



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 11:04 PM UTC

PDB ID : 4A7L / pdb_00004a7l
EMDB ID : EMD-1989
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 1)
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;
Raunser, S.
Deposited on : 2011-11-14
Resolution : 8.10 Å (reported)
Based on initial models : 1LKX, 3MFP

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

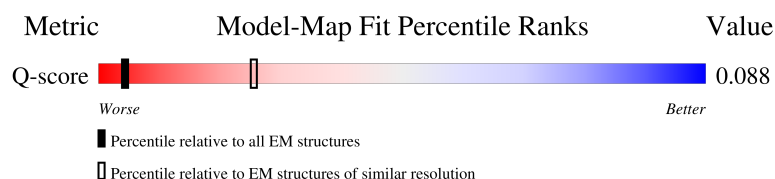
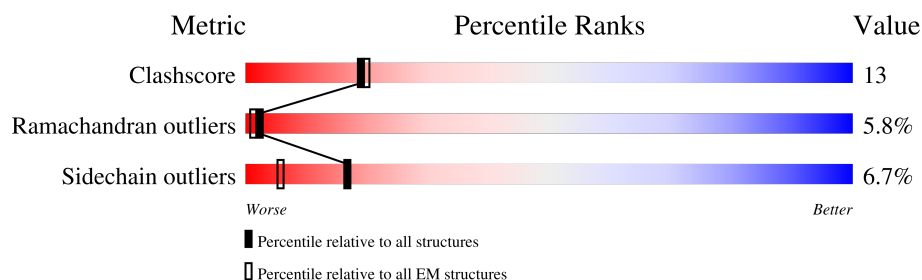
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 8.10 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	342 (7.60 - 8.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	375	 5% 72% 19% 7% .
1	D	375	 6% 70% 21% 6% .
1	E	375	 6% 70% 21% 6% .
1	F	375	 6% 70% 20% 6% .

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Mol	Chain	Length	Quality of chain
1	I	375	6% 71% 20% 6%
2	B	136	18% 97%
2	H	136	26% 96%
3	C	697	31% 77% 17%
3	G	697	30% 76% 18%
3	J	697	29% 77% 18%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 33500 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ACTIN, ALPHA SKELETON MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	F	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
1	I	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1 ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		
2	H	136	Total	C	N	O	S	0	0
			1104	673	189	239	3		

- Molecule 3 is a protein called MYOSIN IE HEAVY CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	G	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		
3	J	689	Total	C	N	O	S	0	0
			5494	3469	946	1048	31		

There are 9 discrepancies between the modelled and reference sequences:

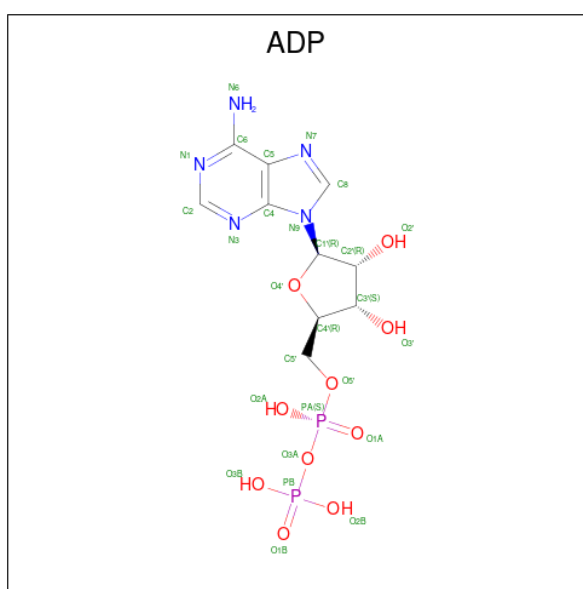
Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	conflict	UNP Q03479

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Chain	Residue	Modelled	Actual	Comment	Reference
C	215	ASP	ASN	conflict	UNP Q03479
C	334	GLU	SER	engineered mutation	UNP Q03479
G	77	MET	ILE	conflict	UNP Q03479
G	215	ASP	ASN	conflict	UNP Q03479
G	334	GLU	SER	engineered mutation	UNP Q03479
J	77	MET	ILE	conflict	UNP Q03479
J	215	ASP	ASN	conflict	UNP Q03479
J	334	GLU	SER	engineered mutation	UNP Q03479

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

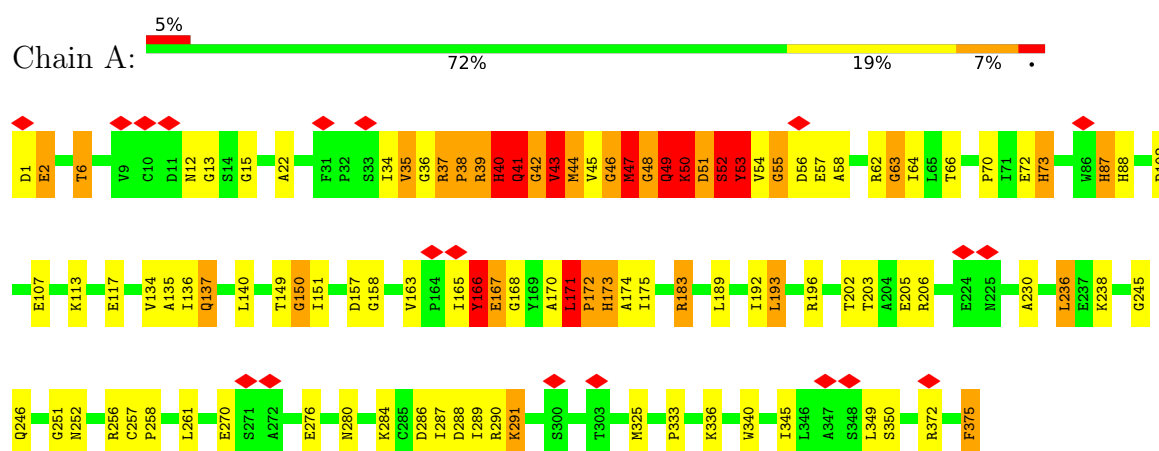


Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	D	1	Total 1	Ca 1	0
5	E	1	Total 1	Ca 1	0
5	F	1	Total 1	Ca 1	0
5	I	1	Total 1	Ca 1	0

