	2.22	0.64
2:L:377:MET:HE3	2:L:406:VAL:HG22	1.78	0.64
3:H:264:LEU:O	3:H:268:LEU:HD13	1.97	0.64
2:D:51:GLU:CD	2:D:51:GLU:H	2.06	0.64
1:I:53:GLN:HB2	1:I:56:LEU:HD12	1.78	0.64
2:L:47:THR:HG22	2:L:52:TYR:CE1	2.33	0.64
2:D:247:MET:HB3	2:D:249:VAL:HG23	1.80	0.64
3:E:156:MET:HE2	3:F:41:LYS:NZ	2.12	0.64
2:J:477:HIS:H	2:L:499:ASN:ND2	1.92	0.64
2:L:205:ALA:HA	2:L:281:MET:CE	2.28	0.64
3:O:72:LEU:HD22	3:O:112:GLU:HB3	1.79	0.64
3:G:237:ALA:HB1	3:G:241:ARG:HH12	1.64	0.63
1:A:420:LEU:HB2	1:A:467:LEU:HD12	1.80	0.63
2:D:296:TRP:HB2	2:D:374:ASP:OD1	1.98	0.63
3:O:192:GLU:O	3:O:196:ILE:HG12	1.97	0.63
1:A:93:ARG:HD2	1:A:113:ASN:HB2	1.79	0.63
1:A:135:ILE:HD13	1:A:178:ILE:HD13	1.80	0.63
1:C:12:LEU:HD13	1:C:415:ARG:HG2	1.80	0.63
1:I:129:LYS:H	1:I:129:LYS:CD	2.05	0.63
2:D:278:GLN:O	2:D:282:LYS:HG3	1.98	0.63
3:F:8:TYR:HB3	3:F:164:ILE:HD13	1.80	0.63
1:K:239:ARG:O	1:K:243:GLU:HG2	1.98	0.63
1:K:420:LEU:HB2	1:K:467:LEU:HD12	1.81	0.63
3:O:3:ARG:HH22	3:O:248:VAL:HA	1.63	0.63
2:B:445:ASN:ND2	2:B:472:PRO:HD2	2.13	0.63
1:K:335:TRP:O	1:K:339:VAL:HG23	1.98	0.63
3:G:6:ALA:HB2	3:G:144:ALA:CB	2.28	0.63
1:I:259:ILE:O	1:I:263:GLU:HG3	1.98	0.63
2:B:499:ASN:ND2	2:D:477:HIS:H	1.89	0.63
3:F:158:MET:HE1	3:F:195:LEU:HD11	1.80	0.63
3:H:33:VAL:HB	3:H:83:VAL:CG1	2.28	0.63
3:O:21:ASN:HB3	3:O:240:TYR:CD2	2.34	0.63
1:A:335:TRP:O	1:A:339:VAL:HG23	1.98	0.62
1:C:372:MET:HE1	1:C:420:LEU:HD13	1.81	0.62
3:E:110:GLU:HG3	3:E:115:TYR:CE2	2.35	0.62
3:M:36:VAL:HA	3:M:86:VAL:HG13	1.79	0.62
1:I:442:HIS:HB3	4:I:494:HCA:O5	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:275:CYS:CA	1:I:358:LEU:HD22	2.29	0.62
3:O:45:THR:HG21	3:O:85:CYS:HB3	1.80	0.62
3:F:10:LYS:HD2	3:F:11:GLY:O	1.99	0.62
3:F:268:LEU:O	3:F:273:ILE:HG12	1.99	0.62
1:K:306:ILE:HG23	1:K:328:ILE:HD13	1.81	0.62
1:A:125:PHE:O	3:F:100:ARG:HD2	2.00	0.62
3:O:60:MET:HB3	3:O:70:LEU:HD11	1.82	0.62
3:F:135:PHE:O	3:F:138:PRO:HD2	1.99	0.62
1:I:42:SER:HA	1:I:391:MET:HE1	1.81	0.62
1:I:429:PHE:CB	2:J:110:PRO:HD3	2.29	0.62
1:A:158:LEU:HD11	2:B:154:MET:CG	2.30	0.62
1:A:428:LYS:HB2	1:A:438:PHE:CE1	2.35	0.62
1:I:35:ASN:HD21	1:I:391:MET:HB3	1.65	0.62
1:K:354:TYR:CZ	1:K:404:VAL:HG12	2.35	0.62
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.81	0.62
3:E:156:MET:HE2	3:F:41:LYS:HZ2	1.65	0.62
1:A:85:PRO:HB2	7:B:1498:CLF:S2B	2.40	0.62
2:J:90:HIS:ND1	2:J:116:ASP:OD1	2.33	0.62
2:L:51:GLU:CD	2:L:51:GLU:H	2.08	0.62
3:N:268:LEU:O	3:N:273:ILE:HG12	2.00	0.61
1:I:426:LYS:HA	2:J:104:ASN:ND2	2.15	0.61
1:C:420:LEU:HB2	1:C:467:LEU:HD12	1.82	0.61
2:D:139:LYS:HE2	2:D:179:PHE:CD1	2.36	0.61
1:I:83:HIS:O	1:I:153:GLU:HB2	2.00	0.61
2:J:445:ASN:ND2	2:J:472:PRO:HD2	2.15	0.61
3:O:158:MET:HE3	3:O:199:LEU:HD12	1.82	0.61
3:E:162:ASN:OD1	3:E:259:ILE:HG12	1.99	0.61
3:G:256:PRO:O	3:G:258:PRO:HD3	2.01	0.61
3:H:215:ASN:N	3:H:215:ASN:ND2	2.46	0.61
1:C:54:PRO:HB3	2:D:116:ASP:O	2.01	0.61
3:G:72:LEU:HD22	3:G:112:GLU:HB3	1.83	0.61
1:I:370:LEU:HD11	1:I:460:ALA:HA	1.82	0.61
2:J:130:ASN:H	2:J:130:ASN:HD22	1.45	0.61
2:B:51:GLU:CD	2:B:51:GLU:H	2.09	0.61
1:K:352:MET:HE3	1:K:413:VAL:HG22	1.82	0.61
1:K:209:LYS:HD3	1:K:263:GLU:OE2	1.99	0.61
1:K:426:LYS:HA	2:L:104:ASN:ND2	2.16	0.61
2:L:205:ALA:HA	2:L:281:MET:HE2	1.82	0.61
3:O:188:ASN:HD21	3:O:213:ARG:HG2	1.66	0.61
3:P:103:ILE:HG12	3:P:137:MET:SD	2.41	0.61
1:K:372:MET:HE1	1:K:420:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:247:MET:HB3	2:J:249:VAL:HG23	1.82	0.61
1:C:437:PRO:HG3	1:C:472:TRP:CE2	2.35	0.60
1:K:12:LEU:HD13	1:K:415:ARG:HG2	1.83	0.60
3:O:178:ARG:HG2	3:O:178:ARG:HH11	1.65	0.60
2:B:125:PHE:CE1	3:E:58:MET:O	2.54	0.60
1:I:10:GLU:HG3	1:I:34:VAL:HG21	1.83	0.60
1:A:372:MET:HE1	1:A:420:LEU:HD13	1.83	0.60
2:B:247:MET:HB3	2:B:249:VAL:HG23	1.82	0.60
3:G:195:LEU:O	3:G:198:ALA:HB3	2.01	0.60
3:P:163:ASN:O	3:P:166:LYS:HB2	2.01	0.60
1:A:433:LYS:NZ	2:B:263:THR:O	2.35	0.60
1:C:259:ILE:O	1:C:263:GLU:HG3	2.01	0.60
1:A:10:GLU:HG3	1:A:34:VAL:HG21	1.84	0.60
1:A:427:GLU:CD	1:A:427:GLU:H	2.10	0.60
3:G:235:LYS:HA	3:G:238:ASP:OD2	2.02	0.60
3:H:38:CYS:HA	3:H:88:SER:HB2	1.82	0.60
3:H:161:ALA:O	3:H:165:SER:OG	2.18	0.60
2:J:74:GLY:HA3	2:J:193:HIS:O	2.02	0.60
2:L:278:GLN:O	2:L:282:LYS:HG3	2.01	0.60
1:A:239:ARG:O	1:A:243:GLU:HG2	2.01	0.60
1:A:354:TYR:CZ	1:A:404:VAL:HG12	2.36	0.60
1:A:465:MET:HG3	1:A:466:THR:N	2.15	0.60
3:E:178:ARG:CB	3:E:253:LEU:HB3	2.31	0.60
1:I:158:LEU:HD11	2:J:154:MET:CG	2.32	0.60
3:M:183:ILE:HG12	3:M:208:ILE:HG21	1.83	0.60
3:O:136:ALA:O	3:O:140:ARG:HG3	2.02	0.60
1:C:306:ILE:HG23	1:C:328:ILE:HD13	1.83	0.60
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.37	0.60
1:K:77:ASP:HB2	1:K:146:LYS:HB2	1.83	0.60
1:A:306:ILE:HG23	1:A:328:ILE:HD13	1.83	0.60
3:O:209:HIS:HD2	3:O:243:LEU:HB2	1.66	0.60
2:B:139:LYS:HE2	2:B:179:PHE:CD1	2.37	0.60
1:K:394:MET:HG3	1:K:400:LEU:HD21	1.84	0.60
3:E:28:GLU:OE1	3:E:241:ARG:NH2	2.25	0.59
2:J:494:LEU:O	2:J:498:VAL:HG12	2.02	0.59
2:L:139:LYS:HE2	2:L:179:PHE:CD1	2.37	0.59
1:A:42:SER:HA	1:A:391:MET:HE1	1.84	0.59
1:A:259:ILE:O	1:A:263:GLU:HG3	2.02	0.59
1:K:465:MET:HG3	1:K:466:THR:N	2.17	0.59
3:M:36:VAL:HA	3:M:86:VAL:CG1	2.33	0.59
3:M:244:ALA:O	3:M:248:VAL:HG23	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:158:MET:CE	3:G:199:LEU:HD12	2.32	0.59
1:I:426:LYS:HA	2:J:104:ASN:HD21	1.67	0.59
3:O:200:ALA:HB1	3:O:205:THR:O	2.02	0.59
2:B:47:THR:HG22	2:B:52:TYR:CE1	2.37	0.59
1:I:245:MET:HG3	1:I:324:CYS:HA	1.85	0.59
2:J:369:LEU:HD12	2:J:379:LEU:HD23	1.84	0.59
2:L:296:TRP:HB2	2:L:374:ASP:OD1	2.03	0.59
3:M:93:PRO:HG2	3:N:163:ASN:HA	1.82	0.59
3:F:97:CYS:O	3:F:100:ARG:HB2	2.02	0.59
1:K:224:ALA:HB3	1:K:271:ASN:ND2	2.17	0.59
3:O:55:ASN:O	3:O:60:MET:HE2	2.03	0.59
1:K:210:ARG:HH11	1:K:264:LEU:HD21	1.67	0.59
1:C:224:ALA:HB3	1:C:271:ASN:ND2	2.17	0.59
2:D:384:LEU:HD11	2:D:410:LEU:HD23	1.84	0.59
1:I:57:MET:HG3	2:J:114:VAL:HG12	1.84	0.59
1:I:354:TYR:CZ	1:I:404:VAL:HG12	2.38	0.59
3:P:243:LEU:O	3:P:247:VAL:HG23	2.02	0.59
3:M:200:ALA:HB1	3:M:205:THR:O	2.03	0.58
1:A:77:ASP:HB2	1:A:146:LYS:HB2	1.85	0.58
1:A:352:MET:HE3	1:A:413:VAL:HG22	1.84	0.58
1:K:352:MET:CE	1:K:413:VAL:HA	2.33	0.58
3:P:225:MET:HG3	3:P:230:TYR:HB2	1.85	0.58
1:A:20:TYR:OH	1:A:408:GLU:HG3	2.03	0.58
1:K:437:PRO:HG3	1:K:472:TRP:CE2	2.37	0.58
1:A:210:ARG:HH11	1:A:264:LEU:HD21	1.68	0.58
1:A:275:CYS:CA	1:A:358:LEU:HD22	2.33	0.58
3:F:165:SER:O	3:F:169:VAL:HG23	2.03	0.58
3:G:160:ALA:O	3:G:164:ILE:HG13	2.03	0.58
1:I:85:PRO:HB2	7:J:5498:CLF:S2B	2.44	0.58
2:J:72:PRO:HB2	2:J:99:PHE:CZ	2.39	0.58
3:P:158:MET:HE3	3:P:199:LEU:HD12	1.83	0.58
2:B:445:ASN:HB2	2:B:472:PRO:O	2.02	0.58
2:L:231:GLU:CD	2:L:236:ASN:HD22	2.11	0.58
2:L:494:LEU:O	2:L:498:VAL:HG12	2.03	0.58
3:P:100:ARG:HD3	3:P:103:ILE:HD12	1.86	0.58
3:G:99:GLY:O	3:G:102:VAL:HB	2.04	0.58
1:K:57:MET:HG3	2:L:114:VAL:HG12	1.84	0.58
3:M:208:ILE:O	3:M:246:LYS:HD2	2.03	0.58
2:B:494:LEU:C	2:B:494:LEU:HD23	2.29	0.58
1:C:158:LEU:HD11	2:D:154:MET:CG	2.33	0.58
1:I:239:ARG:HH11	1:I:252:GLN:HE21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:219:GLY:HA2	2:L:288:LEU:HD23	1.85	0.58
3:F:49:LEU:O	3:F:50:HIS:HB2	2.03	0.58
2:J:139:LYS:HE2	2:J:179:PHE:CD1	2.39	0.58
2:J:219:GLY:HA2	2:J:288:LEU:HD23	1.84	0.58
1:K:358:LEU:HB3	5:K:496:CFN:S4A	2.43	0.58
1:C:83:HIS:O	1:C:153:GLU:HB2	2.04	0.58
1:C:426:LYS:HA	2:D:104:ASN:ND2	2.19	0.58
3:F:21:ASN:HD21	3:F:227:VAL:H	1.52	0.58
3:M:103:ILE:HG12	3:M:137:MET:HG3	1.86	0.58
1:A:245:MET:HG3	1:A:324:CYS:HA	1.86	0.58
3:E:26:LEU:HD23	3:E:29:MET:HE3	1.86	0.58
2:B:219:GLY:HA2	2:B:288:LEU:HD23	1.84	0.57
2:D:219:GLY:HA2	2:D:288:LEU:HD23	1.86	0.57
3:F:159:TYR:O	3:F:163:ASN:HB2	2.04	0.57
2:J:92:SER:HB2	7:J:5498:CLF:S2A	2.43	0.57
1:K:70:VAL:HA	1:K:96:ARG:NH1	2.19	0.57
1:K:100:TYR:CE1	1:K:110:VAL:HB	2.39	0.57
3:O:244:ALA:O	3:O:248:VAL:HG23	2.03	0.57
2:B:74:GLY:HA3	2:B:193:HIS:O	2.04	0.57
1:C:135:ILE:HD13	1:C:178:ILE:HD13	1.86	0.57
2:D:318:ILE:HG23	2:D:318:ILE:O	2.02	0.57
1:K:259:ILE:O	1:K:263:GLU:HG3	2.04	0.57
3:O:158:MET:HE3	3:O:199:LEU:CD1	2.34	0.57
3:O:219:ARG:O	3:O:222:ILE:HG22	2.04	0.57
3:P:103:ILE:HA	3:P:137:MET:SD	2.43	0.57
2:B:232:THR:HG21	2:B:471:PHE:CD1	2.40	0.57
1:C:433:LYS:NZ	2:D:263:THR:O	2.38	0.57
1:K:343:ARG:HD3	1:K:347:GLU:OE2	2.03	0.57
1:K:442:HIS:HB3	4:K:494:HCA:O5	2.04	0.57
1:A:12:LEU:HD13	1:A:415:ARG:HG2	1.86	0.57
2:D:232:THR:HG21	2:D:471:PHE:CD1	2.39	0.57
1:I:229:TYR:OH	1:I:279:MET:HE3	2.03	0.57
1:K:426:LYS:HA	2:L:104:ASN:HD21	1.70	0.57
2:L:445:ASN:HB2	2:L:472:PRO:O	2.04	0.57
3:F:184:CYS:SG	3:F:196:ILE:HG13	2.45	0.57
3:M:231:ASP:HB3	3:M:234:ALA:HB2	1.85	0.57
1:C:343:ARG:N	1:C:344:PRO:HD2	2.19	0.57
3:E:26:LEU:HA	3:E:29:MET:HE3	1.86	0.57
3:G:177:VAL:O	3:G:178:ARG:HD3	2.05	0.57
1:I:97:ARG:O	1:I:231:ILE:HA	2.05	0.57
1:I:394:MET:HG3	1:I:400:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:O	1:C:243:GLU:HG2	2.04	0.57
3:E:47:LEU:HD21	3:E:221:GLU:HG2	1.85	0.57
2:J:67:ALA:HB3	2:J:396:HIS:HB2	1.87	0.57
1:A:70:VAL:HA	1:A:96:ARG:NH1	2.19	0.57
1:A:356:GLY:CA	1:A:380:GLU:HB2	2.30	0.57
2:B:369:LEU:HD12	2:B:379:LEU:HD23	1.86	0.57
1:C:426:LYS:HA	2:D:104:ASN:HD21	1.70	0.57
1:I:437:PRO:HG3	1:I:472:TRP:CE2	2.40	0.57
2:J:477:HIS:N	2:L:499:ASN:HD21	1.92	0.57
1:K:154:CYS:SG	1:K:185:GLY:HA3	2.45	0.57
2:L:443:ILE:HD11	2:L:497:LEU:HD21	1.85	0.57
3:E:26:LEU:HD23	3:E:29:MET:CE	2.35	0.57
3:H:193:ASP:OD2	3:H:193:ASP:N	2.38	0.57
1:I:224:ALA:HB3	1:I:271:ASN:ND2	2.20	0.57
1:K:97:ARG:O	1:K:231:ILE:HA	2.04	0.57
1:K:427:GLU:CD	1:K:427:GLU:H	2.13	0.57
1:K:220:PRO:HA	1:K:269:LYS:HE2	1.87	0.56
1:A:229:TYR:OH	1:A:279:MET:HE3	2.05	0.56
2:D:194:VAL:HB	2:D:297:HIS:CB	2.35	0.56
3:O:21:ASN:HD21	3:O:227:VAL:H	1.52	0.56
2:B:118:MET:HB2	2:B:154:MET:HE1	1.86	0.56
3:E:169:VAL:HG21	3:E:258:PRO:HD3	1.87	0.56
3:F:22:LEU:HD13	3:F:244:ALA:HA	1.87	0.56
3:F:28:GLU:CD	3:F:241:ARG:HE	2.13	0.56
3:H:149:ILE:HG21	3:H:161:ALA:HA	1.87	0.56
1:I:70:VAL:HA	1:I:96:ARG:NH1	2.19	0.56
3:E:76:LEU:HD12	3:E:86:VAL:HB	1.87	0.56
3:G:165:SER:O	3:G:169:VAL:HG23	2.04	0.56
2:J:194:VAL:HB	2:J:297:HIS:CB	2.35	0.56
1:C:10:GLU:HG3	1:C:34:VAL:HG21	1.85	0.56
3:E:49:LEU:HD11	3:E:54:GLN:HE21	1.71	0.56
2:B:420:THR:HG22	2:B:422:TYR:CE1	2.41	0.56
3:E:178:ARG:HB2	3:E:253:LEU:HB3	1.87	0.56
1:I:135:ILE:HD13	1:I:178:ILE:HD13	1.86	0.56
3:N:15:LYS:HD2	3:N:126:VAL:O	2.05	0.56
1:A:370:LEU:HD11	1:A:460:ALA:HA	1.88	0.56
1:C:129:LYS:H	1:C:129:LYS:CD	2.07	0.56
2:D:445:ASN:HB2	2:D:472:PRO:O	2.06	0.56
3:G:20:GLN:NE2	3:G:47:LEU:H	2.03	0.56
3:G:23:VAL:HG11	3:G:35:ILE:HD11	1.88	0.56
1:I:36:ASP:OD1	1:I:38:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:443:ILE:HD11	2:J:497:LEU:HD21	1.88	0.56
1:K:36:ASP:OD1	1:K:38:ALA:HB3	2.05	0.56
3:O:94:GLY:H	3:P:131:VAL:HG12	1.71	0.56
2:D:254:LEU:O	2:D:255:SER:HB3	2.06	0.56
3:E:156:MET:CE	3:F:41:LYS:NZ	2.69	0.56
2:B:16:LEU:O	2:B:21:LYS:HE3	2.06	0.56
2:D:90:HIS:ND1	2:D:116:ASP:OD1	2.37	0.56
3:F:216:VAL:HG11	3:F:236:GLN:HB2	1.87	0.56
3:F:275:GLU:OE1	3:F:275:GLU:N	2.38	0.56
2:L:72:PRO:HB2	2:L:99:PHE:CZ	2.41	0.56
3:O:20:GLN:NE2	3:O:47:LEU:H	2.01	0.56
1:A:97:ARG:O	1:A:231:ILE:HA	2.06	0.55
1:C:343:ARG:HD3	1:C:347:GLU:OE2	2.05	0.55
1:K:245:MET:HG3	1:K:324:CYS:HA	1.87	0.55
2:L:92:SER:HB2	7:L:7498:CLF:S2A	2.45	0.55
1:A:426:LYS:HA	2:B:104:ASN:ND2	2.22	0.55
2:B:445:ASN:HD22	2:B:472:PRO:HD2	1.71	0.55
1:I:239:ARG:O	1:I:243:GLU:HG2	2.05	0.55
1:I:343:ARG:N	1:I:344:PRO:HD2	2.22	0.55
1:I:343:ARG:HD3	1:I:347:GLU:OE2	2.06	0.55
1:K:239:ARG:HH11	1:K:252:GLN:HE21	1.53	0.55
2:L:228:PRO:HA	2:L:293:LEU:HD12	1.89	0.55
3:P:57:ILE:HD12	3:P:105:ALA:HB1	1.88	0.55
2:B:377:MET:HE3	2:B:406:VAL:HG22	1.86	0.55
1:I:230:ASN:HA	1:I:235:ALA:H	1.72	0.55
2:L:148:ALA:HB1	2:L:200:MET:HE2	1.89	0.55
3:M:239:GLU:O	3:M:242:ALA:HB3	2.07	0.55
1:A:352:MET:CE	1:A:413:VAL:HA	2.36	0.55
1:I:427:GLU:H	1:I:427:GLU:CD	2.15	0.55
1:K:354:TYR:C	1:K:355:ILE:HG13	2.31	0.55
2:L:237:PHE:CE1	2:L:257:PRO:HD2	2.41	0.55
2:L:445:ASN:ND2	2:L:472:PRO:HD2	2.21	0.55
3:O:134:GLY:O	3:O:137:MET:HB2	2.06	0.55
3:F:25:ALA:HB2	3:F:228:ILE:CD1	2.36	0.55
2:J:445:ASN:HD22	2:J:472:PRO:HD2	1.72	0.55
3:M:265:GLU:HA	3:M:268:LEU:HD23	1.87	0.55
1:C:77:ASP:HB2	1:C:146:LYS:HB2	1.88	0.55
2:D:72:PRO:HB2	2:D:99:PHE:CZ	2.42	0.55
2:L:118:MET:HB2	2:L:154:MET:HE1	1.89	0.55
3:G:6:ALA:HB3	3:G:147:ILE:HD13	1.88	0.55
1:I:350:ARG:HB3	1:I:375:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:28:GLU:OE2	3:F:241:ARG:NE	2.37	0.55
2:L:369:LEU:HD12	2:L:379:LEU:HD23	1.87	0.55
1:A:36:ASP:OD1	1:A:38:ALA:HB3	2.07	0.55
1:A:224:ALA:HB3	1:A:271:ASN:ND2	2.22	0.55
1:A:230:ASN:HA	1:A:235:ALA:H	1.72	0.55
1:A:239:ARG:HH11	1:A:252:GLN:HE21	1.53	0.55
2:B:330:MET:SD	1:C:478:PRO:HB2	2.47	0.55
1:C:85:PRO:HB2	7:D:3498:CLF:S2B	2.46	0.55
3:F:192:GLU:O	3:F:196:ILE:HG12	2.07	0.55
1:I:433:LYS:NZ	2:J:263:THR:O	2.40	0.55
1:K:430:ILE:HG23	2:L:269:PHE:CD2	2.42	0.55
3:M:38:CYS:HB2	3:M:125:ASP:O	2.07	0.55
3:M:140:ARG:HB3	3:M:171:TYR:CE1	2.41	0.55
2:B:452:GLN:HG3	2:B:464:VAL:O	2.07	0.55
2:J:448:GLY:C	2:J:466:LEU:HD22	2.32	0.55
2:B:125:PHE:HZ	3:E:61:ALA:HB3	1.71	0.54
2:B:194:VAL:HB	2:B:297:HIS:CB	2.37	0.54
2:B:237:PHE:CE1	2:B:257:PRO:HD2	2.43	0.54
2:D:452:GLN:HG3	2:D:464:VAL:O	2.07	0.54
3:F:219:ARG:O	3:F:222:ILE:HG22	2.07	0.54
3:G:58:MET:HE2	3:G:101:GLY:HA2	1.89	0.54
3:N:11:GLY:HA2	3:N:15:LYS:HZ1	1.72	0.54
1:A:343:ARG:N	1:A:344:PRO:HD2	2.22	0.54
1:C:332:LYS:N	1:C:333:PRO:HD2	2.22	0.54
1:C:399:LEU:O	1:C:400:LEU:HD23	2.07	0.54
2:D:92:SER:HB2	7:D:3498:CLF:S2A	2.47	0.54
2:D:445:ASN:ND2	2:D:472:PRO:HD2	2.22	0.54
3:E:225:MET:HE3	3:E:229:GLU:CG	2.34	0.54
2:B:88:TYR:HH	2:B:116:ASP:HB3	1.68	0.54
2:B:90:HIS:ND1	2:B:116:ASP:OD1	2.40	0.54
1:C:394:MET:HG3	1:C:400:LEU:HD21	1.90	0.54
2:J:232:THR:HG21	2:J:471:PHE:CD1	2.42	0.54
2:J:296:TRP:HB2	2:J:374:ASP:OD1	2.07	0.54
3:O:16:SER:O	3:O:20:GLN:HG3	2.08	0.54
1:A:76:LYS:HG2	1:A:257:GLY:O	2.07	0.54
1:A:265:THR:N	1:A:266:PRO:HD2	2.22	0.54
3:E:76:LEU:HD13	3:E:86:VAL:HB	1.89	0.54
3:F:266:GLU:HA	3:F:269:MET:HE2	1.90	0.54
1:K:35:ASN:HD21	1:K:391:MET:HB3	1.72	0.54
2:L:384:LEU:HD11	2:L:410:LEU:HD23	1.89	0.54
1:C:427:GLU:CD	1:C:427:GLU:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:ASP:HB3	1:I:39:VAL:HG23	1.88	0.54
1:I:332:LYS:N	1:I:333:PRO:HD2	2.23	0.54
1:K:153:GLU:O	1:K:184:GLU:HG3	2.06	0.54
3:O:140:ARG:HG2	3:O:171:TYR:CE2	2.43	0.54
3:O:209:HIS:CD2	3:O:243:LEU:HB2	2.42	0.54
1:C:100:TYR:CE1	1:C:110:VAL:HB	2.43	0.54
1:C:229:TYR:OH	1:C:279:MET:HE3	2.07	0.54
2:D:118:MET:HB2	2:D:154:MET:HE1	1.90	0.54
2:D:443:ILE:HD11	2:D:497:LEU:HD21	1.89	0.54
3:H:99:GLY:HA3	3:H:134:GLY:C	2.32	0.54
3:H:164:ILE:O	3:H:168:ILE:HG13	2.08	0.54
2:L:71:GLN:HG2	2:L:192:SER:O	2.08	0.54
3:M:213:ARG:HA	9:M:5292:ADP:N1	2.23	0.54
3:P:19:THR:O	3:P:23:VAL:HG23	2.08	0.54
1:C:352:MET:HG3	1:C:418:PRO:HB3	1.90	0.54
1:C:354:TYR:C	1:C:355:ILE:HG13	2.33	0.54
1:C:442:HIS:HB3	4:C:494:HCA:O5	2.08	0.54
1:K:85:PRO:HB2	7:L:7498:CLF:S2B	2.47	0.54
1:K:229:TYR:OH	1:K:279:MET:HE3	2.07	0.54
2:L:194:VAL:HB	2:L:297:HIS:CB	2.38	0.54
3:P:14:GLY:HA2	9:P:8292:ADP:O2A	2.08	0.54
3:P:38:CYS:HB2	3:P:126:VAL:HG22	1.89	0.54
1:A:158:LEU:HD11	2:B:154:MET:HG3	1.89	0.53
1:C:36:ASP:OD1	1:C:38:ALA:HB3	2.08	0.53
1:C:70:VAL:HA	1:C:96:ARG:NH1	2.23	0.53
1:C:97:ARG:O	1:C:231:ILE:HA	2.07	0.53
1:C:158:LEU:HD11	2:D:154:MET:HG3	1.90	0.53
3:G:4:GLN:OE1	3:G:145:GLN:NE2	2.41	0.53
3:G:45:THR:O	3:G:49:LEU:HB2	2.08	0.53
1:I:352:MET:CE	1:I:413:VAL:HA	2.38	0.53
2:L:90:HIS:ND1	2:L:116:ASP:OD1	2.40	0.53
2:B:67:ALA:HB3	2:B:396:HIS:HB2	1.90	0.53
2:J:237:PHE:CE1	2:J:257:PRO:HD2	2.44	0.53
2:J:394:LEU:HD23	2:J:394:LEU:C	2.33	0.53
3:F:172:ALA:HB1	3:F:255:ILE:HD13	1.90	0.53
3:F:244:ALA:O	3:F:248:VAL:HG23	2.09	0.53
1:K:20:TYR:OH	1:K:408:GLU:HG3	2.08	0.53
1:K:230:ASN:HA	1:K:235:ALA:H	1.74	0.53
3:N:127:LEU:HD21	3:N:129:ASP:HB2	1.90	0.53
3:P:57:ILE:HD12	3:P:105:ALA:CB	2.38	0.53
1:A:100:TYR:CE1	1:A:110:VAL:HB	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:366:ARG:HB3	2:J:391:VAL:CG2	2.38	0.53
2:D:109:GLU:HG3	2:D:261:LEU:O	2.08	0.53
2:D:237:PHE:CE1	2:D:257:PRO:HD2	2.43	0.53
3:M:48:ILE:HD13	3:M:226:THR:HG21	1.91	0.53
3:O:243:LEU:O	3:O:247:VAL:HG23	2.08	0.53
2:B:109:GLU:HG3	2:B:261:LEU:O	2.09	0.53
1:C:230:ASN:HA	1:C:235:ALA:H	1.74	0.53
3:H:6:ALA:HB3	3:H:147:ILE:CD1	2.39	0.53
1:I:352:MET:HE3	1:I:413:VAL:HG22	1.90	0.53
1:K:433:LYS:HE3	2:L:110:PRO:HD2	1.91	0.53
3:M:131:VAL:CG1	3:M:136:ALA:HB2	2.38	0.53
3:O:55:ASN:HB2	3:O:60:MET:HE2	1.90	0.53
1:C:76:LYS:HG2	1:C:257:GLY:O	2.09	0.53
3:H:5:CYS:HB2	3:H:123:PHE:CE1	2.44	0.53
1:K:158:LEU:HD11	2:L:154:MET:CG	2.38	0.53
3:E:94:GLY:N	3:F:131:VAL:HG12	2.23	0.53
2:J:212:SER:O	2:J:216:LYS:HE2	2.09	0.53
2:L:494:LEU:C	2:L:494:LEU:HD23	2.34	0.53
2:B:494:LEU:O	2:B:498:VAL:HG12	2.09	0.53
1:C:370:LEU:HD11	1:C:460:ALA:HA	1.90	0.53
3:F:180:GLY:HA2	3:F:253:LEU:HD23	1.89	0.53
1:A:394:MET:HG3	1:A:400:LEU:HD21	1.90	0.53
3:H:5:CYS:HA	3:H:146:GLU:O	2.09	0.53
1:I:30:LYS:O	1:I:47:ILE:HG22	2.09	0.53
1:K:332:LYS:N	1:K:333:PRO:HD2	2.24	0.53
2:L:96:VAL:CG2	2:L:115:SER:HB2	2.38	0.53
1:A:332:LYS:N	1:A:333:PRO:HD2	2.24	0.52
1:I:100:TYR:CE1	1:I:110:VAL:HB	2.44	0.52
1:K:370:LEU:HD11	1:K:460:ALA:HA	1.90	0.52
3:O:55:ASN:N	3:O:55:ASN:HD22	2.06	0.52
2:B:212:SER:O	2:B:216:LYS:HE2	2.09	0.52
3:F:37:GLY:HA2	3:F:125:ASP:HB3	1.90	0.52
2:J:346:LYS:HE3	2:J:350:ARG:HH22	1.72	0.52
3:G:61:ALA:O	3:G:65:GLY:N	2.42	0.52
3:O:55:ASN:N	3:O:55:ASN:ND2	2.56	0.52
2:B:499:ASN:HD21	2:D:477:HIS:N	1.92	0.52
3:F:55:ASN:HD22	3:F:55:ASN:N	2.07	0.52
1:I:239:ARG:HD2	1:I:252:GLN:HE21	1.72	0.52
1:K:275:CYS:CA	1:K:358:LEU:HD22	2.35	0.52
3:O:132:CYS:O	3:O:136:ALA:N	2.36	0.52
3:P:149:ILE:HD12	3:P:182:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:8:TYR:O	3:O:149:ILE:HA	2.10	0.52
2:B:92:SER:HB2	7:B:1498:CLF:S2A	2.49	0.52
2:B:384:LEU:HD11	2:B:410:LEU:HD23	1.91	0.52
1:K:36:ASP:HB3	1:K:39:VAL:HG23	1.90	0.52
2:L:366:ARG:HB3	2:L:391:VAL:CG2	2.39	0.52
2:B:72:PRO:HB2	2:B:99:PHE:CZ	2.45	0.52
1:C:352:MET:HE3	1:C:413:VAL:HG22	1.91	0.52
1:I:154:CYS:SG	1:I:185:GLY:HA3	2.50	0.52
2:J:47:THR:HG22	2:J:52:TYR:CE1	2.44	0.52
2:J:180:PRO:HA	2:J:207:TYR:OH	2.10	0.52
2:L:220:SER:O	2:L:222:LYS:HE3	2.10	0.52
2:B:236:ASN:CG	2:B:485:LEU:HG	2.35	0.52
3:F:212:PRO:HD2	3:F:236:GLN:HE22	1.75	0.52
3:G:2:MET:CE	3:G:116:GLU:H	2.22	0.52
1:I:430:ILE:HG23	2:J:269:PHE:CG	2.45	0.52
2:J:455:THR:HB	2:J:463:GLU:HA	1.92	0.52
1:K:76:LYS:HG2	1:K:257:GLY:O	2.10	0.52
1:K:220:PRO:O	1:K:269:LYS:HG3	2.09	0.52
1:C:153:GLU:O	1:C:184:GLU:HG3	2.09	0.52
2:D:231:GLU:CD	2:D:236:ASN:HD22	2.18	0.52
3:F:158:MET:HB3	3:F:264:LEU:HD11	1.92	0.52
1:K:430:ILE:HG23	2:L:269:PHE:CG	2.44	0.52
1:A:437:PRO:HG3	1:A:472:TRP:CE2	2.45	0.52
1:C:35:ASN:HD21	1:C:391:MET:HB3	1.75	0.52
1:C:324:CYS:O	1:C:328:ILE:HG13	2.10	0.52
1:K:272:LEU:HD13	1:K:312:ILE:HD13	1.92	0.52
2:L:180:PRO:HA	2:L:207:TYR:OH	2.11	0.52
2:B:264:PRO:HB2	2:D:349:GLY:HA3	1.92	0.51
1:C:275:CYS:CA	1:C:358:LEU:HD22	2.36	0.51
2:D:431:ARG:HG2	2:D:431:ARG:HH11	1.73	0.51
1:I:433:LYS:HE3	2:J:110:PRO:HD2	1.92	0.51
2:J:222:LYS:HA	2:J:288:LEU:HD21	1.91	0.51
2:J:384:LEU:HD11	2:J:410:LEU:HD23	1.91	0.51
3:E:12:GLY:N	3:F:156:MET:HE3	2.25	0.51
3:E:20:GLN:HG2	3:E:48:ILE:HG12	1.91	0.51
3:F:114:ALA:O	3:F:117:ASP:HB2	2.11	0.51
1:I:430:ILE:HG23	2:J:269:PHE:CD2	2.45	0.51
2:L:151:THR:HG23	2:L:162:LEU:HD11	1.92	0.51
1:A:358:LEU:HB3	5:A:496:CFN:S4A	2.50	0.51
1:C:57:MET:HG3	2:D:114:VAL:HG12	1.92	0.51
2:D:194:VAL:HB	2:D:297:HIS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:369:LEU:HD12	2:D:379:LEU:HD23	1.91	0.51
3:E:156:MET:CE	3:F:41:LYS:HZ3	2.22	0.51
1:I:265:THR:N	1:I:266:PRO:HD2	2.25	0.51
2:J:231:GLU:CD	2:J:236:ASN:HD22	2.18	0.51
1:K:352:MET:HG3	1:K:418:PRO:HB3	1.93	0.51
3:O:160:ALA:O	3:O:164:ILE:HG13	2.10	0.51
1:A:62:CYS:SG	1:A:64:TYR:HB3	2.50	0.51
1:A:68:LYS:HD3	1:A:68:LYS:C	2.35	0.51
1:A:343:ARG:HD3	1:A:347:GLU:OE2	2.10	0.51
2:B:130:ASN:ND2	2:B:130:ASN:N	2.56	0.51
1:C:352:MET:CE	1:C:413:VAL:HA	2.41	0.51
3:F:259:ILE:HD11	3:F:264:LEU:HD13	1.93	0.51
3:M:127:LEU:HD21	3:M:129:ASP:HB2	1.93	0.51
3:P:214:ASP:OD1	3:P:216:VAL:HG12	2.10	0.51
2:B:220:SER:O	2:B:222:LYS:HE3	2.10	0.51
2:D:212:SER:O	2:D:216:LYS:HE2	2.10	0.51
2:D:377:MET:HE3	2:D:406:VAL:HG22	1.92	0.51
3:H:262:ASP:O	3:H:265:GLU:HG2	2.10	0.51
3:M:93:PRO:HB3	3:N:131:VAL:HB	1.92	0.51
2:B:10:ALA:O	2:B:11:SER:C	2.53	0.51
3:G:136:ALA:CB	3:H:94:GLY:HA2	2.40	0.51
1:I:62:CYS:SG	1:I:64:TYR:HB3	2.50	0.51
3:M:36:VAL:HG22	3:M:86:VAL:CG1	2.41	0.51
3:P:26:LEU:HD23	3:P:244:ALA:HB1	1.93	0.51
1:A:83:HIS:O	1:A:153:GLU:HB2	2.11	0.51
2:B:448:GLY:C	2:B:466:LEU:HD22	2.36	0.51
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.40	0.51
2:D:448:GLY:C	2:D:466:LEU:HD22	2.35	0.51
3:F:195:LEU:HD13	3:F:271:PHE:HD1	1.75	0.51
3:G:151:CYS:O	3:G:184:CYS:HA	2.11	0.51
3:M:22:LEU:HD13	3:M:243:LEU:HG	1.92	0.51
2:B:302:LYS:O	2:B:306:GLU:HG3	2.11	0.51
1:C:239:ARG:HH11	1:C:252:GLN:HE21	1.57	0.51
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.93	0.51
1:I:220:PRO:HA	1:I:269:LYS:HE2	1.91	0.51
1:I:355:ILE:HB	1:I:360:PRO:HD3	1.93	0.51