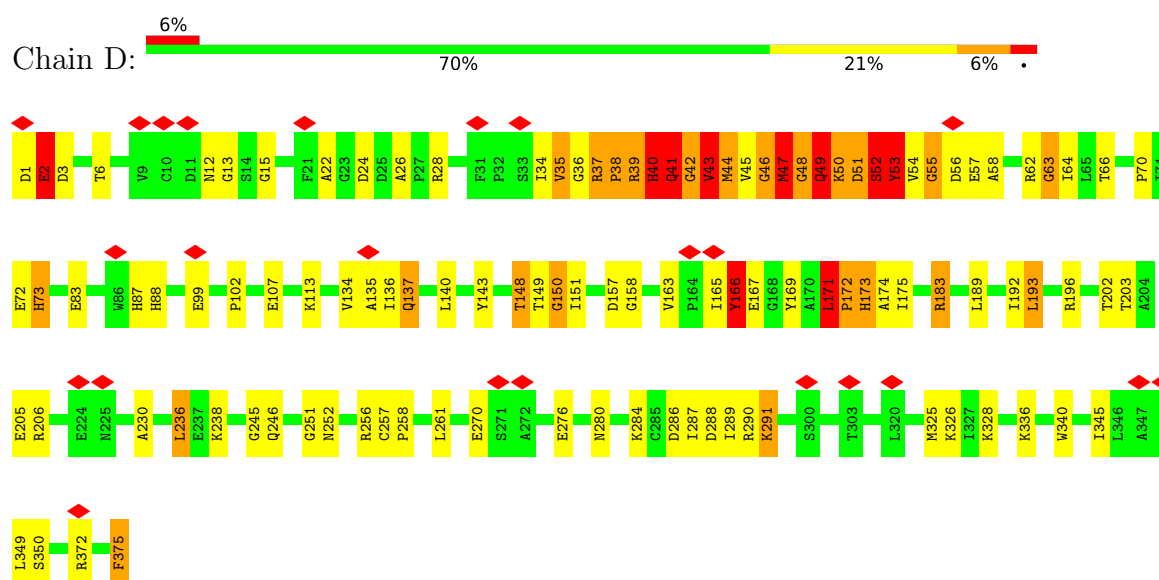
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