1:K:56:LEU:O	1:K:405:THR:HB	2.11	0.51
1:K:356:GLY:HA2	1:K:380:GLU:H	1.76	0.51
2:L:16:LEU:O	2:L:21:LYS:HE3	2.11	0.51
3:M:8:TYR:CB	3:M:164:ILE:HD13	2.35	0.51
1:A:273:VAL:O	1:A:296:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LYS:HE3	2:D:110:PRO:HD2	1.93	0.51
3:F:132:CYS:HB2	10:F:1290:SF4:S2	2.50	0.51
3:H:179:LEU:HG	3:H:205:THR:HG21	1.93	0.51
1:I:158:LEU:HD11	2:J:154:MET:HG3	1.93	0.51
2:J:202:GLU:O	2:J:206:ARG:HB3	2.11	0.51
2:L:266:ASP:OD2	2:L:270:ARG:NH2	2.29	0.51
3:O:140:ARG:HG2	3:O:171:TYR:CZ	2.45	0.51
1:A:352:MET:HE2	1:A:418:PRO:HD3	1.92	0.51
1:C:234:ASP:HB3	1:C:451:HIS:ND1	2.25	0.51
3:E:219:ARG:O	3:E:222:ILE:HG22	2.11	0.51
1:K:343:ARG:N	1:K:344:PRO:HD2	2.25	0.51
2:L:254:LEU:O	2:L:255:SER:HB3	2.11	0.51
3:N:130:VAL:HG22	3:N:132:CYS:SG	2.51	0.51
3:P:156:MET:HE2	3:P:156:MET:HA	1.92	0.51
3:P:214:ASP:O	3:P:217:VAL:HB	2.10	0.51
1:A:426:LYS:HA	2:B:104:ASN:HD21	1.75	0.50
3:E:12:GLY:H	3:F:156:MET:HE3	1.76	0.50
3:H:145:GLN:N	3:H:145:GLN:OE1	2.44	0.50
1:I:30:LYS:HB3	1:I:47:ILE:CG2	2.41	0.50
1:I:153:GLU:O	1:I:184:GLU:HG3	2.11	0.50
1:I:239:ARG:HD2	1:I:252:GLN:HE22	1.72	0.50
1:I:356:GLY:CA	1:I:380:GLU:HB2	2.29	0.50
1:K:433:LYS:NZ	2:L:263:THR:O	2.44	0.50
3:N:219:ARG:O	3:N:222:ILE:HG22	2.10	0.50
1:C:359:ARG:NH1	1:C:444:TRP:CZ2	2.79	0.50
3:F:237:ALA:O	3:F:241:ARG:HG3	2.12	0.50
3:F:264:LEU:O	3:F:268:LEU:HD23	2.10	0.50
3:G:244:ALA:O	3:G:248:VAL:HG23	2.10	0.50
1:I:442:HIS:HE1	5:I:496:CFN:S1B	2.32	0.50
3:M:173:ASN:N	3:M:173:ASN:HD22	2.09	0.50
3:F:206:GLN:NE2	2:L:222:LYS:HD3	2.26	0.50
3:G:5:CYS:HB2	3:G:123:PHE:CD1	2.46	0.50
1:I:134:LEU:O	1:I:138:VAL:HG23	2.11	0.50
2:J:228:PRO:HA	2:J:293:LEU:HD12	1.93	0.50
3:P:214:ASP:CG	3:P:216:VAL:HG12	2.36	0.50
1:A:383:HIS:O	1:A:386:ASP:HB2	2.12	0.50
2:D:10:ALA:O	2:D:11:SER:C	2.54	0.50
3:G:60:MET:HB3	3:G:70:LEU:HD11	1.92	0.50
1:I:220:PRO:O	1:I:269:LYS:HG3	2.12	0.50
2:J:148:ALA:HB1	2:J:200:MET:HE2	1.94	0.50
2:D:213:MET:HE2	2:D:308:THR:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:73:GLU:H	3:G:73:GLU:CD	2.20	0.50
2:J:254:LEU:O	2:J:255:SER:HB3	2.11	0.50
3:O:178:ARG:HG2	3:O:178:ARG:NH1	2.26	0.50
1:C:9:VAL:HG12	1:C:34:VAL:HG22	1.94	0.50
3:F:9:GLY:N	3:F:15:LYS:HD3	2.27	0.50
2:J:170:LYS:HD3	2:J:177:ASP:HA	1.91	0.50
2:J:431:ARG:O	2:J:434:VAL:HG22	2.11	0.50
2:L:80:LEU:HD13	2:L:87:PRO:HG2	1.94	0.50
3:O:146:GLU:C	3:O:147:ILE:HD12	2.37	0.50
3:G:235:LYS:O	3:G:238:ASP:HB2	2.12	0.50
1:I:272:LEU:HD13	1:I:312:ILE:HD13	1.93	0.50
1:K:270:LEU:HD12	1:K:293:PRO:O	2.11	0.50
1:K:420:LEU:C	1:K:420:LEU:HD23	2.37	0.50
3:O:92:GLU:O	3:O:95:VAL:HG22	2.12	0.50
1:A:239:ARG:HD2	1:A:252:GLN:HE22	1.74	0.50
1:C:220:PRO:HA	1:C:269:LYS:HE2	1.94	0.50
2:D:67:ALA:HB3	2:D:396:HIS:HB2	1.94	0.50
3:F:206:GLN:HG2	3:F:252:LEU:HD23	1.94	0.50
3:H:199:LEU:CA	3:H:267:LEU:HD21	2.42	0.50
3:H:214:ASP:HB3	3:H:216:VAL:HG12	1.94	0.50
1:K:352:MET:HE2	1:K:418:PRO:HD3	1.93	0.50
2:L:431:ARG:HH11	2:L:431:ARG:HG2	1.77	0.50
1:A:35:ASN:HD21	1:A:391:MET:HB3	1.77	0.50
1:C:358:LEU:HB3	5:C:496:CFN:S4A	2.52	0.50
1:I:352:MET:HG3	1:I:418:PRO:HB3	1.93	0.50
2:J:16:LEU:O	2:J:21:LYS:HE3	2.12	0.50
1:A:253:TRP:CZ3	1:A:282:ILE:HG12	2.47	0.49
2:B:213:MET:HE2	2:B:308:THR:O	2.12	0.49
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.77	0.49
2:D:47:THR:HG22	2:D:52:TYR:CE1	2.47	0.49
1:I:76:LYS:HG2	1:I:257:GLY:O	2.10	0.49
1:K:158:LEU:HD11	2:L:154:MET:HG3	1.94	0.49
2:B:521:LEU:CD2	1:C:94:ALA:HB3	2.40	0.49
2:D:16:LEU:O	2:D:21:LYS:HE3	2.12	0.49
2:D:220:SER:O	2:D:222:LYS:HE3	2.12	0.49
3:F:195:LEU:HD21	3:F:268:LEU:HD13	1.94	0.49
3:G:234:ALA:O	3:G:237:ALA:HB3	2.12	0.49
1:I:9:VAL:HG12	1:I:34:VAL:HG22	1.93	0.49
2:J:194:VAL:HB	2:J:297:HIS:HB2	1.93	0.49
2:J:302:LYS:O	2:J:306:GLU:HG3	2.12	0.49
2:L:346:LYS:HE3	2:L:350:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:155:MET:HE2	3:P:268:LEU:HD11	1.93	0.49
1:A:220:PRO:HA	1:A:269:LYS:HE2	1.94	0.49
1:A:239:ARG:HD2	1:A:252:GLN:HE21	1.76	0.49
1:A:352:MET:HG3	1:A:418:PRO:HB3	1.93	0.49
1:A:356:GLY:HA2	1:A:380:GLU:H	1.77	0.49
1:C:383:HIS:O	1:C:386:ASP:HB2	2.11	0.49
3:H:199:LEU:HA	3:H:267:LEU:HD21	1.94	0.49
2:L:170:LYS:HD3	2:L:177:ASP:HA	1.94	0.49
3:M:234:ALA:O	3:M:237:ALA:HB3	2.13	0.49
2:B:180:PRO:HA	2:B:207:TYR:OH	2.13	0.49
1:C:210:ARG:HH11	1:C:264:LEU:HD21	1.76	0.49
1:C:356:GLY:HA2	1:C:380:GLU:H	1.78	0.49
3:E:36:VAL:HG22	3:E:86:VAL:CG1	2.42	0.49
3:F:151:CYS:SG	3:F:196:ILE:HD12	2.52	0.49
1:I:444:TRP:CE3	1:I:450:TYR:CD2	3.00	0.49
2:L:222:LYS:HA	2:L:288:LEU:HD21	1.94	0.49
3:M:131:VAL:HG12	3:M:136:ALA:HB2	1.95	0.49
3:P:13:ILE:HD12	3:P:150:VAL:O	2.12	0.49
1:A:354:TYR:C	1:A:355:ILE:HG13	2.36	0.49
2:D:148:ALA:HB1	2:D:200:MET:HE2	1.95	0.49
3:G:19:THR:O	3:G:23:VAL:HG23	2.13	0.49
1:I:253:TRP:CZ2	1:I:262:ILE:HG23	2.47	0.49
3:O:49:LEU:HD11	3:O:54:GLN:NE2	2.27	0.49
3:O:177:VAL:O	3:O:178:ARG:NH1	2.43	0.49
2:D:494:LEU:O	2:D:498:VAL:HG12	2.12	0.49
3:G:114:ALA:O	3:G:117:ASP:HB2	2.12	0.49
1:I:57:MET:HE3	2:J:142:TYR:CZ	2.48	0.49
2:J:71:GLN:HG2	2:J:192:SER:O	2.12	0.49
2:J:445:ASN:HB2	2:J:472:PRO:O	2.11	0.49
1:K:383:HIS:O	1:K:386:ASP:HB2	2.12	0.49
1:K:399:LEU:O	1:K:400:LEU:HD23	2.13	0.49
2:L:455:THR:HB	2:L:463:GLU:HA	1.93	0.49
3:M:45:THR:O	3:M:49:LEU:HB2	2.13	0.49
1:C:265:THR:N	1:C:266:PRO:HD2	2.28	0.49
3:F:56:THR:HG22	3:F:87:GLU:CB	2.38	0.49
2:J:10:ALA:O	2:J:11:SER:C	2.56	0.49
2:B:487:TYR:O	2:B:491:MET:HG3	2.12	0.49
1:C:352:MET:HE2	1:C:416:ILE:HB	1.94	0.49
3:F:10:LYS:O	3:F:15:LYS:HE2	2.12	0.49
3:G:94:GLY:H	3:H:131:VAL:HG12	1.77	0.49
1:I:478:PRO:HB2	2:L:330:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:217:VAL:HG23	3:P:236:GLN:HG2	1.95	0.49
2:B:125:PHE:HE1	3:E:58:MET:O	1.96	0.49
2:B:318:ILE:HG23	2:B:318:ILE:O	2.12	0.49
1:C:245:MET:HG3	1:C:324:CYS:HA	1.95	0.49
1:C:429:PHE:CB	2:D:110:PRO:HD3	2.38	0.49
2:D:277:THR:OG1	2:D:280:GLU:HG3	2.13	0.49
1:I:358:LEU:HB3	5:I:496:CFN:S4A	2.53	0.49
1:A:9:VAL:HG12	1:A:34:VAL:HG22	1.93	0.49
2:B:366:ARG:HB3	2:B:391:VAL:CG2	2.42	0.49
2:D:180:PRO:HA	2:D:207:TYR:OH	2.13	0.49
3:G:94:GLY:N	3:H:131:VAL:HG12	2.28	0.49
3:O:8:TYR:CE2	3:O:126:VAL:HG11	2.48	0.49
3:O:58:MET:HG2	3:O:88:SER:O	2.12	0.49
1:A:36:ASP:HB3	1:A:39:VAL:HG23	1.93	0.48
3:F:256:PRO:O	3:F:258:PRO:HD3	2.13	0.48
1:K:265:THR:N	1:K:266:PRO:HD2	2.28	0.48
2:L:144:PRO:HB3	2:L:272:TYR:OH	2.13	0.48
3:F:195:LEU:HD13	3:F:271:PHE:CD1	2.48	0.48
1:I:77:ASP:OD1	1:I:258:SER:HA	2.13	0.48
3:O:15:LYS:HA	3:O:150:VAL:HG21	1.94	0.48
3:O:134:GLY:O	3:O:137:MET:CB	2.61	0.48
1:A:399:LEU:O	1:A:400:LEU:HD23	2.12	0.48
1:C:36:ASP:HB3	1:C:39:VAL:HG23	1.94	0.48
1:C:220:PRO:O	1:C:269:LYS:HG3	2.13	0.48
3:G:48:ILE:HG22	3:G:79:GLY:HA3	1.95	0.48
1:I:253:TRP:CZ3	1:I:282:ILE:HG12	2.48	0.48
2:J:326:ASP:CG	2:J:348:ARG:HE	2.21	0.48
1:A:478:PRO:HB2	2:D:330:MET:SD	2.52	0.48
2:B:284:ALA:HB3	2:B:285:PRO:HD3	1.95	0.48
1:I:270:LEU:HD12	1:I:293:PRO:O	2.12	0.48
2:J:118:MET:CB	2:J:154:MET:HE1	2.42	0.48
2:L:67:ALA:HB3	2:L:396:HIS:HB2	1.95	0.48
3:M:6:ALA:C	3:M:7:ILE:HD13	2.38	0.48
3:N:7:ILE:O	3:N:126:VAL:HB	2.12	0.48
3:O:147:ILE:HD12	3:O:147:ILE:N	2.28	0.48
2:D:375:PHE:CZ	2:D:379:LEU:HD22	2.49	0.48
3:F:178:ARG:HB3	3:F:253:LEU:HB3	1.95	0.48
2:L:124:VAL:CG2	2:L:125:PHE:N	2.77	0.48
3:M:212:PRO:HG2	3:M:236:GLN:OE1	2.14	0.48
2:B:219:GLY:HA2	2:B:288:LEU:HA	1.94	0.48
3:G:152:SER:OG	3:G:154:GLU:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:135:LEU:HB3	2:L:175:ILE:HG21	1.94	0.48
3:N:245:ARG:O	3:N:249:ASP:HB2	2.14	0.48
3:P:10:LYS:O	3:P:13:ILE:HG12	2.12	0.48
3:P:13:ILE:CD1	3:P:150:VAL:O	2.61	0.48
1:A:77:ASP:OD1	1:A:258:SER:HA	2.13	0.48
2:B:455:THR:HB	2:B:463:GLU:HA	1.95	0.48
2:D:455:THR:HB	2:D:463:GLU:HA	1.94	0.48
2:J:131:MET:HG2	2:J:165:PHE:HB3	1.95	0.48
1:K:426:LYS:HB2	1:K:427:GLU:OE2	2.14	0.48
2:L:109:GLU:HG3	2:L:261:LEU:O	2.13	0.48
2:L:130:ASN:ND2	2:L:130:ASN:N	2.60	0.48
3:M:109:LEU:O	3:M:113:GLY:N	2.47	0.48
1:A:272:LEU:HD13	1:A:312:ILE:HD13	1.95	0.48
2:B:228:PRO:HA	2:B:293:LEU:HD12	1.96	0.48
3:F:213:ARG:HA	9:F:2292:ADP:N1	2.29	0.48
2:B:322:LEU:HD21	1:C:474:LYS:HB3	1.95	0.48
2:D:170:LYS:HD3	2:D:177:ASP:HA	1.96	0.48
1:I:273:VAL:O	1:I:296:GLU:HA	2.12	0.48
2:J:120:GLU:O	2:J:123:ALA:HB3	2.13	0.48
2:J:151:THR:HG23	2:J:162:LEU:HD11	1.95	0.48
2:L:212:SER:O	2:L:216:LYS:HE2	2.13	0.48
2:L:366:ARG:NH2	2:L:437:ASP:OD1	2.47	0.48
1:A:5:SER:O	1:A:9:VAL:HG23	2.13	0.48
2:B:125:PHE:CZ	3:E:61:ALA:HB3	2.49	0.48
1:C:253:TRP:CZ2	1:C:262:ILE:HG23	2.49	0.48
1:C:270:LEU:HD12	1:C:293:PRO:O	2.14	0.48
1:C:352:MET:HE2	1:C:418:PRO:HD3	1.96	0.48
2:D:362:LEU:HD22	2:D:388:CYS:SG	2.54	0.48
3:G:45:THR:CG2	3:G:85:CYS:HB3	2.44	0.48
3:H:36:VAL:HG13	3:H:86:VAL:HG13	1.95	0.48
3:O:189:THR:HG22	3:O:190:ASP:N	2.28	0.48
1:C:359:ARG:NH1	1:C:444:TRP:CH2	2.82	0.47
3:G:142:ASN:HB3	3:G:145:GLN:OE1	2.14	0.47
3:H:199:LEU:HB2	3:H:267:LEU:HD21	1.94	0.47
3:H:200:ALA:HB1	3:H:205:THR:O	2.14	0.47
1:I:30:LYS:HB3	1:I:47:ILE:HG21	1.96	0.47
1:K:30:LYS:HB3	1:K:47:ILE:CG2	2.44	0.47
3:M:99:GLY:HA3	3:M:134:GLY:HA3	1.96	0.47
3:N:21:ASN:N	3:N:21:ASN:HD22	2.10	0.47
1:C:253:TRP:CZ3	1:C:282:ILE:HG12	2.48	0.47
1:C:430:ILE:HG23	2:D:269:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:332:LYS:HA	1:I:335:TRP:NE1	2.29	0.47
1:K:253:TRP:CZ2	1:K:262:ILE:HG23	2.50	0.47
2:L:151:THR:CG2	2:L:162:LEU:HD11	2.43	0.47
3:O:4:GLN:NE2	3:O:145:GLN:HE22	2.13	0.47
1:A:163:ILE:H	1:A:182:ARG:NH2	2.12	0.47
3:F:144:ALA:O	3:F:177:VAL:HG13	2.14	0.47
1:K:239:ARG:HD2	1:K:252:GLN:HE21	1.77	0.47
1:K:428:LYS:HA	1:K:438:PHE:CE2	2.48	0.47
3:N:36:VAL:HA	3:N:86:VAL:O	2.14	0.47
3:O:100:ARG:HA	3:O:103:ILE:HD12	1.96	0.47
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.44	0.47
3:F:11:GLY:HA2	3:F:15:LYS:NZ	2.29	0.47
1:K:253:TRP:CZ3	1:K:282:ILE:HG12	2.49	0.47
1:A:184:GLU:HB2	1:A:187:ARG:HG3	1.96	0.47
3:F:4:GLN:HB3	3:F:144:ALA:HA	1.96	0.47
3:G:36:VAL:HA	3:G:86:VAL:HG13	1.97	0.47
3:G:130:VAL:HG11	3:H:130:VAL:HG11	1.96	0.47
1:I:68:LYS:HD3	1:I:68:LYS:C	2.40	0.47
2:J:151:THR:CG2	2:J:162:LEU:HD11	2.43	0.47
2:J:420:THR:HG22	2:J:422:TYR:CE1	2.50	0.47
3:M:18:THR:O	3:M:22:LEU:HB3	2.14	0.47
3:M:166:LYS:O	3:M:169:VAL:HG23	2.14	0.47
3:P:225:MET:HE2	3:P:230:TYR:HA	1.96	0.47
2:B:231:GLU:CD	2:B:236:ASN:HD22	2.23	0.47
2:B:236:ASN:OD1	2:B:485:LEU:HG	2.14	0.47
2:D:236:ASN:CG	2:D:485:LEU:HG	2.39	0.47
1:I:234:ASP:HB3	1:I:451:HIS:ND1	2.30	0.47
1:K:239:ARG:HD2	1:K:252:GLN:HE22	1.76	0.47
3:M:36:VAL:HG22	3:M:86:VAL:HG11	1.96	0.47
3:N:114:ALA:O	3:N:117:ASP:HB2	2.15	0.47
3:N:165:SER:O	3:N:169:VAL:HG23	2.14	0.47
1:A:352:MET:HE1	1:A:413:VAL:HA	1.97	0.47
2:B:296:TRP:HB2	2:B:374:ASP:OD1	2.15	0.47
1:C:359:ARG:CZ	1:C:444:TRP:CZ2	2.97	0.47
1:C:442:HIS:HE1	5:C:496:CFN:S1B	2.38	0.47
2:D:494:LEU:C	2:D:494:LEU:HD23	2.40	0.47
3:E:170:LYS:HE2	3:F:95:VAL:CG1	2.42	0.47
3:F:206:GLN:HB3	2:L:222:LYS:HG2	1.97	0.47
1:I:383:HIS:O	1:I:386:ASP:HB2	2.15	0.47
1:I:428:LYS:O	1:I:432:GLN:HG3	2.15	0.47
2:L:318:ILE:HG23	2:L:318:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:211:VAL:HA	3:P:212:PRO:HD3	1.76	0.47
1:A:20:TYR:HH	1:A:408:GLU:CD	2.22	0.47
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.96	0.47
1:C:404:VAL:HG22	1:C:405:THR:O	2.15	0.47
3:G:212:PRO:HG2	3:G:239:GLU:HG3	1.96	0.47
1:I:352:MET:HE2	1:I:416:ILE:HB	1.96	0.47
2:J:213:MET:HE2	2:J:308:THR:O	2.15	0.47
1:K:68:LYS:C	1:K:68:LYS:HD3	2.40	0.47
3:O:148:TYR:HA	3:O:181:GLY:O	2.15	0.47
3:O:184:CYS:O	3:O:211:VAL:HG23	2.15	0.47
3:P:6:ALA:O	3:P:7:ILE:HD13	2.15	0.47
3:F:32:LYS:H	3:F:120:ASP:CG	2.23	0.47
3:F:260:THR:HG23	3:F:263:GLU:OE1	2.15	0.47
3:G:138:PRO:HA	3:G:143:LYS:HB2	1.96	0.47
3:G:147:ILE:HG21	3:G:168:ILE:HD11	1.96	0.47
1:I:14:GLN:HA	1:I:14:GLN:NE2	2.30	0.47
2:J:135:LEU:HB3	2:J:175:ILE:HG21	1.97	0.47
1:K:77:ASP:OD1	1:K:258:SER:HA	2.15	0.47
2:L:194:VAL:HB	2:L:297:HIS:HB2	1.97	0.47
2:L:448:GLY:C	2:L:466:LEU:HD22	2.39	0.47
3:M:20:GLN:O	3:M:48:ILE:HD11	2.15	0.47
1:A:97:ARG:HB3	1:A:99:TYR:CE1	2.50	0.47
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.50	0.47
1:C:253:TRP:HA	1:C:254:SER:HA	1.50	0.47
2:D:445:ASN:HD22	2:D:472:PRO:HD2	1.80	0.47
3:E:165:SER:O	3:E:169:VAL:HG23	2.15	0.47
3:F:57:ILE:HD12	3:F:105:ALA:HB1	1.97	0.47
1:I:332:LYS:HA	1:I:335:TRP:CD1	2.50	0.47
1:I:350:ARG:HB3	1:I:375:VAL:HG13	1.97	0.47
1:K:9:VAL:HG12	1:K:34:VAL:HG22	1.97	0.47
1:K:465:MET:O	1:K:469:ASN:HB2	2.15	0.47
2:L:394:LEU:C	2:L:394:LEU:HD23	2.40	0.47
3:O:71:GLU:O	3:O:75:VAL:HG23	2.14	0.47
3:O:137:MET:HA	3:O:140:ARG:HD2	1.97	0.47
1:A:428:LYS:O	1:A:432:GLN:HG3	2.15	0.46
2:B:443:ILE:HD11	2:B:497:LEU:HD21	1.97	0.46
1:I:474:LYS:HB3	2:L:322:LEU:HD21	1.97	0.46
1:K:441:MET:O	1:K:444:TRP:CZ3	2.68	0.46
3:M:20:GLN:HE22	3:M:47:LEU:H	1.62	0.46
3:M:138:PRO:O	3:M:141:GLU:O	2.33	0.46
1:A:47:ILE:HD12	1:A:47:ILE:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:348:ARG:HB2	2:D:487:TYR:CZ	2.50	0.46
3:E:28:GLU:CD	3:E:241:ARG:HH21	2.19	0.46
3:F:267:LEU:HD12	3:F:267:LEU:HA	1.81	0.46
3:G:2:MET:HA	3:G:120:ASP:O	2.14	0.46
3:H:197:ILE:O	3:H:201:ASN:HB2	2.14	0.46
2:J:264:PRO:HB2	2:L:349:GLY:HA3	1.97	0.46
1:K:454:ASP:OD1	2:L:3:GLN:HG2	2.15	0.46
3:M:92:GLU:O	3:M:95:VAL:HG22	2.16	0.46
3:O:20:GLN:HE22	3:O:47:LEU:N	2.06	0.46
3:O:103:ILE:CG1	3:O:137:MET:HG3	2.41	0.46
1:A:199:ASN:HD21	1:A:279:MET:HG2	1.80	0.46
1:A:253:TRP:HA	1:A:254:SER:HA	1.53	0.46
2:D:348:ARG:HB2	2:D:487:TYR:CE2	2.51	0.46
3:E:112:GLU:OE1	3:E:112:GLU:HA	2.15	0.46
3:F:4:GLN:NE2	3:F:143:LYS:O	2.49	0.46
1:I:62:CYS:HB3	2:J:94:GLY:HA3	1.96	0.46
1:I:237:SER:O	1:I:240:ILE:HG22	2.16	0.46
3:M:181:GLY:HA2	3:M:205:THR:OG1	2.15	0.46
3:O:3:ARG:HH22	3:O:248:VAL:CA	2.25	0.46
2:B:468:ARG:HG3	2:B:468:ARG:HH11	1.80	0.46
3:E:9:GLY:N	3:E:15:LYS:HD3	2.31	0.46
3:E:45:THR:O	3:E:49:LEU:HB2	2.15	0.46
3:E:114:ALA:O	3:E:117:ASP:HB2	2.15	0.46
3:F:152:SER:OG	3:F:154:GLU:HG2	2.15	0.46
1:I:350:ARG:HB3	1:I:375:VAL:HG11	1.97	0.46
1:K:253:TRP:HA	1:K:254:SER:HA	1.54	0.46
1:K:265:THR:O	1:K:268:VAL:HG13	2.15	0.46
1:K:273:VAL:O	1:K:296:GLU:HA	2.14	0.46
2:L:326:ASP:CG	2:L:348:ARG:HE	2.23	0.46
3:N:10:LYS:O	3:N:13:ILE:HG12	2.15	0.46
1:C:97:ARG:HB3	1:C:99:TYR:CE1	2.51	0.46
3:F:2:MET:CG	3:F:119:LEU:O	2.63	0.46
3:F:252:LEU:HD12	3:F:254:VAL:HG13	1.97	0.46
1:I:354:TYR:C	1:I:355:ILE:HG13	2.39	0.46
1:I:428:LYS:HA	1:I:438:PHE:CE2	2.51	0.46
1:K:190:SER:HB2	1:K:381:PHE:HB3	1.96	0.46
1:K:332:LYS:HA	1:K:335:TRP:CD1	2.51	0.46
1:K:429:PHE:CB	2:L:110:PRO:HD3	2.40	0.46
1:K:442:HIS:HE1	5:K:496:CFN:S1B	2.38	0.46
2:L:198:ASP:HB2	2:L:297:HIS:O	2.15	0.46
2:L:277:THR:OG1	2:L:280:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:165:SER:OG	3:M:256:PRO:HB2	2.14	0.46
1:A:54:PRO:HB3	2:B:116:ASP:C	2.41	0.46
1:A:152:SER:HB2	1:A:184:GLU:OE1	2.16	0.46
2:B:431:ARG:O	2:B:434:VAL:HG22	2.16	0.46
1:C:272:LEU:HD13	1:C:312:ILE:HD13	1.98	0.46
1:I:210:ARG:HH11	1:I:264:LEU:CD2	2.28	0.46
1:K:42:SER:HA	1:K:391:MET:CE	2.45	0.46
1:K:428:LYS:O	1:K:432:GLN:HG3	2.16	0.46
2:L:72:PRO:O	2:L:76:VAL:HG23	2.15	0.46
2:L:232:THR:HG21	2:L:471:PHE:CD1	2.50	0.46
1:A:430:ILE:HG23	2:B:269:PHE:CG	2.51	0.46
2:B:103:PHE:HB3	2:B:111:VAL:HG21	1.97	0.46
1:C:423:SER:O	1:C:440:GLU:HA	2.16	0.46
1:I:47:ILE:HD12	1:I:47:ILE:HA	1.84	0.46
1:I:190:SER:HB2	1:I:381:PHE:HB3	1.98	0.46
1:K:203:ARG:HH11	1:K:204:ASP:CG	2.24	0.46
2:L:10:ALA:O	2:L:11:SER:C	2.58	0.46
2:L:355:MET:HE3	2:L:386:LEU:HD23	1.97	0.46
2:B:198:ASP:HB2	2:B:297:HIS:O	2.16	0.46
1:C:430:ILE:HG23	2:D:269:PHE:CG	2.50	0.46
2:D:202:GLU:O	2:D:206:ARG:HB3	2.15	0.46
3:E:10:LYS:O	3:E:13:ILE:HG12	2.16	0.46
3:F:158:MET:SD	3:F:268:LEU:HD21	2.56	0.46
3:G:237:ALA:HB1	3:G:241:ARG:NH1	2.28	0.46
2:J:362:LEU:HD22	2:J:388:CYS:SG	2.56	0.46
2:L:298:LEU:HD23	2:L:298:LEU:HA	1.78	0.46
3:P:216:VAL:HG22	3:P:227:VAL:HG13	1.96	0.46
1:A:220:PRO:O	1:A:269:LYS:HG3	2.16	0.46
2:B:170:LYS:HD3	2:B:177:ASP:HA	1.97	0.46
3:E:23:VAL:HG11	3:E:83:VAL:HG11	1.98	0.46
3:F:186:SER:O	3:F:213:ARG:HD3	2.15	0.46
3:G:138:PRO:O	3:G:141:GLU:O	2.34	0.46
1:I:70:VAL:HG13	1:I:96:ARG:NH2	2.31	0.46
1:I:97:ARG:HB3	1:I:99:TYR:CE1	2.51	0.46
1:I:163:ILE:H	1:I:182:ARG:NH2	2.14	0.46
2:J:236:ASN:CG	2:J:485:LEU:HG	2.41	0.46
2:J:314:PRO:HB3	2:J:331:LYS:HE2	1.97	0.46
1:K:352:MET:HE1	1:K:413:VAL:HA	1.97	0.46
2:L:362:LEU:HD22	2:L:388:CYS:SG	2.56	0.46
2:L:377:MET:HE3	2:L:406:VAL:CG2	2.46	0.46
3:M:134:GLY:O	3:M:137:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:165:SER:O	3:P:169:VAL:HG23	2.14	0.46
2:D:219:GLY:HA2	2:D:288:LEU:HA	1.98	0.46
3:E:48:ILE:HG22	3:E:80:TYR:H	1.81	0.46
3:F:32:LYS:O	3:F:120:ASP:N	2.49	0.46
1:K:47:ILE:HD12	1:K:47:ILE:HA	1.82	0.46
1:K:224:ALA:HB3	1:K:271:ASN:HD22	1.80	0.46
3:O:4:GLN:NE2	3:O:145:GLN:NE2	2.64	0.46
3:O:35:ILE:HA	3:O:123:PHE:O	2.16	0.46
1:A:14:GLN:HA	1:A:14:GLN:NE2	2.31	0.45
1:C:273:VAL:O	1:C:296:GLU:HA	2.15	0.45
3:E:145:GLN:N	3:E:145:GLN:CD	2.74	0.45
3:F:149:ILE:HG21	3:F:161:ALA:HA	1.97	0.45
3:F:195:LEU:HA	3:F:271:PHE:CE1	2.51	0.45
3:G:238:ASP:O	3:G:241:ARG:HB2	2.15	0.45
1:I:399:LEU:O	1:I:400:LEU:HD23	2.15	0.45
1:K:57:MET:CE	2:L:86:MET:HE1	2.47	0.45
1:K:354:TYR:C	1:K:355:ILE:CG1	2.89	0.45
1:K:423:SER:O	1:K:440:GLU:HA	2.16	0.45
2:L:213:MET:HE2	2:L:308:THR:O	2.16	0.45
3:P:54:GLN:OE1	3:P:87:GLU:HG2	2.16	0.45
2:B:331:LYS:HD2	2:B:331:LYS:HA	1.72	0.45
1:C:56:LEU:O	1:C:405:THR:HB	2.17	0.45
3:F:152:SER:H	3:F:157:ALA:CB	2.29	0.45
3:G:12:GLY:H	9:G:3292:ADP:PB	2.40	0.45
2:J:109:GLU:HG3	2:J:261:LEU:O	2.16	0.45
2:B:202:GLU:O	2:B:206:ARG:HB3	2.17	0.45
2:B:254:LEU:O	2:B:255:SER:HB3	2.16	0.45
1:C:428:LYS:O	1:C:432:GLN:HG3	2.16	0.45
2:D:284:ALA:HB3	2:D:285:PRO:HD3	1.98	0.45
3:E:7:ILE:HD13	3:E:148:TYR:HB2	1.97	0.45
3:E:22:LEU:HB2	3:E:243:LEU:HD23	1.98	0.45
3:F:14:GLY:HA2	9:F:2292:ADP:O5'	2.16	0.45
3:F:137:MET:HB3	3:F:138:PRO:HD3	1.98	0.45
1:I:35:ASN:HD21	1:I:391:MET:CB	2.28	0.45
2:L:426:ASP:O	2:L:429:HIS:HB2	2.15	0.45
3:M:93:PRO:HB2	3:N:163:ASN:O	2.15	0.45
3:M:219:ARG:O	3:M:222:ILE:HG22	2.16	0.45
3:O:189:THR:CG2	3:O:190:ASP:N	2.79	0.45
1:A:270:LEU:HD12	1:A:293:PRO:O	2.16	0.45
1:A:324:CYS:O	1:A:328:ILE:HG13	2.16	0.45
2:B:148:ALA:HB1	2:B:200:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:366:ARG:NH2	2:D:437:ASP:OD1	2.50	0.45
3:G:154:GLU:HG3	3:G:157:ALA:H	1.82	0.45
3:P:217:VAL:CG2	3:P:236:GLN:HG2	2.46	0.45
1:A:237:SER:O	1:A:240:ILE:HG22	2.17	0.45
3:E:131:VAL:HG11	3:F:93:PRO:HB3	1.97	0.45
3:E:225:MET:HE2	3:E:230:TYR:CA	2.45	0.45
1:I:56:LEU:O	1:I:405:THR:HB	2.15	0.45
2:J:430:LEU:O	2:J:431:ARG:C	2.59	0.45
2:L:445:ASN:HD22	2:L:472:PRO:HD2	1.82	0.45
3:M:217:VAL:HA	3:M:227:VAL:CG2	2.45	0.45
1:A:56:LEU:O	1:A:405:THR:HB	2.15	0.45
2:B:277:THR:OG1	2:B:280:GLU:HG3	2.15	0.45
2:D:78:CYS:HB2	2:D:197:TRP:CD1	2.51	0.45
2:D:131:MET:HG2	2:D:165:PHE:HB3	1.99	0.45
3:G:136:ALA:O	3:G:139:ILE:HB	2.16	0.45
3:G:200:ALA:O	3:G:205:THR:O	2.33	0.45
2:J:80:LEU:HD13	2:J:87:PRO:HG2	1.98	0.45
2:J:198:ASP:HB2	2:J:297:HIS:O	2.17	0.45
2:J:431:ARG:HG2	2:J:431:ARG:HH11	1.82	0.45
3:M:93:PRO:HG2	3:N:163:ASN:CA	2.45	0.45
3:M:140:ARG:HA	3:M:171:TYR:CD1	2.51	0.45
3:M:231:ASP:OD2	3:M:234:ALA:HB2	2.17	0.45
3:P:9:GLY:HA3	3:P:13:ILE:HD11	1.97	0.45
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.99	0.45
2:D:80:LEU:HD13	2:D:87:PRO:HG2	1.99	0.45
2:D:198:ASP:HB2	2:D:297:HIS:O	2.17	0.45
3:F:138:PRO:HA	3:F:143:LYS:HB2	1.99	0.45
3:O:179:LEU:CD2	3:O:205:THR:HG21	2.47	0.45
3:O:222:ILE:CG2	3:O:223:ARG:N	2.79	0.45
3:P:156:MET:HA	3:P:156:MET:CE	2.47	0.45
2:B:366:ARG:HA	2:B:389:GLU:O	2.17	0.45
1:C:9:VAL:CG1	1:C:34:VAL:HG22	2.47	0.45
1:C:14:GLN:NE2	1:C:14:GLN:HA	2.32	0.45
1:C:30:LYS:O	1:C:47:ILE:HG22	2.17	0.45
1:C:47:ILE:HD12	1:C:47:ILE:HA	1.82	0.45
1:C:199:ASN:HD21	1:C:279:MET:HG2	1.81	0.45
1:C:332:LYS:HA	1:C:335:TRP:CD1	2.52	0.45
3:G:103:ILE:HA	3:G:137:MET:HE2	1.98	0.45
2:J:499:ASN:HD21	2:L:477:HIS:N	1.97	0.45
1:A:184:GLU:CD	1:A:187:ARG:HE	2.25	0.45
1:A:322:LYS:O	1:A:326:GLU:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:LYS:HA	2:D:288:LEU:HD21	1.99	0.45
2:D:299:GLU:CD	2:D:401:ARG:HH22	2.25	0.45
1:I:158:LEU:HD11	2:J:154:MET:HG2	1.98	0.45
3:M:160:ALA:O	3:M:164:ILE:HG13	2.17	0.45
3:N:130:VAL:HG13	3:N:130:VAL:O	2.16	0.45
1:C:126:GLY:HA2	1:C:159:ILE:HD12	1.99	0.45
1:C:163:ILE:H	1:C:182:ARG:NH2	2.14	0.45
1:C:441:MET:O	1:C:444:TRP:CZ3	2.70	0.45
2:D:254:LEU:O	2:D:255:SER:CB	2.64	0.45
3:E:22:LEU:O	3:E:26:LEU:HG	2.17	0.45
3:E:23:VAL:CG1	3:E:83:VAL:HG11	2.47	0.45
3:G:259:ILE:HD12	3:G:260:THR:O	2.17	0.45
1:K:332:LYS:HA	1:K:335:TRP:NE1	2.31	0.45
3:O:34:MET:HA	3:O:84:LYS:O	2.16	0.45
3:O:139:ILE:HG23	3:O:177:VAL:HG11	1.98	0.45
3:O:152:SER:H	3:O:157:ALA:CB	2.29	0.45
1:A:9:VAL:CG1	1:A:34:VAL:HG22	2.48	0.44
1:A:30:LYS:O	1:A:47:ILE:HG22	2.18	0.44
3:G:60:MET:HE1	3:G:74:ASP:O	2.17	0.44
2:J:144:PRO:HB3	2:J:272:TYR:OH	2.17	0.44
1:A:224:ALA:HB3	1:A:271:ASN:HD22	1.82	0.44
1:A:279:MET:O	1:A:282:ILE:HG22	2.16	0.44
1:A:426:LYS:HB2	1:A:427:GLU:OE2	2.18	0.44
1:A:465:MET:O	1:A:469:ASN:HB2	2.17	0.44
2:B:194:VAL:HB	2:B:297:HIS:HB2	1.98	0.44
2:D:160:ASP:HB3	2:D:165:PHE:CE2	2.52	0.44
3:E:70:LEU:HD21	3:E:75:VAL:CG2	2.45	0.44
1:I:76:LYS:HD3	1:I:100:TYR:HB2	1.99	0.44