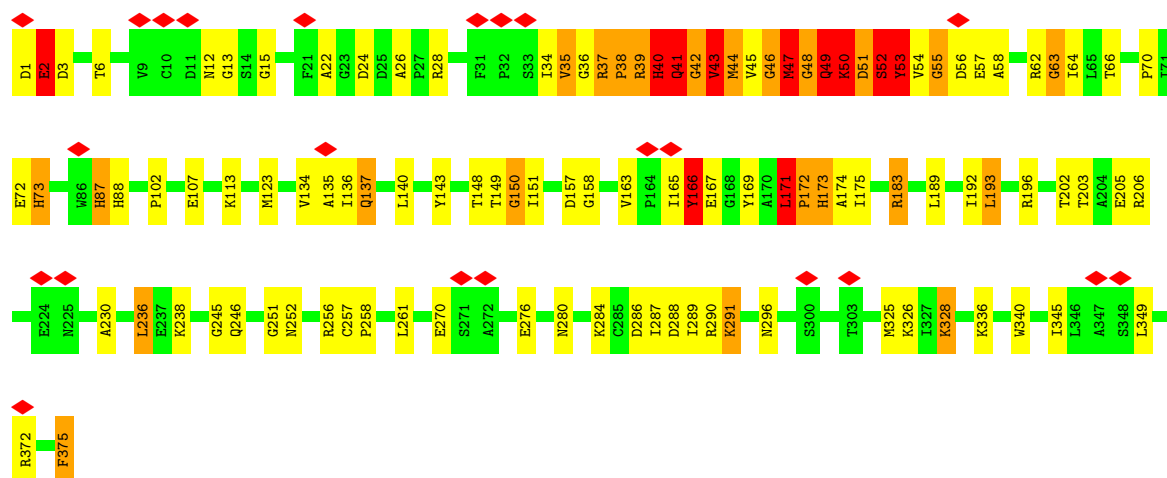


- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

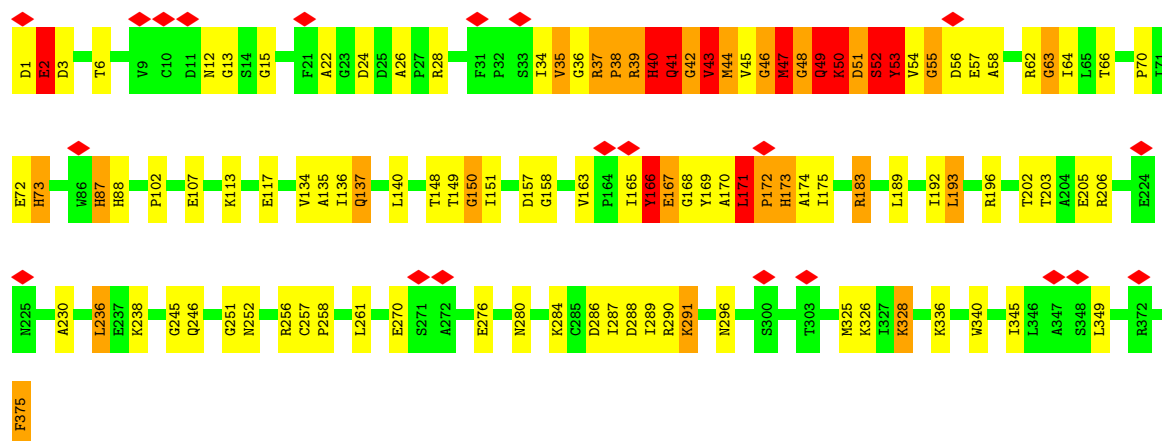


- Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

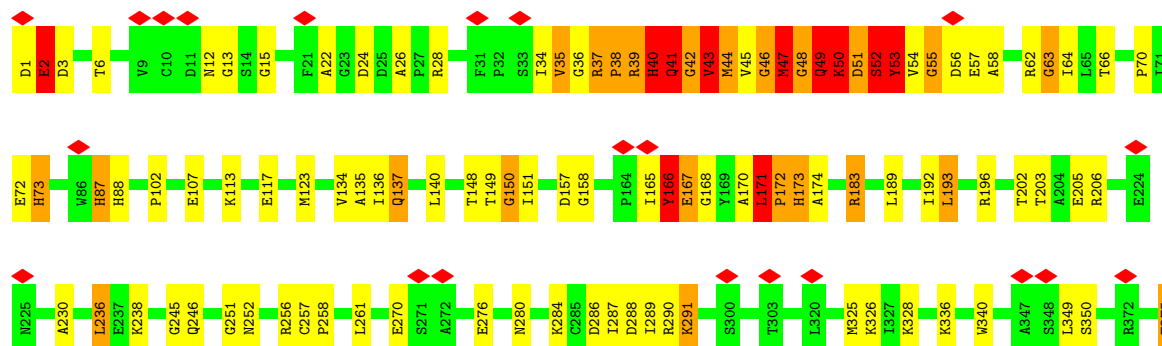




• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

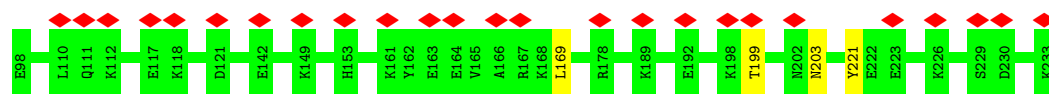


• Molecule 1: ACTIN, ALPHA SKELETON MUSCLE

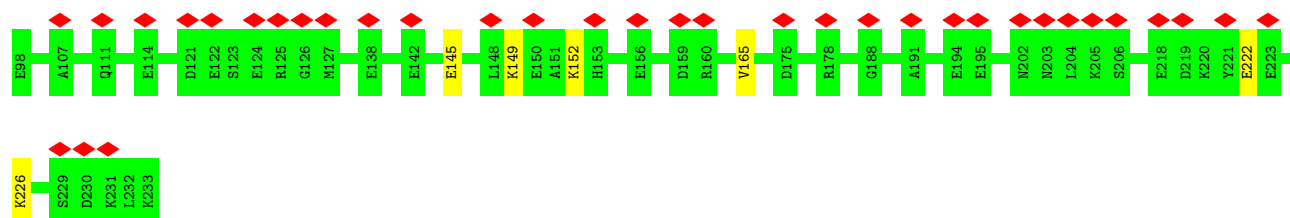


• Molecule 2: TROPOMYOSIN 1 ALPHA

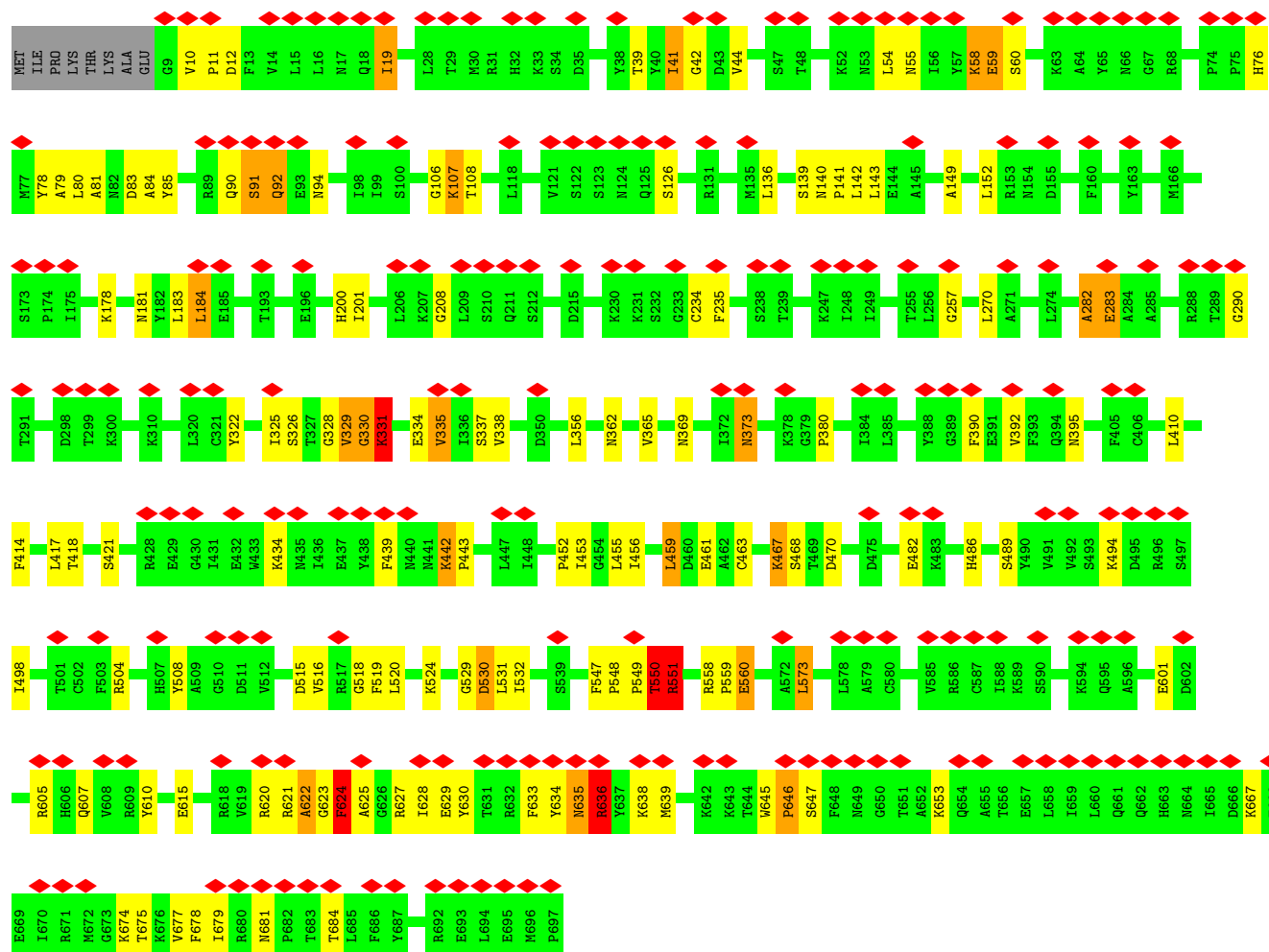
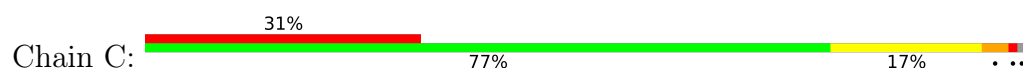