2:L:202:GLU:O	2:L:206:ARG:HB3	2.16	0.44
3:M:209:HIS:HD1	3:M:246:LYS:HE3	1.78	0.44
3:N:7:ILE:HG13	3:N:19:THR:OG1	2.17	0.44
1:A:265:THR:O	1:A:268:VAL:HG13	2.17	0.44
2:B:187:PRO:HG2	2:B:190:VAL:HB	1.97	0.44
2:B:322:LEU:HD23	1:C:474:LYS:HG3	1.99	0.44
1:C:239:ARG:HD2	1:C:252:GLN:HE21	1.80	0.44
1:C:265:THR:O	1:C:268:VAL:HG13	2.17	0.44
2:J:370:TRP:CZ2	2:J:444:GLY:HA3	2.52	0.44
1:K:322:LYS:O	1:K:326:GLU:HG3	2.18	0.44
2:B:78:CYS:HB2	2:B:197:TRP:CD1	2.53	0.44
2:B:326:ASP:CG	2:B:348:ARG:HE	2.26	0.44
1:C:332:LYS:N	1:C:333:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:20:GLN:CD	3:E:44:SER:O	2.61	0.44
3:E:38:CYS:HA	3:E:88:SER:HB2	1.99	0.44
1:I:152:SER:HB2	1:I:184:GLU:OE1	2.18	0.44
2:J:331:LYS:HD2	2:J:331:LYS:HA	1.71	0.44
1:K:59:ILE:HG23	1:K:426:LYS:HE2	1.99	0.44
2:L:320:MET:O	2:L:324:TRP:HB2	2.18	0.44
1:A:234:ASP:HB3	1:A:451:HIS:ND1	2.32	0.44
2:B:431:ARG:HH11	2:B:431:ARG:HG2	1.82	0.44
3:F:168:ILE:HD13	3:F:179:LEU:HB2	2.00	0.44
3:G:31:LYS:O	3:G:33:VAL:HG23	2.17	0.44
3:G:193:ASP:OD2	3:G:193:ASP:N	2.50	0.44
1:I:322:LYS:O	1:I:326:GLU:HG3	2.17	0.44
1:K:70:VAL:HG13	1:K:96:ARG:NH2	2.32	0.44
1:K:97:ARG:HB3	1:K:99:TYR:CE1	2.53	0.44
1:K:392:LYS:H	1:K:392:LYS:HG3	1.62	0.44
1:A:190:SER:HB2	1:A:381:PHE:HB3	1.99	0.44
1:C:23:LYS:NZ	2:D:133:ASP:OD2	2.49	0.44
1:C:57:MET:CE	2:D:86:MET:HE1	2.48	0.44
1:C:62:CYS:HB3	2:D:94:GLY:HA3	1.98	0.44
2:D:239:VAL:HG22	2:D:243:MET:HE2	1.99	0.44
1:I:35:ASN:HB2	1:I:400:LEU:HG	1.98	0.44
1:K:350:ARG:HB3	1:K:375:VAL:CG1	2.48	0.44
2:B:248:GLY:C	2:B:338:GLN:HE21	2.26	0.44
2:B:294:GLN:HG2	2:B:318:ILE:HD12	2.00	0.44
2:D:144:PRO:HB3	2:D:272:TYR:OH	2.18	0.44
2:D:318:ILE:O	2:D:318:ILE:CG2	2.65	0.44
2:D:379:LEU:HD21	2:D:443:ILE:HG21	2.00	0.44
3:E:20:GLN:HE21	3:E:20:GLN:HB2	1.65	0.44
3:G:142:ASN:OD1	3:G:177:VAL:HG23	2.17	0.44
1:I:20:TYR:OH	1:I:408:GLU:HG3	2.18	0.44
1:I:253:TRP:HA	1:I:254:SER:HA	1.56	0.44
1:I:265:THR:O	1:I:268:VAL:HG13	2.17	0.44
1:I:465:MET:O	1:I:469:ASN:HB2	2.17	0.44
2:J:330:MET:SD	1:K:478:PRO:HB2	2.58	0.44
1:K:152:SER:HB2	1:K:184:GLU:OE1	2.18	0.44
1:K:352:MET:HE2	1:K:416:ILE:HB	1.99	0.44
3:O:149:ILE:HG21	3:O:161:ALA:HA	2.00	0.44
3:G:200:ALA:HB1	3:G:205:THR:O	2.18	0.44
1:I:94:ALA:HB3	2:L:521:LEU:HD22	2.00	0.44
1:I:258:SER:HG	1:I:261:GLU:HG3	1.83	0.44
1:I:279:MET:O	1:I:282:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:318:ILE:O	2:J:318:ILE:HG23	2.16	0.44
2:J:366:ARG:HA	2:J:389:GLU:O	2.18	0.44
1:K:199:ASN:HD21	1:K:279:MET:HG2	1.83	0.44
3:M:192:GLU:O	3:M:196:ILE:HG12	2.18	0.44
3:N:9:GLY:HA3	3:N:13:ILE:HD11	2.00	0.44
3:N:138:PRO:O	3:N:141:GLU:O	2.35	0.44
1:A:428:LYS:HA	1:A:438:PHE:CE2	2.53	0.44
1:C:389:ARG:HG3	1:C:389:ARG:HH11	1.83	0.44
3:E:25:ALA:HB2	3:E:228:ILE:HD12	1.99	0.44
2:J:160:ASP:HB3	2:J:165:PHE:CE2	2.52	0.44
3:M:8:TYR:O	3:M:149:ILE:HA	2.18	0.44
1:A:423:SER:O	1:A:440:GLU:HA	2.18	0.43
2:B:346:LYS:HE3	2:B:350:ARG:HH22	1.74	0.43
1:C:203:ARG:HH11	1:C:204:ASP:CG	2.26	0.43
2:D:151:THR:HG23	2:D:162:LEU:HD11	2.00	0.43
2:D:331:LYS:HD2	2:D:331:LYS:HA	1.73	0.43
2:D:507:GLU:HA	2:D:510:ARG:NH1	2.33	0.43
3:E:4:GLN:HE21	3:E:145:GLN:NE2	2.16	0.43
3:F:208:ILE:HG23	3:F:209:HIS:N	2.33	0.43
2:J:249:VAL:HG13	2:J:336:SER:HB3	1.99	0.43
2:J:443:ILE:CD1	2:J:497:LEU:HD21	2.48	0.43
2:L:118:MET:HE1	2:L:158:ILE:HD11	2.00	0.43
3:M:144:ALA:O	3:M:177:VAL:HG13	2.18	0.43
3:O:3:ARG:HE	3:O:121:PHE:HE2	1.65	0.43
3:P:18:THR:HG21	3:P:183:ILE:HG21	2.00	0.43
1:A:62:CYS:HB3	2:B:94:GLY:HA3	1.99	0.43
1:A:153:GLU:O	1:A:184:GLU:HG3	2.18	0.43
1:A:442:HIS:HE1	5:A:496:CFN:S1B	2.39	0.43
1:A:444:TRP:CE3	1:A:450:TYR:CD2	3.06	0.43
1:C:354:TYR:C	1:C:355:ILE:CG1	2.91	0.43
2:D:248:GLY:C	2:D:338:GLN:HE21	2.26	0.43
2:D:355:MET:HE3	2:D:386:LEU:HD23	1.99	0.43
3:F:187:ARG:O	3:F:188:ASN:HB2	2.18	0.43
3:G:189:THR:HG22	3:G:190:ASP:N	2.33	0.43
3:G:217:VAL:HG22	3:G:227:VAL:HG21	2.00	0.43
2:J:377:MET:HE3	2:J:406:VAL:CG2	2.47	0.43
1:K:54:PRO:HB3	2:L:116:ASP:C	2.43	0.43
3:O:78:ALA:HA	3:O:84:LYS:HA	2.00	0.43
3:P:149:ILE:HG21	3:P:161:ALA:HA	1.99	0.43
1:A:76:LYS:HD3	1:A:100:TYR:HB2	2.00	0.43
1:C:465:MET:O	1:C:469:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:GLN:HE21	3:E:145:GLN:HE21	1.65	0.43
3:E:45:THR:HB	3:E:85:CYS:HB3	2.00	0.43
3:E:163:ASN:HD22	3:E:163:ASN:HA	1.51	0.43
1:I:97:ARG:NH2	1:I:447:SER:O	2.35	0.43
2:J:248:GLY:C	2:J:338:GLN:HE21	2.26	0.43
2:J:521:LEU:CD2	1:K:94:ALA:HB3	2.45	0.43
2:L:236:ASN:CG	2:L:485:LEU:HG	2.42	0.43
3:M:6:ALA:HB3	3:M:147:ILE:HD12	2.00	0.43
3:M:137:MET:N	3:M:138:PRO:HD2	2.34	0.43
3:O:135:PHE:C	3:O:137:MET:H	2.25	0.43
3:O:144:ALA:O	3:O:177:VAL:HG13	2.18	0.43
3:P:244:ALA:O	3:P:248:VAL:HG23	2.18	0.43
1:A:75:ILE:HD12	1:A:254:SER:HB2	2.00	0.43
1:C:166:VAL:O	1:C:170:LYS:HG2	2.18	0.43
2:D:326:ASP:CG	2:D:348:ARG:HE	2.25	0.43
3:E:61:ALA:O	3:E:65:GLY:N	2.47	0.43
3:F:6:ALA:HB3	3:F:147:ILE:HG23	2.01	0.43
3:F:268:LEU:CD1	3:F:273:ILE:HG13	2.46	0.43
3:G:10:LYS:H	3:G:13:ILE:HD13	1.84	0.43
3:H:150:VAL:HA	3:H:183:ILE:O	2.18	0.43
1:I:9:VAL:CG1	1:I:34:VAL:HG22	2.49	0.43
2:J:219:GLY:HA2	2:J:288:LEU:HA	1.99	0.43
2:L:379:LEU:HD21	2:L:443:ILE:HG21	2.00	0.43
2:L:518:ASN:O	2:L:518:ASN:CG	2.62	0.43
3:M:8:TYR:HB3	3:M:164:ILE:CD1	2.39	0.43
3:O:147:ILE:O	3:O:180:GLY:N	2.51	0.43
3:O:150:VAL:HA	3:O:183:ILE:O	2.18	0.43
3:P:137:MET:O	3:P:138:PRO:C	2.61	0.43
2:B:394:LEU:C	2:B:394:LEU:HD23	2.43	0.43
1:C:77:ASP:OD1	1:C:258:SER:HA	2.18	0.43
1:C:141:LEU:HD23	1:C:141:LEU:HA	1.87	0.43
3:E:33:VAL:HB	3:E:83:VAL:HG13	1.99	0.43
3:E:131:VAL:CB	3:F:93:PRO:HB3	2.48	0.43
3:G:150:VAL:HA	3:G:183:ILE:O	2.19	0.43
1:K:35:ASN:HD21	1:K:391:MET:CB	2.32	0.43
3:M:86:VAL:HG22	3:M:87:GLU:N	2.32	0.43
3:O:21:ASN:HB3	3:O:240:TYR:CG	2.53	0.43
1:A:125:PHE:O	3:F:100:ARG:CD	2.66	0.43
2:B:135:LEU:HB3	2:B:175:ILE:HG21	2.01	0.43
1:C:426:LYS:HB2	1:C:427:GLU:OE2	2.19	0.43
3:G:178:ARG:CB	3:G:253:LEU:HB3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:5:CYS:HB2	3:H:123:PHE:CD1	2.53	0.43
3:H:124:TYR:CD2	3:H:144:ALA:HB2	2.53	0.43
1:K:30:LYS:HB3	1:K:47:ILE:HG21	2.00	0.43
1:K:166:VAL:O	1:K:170:LYS:HG2	2.17	0.43
1:K:234:ASP:HB3	1:K:451:HIS:ND1	2.32	0.43
1:K:424:GLY:HA2	1:K:442:HIS:HD2	1.84	0.43
2:L:187:PRO:HG2	2:L:190:VAL:HB	2.01	0.43
2:L:237:PHE:CZ	2:L:257:PRO:HD2	2.54	0.43
3:M:32:LYS:O	3:M:120:ASP:N	2.51	0.43
1:A:360:PRO:HB3	1:A:377:THR:OG1	2.19	0.43
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.59	0.43
1:C:239:ARG:HD2	1:C:252:GLN:HE22	1.80	0.43
3:F:204:GLY:O	3:F:254:VAL:HG21	2.19	0.43
1:I:199:ASN:HD21	1:I:279:MET:HG2	1.83	0.43
2:L:285:PRO:HG3	2:L:309:TRP:CE2	2.54	0.43
2:L:420:THR:HG22	2:L:422:TYR:CE1	2.54	0.43
3:M:23:VAL:O	3:M:26:LEU:HB2	2.17	0.43
3:M:78:ALA:HA	3:M:84:LYS:HA	2.00	0.43
3:M:161:ALA:O	3:M:165:SER:HB3	2.18	0.43
1:A:350:ARG:HB3	1:A:375:VAL:CG1	2.47	0.43
1:A:420:LEU:C	1:A:420:LEU:HD23	2.44	0.43
1:C:35:ASN:HB2	1:C:400:LEU:HG	2.01	0.43
3:E:6:ALA:HB3	3:E:147:ILE:HD12	1.99	0.43
3:F:16:SER:HB2	9:F:2292:ADP:O2A	2.19	0.43
1:I:78:MET:HG2	1:I:147:GLY:HA3	2.00	0.43
1:I:203:ARG:HH11	1:I:204:ASP:CG	2.26	0.43
1:I:324:CYS:O	1:I:328:ILE:HG13	2.19	0.43
2:L:154:MET:HE2	2:L:154:MET:HB3	1.63	0.43
1:A:57:MET:HE3	2:B:142:TYR:CZ	2.54	0.43
2:L:431:ARG:O	2:L:434:VAL:HG22	2.19	0.43
3:M:7:ILE:CD1	3:M:148:TYR:HB2	2.45	0.43
3:M:57:ILE:HD12	3:M:105:ALA:CB	2.48	0.43
3:N:33:VAL:HA	3:N:121:PHE:O	2.19	0.43
3:O:4:GLN:HA	3:O:122:VAL:HB	2.00	0.43
3:O:231:ASP:CG	3:O:234:ALA:HB2	2.43	0.43
1:A:164:GLU:N	1:A:164:GLU:OE1	2.51	0.43
1:C:20:TYR:OH	1:C:408:GLU:HG3	2.19	0.43
2:D:314:PRO:HB3	2:D:331:LYS:HE2	2.00	0.43
1:I:352:MET:HE2	1:I:418:PRO:HD3	2.00	0.43
1:I:423:SER:O	1:I:440:GLU:HA	2.19	0.43
1:K:437:PRO:HG3	1:K:472:TRP:NE1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:131:MET:HG2	2:L:165:PHE:HB3	2.01	0.43
3:O:107:ASN:N	3:O:107:ASN:HD22	2.17	0.43
2:B:71:GLN:HG2	2:B:192:SER:O	2.19	0.42
1:C:148:ILE:HB	1:C:178:ILE:HG12	2.01	0.42
1:C:184:GLU:HB2	1:C:187:ARG:HG3	2.00	0.42
1:C:352:MET:HG3	1:C:418:PRO:CB	2.49	0.42
1:C:381:PHE:HZ	5:C:496:CFN:S2B	2.41	0.42
1:C:439:ARG:HD2	1:C:439:ARG:HA	1.87	0.42
2:J:452:GLN:HG3	2:J:464:VAL:O	2.18	0.42
2:L:23:MET:HE2	2:L:23:MET:HB3	1.93	0.42
3:M:136:ALA:O	3:M:139:ILE:HB	2.18	0.42
3:M:209:HIS:CG	3:M:246:LYS:HE3	2.54	0.42
1:A:154:CYS:SG	1:A:185:GLY:HA3	2.59	0.42
2:B:299:GLU:CD	2:B:401:ARG:HH22	2.27	0.42
1:C:322:LYS:O	1:C:326:GLU:HG3	2.19	0.42
3:F:25:ALA:O	3:F:28:GLU:HB3	2.19	0.42
1:I:352:MET:HE1	1:I:413:VAL:HA	2.01	0.42
1:K:332:LYS:N	1:K:333:PRO:CD	2.82	0.42
3:O:55:ASN:HA	3:O:59:GLU:OE2	2.19	0.42
3:O:103:ILE:HG12	3:O:137:MET:CG	2.43	0.42
3:O:152:SER:H	3:O:157:ALA:HB1	1.84	0.42
2:B:131:MET:HG2	2:B:165:PHE:HB3	2.00	0.42
2:B:314:PRO:HB3	2:B:331:LYS:HE2	2.01	0.42
2:D:394:LEU:C	2:D:394:LEU:HD23	2.44	0.42
1:I:203:ARG:HD2	1:I:204:ASP:OD1	2.20	0.42
1:K:14:GLN:NE2	1:K:14:GLN:HA	2.34	0.42
1:K:126:GLY:HA2	1:K:159:ILE:HD12	2.01	0.42
1:K:265:THR:O	1:K:268:VAL:HG22	2.20	0.42
2:L:379:LEU:O	2:L:383:LEU:HG	2.20	0.42
2:L:468:ARG:HG3	2:L:468:ARG:HH11	1.84	0.42
3:M:22:LEU:HB2	3:M:243:LEU:HD23	2.00	0.42
3:M:149:ILE:HG21	3:M:161:ALA:HA	2.01	0.42
2:B:9:LYS:HD3	2:B:13:PRO:HG2	2.01	0.42
1:C:279:MET:O	1:C:282:ILE:HG22	2.19	0.42
1:I:389:ARG:HG3	1:I:389:ARG:HH11	1.84	0.42
1:I:426:LYS:HB2	1:I:427:GLU:OE2	2.20	0.42
2:J:103:PHE:HB3	2:J:111:VAL:HG21	2.02	0.42
3:P:56:THR:HG22	3:P:87:GLU:HB3	2.01	0.42
3:P:102:VAL:O	3:P:106:ILE:HG13	2.19	0.42
1:A:332:LYS:HA	1:A:335:TRP:NE1	2.35	0.42
2:B:151:THR:CG2	2:B:162:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:LYS:HA	1:C:335:TRP:NE1	2.34	0.42
2:D:124:VAL:CG2	2:D:125:PHE:N	2.82	0.42
2:D:452:GLN:CD	2:D:465:PRO:HA	2.45	0.42
3:E:182:LEU:HD12	3:E:182:LEU:HA	1.90	0.42
1:I:42:SER:HA	1:I:391:MET:CE	2.49	0.42
1:I:420:LEU:HD23	1:I:420:LEU:C	2.45	0.42
2:J:277:THR:OG1	2:J:280:GLU:HG3	2.19	0.42
2:J:284:ALA:HB3	2:J:285:PRO:HD3	2.01	0.42
1:K:62:CYS:SG	1:K:64:TYR:HB3	2.59	0.42
3:M:201:ASN:HD22	3:M:201:ASN:HA	1.64	0.42
3:M:265:GLU:O	3:M:268:LEU:HD23	2.19	0.42
3:P:199:LEU:HD23	3:P:199:LEU:O	2.19	0.42
3:F:275:GLU:CD	3:F:275:GLU:H	2.23	0.42
3:G:201:ASN:HD22	3:G:201:ASN:HA	1.55	0.42
1:K:237:SER:O	1:K:240:ILE:HG22	2.20	0.42
3:O:27:ALA:HB2	3:O:83:VAL:CG1	2.50	0.42
1:C:59:ILE:HG23	1:C:426:LYS:HE2	2.01	0.42
3:E:7:ILE:HG13	3:E:19:THR:OG1	2.19	0.42
3:H:195:LEU:O	3:H:267:LEU:HD11	2.19	0.42
3:H:211:VAL:HA	3:H:212:PRO:HD3	1.89	0.42
1:I:59:ILE:HG22	1:I:59:ILE:O	2.19	0.42
1:I:126:GLY:HA2	1:I:159:ILE:HD12	2.01	0.42
1:K:61:GLY:H	1:K:191:GLN:CD	2.27	0.42
3:M:99:GLY:O	3:M:103:ILE:HG13	2.20	0.42
3:M:137:MET:HA	3:M:140:ARG:HG3	2.01	0.42
1:A:148:ILE:HB	1:A:178:ILE:HG12	2.02	0.42
2:D:427:LEU:HD23	2:D:430:LEU:HD12	2.02	0.42
3:F:10:LYS:O	3:F:13:ILE:HG12	2.19	0.42
3:F:154:GLU:OE1	3:F:156:MET:HB3	2.20	0.42
3:H:126:VAL:HG12	3:H:127:LEU:N	2.35	0.42
2:J:379:LEU:HD21	2:J:443:ILE:HG21	2.01	0.42
2:L:331:LYS:HD2	2:L:331:LYS:HA	1.69	0.42
2:L:458:LYS:HD3	2:L:462:PHE:CG	2.54	0.42
3:N:159:TYR:O	3:N:162:ASN:HB3	2.20	0.42
3:O:19:THR:O	3:O:23:VAL:HG23	2.20	0.42
1:C:190:SER:HB2	1:C:381:PHE:HB3	2.01	0.42
2:J:249:VAL:HG13	2:J:336:SER:CB	2.49	0.42
2:J:494:LEU:HD23	2:J:494:LEU:C	2.45	0.42
1:K:76:LYS:HD3	1:K:100:TYR:HB2	2.01	0.42
1:K:324:CYS:O	1:K:328:ILE:HG13	2.19	0.42
2:L:120:GLU:O	2:L:123:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:21:ASN:ND2	3:O:227:VAL:H	2.17	0.42
3:P:55:ASN:HD22	3:P:55:ASN:HA	1.48	0.42
1:A:203:ARG:HH11	1:A:204:ASP:CG	2.28	0.42
1:C:350:ARG:HB3	1:C:375:VAL:CG1	2.50	0.42
2:D:71:GLN:HB3	2:D:186:THR:HB	2.01	0.42
3:E:131:VAL:HB	3:F:93:PRO:HB3	2.02	0.42
3:G:206:GLN:H	3:G:206:GLN:HG3	1.56	0.42
1:I:5:SER:O	1:I:9:VAL:HG23	2.20	0.42
1:I:164:GLU:OE1	1:I:164:GLU:N	2.52	0.42
1:I:360:PRO:HB3	1:I:377:THR:OG1	2.20	0.42
2:J:78:CYS:HB2	2:J:197:TRP:CD1	2.55	0.42
1:K:57:MET:HE3	2:L:142:TYR:CZ	2.55	0.42
3:O:17:THR:O	3:O:21:ASN:OD1	2.38	0.42
1:C:75:ILE:HD12	1:C:254:SER:HB2	2.02	0.41
1:C:133:LYS:HA	1:C:133:LYS:HD2	1.81	0.41
2:D:23:MET:HE2	2:D:23:MET:HB3	1.95	0.41
3:F:189:THR:HG22	3:F:190:ASP:N	2.35	0.41
3:H:24:ALA:O	3:H:27:ALA:HB3	2.20	0.41
3:H:199:LEU:CB	3:H:267:LEU:HD21	2.50	0.41
1:I:437:PRO:HG3	1:I:472:TRP:NE1	2.34	0.41
2:J:240:ILE:HD13	2:J:240:ILE:HA	1.93	0.41
2:J:285:PRO:HG3	2:J:309:TRP:CE2	2.55	0.41
3:O:178:ARG:NE	3:O:255:ILE:HG12	2.34	0.41
3:O:193:ASP:O	3:O:197:ILE:CG1	2.66	0.41
2:B:71:GLN:HB3	2:B:186:THR:HB	2.01	0.41
2:B:73:LEU:HG	2:B:103:PHE:CZ	2.55	0.41
2:B:120:GLU:O	2:B:123:ALA:HB3	2.20	0.41
2:B:222:LYS:HA	2:B:288:LEU:HD21	2.01	0.41
1:C:57:MET:HE3	2:D:142:TYR:CZ	2.55	0.41
2:D:71:GLN:HG2	2:D:192:SER:O	2.19	0.41
3:E:108:PHE:O	3:E:112:GLU:HG2	2.20	0.41
1:I:275:CYS:CB	1:I:358:LEU:HD22	2.49	0.41
1:I:332:LYS:N	1:I:333:PRO:CD	2.83	0.41
2:J:298:LEU:HA	2:J:298:LEU:HD23	1.86	0.41
2:L:219:GLY:HA2	2:L:288:LEU:HA	2.02	0.41
1:A:158:LEU:HD11	2:B:154:MET:HG2	1.98	0.41
1:C:355:ILE:HB	1:C:360:PRO:HD3	2.01	0.41
2:D:120:GLU:O	2:D:123:ALA:HB3	2.21	0.41
3:F:2:MET:HE3	3:F:122:VAL:CG2	2.50	0.41
3:G:39:ASP:HA	3:G:40:PRO:HD3	1.90	0.41
1:I:125:PHE:CD2	1:I:125:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:13:ILE:HD12	3:M:150:VAL:HG12	2.02	0.41
3:M:39:ASP:HA	3:M:40:PRO:HD3	1.93	0.41
3:O:95:VAL:HG23	3:O:95:VAL:O	2.20	0.41
1:A:70:VAL:HG13	1:A:96:ARG:NH2	2.35	0.41
1:A:354:TYR:C	1:A:355:ILE:CG1	2.93	0.41
3:E:239:GLU:O	3:E:242:ALA:HB3	2.20	0.41
3:F:34:MET:HB2	3:F:119:LEU:HD13	2.03	0.41
3:H:7:ILE:HG13	3:H:19:THR:OG1	2.20	0.41
3:H:27:ALA:HB1	3:H:81:GLY:HA3	2.02	0.41
1:I:75:ILE:HD12	1:I:254:SER:HB2	2.02	0.41
2:J:124:VAL:CG2	2:J:125:PHE:N	2.83	0.41
2:J:427:LEU:HD23	2:J:427:LEU:HA	1.94	0.41
1:A:125:PHE:N	1:A:125:PHE:CD2	2.88	0.41
1:A:166:VAL:O	1:A:170:LYS:HG2	2.21	0.41
2:B:154:MET:HB3	2:B:154:MET:HE2	1.82	0.41
2:B:249:VAL:HG13	2:B:336:SER:CB	2.50	0.41
2:D:206:ARG:HA	2:D:304:PHE:CZ	2.55	0.41
3:G:180:GLY:HA2	3:G:253:LEU:HD23	2.02	0.41
3:H:152:SER:H	3:H:157:ALA:HB1	1.83	0.41
3:H:214:ASP:CG	3:H:216:VAL:HG12	2.45	0.41
1:I:334:GLU:OE2	2:J:2:SER:HB3	2.20	0.41
1:I:474:LYS:HB3	2:L:322:LEU:CD2	2.50	0.41
2:L:314:PRO:HB3	2:L:331:LYS:HE2	2.02	0.41
2:L:375:PHE:CZ	2:L:379:LEU:HD22	2.56	0.41
3:M:38:CYS:SG	3:M:126:VAL:HG22	2.59	0.41
2:B:124:VAL:CG2	2:B:125:PHE:N	2.84	0.41
1:C:42:SER:HA	1:C:391:MET:CE	2.48	0.41
1:C:237:SER:O	1:C:240:ILE:HG22	2.20	0.41
1:C:392:LYS:H	1:C:392:LYS:HG3	1.65	0.41
3:F:12:GLY:N	9:F:2292:ADP:O1B	2.54	0.41
3:F:16:SER:O	3:F:20:GLN:HG3	2.20	0.41
3:G:6:ALA:HB2	3:G:144:ALA:HB2	2.00	0.41
2:J:154:MET:HE2	2:J:154:MET:HB3	1.87	0.41
1:K:5:SER:O	1:K:9:VAL:HG23	2.21	0.41
1:K:9:VAL:CG1	1:K:34:VAL:HG22	2.51	0.41
2:L:484:THR:C	2:L:489:GLY:HA3	2.46	0.41
1:A:332:LYS:HA	1:A:335:TRP:CD1	2.55	0.41
1:A:430:ILE:HG23	2:B:269:PHE:CD2	2.55	0.41
1:C:56:LEU:HD23	1:C:56:LEU:HA	1.86	0.41
2:D:47:THR:HA	2:D:52:TYR:CG	2.56	0.41
3:M:8:TYR:O	3:M:149:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:225:MET:HE2	3:M:229:GLU:OE1	2.20	0.41
3:N:268:LEU:HA	3:N:273:ILE:HD11	2.01	0.41
3:O:230:TYR:CD1	3:O:230:TYR:C	2.98	0.41
2:B:48:THR:HG22	2:B:435:PHE:CE1	2.56	0.41
3:G:36:VAL:HA	3:G:86:VAL:CG1	2.50	0.41
3:G:102:VAL:O	3:G:106:ILE:HG13	2.21	0.41
1:I:141:LEU:HA	1:I:141:LEU:HD23	1.89	0.41
1:I:224:ALA:HB3	1:I:271:ASN:HD22	1.83	0.41
1:I:234:ASP:HA	1:I:449:PRO:HB2	2.02	0.41
2:J:426:ASP:O	2:J:429:HIS:HB2	2.21	0.41
2:J:516:ASP:HA	2:J:519:HIS:HB2	2.03	0.41
1:K:381:PHE:HZ	5:K:496:CFN:S2B	2.43	0.41
2:L:47:THR:HA	2:L:52:TYR:CG	2.56	0.41
3:M:173:ASN:N	3:M:173:ASN:ND2	2.69	0.41
3:O:9:GLY:N	3:O:15:LYS:HD3	2.35	0.41
3:O:188:ASN:HD21	3:O:213:ARG:CG	2.31	0.41
1:A:424:GLY:HA2	1:A:442:HIS:HD2	1.86	0.41
2:B:260:VAL:HA	2:B:273:ALA:HB3	2.03	0.41
2:B:375:PHE:CZ	2:B:379:LEU:HD22	2.56	0.41
2:B:401:ARG:HG2	2:B:401:ARG:HH11	1.86	0.41
1:C:420:LEU:C	1:C:420:LEU:HD23	2.46	0.41
2:D:302:LYS:O	2:D:306:GLU:HG3	2.21	0.41
3:E:254:VAL:O	3:E:256:PRO:HD3	2.21	0.41
3:F:197:ILE:HD13	2:L:220:SER:HB3	2.02	0.41
1:I:128:ASP:HB2	1:I:129:LYS:NZ	2.36	0.41
1:I:354:TYR:C	1:I:355:ILE:CG1	2.94	0.41
1:I:370:LEU:HD11	1:I:460:ALA:CB	2.51	0.41
1:K:30:LYS:O	1:K:47:ILE:HG22	2.21	0.41
1:K:35:ASN:HB2	1:K:400:LEU:HG	2.03	0.41
1:K:358:LEU:HD11	1:K:362:HIS:CD2	2.56	0.41
1:K:359:ARG:CZ	1:K:444:TRP:CZ2	3.03	0.41
1:K:439:ARG:HD2	1:K:439:ARG:HA	1.90	0.41
2:L:258:GLU:HG3	2:L:259:GLU:N	2.36	0.41
2:L:368:ALA:O	2:L:442:MET:HA	2.19	0.41
3:M:209:HIS:NE2	3:M:242:ALA:HB3	2.35	0.41
1:C:424:GLY:HA2	1:C:442:HIS:HD2	1.86	0.41
2:D:417:LYS:HG3	2:D:418:ASN:N	2.35	0.41
3:E:100:ARG:HA	3:E:103:ILE:HD12	2.03	0.41
3:F:172:ALA:HB1	3:F:255:ILE:CD1	2.50	0.41
3:G:80:TYR:CD1	3:G:80:TYR:C	2.98	0.41
1:I:284:ARG:HH11	1:I:284:ARG:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:48:THR:HG22	2:J:435:PHE:CE1	2.56	0.41
2:J:254:LEU:O	2:J:255:SER:CB	2.69	0.41
1:K:163:ILE:H	1:K:182:ARG:NH2	2.19	0.41
1:K:203:ARG:HD2	1:K:204:ASP:OD1	2.21	0.41
1:K:404:VAL:HG22	1:K:405:THR:O	2.21	0.41
2:L:160:ASP:HB3	2:L:165:PHE:CE2	2.55	0.41
3:M:57:ILE:HD12	3:M:105:ALA:HA	2.03	0.41
1:A:234:ASP:HA	1:A:449:PRO:HB2	2.02	0.40
2:B:362:LEU:HD22	2:B:388:CYS:SG	2.62	0.40
2:D:78:CYS:HB2	2:D:197:TRP:NE1	2.35	0.40
2:D:130:ASN:ND2	2:D:130:ASN:N	2.55	0.40
2:D:431:ARG:O	2:D:434:VAL:HG22	2.21	0.40
3:F:8:TYR:CB	3:F:164:ILE:HD13	2.50	0.40
3:F:147:ILE:O	3:F:179:LEU:HD12	2.21	0.40
2:J:260:VAL:HA	2:J:273:ALA:HB3	2.03	0.40
2:J:322:LEU:HD23	1:K:474:LYS:HG3	2.03	0.40
1:K:275:CYS:CB	1:K:358:LEU:HD22	2.51	0.40
1:K:279:MET:O	1:K:282:ILE:HG22	2.21	0.40
2:L:78:CYS:HB2	2:L:197:TRP:CD1	2.55	0.40
3:O:94:GLY:N	3:P:131:VAL:HG12	2.34	0.40
1:A:42:SER:HA	1:A:391:MET:CE	2.51	0.40
1:A:57:MET:CE	2:B:86:MET:HE1	2.50	0.40
1:C:206:VAL:O	1:C:206:VAL:HG12	2.20	0.40
1:C:266:PRO:O	1:C:292:ILE:HD11	2.22	0.40
3:E:151:CYS:O	3:E:184:CYS:HA	2.21	0.40
3:F:99:GLY:O	3:F:102:VAL:HB	2.22	0.40
3:G:5:CYS:HA	3:G:146:GLU:O	2.22	0.40
3:G:6:ALA:HB2	3:G:144:ALA:HB1	2.00	0.40
1:I:334:GLU:OE1	2:J:2:SER:HA	2.22	0.40
1:I:359:ARG:NH1	1:I:441:MET:O	2.54	0.40
1:I:465:MET:CG	1:I:466:THR:N	2.81	0.40
2:B:13:PRO:O	2:B:16:LEU:HB2	2.21	0.40
1:C:352:MET:HG3	1:C:418:PRO:HG3	2.02	0.40
3:E:268:LEU:HD23	3:E:268:LEU:HA	1.73	0.40
3:F:212:PRO:HD3	3:F:239:GLU:OE1	2.22	0.40
1:I:56:LEU:HA	1:I:56:LEU:HD23	1.84	0.40
2:L:146:MET:HA	2:L:180:PRO:HG2	2.04	0.40
2:L:366:ARG:HA	2:L:389:GLU:O	2.22	0.40
3:M:236:GLN:O	3:M:239:GLU:HB2	2.21	0.40
3:M:256:PRO:O	3:M:258:PRO:HD3	2.22	0.40
3:P:98:ALA:HB3	3:P:135:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:HG13	2:B:189:PHE:CD2	2.57	0.40
1:A:275:CYS:CB	1:A:358:LEU:HD22	2.51	0.40
2:B:144:PRO:HB3	2:B:272:TYR:OH	2.21	0.40
2:B:285:PRO:HG3	2:B:309:TRP:CE2	2.57	0.40
1:C:125:PHE:N	1:C:125:PHE:CD2	2.87	0.40
3:E:137:MET:O	3:E:138:PRO:C	2.61	0.40
3:F:103:ILE:HA	3:F:106:ILE:HD12	2.04	0.40
3:F:202:LYS:HB3	3:F:259:ILE:CG2	2.43	0.40
3:H:95:VAL:O	3:H:95:VAL:HG23	2.22	0.40
2:J:47:THR:HA	2:J:52:TYR:CG	2.57	0.40
2:J:401:ARG:HG2	2:J:401:ARG:HH11	1.87	0.40
2:J:417:LYS:HG3	2:J:418:ASN:N	2.36	0.40
3:O:32:LYS:O	3:O:120:ASP:N	2.55	0.40
1:C:131:LEU:O	1:C:135:ILE:HG13	2.22	0.40
1:C:258:SER:HG	1:C:261:GLU:HG3	1.85	0.40
2:D:135:LEU:HB3	2:D:175:ILE:HG21	2.03	0.40
3:E:262:ASP:O	3:E:265:GLU:N	2.54	0.40
3:G:15:LYS:O	3:G:19:THR:OG1	2.39	0.40
2:J:73:LEU:HG	2:J:103:PHE:CZ	2.57	0.40
1:K:319:SER:O	1:K:323:LYS:HG3	2.22	0.40
2:L:248:GLY:C	2:L:338:GLN:HE21	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	43 73
1	C	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	43 73
1	I	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	43 73
1	K	474/491 (96%)	467 (98%)	6 (1%)	1 (0%)	43 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	520/522 (100%)	514 (99%)	6 (1%)	0	100	100
2	D	520/522 (100%)	514 (99%)	6 (1%)	0	100	100
2	J	520/522 (100%)	514 (99%)	6 (1%)	0	100	100
2	L	520/522 (100%)	513 (99%)	7 (1%)	0	100	100
3	E	269/289 (93%)	268 (100%)	1 (0%)	0	100	100
3	F	273/289 (94%)	270 (99%)	3 (1%)	0	100	100
3	G	261/289 (90%)	259 (99%)	2 (1%)	0	100	100
3	H	267/289 (92%)	265 (99%)	2 (1%)	0	100	100
3	M	266/289 (92%)	264 (99%)	2 (1%)	0	100	100
3	N	268/289 (93%)	267 (100%)	1 (0%)	0	100	100
3	O	260/289 (90%)	259 (100%)	1 (0%)	0	100	100
3	P	265/289 (92%)	264 (100%)	1 (0%)	0	100	100
All	All	6105/6364 (96%)	6039 (99%)	62 (1%)	4 (0%)	48	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	357	GLY
1	A	357	GLY
1	K	357	GLY
1	I	357	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/414 (98%)	386 (95%)	20 (5%)	22	53
1	C	406/414 (98%)	383 (94%)	23 (6%)	18	49
1	I	406/414 (98%)	386 (95%)	20 (5%)	22	53
1	K	406/414 (98%)	383 (94%)	23 (6%)	18	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	454/454 (100%)	430 (95%)	24 (5%)	20	51
2	D	454/454 (100%)	427 (94%)	27 (6%)	18	48
2	J	454/454 (100%)	429 (94%)	25 (6%)	19	50
2	L	454/454 (100%)	430 (95%)	24 (5%)	20	51
3	E	218/233 (94%)	188 (86%)	30 (14%)	3	15
3	F	221/233 (95%)	194 (88%)	27 (12%)	5	20
3	G	210/233 (90%)	183 (87%)	27 (13%)	4	18
3	H	217/233 (93%)	187 (86%)	30 (14%)	3	15
3	M	216/233 (93%)	188 (87%)	28 (13%)	4	18
3	N	217/233 (93%)	189 (87%)	28 (13%)	4	18
3	O	210/233 (90%)	193 (92%)	17 (8%)	11	36
3	P	214/233 (92%)	191 (89%)	23 (11%)	6	25
All	All	5163/5336 (97%)	4767 (92%)	396 (8%)	12	38