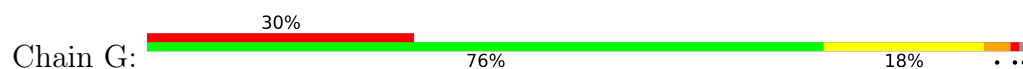
• Molecule 2: TROPOMYOSIN 1 ALPHA

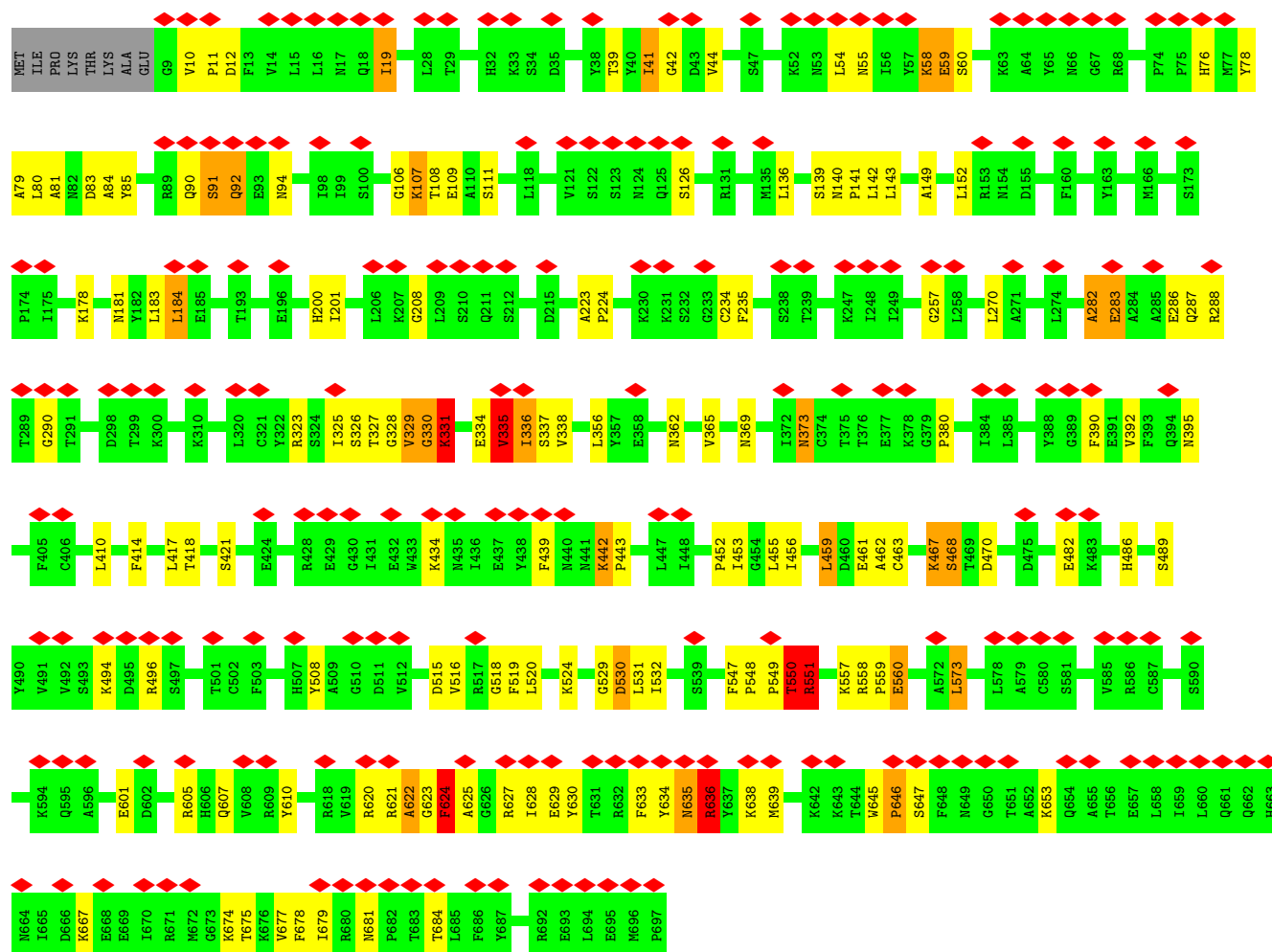


• Molecule 3: MYOSIN IE HEAVY CHAIN



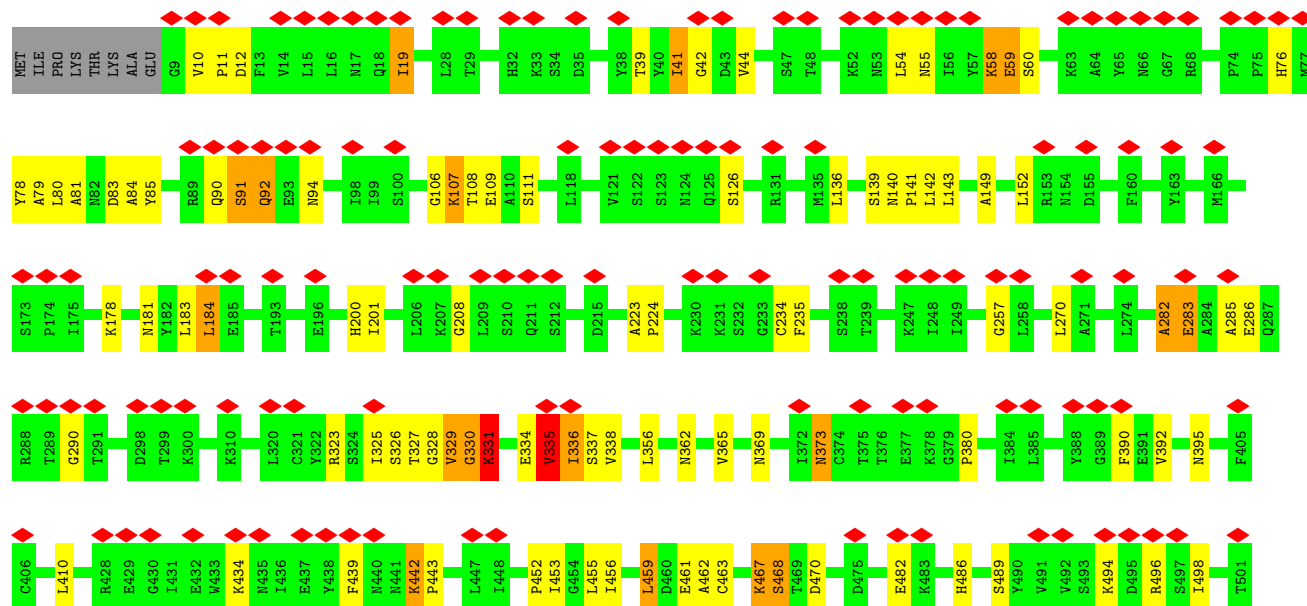
• Molecule 3: MYOSIN IE HEAVY CHAIN

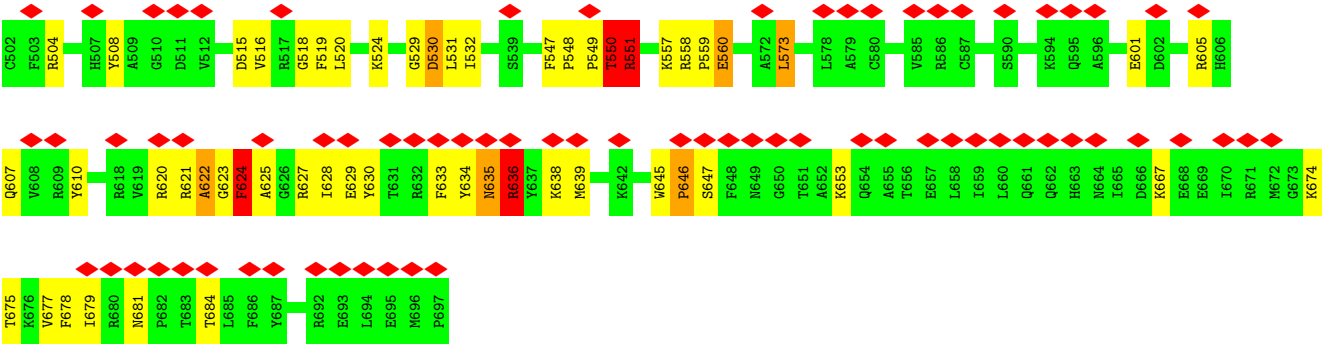




● Molecule 3: MYOSIN IE HEAVY CHAIN

Chain J: 29% 77% 18%





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	5555	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	169644	Depositor
Image detector	TVIPS TEMCAM-F816 (8k x 8k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	0.000	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	294.4, 294.4, 404.80002	wwPDB
Map dimensions	160, 160, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.84, 1.84, 1.84	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HIC, ADP

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	0.93	24/2984 (0.8%)	0.97	26/4040 (0.6%)
1	D	0.89	21/2984 (0.7%)	0.95	24/4040 (0.6%)
1	E	0.90	23/2984 (0.8%)	0.97	26/4040 (0.6%)
1	F	0.90	23/2984 (0.8%)	0.97	26/4040 (0.6%)
1	I	0.90	23/2984 (0.8%)	0.97	26/4040 (0.6%)
2	B	0.30	0/1107	0.59	0/1471
2	H	0.27	0/1107	0.60	0/1471
3	C	0.29	0/5594	0.62	0/7539
3	G	0.27	0/5594	0.62	1/7539 (0.0%)
3	J	0.27	0/5594	0.62	1/7539 (0.0%)
All	All	0.63	114/33916 (0.3%)	0.79	130/45759 (0.3%)

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	1
1	D	0	1
1	E	0	1
1	F	0	1
1	I	0	1
All	All	0	5

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	150	GLY	N-CA	14.65	1.60	1.45
1	F	150	GLY	N-CA	14.65	1.60	1.45
1	I	150	GLY	N-CA	14.65	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	150	GLY	N-CA	14.64	1.60	1.45
1	A	150	GLY	N-CA	14.63	1.60	1.45
1	D	41	GLN	N-CA	13.29	1.63	1.46
1	F	41	GLN	N-CA	13.28	1.63	1.46
1	A	41	GLN	N-CA	13.27	1.63	1.46
1	I	41	GLN	N-CA	13.27	1.63	1.46
1	E	41	GLN	N-CA	13.25	1.63	1.46
1	A	166	TYR	CE2-CZ	10.16	1.62	1.38
1	I	166	TYR	CE2-CZ	10.16	1.62	1.38
1	D	166	TYR	CE2-CZ	10.15	1.62	1.38
1	E	166	TYR	CE2-CZ	10.14	1.62	1.38
1	F	166	TYR	CE2-CZ	10.12	1.62	1.38
1	I	166	TYR	CD2-CE2	9.78	1.68	1.38
1	E	166	TYR	CD2-CE2	9.77	1.68	1.38
1	A	166	TYR	CD2-CE2	9.77	1.68	1.38
1	F	166	TYR	CD2-CE2	9.76	1.68	1.38
1	D	166	TYR	CD2-CE2	9.75	1.67	1.38
1	D	166	TYR	CD1-CE1	9.41	1.66	1.38
1	I	166	TYR	CD1-CE1	9.40	1.66	1.38
1	E	166	TYR	CD1-CE1	9.40	1.66	1.38
1	F	166	TYR	CD1-CE1	9.39	1.66	1.38
1	A	166	TYR	CD1-CE1	9.38	1.66	1.38
1	A	333	PRO	N-CD	9.20	1.60	1.47
1	E	149	THR	C-N	8.67	1.45	1.33
1	A	149	THR	C-N	8.66	1.45	1.33
1	D	149	THR	C-N	8.66	1.45	1.33
1	F	149	THR	C-N	8.63	1.45	1.33
1	I	149	THR	C-N	8.62	1.45	1.33
1	D	166	TYR	CE1-CZ	8.55	1.58	1.38
1	I	166	TYR	CE1-CZ	8.55	1.58	1.38
1	F	166	TYR	CE1-CZ	8.55	1.58	1.38
1	D	40	HIS	C-N	8.55	1.45	1.33
1	E	40	HIS	C-N	8.55	1.45	1.33
1	A	166	TYR	CE1-CZ	8.54	1.58	1.38
1	F	40	HIS	C-N	8.53	1.45	1.33
1	A	40	HIS	C-N	8.53	1.45	1.33
1	E	166	TYR	CE1-CZ	8.51	1.58	1.38
1	I	40	HIS	C-N	8.50	1.45	1.33
1	F	40	HIS	CA-CB	8.22	1.66	1.53
1	I	40	HIS	CA-CB	8.21	1.66	1.53
1	E	40	HIS	CA-CB	8.21	1.66	1.53
1	A	40	HIS	CA-CB	8.21	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	HIS	CA-CB	8.20	1.66	1.53
1	D	43	VAL	CA-CB	8.16	1.65	1.54
1	I	43	VAL	CA-CB	8.13	1.65	1.54
1	F	43	VAL	CA-CB	8.11	1.65	1.54
1	A	43	VAL	CA-CB	8.10	1.65	1.54
1	E	43	VAL	CA-CB	8.10	1.65	1.54
1	F	40	HIS	CB-CG	7.75	1.60	1.50
1	D	40	HIS	CB-CG	7.71	1.60	1.50
1	I	40	HIS	CB-CG	7.71	1.60	1.50
1	A	40	HIS	CB-CG	7.69	1.60	1.50
1	E	40	HIS	CB-CG	7.66	1.60	1.50
1	I	47	MET	C-N	7.53	1.44	1.33
1	A	47	MET	C-N	7.52	1.44	1.33
1	D	47	MET	C-N	7.51	1.44	1.33
1	E	47	MET	C-N	7.51	1.44	1.33
1	F	47	MET	C-N	7.49	1.44	1.33