All (396) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	58	THR
1	A	75	ILE
1	A	77	ASP
1	A	98	ASN
1	A	129	LYS
1	A	140	THR
1	A	161	ASP
1	A	168	LYS
1	A	199	ASN
1	A	218	SER
1	A	219	THR
1	A	268	VAL
1	A	271	ASN
1	A	310	ARG
1	A	352	MET
1	A	355	ILE
1	A	362	HIS
1	A	420	LEU
1	A	437	PRO
2	B	4	GLN

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Mol	Chain	Res	Type
2	B	13	PRO
2	B	16	LEU
2	B	45	GLN
2	B	62	LEU
2	B	80	LEU
2	B	92	SER
2	B	119	THR
2	B	124	VAL
2	B	130	ASN
2	B	150	SER
2	B	189	PHE
2	B	192	SER
2	B	194	VAL
2	B	202	GLU
2	B	206	ARG
2	B	222	LYS
2	B	247	MET
2	B	252	SER
2	B	258	GLU
2	B	264	PRO
2	B	391	VAL
2	B	430	LEU
2	B	432	SER
1	C	14	GLN
1	C	58	THR
1	C	75	ILE
1	C	77	ASP
1	C	98	ASN
1	C	104	THR
1	C	129	LYS
1	C	140	THR
1	C	161	ASP
1	C	168	LYS
1	C	199	ASN
1	C	218	SER
1	C	219	THR
1	C	268	VAL
1	C	271	ASN
1	C	305	THR
1	C	310	ARG
1	C	352	MET
1	C	355	ILE