1	I	40	HIS	CA-C	7.42	1.62	1.52
1	A	40	HIS	CA-C	7.39	1.62	1.52
1	D	40	HIS	CA-C	7.36	1.62	1.52
1	E	40	HIS	CA-C	7.36	1.62	1.52
1	F	40	HIS	CA-C	7.34	1.62	1.52
1	F	166	TYR	CG-CD1	7.18	1.54	1.39
1	A	166	TYR	CG-CD1	7.17	1.54	1.39
1	I	166	TYR	CG-CD1	7.16	1.54	1.39
1	D	166	TYR	CG-CD1	7.14	1.54	1.39
1	E	166	TYR	CG-CD1	7.14	1.54	1.39
1	D	166	TYR	CG-CD2	7.00	1.54	1.39
1	E	166	TYR	CG-CD2	6.99	1.54	1.39
1	I	166	TYR	CG-CD2	6.98	1.54	1.39
1	F	166	TYR	CG-CD2	6.97	1.53	1.39
1	A	166	TYR	CG-CD2	6.97	1.53	1.39
1	F	40	HIS	CE1-NE2	-6.83	1.25	1.32
1	E	40	HIS	CE1-NE2	-6.78	1.25	1.32
1	A	40	HIS	CE1-NE2	-6.78	1.25	1.32
1	I	40	HIS	CE1-NE2	-6.77	1.25	1.32
1	D	40	HIS	CE1-NE2	-6.77	1.25	1.32
1	F	52	SER	N-CA	6.28	1.54	1.46
1	I	52	SER	N-CA	6.26	1.54	1.46
1	E	52	SER	N-CA	6.24	1.54	1.46
1	A	52	SER	N-CA	6.22	1.54	1.46
1	D	52	SER	N-CA	6.17	1.54	1.46
1	D	43	VAL	C-N	6.00	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	43	VAL	C-N	5.99	1.42	1.33
1	A	43	VAL	C-N	5.98	1.42	1.33
1	F	43	VAL	C-N	5.96	1.42	1.33
1	E	43	VAL	C-N	5.95	1.42	1.33
1	F	48	GLY	N-CA	5.85	1.53	1.45
1	E	48	GLY	N-CA	5.83	1.53	1.45
1	A	48	GLY	N-CA	5.80	1.53	1.45
1	I	40	HIS	ND1-CE1	-5.79	1.26	1.32
1	D	40	HIS	ND1-CE1	-5.78	1.26	1.32
1	D	46	GLY	N-CA	5.78	1.53	1.45
1	E	46	GLY	N-CA	5.78	1.53	1.45
1	F	40	HIS	ND1-CE1	-5.78	1.26	1.32
1	I	48	GLY	N-CA	5.77	1.53	1.45
1	D	48	GLY	N-CA	5.75	1.53	1.45
1	A	40	HIS	ND1-CE1	-5.75	1.26	1.32
1	F	46	GLY	N-CA	5.75	1.53	1.45
1	E	40	HIS	ND1-CE1	-5.74	1.26	1.32
1	A	46	GLY	N-CA	5.74	1.53	1.45
1	I	46	GLY	N-CA	5.74	1.53	1.45
1	A	47	MET	CA-CB	5.50	1.62	1.53
1	F	47	MET	CA-CB	5.50	1.62	1.53
1	E	47	MET	CA-CB	5.47	1.62	1.53
1	I	47	MET	CA-CB	5.46	1.62	1.53
1	A	50	LYS	CA-CB	5.36	1.62	1.53
1	E	50	LYS	CA-CB	5.34	1.62	1.53
1	F	50	LYS	CA-CB	5.34	1.62	1.53
1	I	50	LYS	CA-CB	5.33	1.62	1.53

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	THR	CA-C-N	12.59	142.07	121.17
1	E	149	THR	C-N-CA	12.59	142.07	121.17
1	I	149	THR	CA-C-N	12.57	142.04	121.17
1	I	149	THR	C-N-CA	12.57	142.04	121.17
1	A	149	THR	CA-C-N	12.57	142.04	121.17
1	A	149	THR	C-N-CA	12.57	142.04	121.17
1	F	149	THR	CA-C-N	12.57	142.03	121.17
1	F	149	THR	C-N-CA	12.57	142.03	121.17
1	D	149	THR	CA-C-N	12.56	142.02	121.17
1	D	149	THR	C-N-CA	12.56	142.02	121.17
1	F	40	HIS	CA-CB-CG	10.79	124.59	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	HIS	CA-CB-CG	10.79	124.59	113.80
1	E	40	HIS	CA-CB-CG	10.79	124.59	113.80
1	I	40	HIS	CA-CB-CG	10.78	124.58	113.80
3	G	107	LYS	N-CA-C	-10.73	100.14	113.01
1	D	40	HIS	CA-CB-CG	10.72	124.52	113.80
3	J	107	LYS	N-CA-C	-10.69	100.18	113.01
1	A	53	TYR	CB-CA-C	9.17	128.66	110.42
1	F	53	TYR	CB-CA-C	9.16	128.66	110.42
1	I	53	TYR	CB-CA-C	9.16	128.66	110.42
1	D	53	TYR	CB-CA-C	9.16	128.64	110.42
1	E	53	TYR	CB-CA-C	9.15	128.63	110.42
1	E	43	VAL	CA-CB-CG1	8.41	124.70	110.40
1	A	43	VAL	CA-CB-CG1	8.40	124.67	110.40
1	F	43	VAL	CA-CB-CG1	8.39	124.67	110.40
1	D	43	VAL	CA-CB-CG1	8.38	124.65	110.40
1	I	43	VAL	CA-CB-CG1	8.38	124.64	110.40
1	D	40	HIS	CB-CA-C	7.76	123.68	110.79
1	E	40	HIS	CB-CA-C	7.75	123.65	110.79
1	F	40	HIS	CB-CA-C	7.75	123.65	110.79
1	I	40	HIS	CB-CA-C	7.73	123.63	110.79
1	A	40	HIS	CB-CA-C	7.73	123.62	110.79
1	A	171	LEU	CA-C-N	-7.68	110.24	119.84
1	A	171	LEU	C-N-CA	-7.68	110.24	119.84
1	E	171	LEU	CA-C-N	-7.68	110.24	119.84
1	E	171	LEU	C-N-CA	-7.68	110.24	119.84
1	I	171	LEU	CA-C-N	-7.67	110.25	119.84
1	I	171	LEU	C-N-CA	-7.67	110.25	119.84
1	D	171	LEU	CA-C-N	-7.67	110.25	119.84
1	D	171	LEU	C-N-CA	-7.67	110.25	119.84
1	F	171	LEU	CA-C-N	-7.65	110.28	119.84
1	F	171	LEU	C-N-CA	-7.65	110.28	119.84
1	F	47	MET	CB-CA-C	7.28	124.92	110.42
1	E	47	MET	CB-CA-C	7.28	124.90	110.42
1	I	47	MET	CB-CA-C	7.27	124.90	110.42
1	A	47	MET	CB-CA-C	7.27	124.88	110.42
1	F	43	VAL	N-CA-CB	7.11	122.97	111.23
1	D	43	VAL	N-CA-CB	7.11	122.96	111.23
1	A	43	VAL	N-CA-CB	7.11	122.95	111.23
1	E	43	VAL	N-CA-CB	7.10	122.94	111.23
1	I	43	VAL	N-CA-CB	7.10	122.94	111.23
1	D	52	SER	CA-C-N	7.08	135.07	121.54
1	D	52	SER	C-N-CA	7.08	135.07	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	52	SER	CA-C-N	7.07	135.04	121.54
1	I	52	SER	C-N-CA	7.07	135.04	121.54
1	A	52	SER	CA-C-N	7.07	135.04	121.54
1	A	52	SER	C-N-CA	7.07	135.04	121.54
1	E	52	SER	CA-C-N	7.06	135.03	121.54
1	E	52	SER	C-N-CA	7.06	135.03	121.54
1	F	52	SER	CA-C-N	7.04	134.99	121.54
1	F	52	SER	C-N-CA	7.04	134.99	121.54
1	E	53	TYR	N-CA-CB	6.75	121.90	110.49
1	F	53	TYR	N-CA-CB	6.74	121.88	110.49
1	I	53	TYR	N-CA-CB	6.73	121.87	110.49
1	D	53	TYR	N-CA-CB	6.73	121.87	110.49
1	A	53	TYR	N-CA-CB	6.72	121.86	110.49
1	I	40	HIS	CA-C-O	-6.65	113.50	120.55
1	E	40	HIS	CA-C-O	-6.63	113.52	120.55
1	A	40	HIS	CA-C-O	-6.63	113.52	120.55
1	F	40	HIS	CA-C-O	-6.61	113.55	120.55
1	D	40	HIS	CA-C-O	-6.60	113.55	120.55
1	I	43	VAL	CA-C-N	6.43	133.83	121.54
1	I	43	VAL	C-N-CA	6.43	133.83	121.54
1	F	43	VAL	CA-C-N	6.43	133.82	121.54
1	F	43	VAL	C-N-CA	6.43	133.82	121.54
1	D	43	VAL	CA-C-N	6.43	133.82	121.54
1	D	43	VAL	C-N-CA	6.43	133.82	121.54
1	E	43	VAL	CA-C-N	6.42	133.81	121.54
1	E	43	VAL	C-N-CA	6.42	133.81	121.54
1	A	43	VAL	CA-C-N	6.41	133.79	121.54
1	A	43	VAL	C-N-CA	6.41	133.79	121.54
1	E	47	MET	CA-CB-CG	6.18	126.47	114.10
1	A	47	MET	CA-CB-CG	6.18	126.46	114.10
1	F	47	MET	CA-CB-CG	6.18	126.46	114.10
1	I	47	MET	CA-CB-CG	6.17	126.45	114.10
1	D	41	GLN	CB-CA-C	-6.13	98.22	110.42
1	E	41	GLN	CB-CA-C	-6.13	98.23	110.42
1	I	41	GLN	CB-CA-C	-6.13	98.22	110.42
1	A	41	GLN	CB-CA-C	-6.12	98.25	110.42
1	F	41	GLN	CB-CA-C	-6.12	98.25	110.42
1	D	46	GLY	CA-C-N	6.05	133.09	121.54
1	D	46	GLY	C-N-CA	6.05	133.09	121.54
1	A	46	GLY	CA-C-N	6.02	133.04	121.54
1	A	46	GLY	C-N-CA	6.02	133.04	121.54
1	D	50	LYS	CA-C-N	6.02	133.04	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	LYS	C-N-CA	6.02	133.04	121.54
1	E	46	GLY	CA-C-N	6.02	133.04	121.54
1	E	46	GLY	C-N-CA	6.02	133.04	121.54
1	F	46	GLY	CA-C-N	6.02	133.04	121.54
1	F	46	GLY	C-N-CA	6.02	133.04	121.54
1	A	50	LYS	CA-C-N	6.01	133.01	121.54
1	A	50	LYS	C-N-CA	6.01	133.01	121.54
1	F	41	GLN	N-CA-CB	6.01	120.64	110.49
1	E	50	LYS	CA-C-N	6.00	133.01	121.54
1	E	50	LYS	C-N-CA	6.00	133.01	121.54
1	I	46	GLY	CA-C-N	6.00	133.01	121.54
1	I	46	GLY	C-N-CA	6.00	133.01	121.54
1	F	50	LYS	CA-C-N	6.00	133.00	121.54
1	F	50	LYS	C-N-CA	6.00	133.00	121.54
1	I	50	LYS	CA-C-N	6.00	132.99	121.54
1	I	50	LYS	C-N-CA	6.00	132.99	121.54
1	A	41	GLN	N-CA-CB	5.99	120.61	110.49
1	I	41	GLN	N-CA-CB	5.98	120.59	110.49
1	D	41	GLN	N-CA-CB	5.97	120.58	110.49
1	E	41	GLN	N-CA-CB	5.97	120.58	110.49
1	D	41	GLN	CB-CG-CD	-5.59	103.10	112.60
1	A	41	GLN	CB-CG-CD	-5.58	103.11	112.60
1	I	41	GLN	CB-CG-CD	-5.58	103.11	112.60
1	E	41	GLN	CB-CG-CD	-5.57	103.13	112.60
1	F	41	GLN	CB-CG-CD	-5.56	103.14	112.60
1	E	40	HIS	CA-C-N	5.09	131.27	121.54
1	E	40	HIS	C-N-CA	5.09	131.27	121.54
1	I	40	HIS	CA-C-N	5.09	131.26	121.54
1	I	40	HIS	C-N-CA	5.09	131.26	121.54
1	D	40	HIS	CA-C-N	5.08	131.25	121.54
1	D	40	HIS	C-N-CA	5.08	131.25	121.54
1	A	40	HIS	CA-C-N	5.08	131.24	121.54
1	A	40	HIS	C-N-CA	5.08	131.24	121.54
1	F	40	HIS	CA-C-N	5.08	131.24	121.54
1	F	40	HIS	C-N-CA	5.08	131.24	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	HIS	Sidechain
1	D	40	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	E	40	HIS	Sidechain
1	F	40	HIS	Sidechain
1	I	40	HIS	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	2934	0	2895	151	0
1	D	2934	0	2895	132	0
1	E	2934	0	2895	125	0
1	F	2934	0	2895	124	0
1	I	2934	0	2895	128	0
2	B	1104	0	1104	3	0
2	H	1104	0	1104	18	0
3	C	5494	0	5492	84	0
3	G	5494	0	5492	94	0
3	J	5494	0	5492	102	0
4	A	27	0	12	4	0
4	D	27	0	12	4	0
4	E	27	0	12	4	0
4	F	27	0	12	4	0
4	I	27	0	12	4	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
All	All	33500	0	33219	853	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 13.