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Mol	Chain	Res	Type
1	C	362	HIS
1	C	401	TYR
1	C	420	LEU
1	C	437	PRO
2	D	4	GLN
2	D	13	PRO
2	D	16	LEU
2	D	19	ASP
2	D	45	GLN
2	D	62	LEU
2	D	80	LEU
2	D	92	SER
2	D	119	THR
2	D	124	VAL
2	D	130	ASN
2	D	150	SER
2	D	189	PHE
2	D	192	SER
2	D	194	VAL
2	D	202	GLU
2	D	214	ASP
2	D	222	LYS
2	D	252	SER
2	D	258	GLU
2	D	264	PRO
2	D	389	GLU
2	D	391	VAL
2	D	401	ARG
2	D	430	LEU
2	D	432	SER
2	D	472	PRO
3	E	4	GLN
3	E	5	CYS
3	E	20	GLN
3	E	22	LEU
3	E	29	MET
3	E	33	VAL
3	E	41	LYS
3	E	55	ASN
3	E	57	ILE
3	E	67	VAL
3	E	75	VAL

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Mol	Chain	Res	Type
3	E	83	VAL
3	E	112	GLU
3	E	145	GLN
3	E	151	CYS
3	E	156	MET
3	E	163	ASN
3	E	199	LEU
3	E	201	ASN
3	E	206	GLN
3	E	211	VAL
3	E	222	ILE
3	E	228	ILE
3	E	233	LYS
3	E	246	LYS
3	E	254	VAL
3	E	260	THR
3	E	263	GLU
3	E	268	LEU
3	E	269	MET
3	F	22	LEU
3	F	35	ILE
3	F	47	LEU
3	F	63	GLU
3	F	66	THR
3	F	67	VAL
3	F	69	ASP
3	F	86	VAL
3	F	132	CYS
3	F	139	ILE
3	F	145	GLN
3	F	163	ASN
3	F	174	SER
3	F	178	ARG
3	F	179	LEU
3	F	182	LEU
3	F	185	ASN
3	F	192	GLU
3	F	206	GLN
3	F	207	MET
3	F	217	VAL
3	F	228	ILE
3	F	236	GLN

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Mol	Chain	Res	Type
3	F	249	ASP
3	F	264	LEU
3	F	269	MET
3	F	275	GLU
3	G	19	THR
3	G	22	LEU
3	G	41	LYS
3	G	43	ASP
3	G	58	MET
3	G	66	THR
3	G	80	TYR
3	G	83	VAL
3	G	88	SER
3	G	145	GLN
3	G	146	GLU
3	G	163	ASN
3	G	170	LYS
3	G	178	ARG
3	G	187	ARG
3	G	199	LEU
3	G	201	ASN
3	G	206	GLN
3	G	218	GLN
3	G	225	MET
3	G	233	LYS
3	G	249	ASP
3	G	250	ASN
3	G	251	LYS
3	G	259	ILE
3	G	262	ASP
3	G	263	GLU
3	H	13	ILE
3	H	22	LEU
3	H	44	SER
3	H	49	LEU
3	H	56	THR
3	H	58	MET
3	H	63	GLU
3	H	66	THR
3	H	84	LYS
3	H	115	TYR
3	H	117	ASP

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Mol	Chain	Res	Type
3	H	126	VAL
3	H	132	CYS
3	H	140	ARG
3	H	145	GLN
3	H	163	ASN
3	H	165	SER
3	H	187	ARG
3	H	199	LEU
3	H	201	ASN
3	H	215	ASN
3	H	233	LYS
3	H	246	LYS
3	H	247	VAL
3	H	250	ASN
3	H	261	MET
3	H	264	LEU
3	H	265	GLU
3	H	267	LEU
3	H	268	LEU
1	I	58	THR
1	I	75	ILE
1	I	77	ASP
1	I	98	ASN
1	I	129	LYS
1	I	140	THR
1	I	161	ASP
1	I	168	LYS
1	I	199	ASN
1	I	218	SER
1	I	219	THR
1	I	268	VAL
1	I	271	ASN
1	I	305	THR
1	I	310	ARG
1	I	352	MET
1	I	355	ILE
1	I	362	HIS
1	I	420	LEU
1	I	437	PRO
2	J	4	GLN
2	J	6	ASP
2	J	13	PRO

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Mol	Chain	Res	Type
2	J	16	LEU
2	J	45	GLN
2	J	62	LEU
2	J	80	LEU
2	J	92	SER
2	J	119	THR
2	J	124	VAL
2	J	130	ASN
2	J	150	SER
2	J	189	PHE
2	J	192	SER
2	J	194	VAL
2	J	202	GLU
2	J	206	ARG
2	J	214	ASP
2	J	222	LYS
2	J	252	SER
2	J	258	GLU
2	J	341	PRO
2	J	391	VAL
2	J	430	LEU
2	J	432	SER
1	K	14	GLN
1	K	58	THR
1	K	75	ILE
1	K	77	ASP
1	K	98	ASN
1	K	104	THR
1	K	129	LYS
1	K	140	THR
1	K	161	ASP
1	K	168	LYS
1	K	199	ASN
1	K	218	SER
1	K	219	THR
1	K	268	VAL
1	K	271	ASN
1	K	305	THR
1	K	310	ARG
1	K	352	MET
1	K	355	ILE
1	K	362	HIS

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Mol	Chain	Res	Type
1	K	401	TYR
1	K	420	LEU
1	K	437	PRO
2	L	4	GLN
2	L	13	PRO
2	L	16	LEU
2	L	45	GLN
2	L	62	LEU
2	L	80	LEU
2	L	92	SER
2	L	119	THR
2	L	124	VAL
2	L	130	ASN
2	L	144	PRO
2	L	150	SER
2	L	189	PHE
2	L	192	SER
2	L	194	VAL
2	L	202	GLU
2	L	214	ASP
2	L	222	LYS
2	L	252	SER
2	L	258	GLU
2	L	264	PRO
2	L	391	VAL
2	L	430	LEU
2	L	432	SER
3	M	7	ILE
3	M	39	ASP
3	M	63	GLU
3	M	67	VAL
3	M	92	GLU
3	M	95	VAL
3	M	112	GLU
3	M	119	LEU
3	M	140	ARG
3	M	143	LYS
3	M	145	GLN
3	M	163	ASN
3	M	169	VAL
3	M	174	SER
3	M	177	VAL

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Mol	Chain	Res	Type
3	M	179	LEU
3	M	182	LEU
3	M	193	ASP
3	M	199	LEU
3	M	205	THR
3	M	207	MET
3	M	247	VAL
3	M	249	ASP
3	M	254	VAL
3	M	260	THR
3	M	266	GLU
3	M	268	LEU
3	M	271	PHE
3	N	18	THR
3	N	23	VAL
3	N	63	GLU
3	N	85	CYS
3	N	95	VAL
3	N	100	ARG
3	N	126	VAL
3	N	145	GLN
3	N	146	GLU
3	N	147	ILE
3	N	168	ILE
3	N	179	LEU
3	N	182	LEU
3	N	194	GLU
3	N	201	ASN
3	N	206	GLN
3	N	226	THR
3	N	231	ASP
3	N	233	LYS
3	N	243	LEU
3	N	247	VAL
3	N	249	ASP
3	N	254	VAL
3	N	264	LEU
3	N	267	LEU
3	N	268	LEU
3	N	269	MET
3	N	273	ILE
3	O	44	SER

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Mol	Chain	Res	Type
3	O	45	THR
3	O	55	ASN
3	O	66	THR
3	O	83	VAL
3	O	120	ASP
3	O	145	GLN
3	O	146	GLU
3	O	163	ASN
3	O	195	LEU
3	O	201	ASN
3	O	205	THR
3	O	206	GLN
3	O	208	ILE
3	O	211	VAL
3	O	236	GLN
3	O	249	ASP
3	P	16	SER
3	P	22	LEU
3	P	28	GLU
3	P	44	SER
3	P	55	ASN
3	P	63	GLU
3	P	66	THR
3	P	92	GLU
3	P	93	PRO
3	P	95	VAL
3	P	117	ASP
3	P	132	CYS
3	P	137	MET
3	P	145	GLN
3	P	152	SER
3	P	156	MET
3	P	163	ASN
3	P	179	LEU
3	P	199	LEU
3	P	205	THR
3	P	208	ILE
3	P	233	LYS
3	P	249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	29	ASN
1	A	35	ASN
1	A	49	ASN
1	A	252	GLN
1	A	271	ASN
2	B	18	GLN
2	B	37	GLN
2	B	45	GLN
2	B	130	ASN
2	B	163	ASN
2	B	278	GLN
2	B	338	GLN
2	B	499	ASN
2	B	518	ASN
1	C	14	GLN
1	C	29	ASN
1	C	35	ASN
1	C	49	ASN
1	C	252	GLN
1	C	271	ASN
1	C	362	HIS
2	D	18	GLN
2	D	37	GLN
2	D	45	GLN
2	D	130	ASN
2	D	136	GLN
2	D	163	ASN
2	D	278	GLN
2	D	317	ASN
2	D	338	GLN
2	D	478	HIS
2	D	499	ASN
2	D	518	ASN
3	E	4	GLN
3	E	21	ASN
3	E	55	ASN
3	E	107	ASN
3	E	163	ASN
3	E	257	ASN
3	F	21	ASN
3	F	54	GLN
3	F	55	ASN

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Mol	Chain	Res	Type
3	F	163	ASN
3	F	173	ASN
3	F	201	ASN
3	F	206	GLN
3	F	215	ASN
3	F	218	GLN
3	F	236	GLN
3	F	257	ASN
3	G	21	ASN
3	G	107	ASN
3	G	163	ASN
3	G	173	ASN
3	G	201	ASN
3	H	201	ASN
3	H	215	ASN
1	I	14	GLN
1	I	29	ASN
1	I	35	ASN
1	I	41	GLN
1	I	49	ASN
1	I	252	GLN
1	I	271	ASN
1	I	362	HIS
2	J	18	GLN
2	J	37	GLN
2	J	45	GLN
2	J	130	ASN
2	J	136	GLN
2	J	163	ASN
2	J	338	GLN
2	J	457	HIS
2	J	499	ASN
2	J	518	ASN
1	K	14	GLN
1	K	29	ASN
1	K	35	ASN
1	K	49	ASN
1	K	252	GLN
1	K	271	ASN
1	K	362	HIS
2	L	18	GLN
2	L	37	GLN

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Mol	Chain	Res	Type
2	L	45	GLN
2	L	130	ASN
2	L	136	GLN
2	L	163	ASN
2	L	338	GLN
2	L	457	HIS
2	L	499	ASN
2	L	518	ASN
3	M	20	GLN
3	M	163	ASN
3	M	173	ASN
3	M	201	ASN
3	M	257	ASN
3	N	163	ASN
3	N	257	ASN
3	O	4	GLN
3	O	20	GLN
3	O	21	ASN
3	O	50	HIS
3	O	55	ASN
3	O	107	ASN
3	O	163	ASN
3	O	185	ASN
3	O	188	ASN
3	O	201	ASN
3	O	215	ASN
3	O	257	ASN
3	P	55	ASN
3	P	107	ASN
3	P	201	ASN
3	P	215	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
5	CFN	K	496	4,1	18,30,30	3.01	9 (50%)	-		
10	SF4	G	3290	3	0,12,12	-	-	-		
9	ADP	N	6292	8	28,29,29	1.37	5 (17%)	43,45,45	1.36	7 (16%)
9	ADP	M	5292	8	28,29,29	1.41	6 (21%)	43,45,45	1.27	4 (9%)
9	ADP	G	3292	8	28,29,29	1.94	5 (17%)	43,45,45	1.28	4 (9%)
9	ADP	E	1292	-	28,29,29	1.21	2 (7%)	43,45,45	1.28	5 (11%)
9	ADP	P	8292	8	28,29,29	1.36	4 (14%)	43,45,45	1.27	4 (9%)
7	CLF	L	7498	2,1	0,24,24	-	-	-		
4	HCA	K	494	5	13,13,13	3.96	5 (38%)	15,18,18	1.42	3 (20%)
5	CFN	A	496	4,1	18,30,30	2.46	9 (50%)	-		
7	CLF	B	1498	2,1	0,24,24	-	-	-		
7	CLF	D	3498	2,1	0,24,24	-	-	-		
4	HCA	I	494	5	13,13,13	4.10	4 (30%)	15,18,18	1.17	1 (6%)
4	HCA	A	494	5	13,13,13	3.90	4 (30%)	15,18,18	1.28	1 (6%)
4	HCA	C	494	5	13,13,13	3.00	5 (38%)	15,18,18	1.50	4 (26%)
10	SF4	F	1290	3	0,12,12	-	-	-		
9	ADP	O	7292	8	28,29,29	1.56	4 (14%)	43,45,45	1.22	2 (4%)
5	CFN	I	496	4,1	18,30,30	2.77	12 (66%)	-		
7	CLF	J	5498	2,1	0,24,24	-	-	-		
10	SF4	N	5290	3	0,12,12	-	-	-		
9	ADP	F	2292	8	28,29,29	1.51	7 (25%)	43,45,45	1.18	4 (9%)
10	SF4	P	7290	3	0,12,12	-	-	-		
5	CFN	C	496	4,1	18,30,30	3.26	12 (66%)	-		
9	ADP	H	4292	-	28,29,29	1.50	3 (10%)	43,45,45	1.35	5 (11%)

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	SF4	G	3290	3	-	-	0/6/5/5
9	ADP	N	6292	8	-	4/16/32/32	0/3/3/3
9	ADP	M	5292	8	-	4/16/32/32	0/3/3/3
9	ADP	G	3292	8	-	0/16/32/32	0/3/3/3
9	ADP	E	1292	-	-	3/16/32/32	0/3/3/3
9	ADP	P	8292	8	-	4/16/32/32	0/3/3/3
7	CLF	L	7498	2,1	-	-	0/12/10/10
4	HCA	K	494	5	-	8/17/17/17	-
7	CLF	B	1498	2,1	-	-	0/12/10/10
7	CLF	D	3498	2,1	-	-	0/12/10/10
4	HCA	I	494	5	-	8/17/17/17	-
4	HCA	C	494	5	-	8/17/17/17	-
10	SF4	F	1290	3	-	-	0/6/5/5
9	ADP	O	7292	8	-	1/16/32/32	0/3/3/3
7	CLF	J	5498	2,1	-	-	0/12/10/10
10	SF4	N	5290	3	-	-	0/6/5/5
9	ADP	F	2292	8	-	7/16/32/32	0/3/3/3
10	SF4	P	7290	3	-	-	0/6/5/5
4	HCA	A	494	5	-	8/17/17/17	-
9	ADP	H	4292	-	-	3/16/32/32	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	494	HCA	C3-C7	-13.02	1.39	1.53
4	A	494	HCA	C3-C7	-11.49	1.41	1.53
4	K	494	HCA	C3-C7	-10.83	1.42	1.53
9	G	3292	ADP	PA-O3A	-6.68	1.52	1.59
4	C	494	HCA	C3-C7	-6.42	1.46	1.53
4	C	494	HCA	C2-C3	-6.31	1.46	1.54
4	K	494	HCA	C2-C3	-5.89	1.46	1.54
5	C	496	CFN	S2A-FE3	-5.55	2.18	2.29
5	C	496	CFN	S4B-FE5	-5.35	2.19	2.29
4	A	494	HCA	C2-C3	-5.09	1.47	1.54
5	A	496	CFN	S4B-FE7	-4.72	2.20	2.29
5	K	496	CFN	S2A-FE3	-4.72	2.20	2.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	496	CFN	S1B-FE6	-4.67	2.20	2.29
5	K	496	CFN	S4B-FE7	-4.61	2.20	2.29
5	K	496	CFN	S2A-FE2	-4.52	2.20	2.29
5	K	496	CFN	S4A-FE4	-4.52	2.20	2.29
5	A	496	CFN	S3B-FE6	-4.51	2.20	2.29
4	K	494	HCA	C4-C3	-4.38	1.42	1.53
9	O	7292	ADP	C2-N1	4.31	1.41	1.33
4	K	494	HCA	O7-C3	4.30	1.51	1.43
4	A	494	HCA	O7-C3	4.27	1.51	1.43
5	I	496	CFN	S1B-FE6	-4.14	2.21	2.29
5	K	496	CFN	S3B-FE7	-4.14	2.21	2.29
5	C	496	CFN	S2A-FE2	-4.03	2.21	2.29
5	C	496	CFN	S1B-FE6	-3.98	2.21	2.29
5	C	496	CFN	S3B-FE6	-3.90	2.21	2.29
5	C	496	CFN	S4B-FE7	-3.90	2.21	2.29
5	I	496	CFN	S2A-FE2	-3.86	2.22	2.29
9	H	4292	ADP	C2-N1	3.84	1.40	1.33
4	I	494	HCA	C4-C3	-3.81	1.43	1.53
5	A	496	CFN	S3B-FE7	-3.77	2.22	2.29
5	C	496	CFN	S4A-FE4	-3.77	2.22	2.29
5	C	496	CFN	S3B-FE7	-3.68	2.22	2.29
5	I	496	CFN	S2A-FE3	-3.67	2.22	2.29
5	I	496	CFN	S3B-FE7	-3.62	2.22	2.29
5	I	496	CFN	S4B-FE5	-3.62	2.22	2.29
9	N	6292	ADP	C2-N1	3.57	1.40	1.33
5	C	496	CFN	S1A-FE2	-3.56	2.22	2.29
5	C	496	CFN	S4A-FE3	-3.53	2.22	2.29
4	I	494	HCA	C2-C3	-3.51	1.49	1.54
4	C	494	HCA	C4-C3	-3.42	1.44	1.53
5	A	496	CFN	S1B-FE5	-3.42	2.22	2.29
9	F	2292	ADP	C2-N1	3.39	1.40	1.33
9	P	8292	ADP	C2-N1	3.37	1.39	1.33
5	K	496	CFN	S4B-FE5	-3.34	2.23	2.29
9	O	7292	ADP	PA-O3A	-3.32	1.55	1.59
5	K	496	CFN	S1B-FE5	-3.19	2.23	2.29
9	G	3292	ADP	C6-N6	-3.15	1.26	1.34
9	E	1292	ADP	C2-N1	3.14	1.39	1.33
9	F	2292	ADP	C1'-N9	3.13	1.55	1.46
5	I	496	CFN	S3B-FE6	-3.10	2.23	2.29
4	A	494	HCA	C4-C3	-3.08	1.45	1.53
9	M	5292	ADP	C5-N7	-3.05	1.33	1.39
9	H	4292	ADP	C1'-N9	2.96	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	3292	ADP	C5-N7	-2.95	1.33	1.39
5	I	496	CFN	S4A-FE4	-2.93	2.23	2.29
9	M	5292	ADP	C2-N1	2.90	1.39	1.33
5	I	496	CFN	S1B-FE5	-2.87	2.23	2.29
5	I	496	CFN	S1A-FE4	-2.87	2.23	2.29
9	G	3292	ADP	C2-N1	2.85	1.39	1.33
5	I	496	CFN	S4A-FE3	-2.83	2.24	2.29
9	M	5292	ADP	C6-N6	-2.83	1.27	1.34
9	F	2292	ADP	C8-N7	2.82	1.37	1.31
9	P	8292	ADP	C1'-N9	2.77	1.54	1.46
9	O	7292	ADP	C1'-N9	2.75	1.54	1.46
5	I	496	CFN	S4B-FE7	-2.75	2.24	2.29
5	I	496	CFN	S1A-FE2	-2.74	2.24	2.29
4	C	494	HCA	O7-C3	2.69	1.48	1.43
9	E	1292	ADP	C5-N7	-2.68	1.34	1.39
9	M	5292	ADP	C1'-N9	2.68	1.53	1.46
9	F	2292	ADP	C6-N6	-2.66	1.27	1.34
9	H	4292	ADP	C5-N7	-2.63	1.34	1.39
9	F	2292	ADP	PA-O3A	-2.63	1.56	1.59
5	A	496	CFN	S1A-FE2	-2.62	2.24	2.29
9	N	6292	ADP	C5-N7	-2.62	1.34	1.39
5	C	496	CFN	S1A-FE4	-2.62	2.24	2.29
9	O	7292	ADP	C5-N7	-2.60	1.34	1.39
9	P	8292	ADP	C5-N7	-2.58	1.34	1.39
5	K	496	CFN	S3B-FE6	-2.54	2.24	2.29
5	A	496	CFN	S2A-FE2	-2.53	2.24	2.29
5	A	496	CFN	S2A-FE3	-2.43	2.24	2.29
9	P	8292	ADP	C6-N6	-2.40	1.28	1.34
4	I	494	HCA	O7-C3	2.37	1.47	1.43
9	G	3292	ADP	O4'-C4'	2.30	1.50	1.45
9	F	2292	ADP	C5-C6	2.28	1.47	1.41
9	N	6292	ADP	C5-C6	2.22	1.47	1.41
9	N	6292	ADP	C6-N6	-2.19	1.28	1.34
5	A	496	CFN	S4B-FE5	-2.17	2.25	2.29
9	M	5292	ADP	C8-N7	2.13	1.35	1.31
4	K	494	HCA	O2-C1	-2.13	1.23	1.30
5	A	496	CFN	S4A-FE3	-2.11	2.25	2.29
5	C	496	CFN	S3A-FE4	2.10	2.30	2.24
9	N	6292	ADP	C1'-N9	2.07	1.52	1.46
9	M	5292	ADP	PA-O3A	-2.05	1.57	1.59
4	C	494	HCA	C5-C6	2.05	1.55	1.50
9	F	2292	ADP	C5-N7	-2.00	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	1292	ADP	N3-C2-N1	-3.84	122.78	128.58
9	G	3292	ADP	N3-C2-N1	-3.58	123.16	128.58
9	P	8292	ADP	N3-C2-N1	-3.37	123.48	128.58
9	M	5292	ADP	N3-C2-N1	-3.28	123.62	128.58
9	H	4292	ADP	N3-C2-N1	-3.23	123.70	128.58
9	N	6292	ADP	N3-C2-N1	-3.19	123.75	128.58
9	P	8292	ADP	C2-N1-C6	3.19	123.97	118.73
9	G	3292	ADP	C2-N1-C6	3.15	123.91	118.73
9	H	4292	ADP	C2-N1-C6	3.13	123.87	118.73
9	N	6292	ADP	O5'-C5'-C4'	3.07	119.45	108.99
4	C	494	HCA	O7-C3-C7	3.07	113.31	108.96
9	O	7292	ADP	C2-N1-C6	3.07	123.77	118.73
9	E	1292	ADP	C2-N1-C6	3.06	123.75	118.73
9	O	7292	ADP	N3-C2-N1	-3.04	123.98	128.58
9	F	2292	ADP	N3-C2-N1	-2.97	124.09	128.58
4	K	494	HCA	O7-C3-C7	2.93	113.11	108.96
9	H	4292	ADP	C3'-C2'-C1'	2.89	106.94	101.46
4	A	494	HCA	O7-C3-C7	2.88	113.04	108.96
9	G	3292	ADP	O4'-C1'-N9	2.73	113.34	108.09
9	E	1292	ADP	O5'-C5'-C4'	2.66	118.05	108.99
9	N	6292	ADP	C2-N1-C6	2.61	123.02	118.73
9	N	6292	ADP	C3'-C2'-C1'	2.61	106.39	101.46
9	F	2292	ADP	C2-N1-C6	2.60	123.00	118.73
9	M	5292	ADP	C2-N1-C6	2.49	122.82	118.73
9	M	5292	ADP	O4'-C1'-N9	2.41	112.72	108.09
9	P	8292	ADP	O5'-C5'-C4'	2.35	116.99	108.99
9	H	4292	ADP	O4'-C1'-N9	2.31	112.53	108.09
9	E	1292	ADP	C3'-C2'-C1'	2.31	105.83	101.46
9	P	8292	ADP	O4'-C1'-N9	2.30	112.50	108.09
4	C	494	HCA	O4-C6-C5	2.28	121.19	114.00
9	G	3292	ADP	O3B-PB-O2B	2.24	116.20	107.80
4	C	494	HCA	C2-C3-C7	-2.24	105.08	110.03
4	K	494	HCA	O4-C6-C5	2.21	120.99	114.00
4	K	494	HCA	O6-C7-C3	2.21	117.38	113.14
9	M	5292	ADP	O3B-PB-O2B	2.20	116.06	107.80
9	N	6292	ADP	C4'-O4'-C1'	2.20	114.32	109.47
9	N	6292	ADP	O5'-PA-O1A	-2.17	100.34	108.94
9	H	4292	ADP	O3B-PB-O2B	2.16	115.90	107.80
9	E	1292	ADP	C4'-O4'-C1'	2.12	114.16	109.47
4	I	494	HCA	O7-C3-C7	2.12	111.96	108.96
9	F	2292	ADP	C3'-C2'-C1'	2.08	105.39	101.46
4	C	494	HCA	O6-C7-C3	2.06	117.09	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	2292	ADP	C4'-O4'-C1'	2.04	113.98	109.47
9	N	6292	ADP	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	494	HCA	C2-C3-C4-C5
4	A	494	HCA	C7-C3-C4-C5
4	A	494	HCA	O7-C3-C4-C5
4	C	494	HCA	C2-C3-C4-C5
4	C	494	HCA	C7-C3-C4-C5
4	C	494	HCA	O7-C3-C4-C5
4	I	494	HCA	C2-C3-C4-C5
4	I	494	HCA	C7-C3-C4-C5
4	I	494	HCA	O7-C3-C4-C5
4	K	494	HCA	C2-C3-C4-C5
4	K	494	HCA	C7-C3-C4-C5
4	K	494	HCA	O7-C3-C4-C5
9	F	2292	ADP	PA-O3A-PB-O3B
9	H	4292	ADP	C5'-O5'-PA-O1A
9	H	4292	ADP	C5'-O5'-PA-O3A
9	H	4292	ADP	C4'-C5'-O5'-PA
9	N	6292	ADP	C5'-O5'-PA-O3A
9	P	8292	ADP	C5'-O5'-PA-O3A
9	M	5292	ADP	O4'-C4'-C5'-O5'
4	A	494	HCA	C3-C4-C5-C6
4	C	494	HCA	C3-C4-C5-C6
4	I	494	HCA	C3-C4-C5-C6
4	K	494	HCA	C3-C4-C5-C6
9	F	2292	ADP	O4'-C4'-C5'-O5'
9	F	2292	ADP	C3'-C4'-C5'-O5'
9	P	8292	ADP	PB-O3A-PA-O5'
9	F	2292	ADP	PA-O3A-PB-O1B
9	M	5292	ADP	C3'-C4'-C5'-O5'
9	F	2292	ADP	C5'-O5'-PA-O1A
9	N	6292	ADP	C5'-O5'-PA-O1A
9	P	8292	ADP	C5'-O5'-PA-O1A
9	P	8292	ADP	C4'-C5'-O5'-PA
9	E	1292	ADP	PB-O3A-PA-O2A
9	N	6292	ADP	C4'-C5'-O5'-PA
9	E	1292	ADP	C4'-C5'-O5'-PA

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Mol	Chain	Res	Type	Atoms
4	A	494	HCA	C4-C5-C6-O4
4	C	494	HCA	C4-C5-C6-O4
4	I	494	HCA	C4-C5-C6-O4
4	A	494	HCA	C4-C5-C6-O3
4	K	494	HCA	C4-C5-C6-O4
4	C	494	HCA	C4-C5-C6-O3
4	K	494	HCA	C4-C5-C6-O3
4	C	494	HCA	O2-C1-C2-C3
4	I	494	HCA	O2-C1-C2-C3
4	K	494	HCA	O2-C1-C2-C3
4	I	494	HCA	C4-C5-C6-O3
9	F	2292	ADP	PB-O3A-PA-O2A
9	M	5292	ADP	PB-O3A-PA-O1A
9	O	7292	ADP	PB-O3A-PA-O2A
4	A	494	HCA	O1-C1-C2-C3
4	A	494	HCA	O2-C1-C2-C3
4	K	494	HCA	O1-C1-C2-C3
4	C	494	HCA	O1-C1-C2-C3
4	I	494	HCA	O1-C1-C2-C3
9	E	1292	ADP	PB-O3A-PA-O1A
9	F	2292	ADP	PB-O3A-PA-O1A
9	M	5292	ADP	PB-O3A-PA-O2A
9	N	6292	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

17 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	496	CFN	3	0
9	M	5292	ADP	2	0
9	G	3292	ADP	1	0
9	P	8292	ADP	1	0
7	L	7498	CLF	2	0
4	K	494	HCA	1	0
5	A	496	CFN	2	0
7	B	1498	CLF	2	0
7	D	3498	CLF	2	0
4	I	494	HCA	1	0
4	A	494	HCA	1	0
4	C	494	HCA	1	0
10	F	1290	SF4	1	0
5	I	496	CFN	2	0

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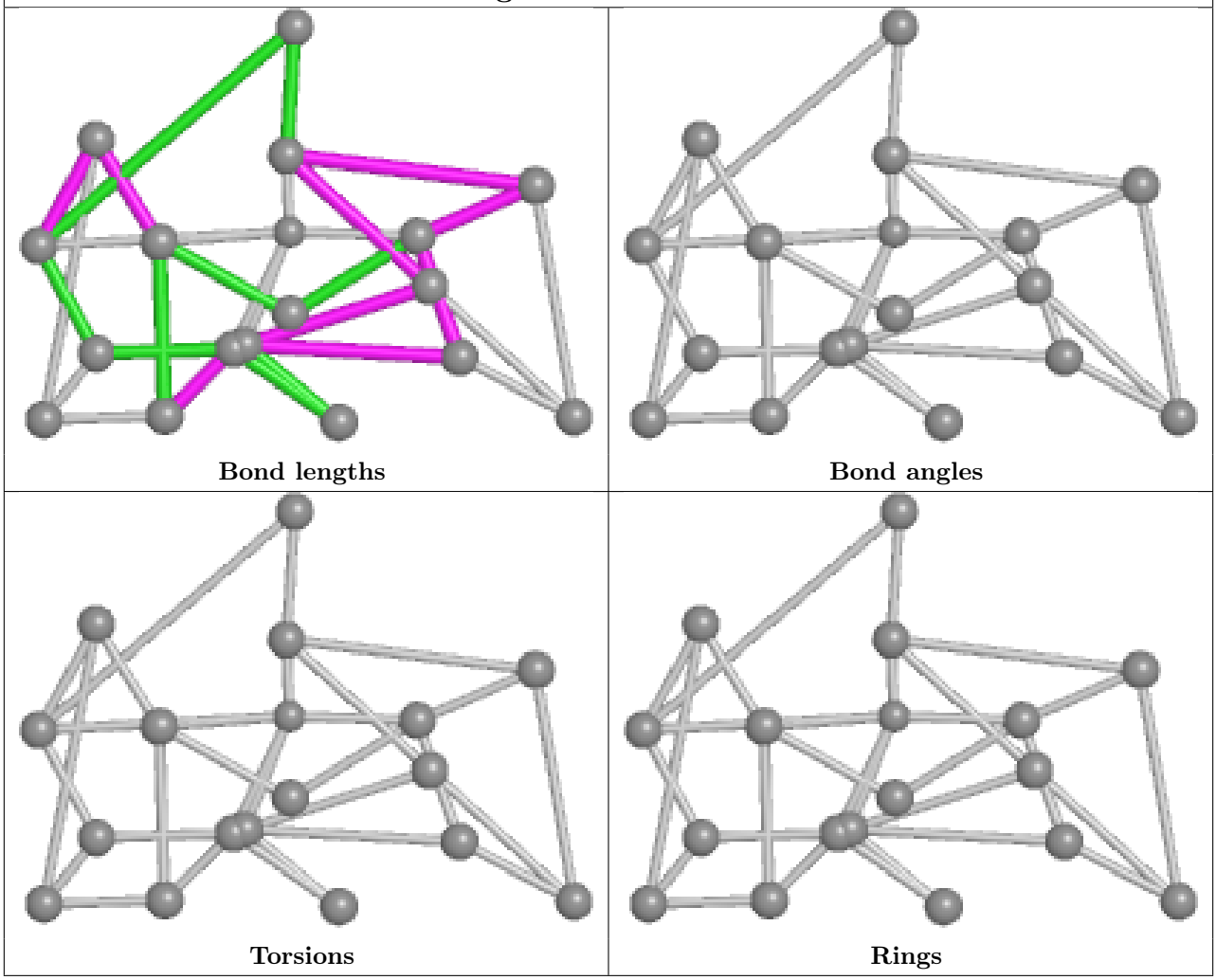
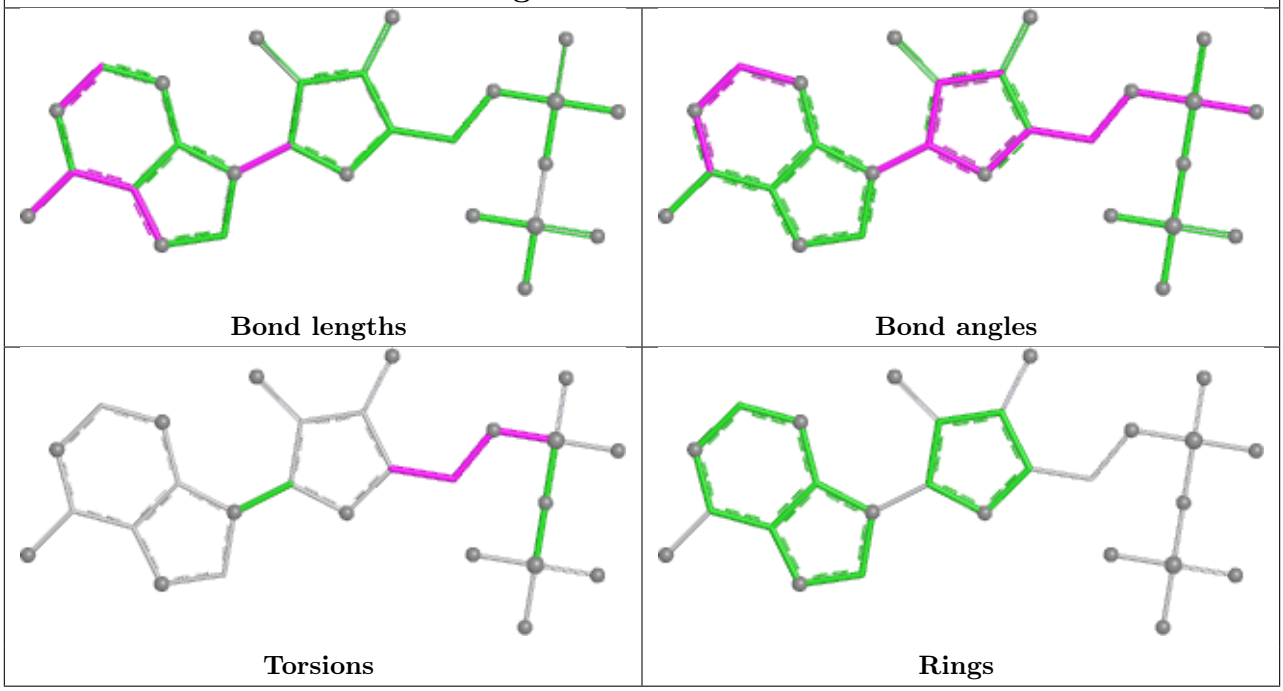
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	J	5498	CLF	2	0
9	F	2292	ADP	4	0
5	C	496	CFN	3	0

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.

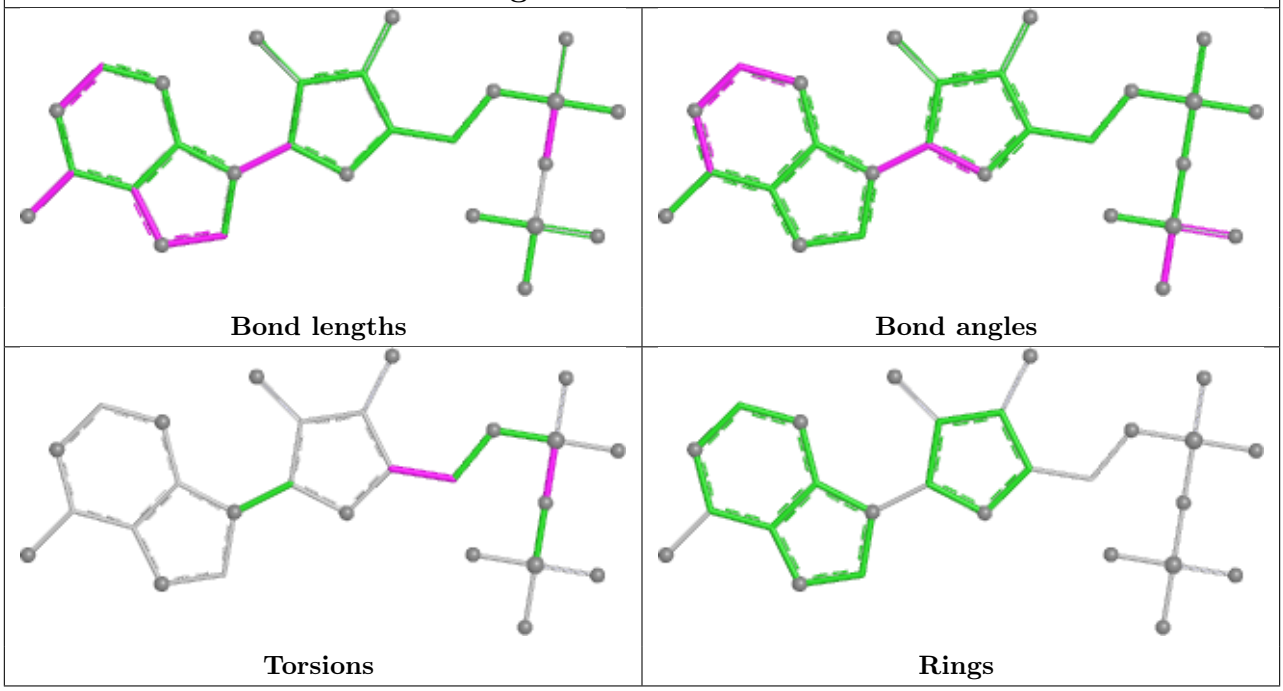
Ligand CFN K 496



Ligand ADP N 6292



Ligand ADP M 5292



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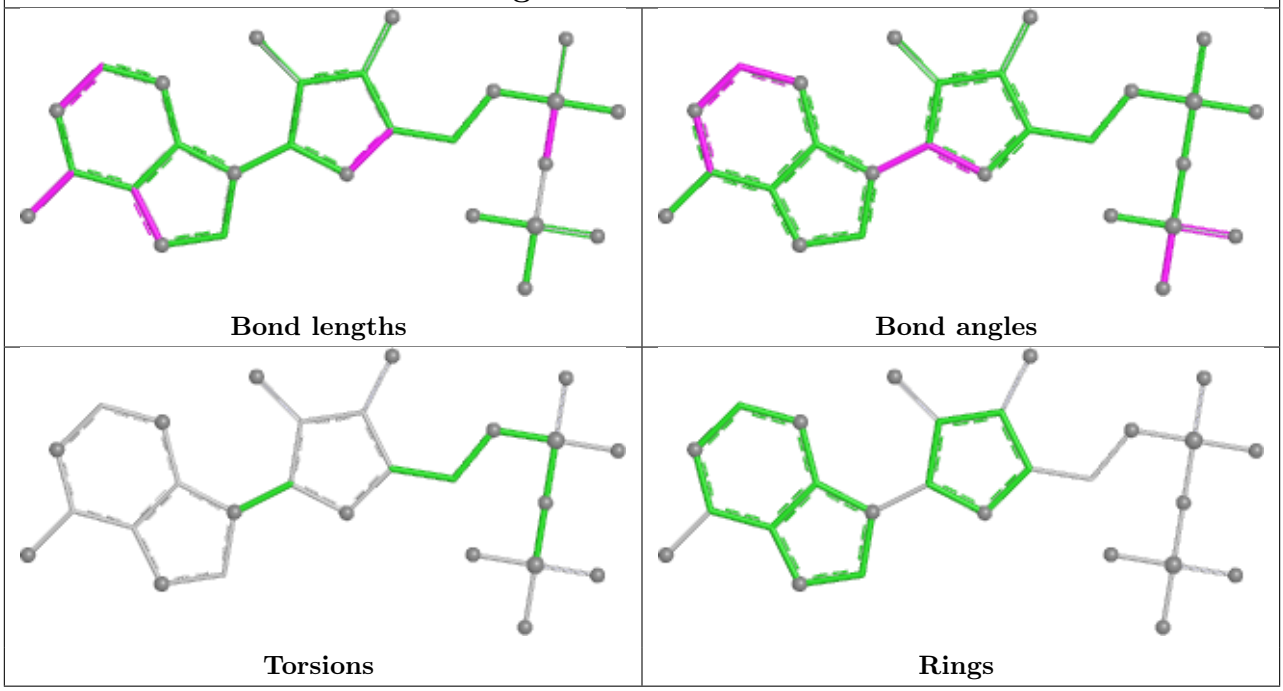

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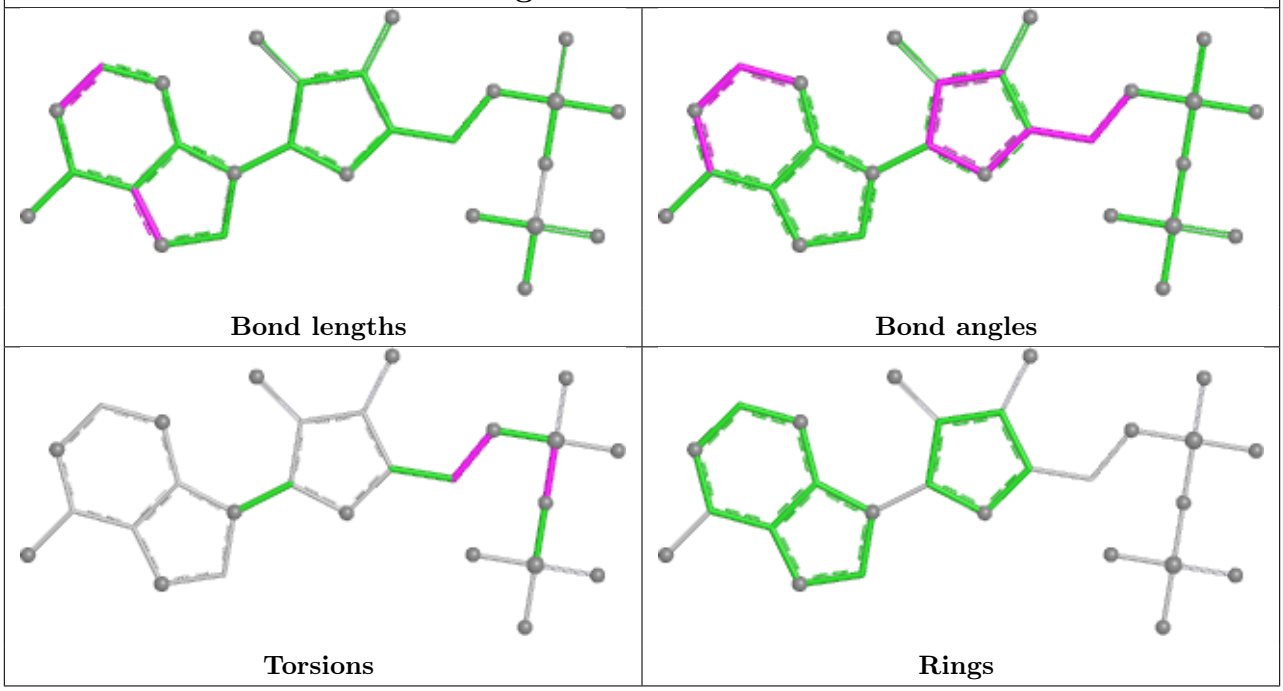

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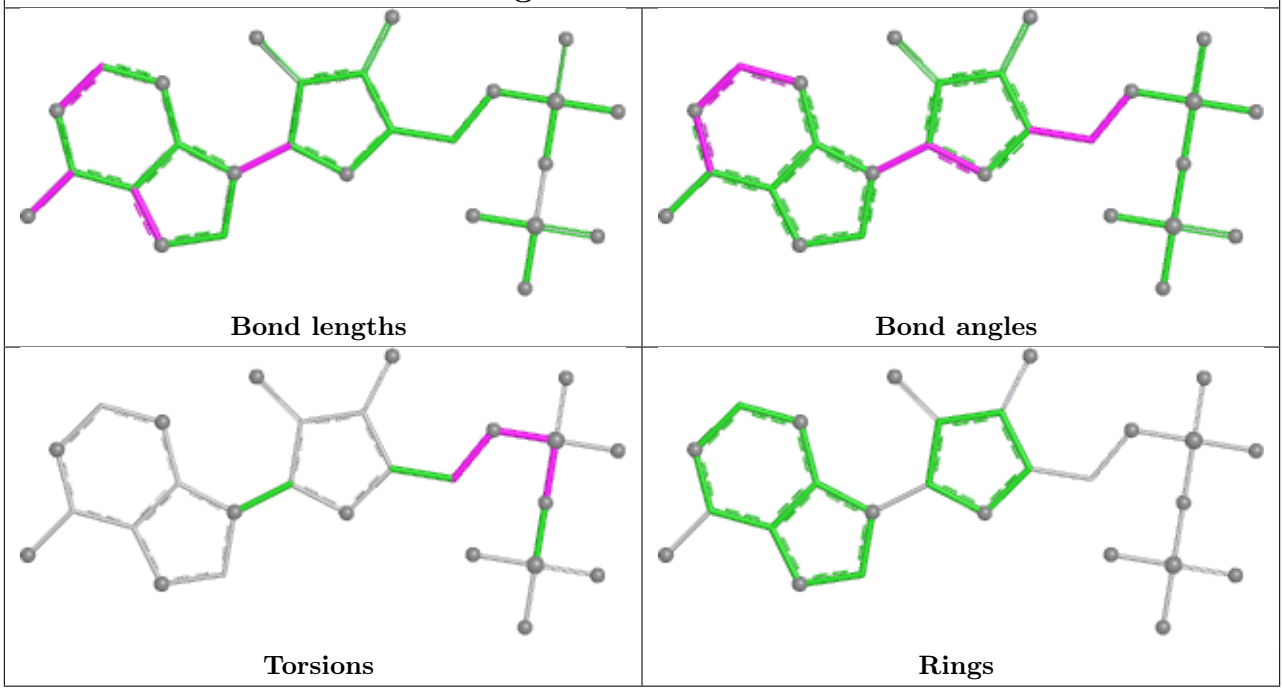

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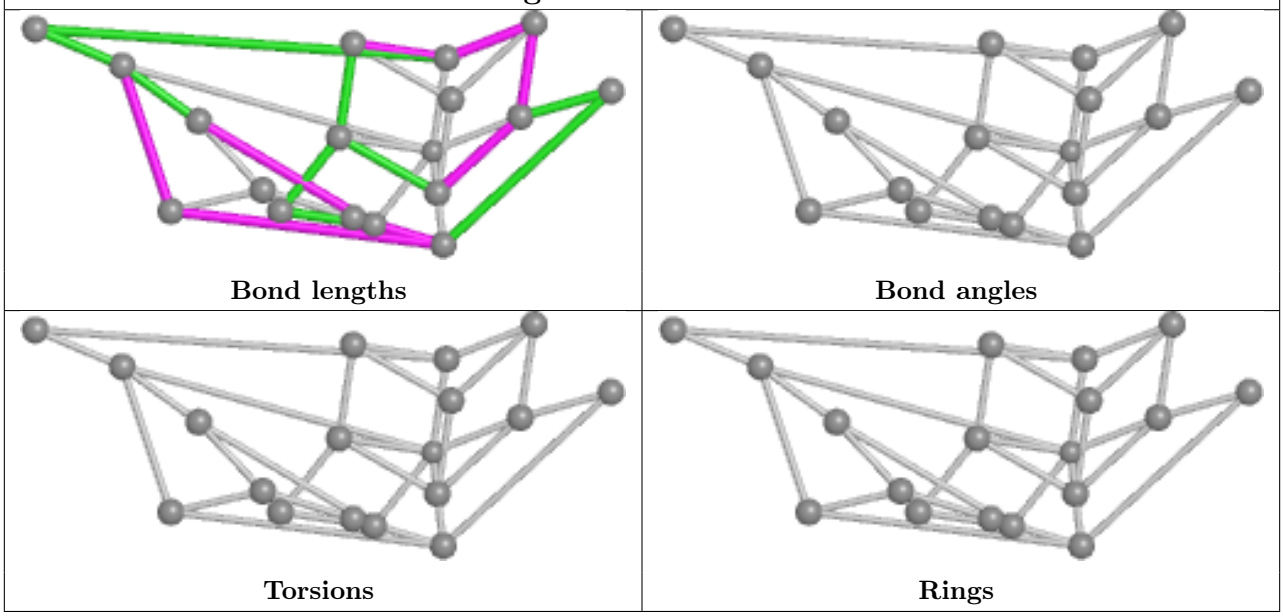
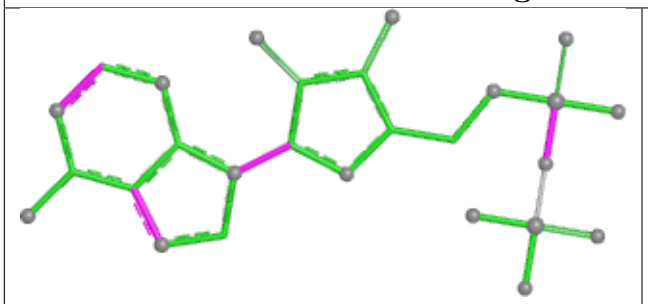
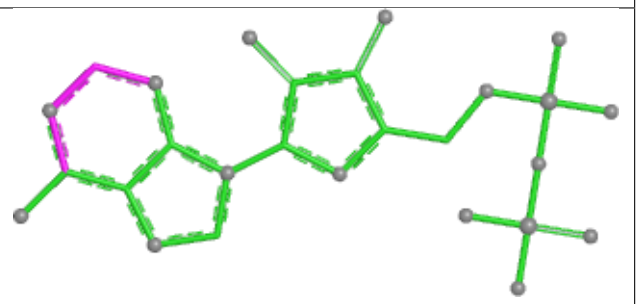


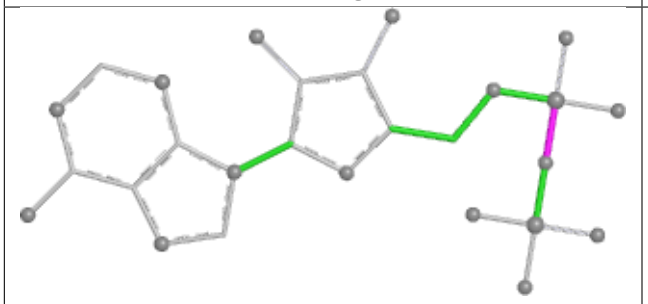
Ligand ADP O 7292



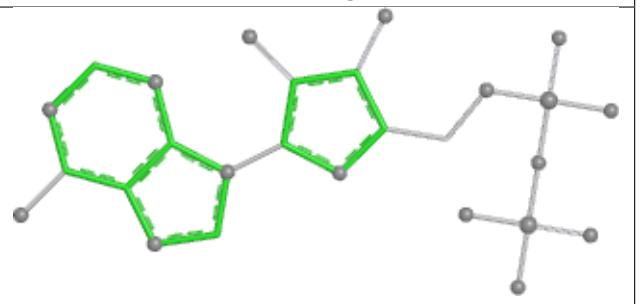
Bond lengths



Bond angles

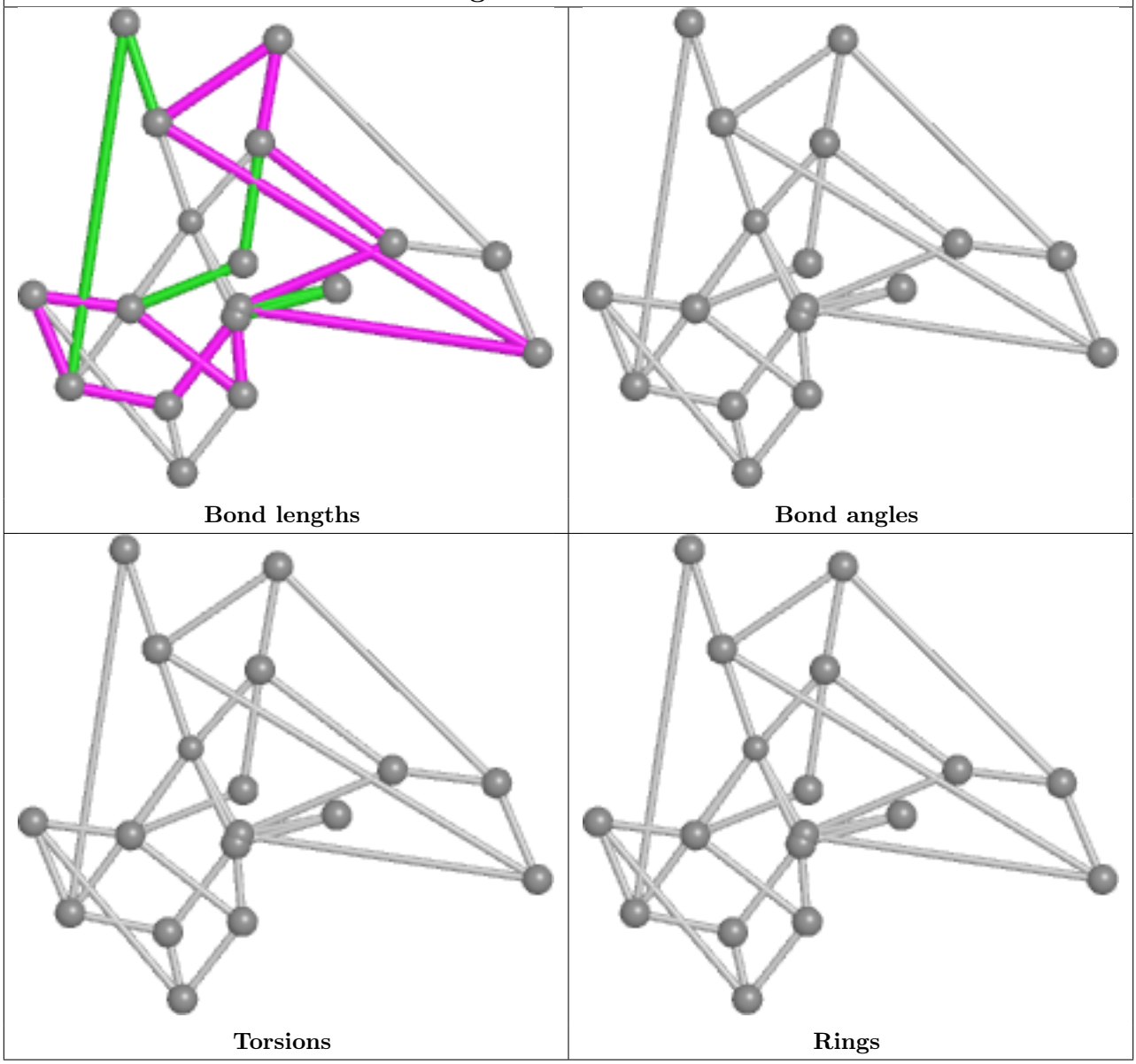


Torsions

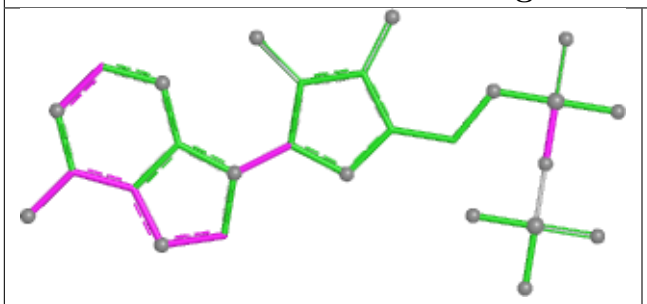


Rings

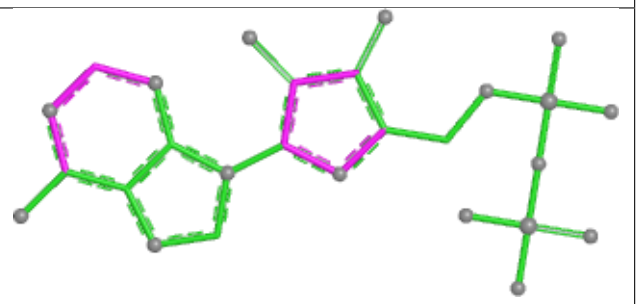
Ligand CFN I 496



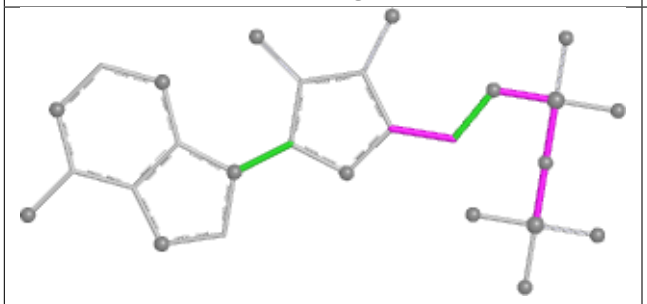
Ligand ADP F 2292



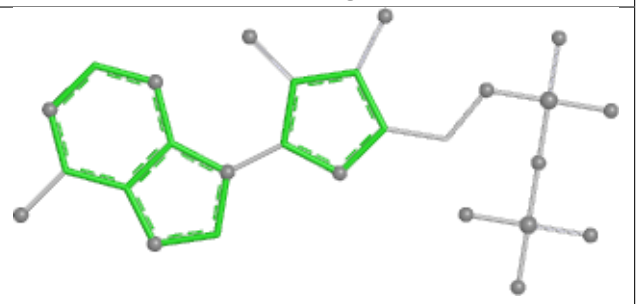
Bond lengths



Bond angles

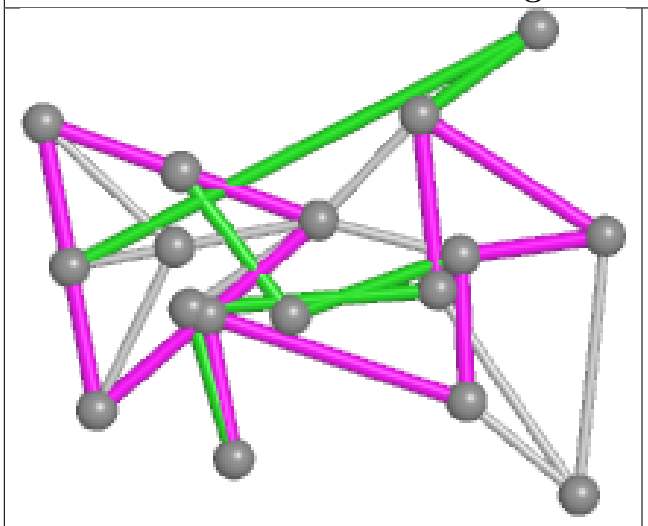


Torsions

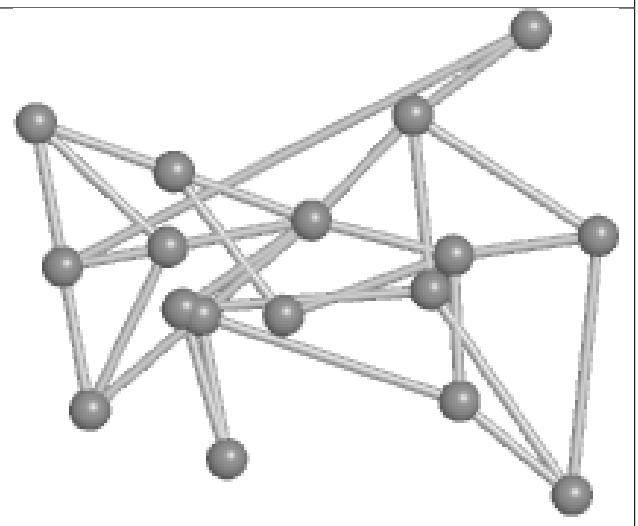


Rings

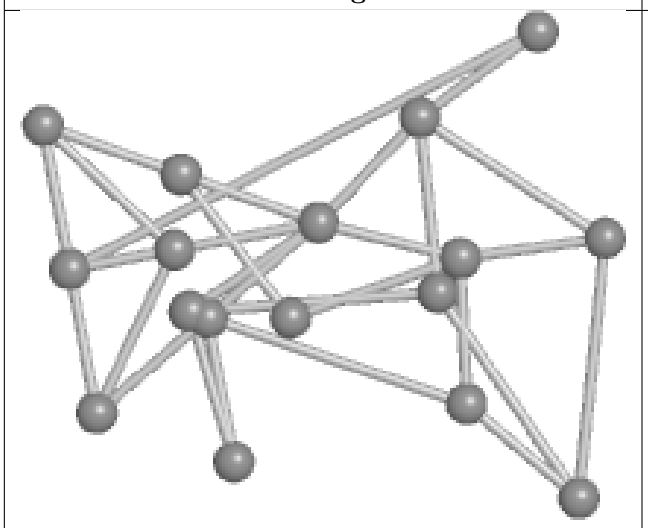
Ligand CFN C 496



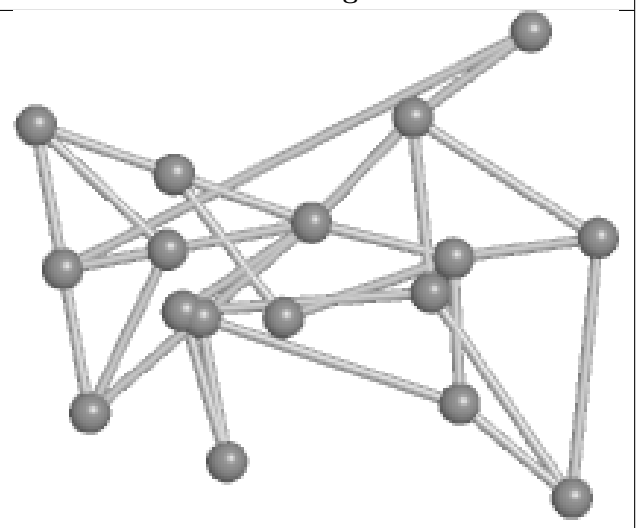
Bond lengths



Bond angles

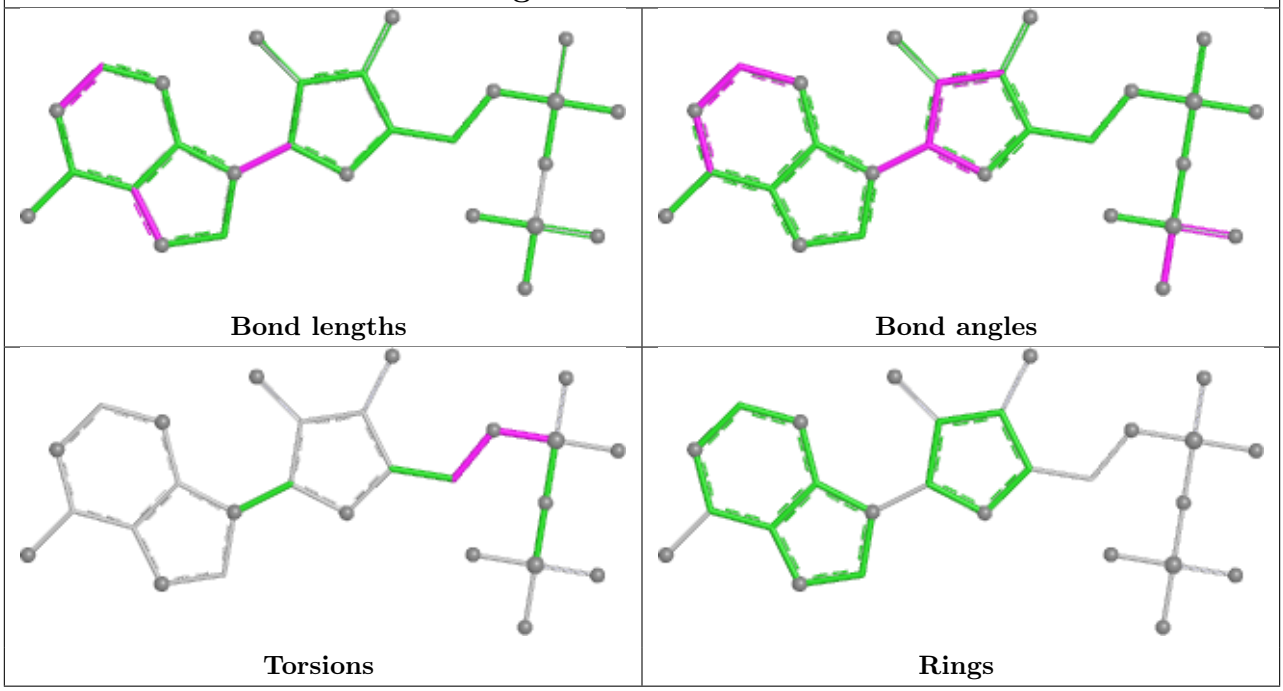


Torsions



Rings

Ligand ADP H 4292



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	476/491 (96%)	-0.29	0	100	100	16, 34, 57, 86	7 (1%)
1	C	476/491 (96%)	-0.29	0	100	100	13, 33, 56, 85	6 (1%)
1	I	476/491 (96%)	-0.23	0	100	100	18, 35, 59, 86	0
1	K	476/491 (96%)	-0.27	1 (0%)	91	83	15, 34, 58, 85	3 (0%)
2	B	522/522 (100%)	-0.43	1 (0%)	91	83	9, 28, 49, 69	8 (1%)
2	D	522/522 (100%)	-0.46	1 (0%)	91	83	9, 28, 49, 69	2 (0%)
2	J	522/522 (100%)	-0.47	0	100	100	10, 29, 50, 69	1 (0%)
2	L	522/522 (100%)	-0.47	0	100	100	9, 29, 50, 70	1 (0%)
3	E	252/289 (87%)	0.70	20 (7%)	18	10	24, 77, 110, 127	65 (25%)
3	F	270/289 (93%)	0.39	9 (3%)	49	29	23, 75, 107, 130	43 (15%)
3	G	257/289 (88%)	0.52	16 (6%)	26	14	23, 65, 107, 128	49 (19%)
3	H	170/289 (58%)	0.66	8 (4%)	36	19	25, 78, 109, 121	55 (32%)
3	M	253/289 (87%)	0.67	19 (7%)	20	11	25, 80, 115, 134	72 (28%)
3	N	157/289 (54%)	1.03	23 (14%)	6	3	32, 74, 118, 130	77 (49%)
3	O	260/289 (89%)	0.57	19 (7%)	21	11	25, 74, 114, 131	61 (23%)
3	P	190/289 (65%)	0.55	6 (3%)	50	30	30, 90, 119, 131	54 (28%)
All	All	5801/6364 (91%)	-0.06	123 (2%)	63	42	9, 37, 98, 134	504 (8%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	N	18	THR	6.6
3	N	19	THR	5.4
3	F	149	ILE	5.3
3	M	88	SER	4.7
3	E	88	SER	4.5

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Mol	Chain	Res	Type	RSRZ
3	E	38	CYS	4.4
3	E	79	GLY	4.4
3	H	18	THR	4.3
3	O	128	GLY	4.0
3	O	183	ILE	3.9
2	B	122	ALA	3.7
3	O	227	VAL	3.7
3	P	227	VAL	3.7
3	H	151	CYS	3.6
3	F	88	SER	3.5
3	M	58	MET	3.5
3	M	38	CYS	3.4
3	G	64	ALA	3.3
3	O	129	ASP	3.3
3	F	8	TYR	3.3
3	O	36	VAL	3.3
3	E	67	VAL	3.2
3	M	113	GLY	3.1
3	N	20	GLN	3.1
3	F	53	ALA	3.1
3	N	14	GLY	3.1
3	N	168	ILE	3.1
3	G	12	GLY	3.1
3	N	162	ASN	3.0
3	N	158	MET	3.0
3	G	94	GLY	3.0
3	P	164	ILE	3.0
3	G	137	MET	2.9
3	P	147	ILE	2.9
3	N	8	TYR	2.9
3	M	76	LEU	2.8
3	O	163	ASN	2.8
3	N	156	MET	2.7
3	N	217	VAL	2.7
3	P	236	GLN	2.7
3	N	9	GLY	2.7
3	M	271	PHE	2.7
3	E	76	LEU	2.7
3	H	169	VAL	2.7
3	E	22	LEU	2.6
3	G	244	ALA	2.6
3	G	192	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	227	VAL	2.6
3	H	88	SER	2.6
3	O	58	MET	2.6
3	E	63	GLU	2.6
3	M	71	GLU	2.6
3	N	150	VAL	2.6
3	F	76	LEU	2.6
3	M	161	ALA	2.6
3	E	66	THR	2.5
3	O	185	ASN	2.5
3	H	149	ILE	2.5
3	E	156	MET	2.5
3	G	135	PHE	2.5
3	G	70	LEU	2.5
3	O	64	ALA	2.4
3	M	61	ALA	2.4
3	F	151	CYS	2.4
3	H	19	THR	2.4
3	G	6	ALA	2.4
3	O	184	CYS	2.4
3	E	227	VAL	2.4
3	P	113	GLY	2.4
3	N	7	ILE	2.4
3	O	135	PHE	2.3
3	P	104	THR	2.3
3	E	102	VAL	2.3
1	K	423	SER	2.3
3	M	174	SER	2.3
2	D	160	ASP	2.3
3	O	117	ASP	2.3
3	N	86	VAL	2.3
3	O	90	GLY	2.3
3	E	165	SER	2.3
3	N	220	ALA	2.2
3	H	22	LEU	2.2
3	O	19	THR	2.2
3	E	134	GLY	2.2
3	G	27	ALA	2.2
3	O	35	ILE	2.2
3	E	32	LYS	2.2
3	G	66	THR	2.2
3	M	67	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	183	ILE	2.2
3	F	146	GLU	2.2
3	H	155	MET	2.2
3	E	90	GLY	2.2
3	N	40	PRO	2.2
3	M	83	VAL	2.1
3	O	114	ALA	2.1
3	G	11	GLY	2.1
3	F	38	CYS	2.1
3	N	157	ALA	2.1
3	M	164	ILE	2.1
3	O	228	ILE	2.1
3	M	4	GLN	2.1
3	M	91	PRO	2.1
3	M	152	SER	2.1
3	N	163	ASN	2.1
3	F	95	VAL	2.1
3	M	267	LEU	2.1
3	N	22	LEU	2.1
3	E	114	ALA	2.1
3	G	79	GLY	2.1
3	E	23	VAL	2.1
3	N	130	VAL	2.0
3	G	182	LEU	2.0
3	O	237	ALA	2.0
3	N	228	ILE	2.0
3	G	29	MET	2.0
3	G	198	ALA	2.0
3	E	171	TYR	2.0
3	M	171	TYR	2.0
3	O	214	ASP	2.0
3	M	94	GLY	2.0
3	E	147	ILE	2.0
3	N	273	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	ADP	N	6292	27/27	0.61	0.13	139,148,148,149	10
9	ADP	H	4292	27/27	0.62	0.14	124,133,136,136	10
9	ADP	P	8292	27/27	0.65	0.15	114,122,127,128	0
8	MG	G	3291	1/1	0.75	0.09	41,41,41,41	0
8	MG	H	4291	1/1	0.78	0.22	68,68,68,68	0
8	MG	N	6291	1/1	0.84	0.09	46,46,46,46	0
8	MG	O	7291	1/1	0.85	0.16	39,39,39,39	0
9	ADP	O	7292	27/27	0.88	0.09	66,81,93,96	0
8	MG	M	5291	1/1	0.88	0.14	47,47,47,47	0
9	ADP	M	5292	27/27	0.89	0.08	78,82,85,87	0
9	ADP	E	1292	27/27	0.89	0.09	61,68,71,73	0
8	MG	P	8291	1/1	0.90	0.11	66,66,66,66	0
9	ADP	F	2292	27/27	0.91	0.08	68,75,91,93	0
9	ADP	G	3292	27/27	0.92	0.09	50,56,59,60	0
8	MG	F	2291	1/1	0.93	0.13	23,23,23,23	0
8	MG	E	1291	1/1	0.94	0.17	44,44,44,44	0
4	HCA	I	494	14/14	0.94	0.09	19,27,32,37	0
4	HCA	K	494	14/14	0.95	0.09	17,23,31,33	0
4	HCA	A	494	14/14	0.96	0.08	21,25,29,30	0
4	HCA	C	494	14/14	0.96	0.09	18,22,30,32	0
10	SF4	P	7290	8/8	0.96	0.06	74,76,80,82	0
10	SF4	F	1290	8/8	0.97	0.04	55,59,61,62	0
6	CA	J	8492	1/1	0.97	0.04	42,42,42,42	0
10	SF4	N	5290	8/8	0.98	0.05	53,57,60,63	0
10	SF4	G	3290	8/8	0.98	0.06	42,46,48,49	0
5	CFN	I	496	18/18	0.99	0.03	17,22,25,27	0
5	CFN	K	496	18/18	0.99	0.03	12,21,25,26	0
6	CA	B	2492	1/1	0.99	0.03	34,34,34,34	0
6	CA	B	4492	1/1	0.99	0.04	32,32,32,32	0
5	CFN	C	496	18/18	0.99	0.04	9,15,18,18	0
6	CA	L	6492	1/1	0.99	0.02	37,37,37,37	0
7	CLF	B	1498	15/15	0.99	0.03	17,21,30,33	0

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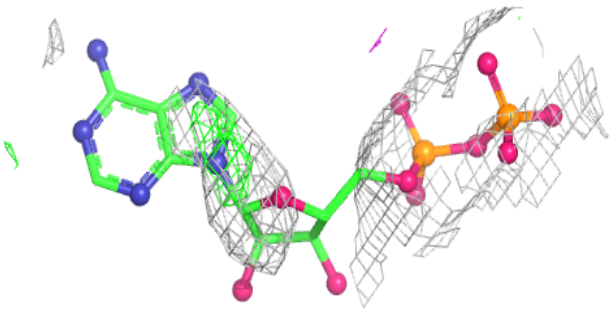
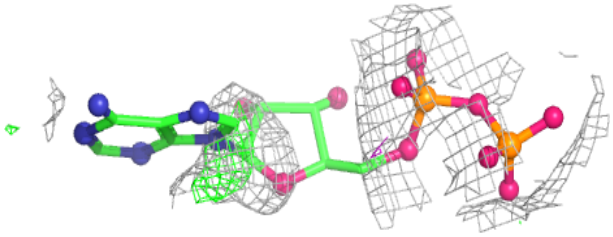
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CLF	D	3498	15/15	0.99	0.04	15,20,28,29	0
7	CLF	J	5498	15/15	0.99	0.04	21,27,34,35	0
7	CLF	L	7498	15/15	0.99	0.03	24,28,34,35	0
5	CFN	A	496	18/18	1.00	0.02	14,19,23,28	0

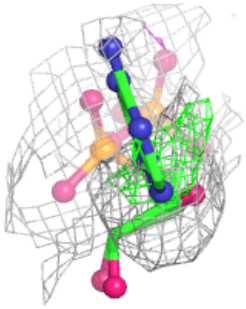
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP N 6292:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

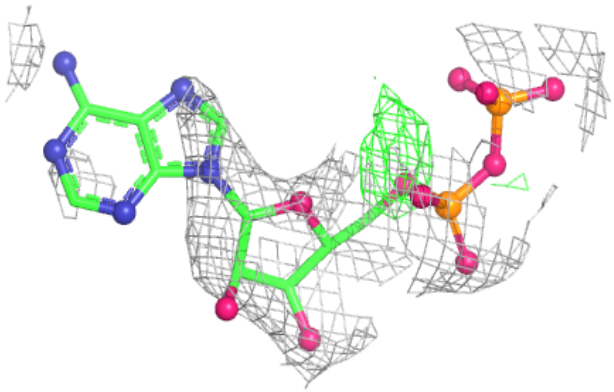


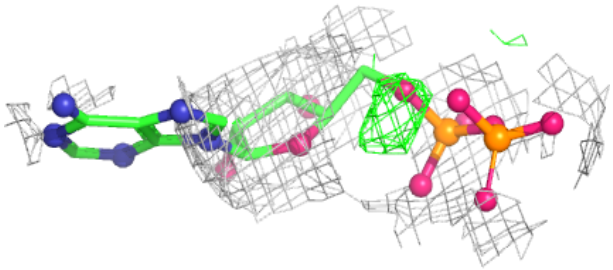


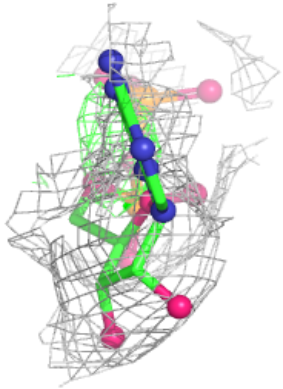


Electron density around ADP H 4292:

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

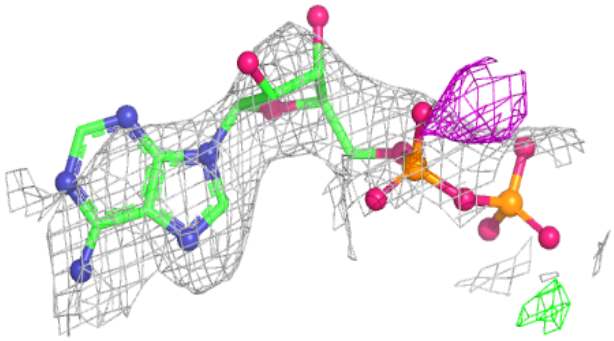


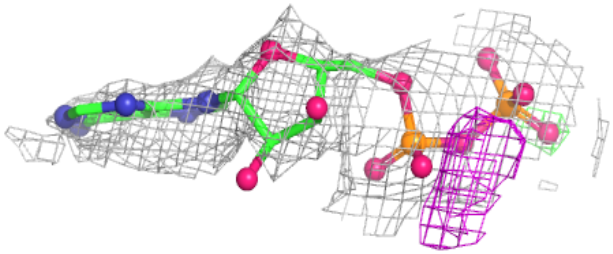


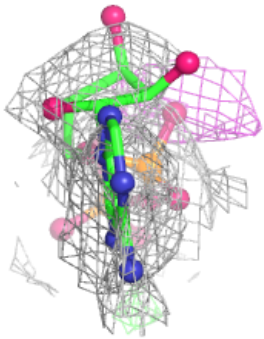


Electron density around ADP P 8292:

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

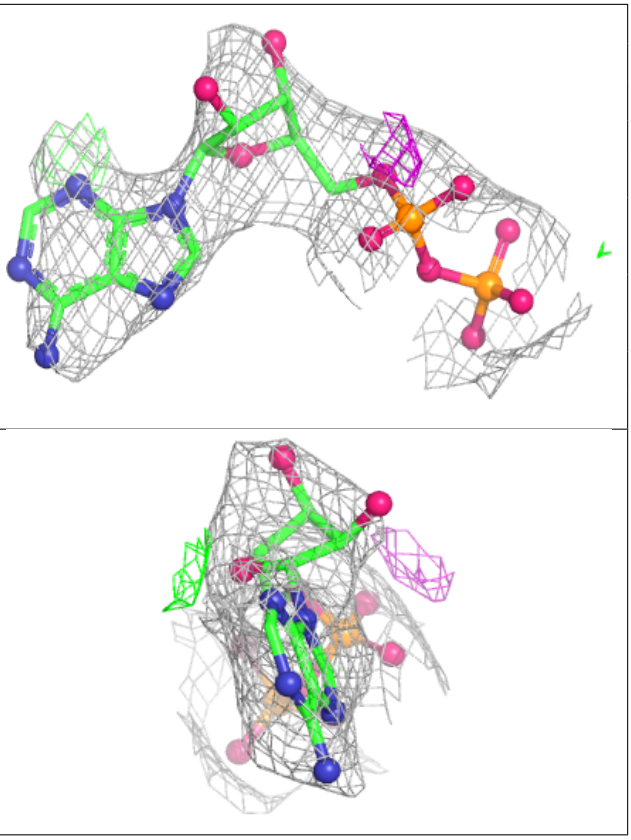






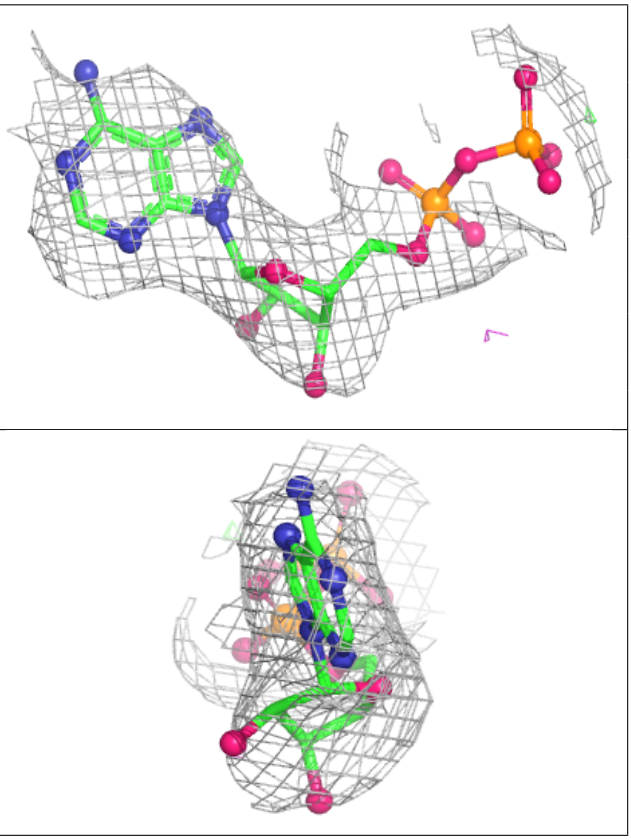
Electron density around ADP O 7292:

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



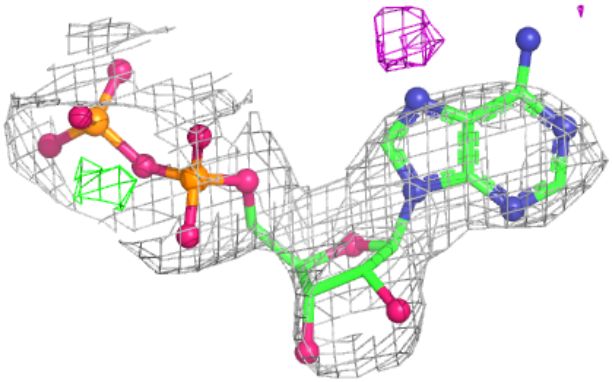
Electron density around ADP M 5292:

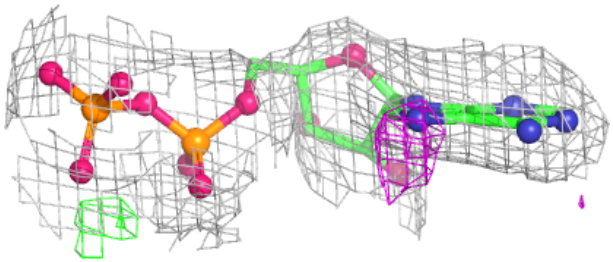
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

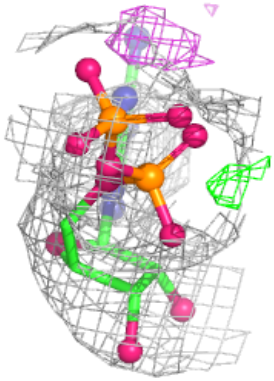


Electron density around ADP E 1292:

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

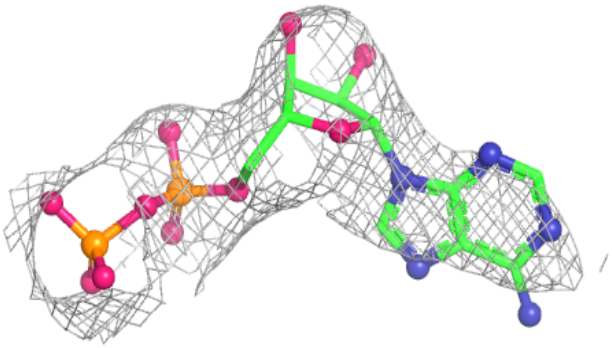


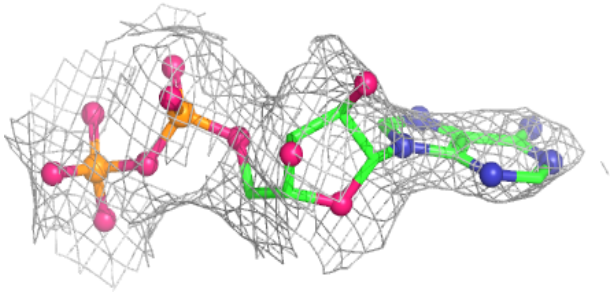


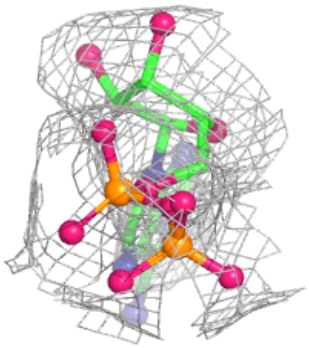


Electron density around ADP F 2292:

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

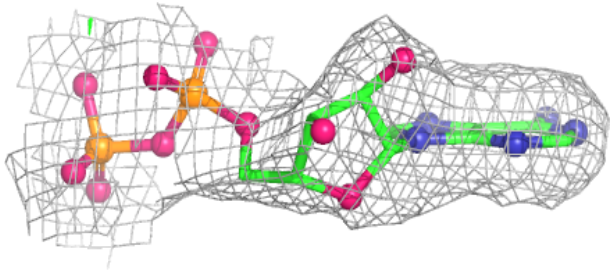


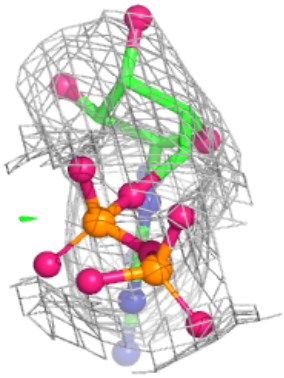




Electron density around ADP G 3292:

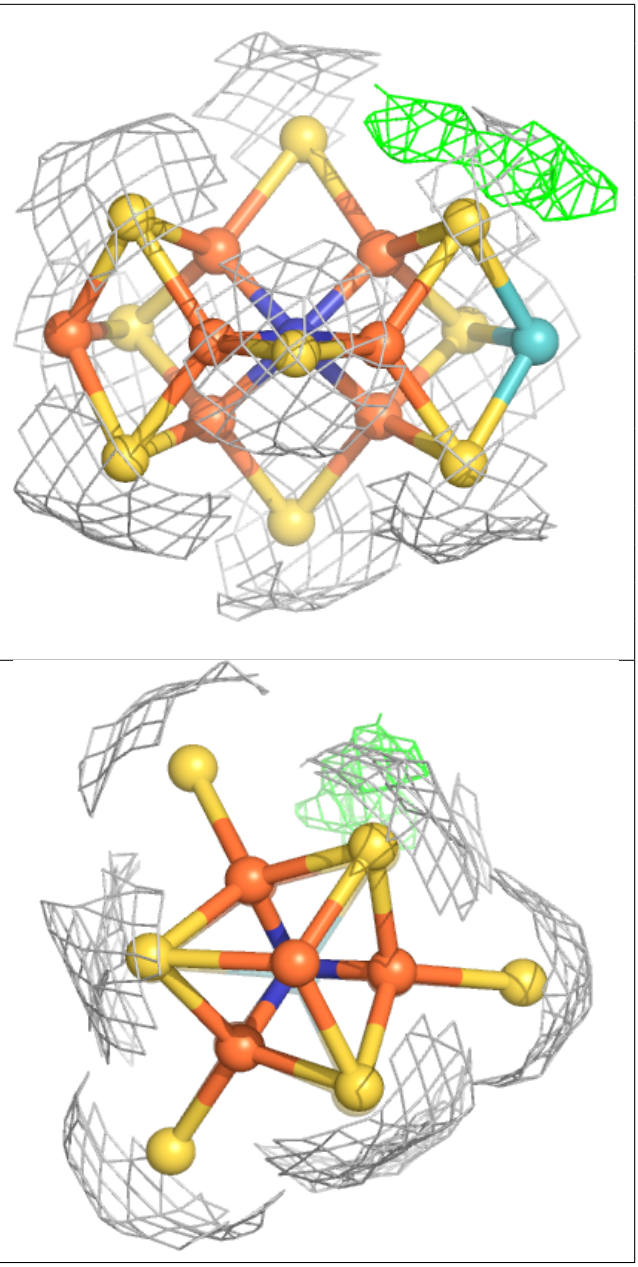
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





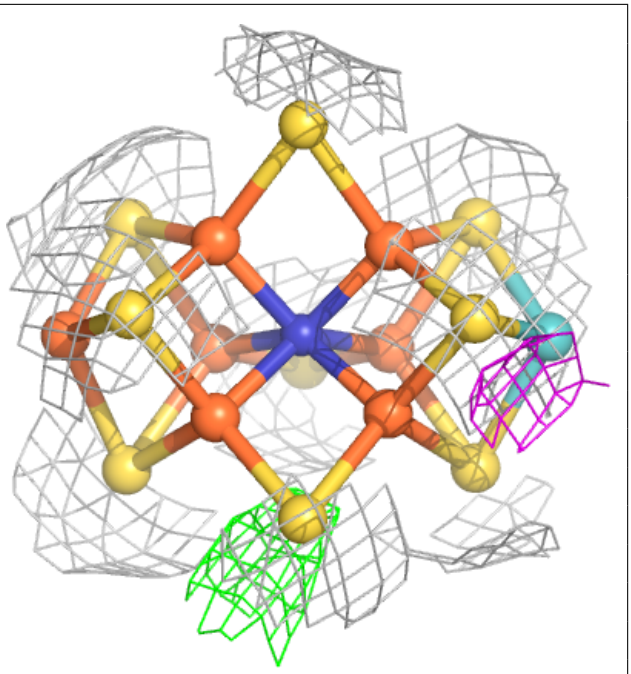
Electron density around CFN I 496:

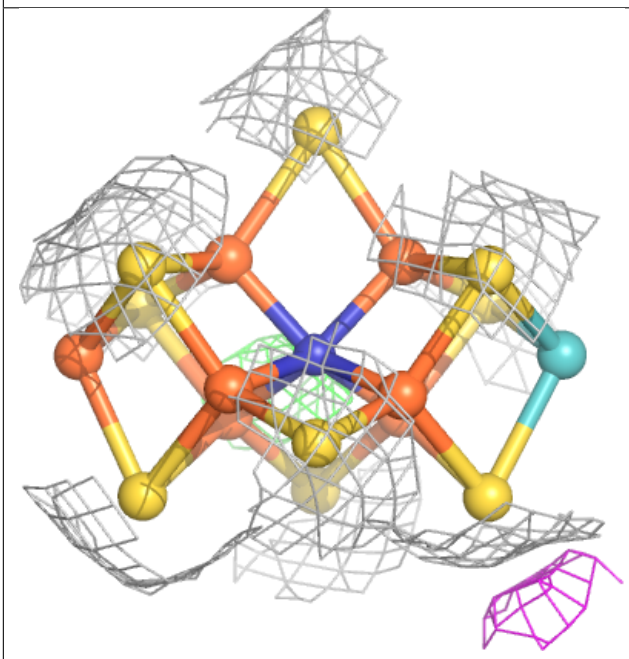
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

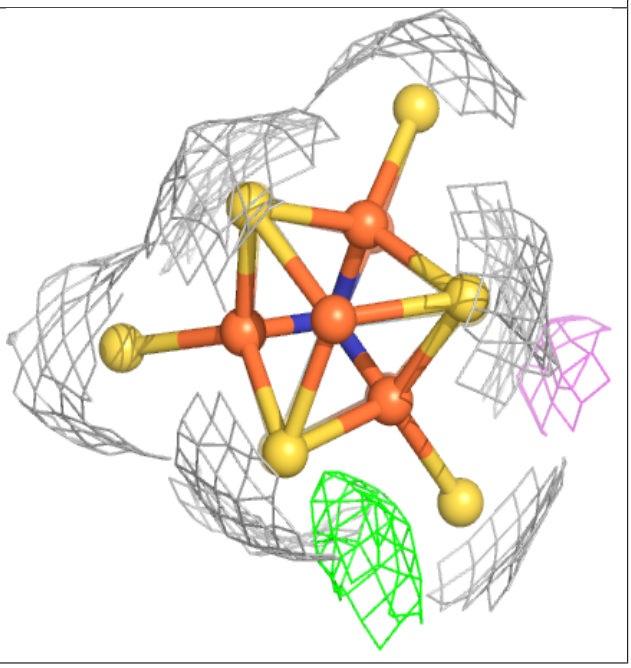


Electron density around CFN K 496:

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

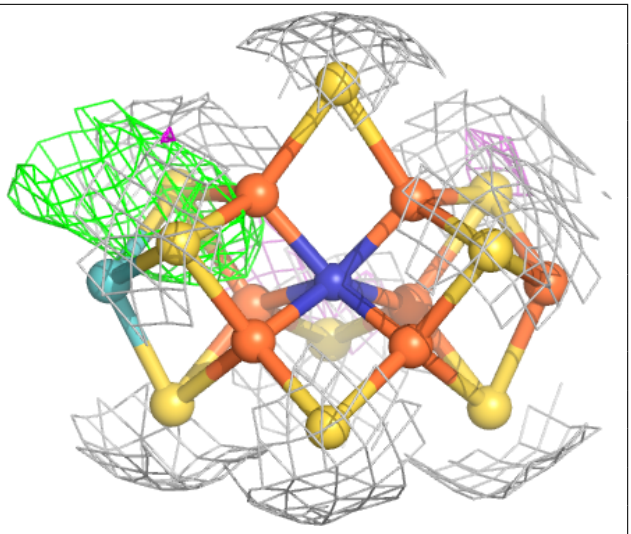


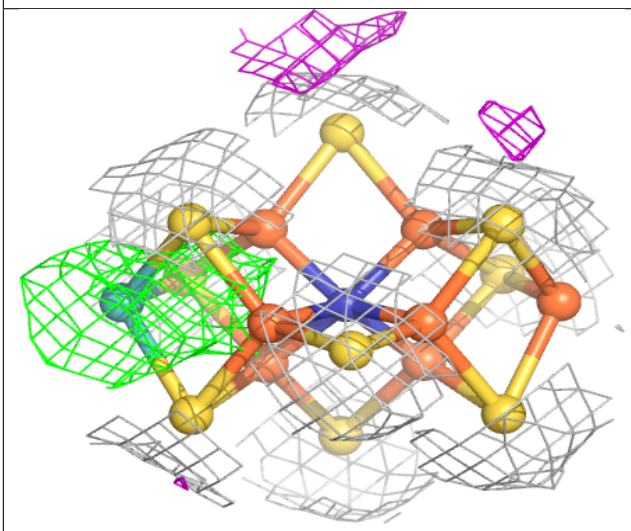


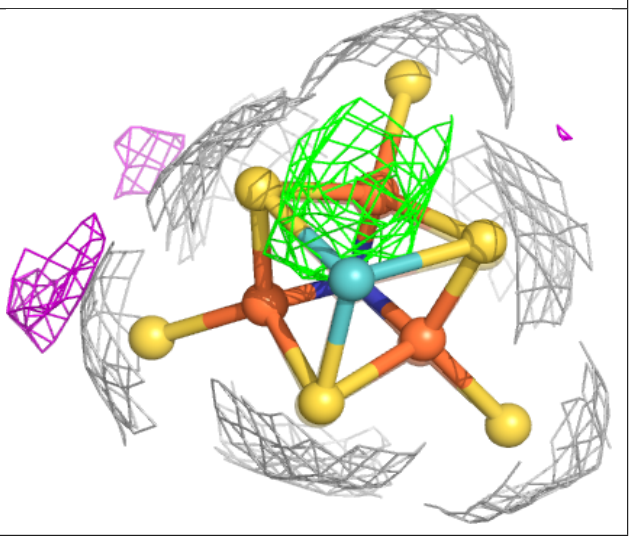


Electron density around CFN C 496:

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

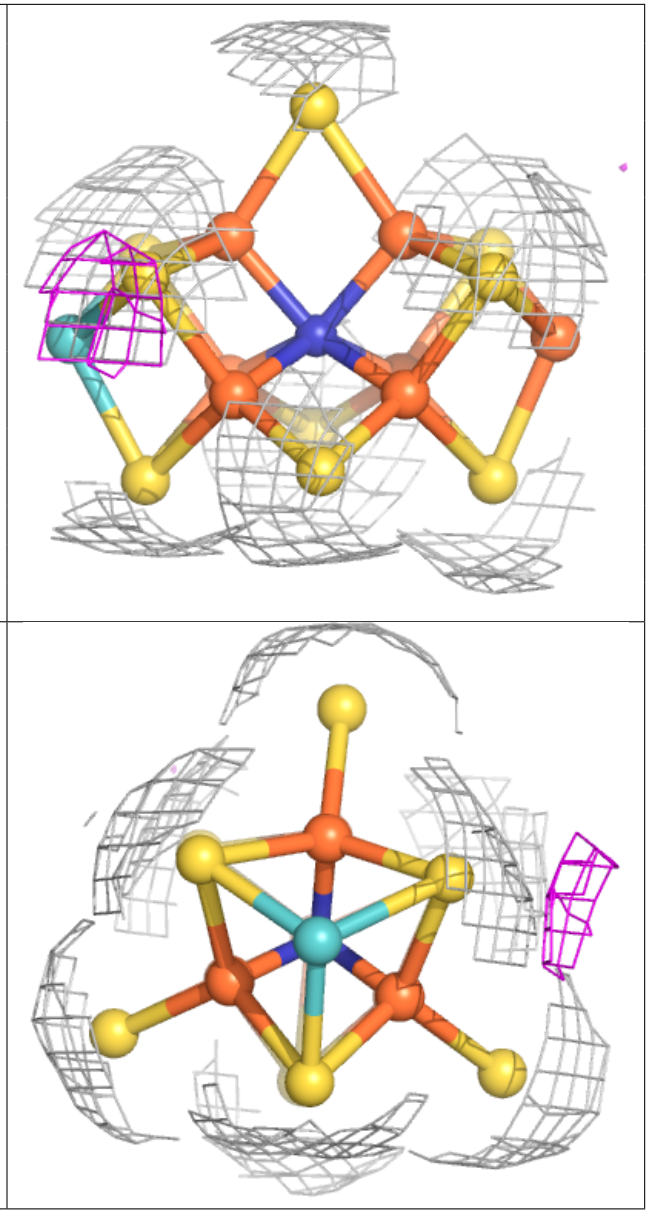






Electron density around CFN A 496:

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



6.5 Other polymers (i)

There are no such residues in this entry.