All (853) 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:D:54:VAL:HG22	1:D:55:GLY:H	1.10	1.14
1:A:54:VAL:HG22	1:A:55:GLY:H	1.10	1.10
1:I:54:VAL:HG22	1:I:55:GLY:H	1.10	1.10
1:F:54:VAL:HG22	1:F:55:GLY:H	1.10	1.08
1:E:54:VAL:HG22	1:E:55:GLY:H	1.10	1.07
1:F:54:VAL:HG22	1:F:55:GLY:N	1.73	1.02
1:I:54:VAL:HG22	1:I:55:GLY:N	1.73	1.02
1:A:54:VAL:HG22	1:A:55:GLY:N	1.73	1.01
1:E:40:HIS:CD2	1:F:167:GLU:HB3	1.95	1.01
1:D:54:VAL:HG22	1:D:55:GLY:N	1.73	1.01
1:A:55:GLY:HA3	1:A:88:HIS:CE1	1.96	1.00
1:F:55:GLY:HA3	1:F:88:HIS:CE1	1.96	1.00
1:I:55:GLY:HA3	1:I:88:HIS:CE1	1.96	1.00
1:E:55:GLY:HA3	1:E:88:HIS:CE1	1.96	0.99
1:D:55:GLY:HA3	1:D:88:HIS:CE1	1.96	0.99
1:A:40:HIS:CD2	1:I:167:GLU:HB3	1.99	0.98
2:H:226:LYS:HG3	3:J:285:ALA:HB3	1.45	0.98
1:A:167:GLU:HB3	1:D:40:HIS:CD2	1.98	0.98
1:E:54:VAL:HG22	1:E:55:GLY:N	1.73	0.98
1:A:54:VAL:CG2	1:A:55:GLY:H	1.78	0.97
1:I:54:VAL:CG2	1:I:55:GLY:H	1.78	0.97
1:D:54:VAL:CG2	1:D:55:GLY:H	1.78	0.96
1:F:54:VAL:CG2	1:F:55:GLY:H	1.78	0.96
1:E:54:VAL:CG2	1:E:55:GLY:H	1.78	0.95
1:A:170:ALA:HB3	1:D:41:GLN:NE2	1.84	0.93
1:D:43:VAL:HG23	1:D:46:GLY:H	1.33	0.93
1:A:41:GLN:NE2	1:I:170:ALA:HB3	1.83	0.93
1:A:43:VAL:HG23	1:A:46:GLY:H	1.33	0.92
3:G:107:LYS:HD3	3:G:107:LYS:N	1.85	0.91
1:I:43:VAL:HG23	1:I:46:GLY:H	1.33	0.91
3:C:106:GLY:C	3:C:108:THR:H	1.66	0.90
1:F:43:VAL:HG23	1:F:46:GLY:H	1.33	0.90
3:J:107:LYS:HD3	3:J:107:LYS:N	1.86	0.90
1:D:51:ASP:O	1:D:53:TYR:N	2.05	0.90
1:A:51:ASP:O	1:A:53:TYR:N	2.05	0.90
1:A:42:GLY:C	1:I:167:GLU:O	2.14	0.90
1:E:43:VAL:HG23	1:E:46:GLY:H	1.33	0.90
1:I:51:ASP:O	1:I:53:TYR:N	2.05	0.90
1:F:51:ASP:O	1:F:53:TYR:N	2.05	0.89
1:I:51:ASP:C	1:I:53:TYR:H	1.81	0.88
1:E:51:ASP:O	1:E:53:TYR:N	2.05	0.88
1:A:51:ASP:C	1:A:53:TYR:H	1.81	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLU:O	1:D:42:GLY:C	2.17	0.88
1:E:41:GLN:NE2	1:F:170:ALA:HB3	1.87	0.87
3:G:107:LYS:HD3	3:G:107:LYS:H	1.39	0.87
1:D:51:ASP:C	1:D:53:TYR:H	1.81	0.87
3:J:107:LYS:HD3	3:J:107:LYS:H	1.39	0.86
1:E:41:GLN:HE22	1:F:169:TYR:C	1.81	0.85
1:I:38:PRO:HG3	1:I:49:GLN:HG2	1.59	0.85
1:A:38:PRO:HG3	1:A:49:GLN:HG2	1.58	0.85
1:E:42:GLY:C	1:F:167:GLU:O	2.19	0.84
1:D:38:PRO:HG3	1:D:49:GLN:HG2	1.58	0.84
1:F:51:ASP:C	1:F:53:TYR:H	1.81	0.84
1:F:38:PRO:HG3	1:F:49:GLN:HG2	1.58	0.84
1:E:51:ASP:C	1:E:53:TYR:H	1.81	0.83
1:E:38:PRO:HG3	1:E:49:GLN:HG2	1.58	0.83
1:F:157:ASP:HB3	4:F:376:ADP:O3B	1.80	0.82
1:E:171:LEU:HB2	1:E:172:PRO:HD2	1.63	0.81
1:F:171:LEU:HB2	1:F:172:PRO:HD2	1.63	0.81
1:I:157:ASP:HB3	4:I:376:ADP:O3B	1.80	0.81
1:A:157:ASP:HB3	4:A:376:ADP:O3B	1.80	0.81
1:I:38:PRO:HG3	1:I:49:GLN:CG	2.11	0.81
1:D:157:ASP:HB3	4:D:376:ADP:O3B	1.80	0.81
1:A:38:PRO:HG3	1:A:49:GLN:CG	2.11	0.81
1:E:157:ASP:HB3	4:E:376:ADP:O3B	1.80	0.80
1:D:171:LEU:HB2	1:D:172:PRO:HD2	1.63	0.80
2:H:222:GLU:OE1	3:J:286:GLU:HG3	1.82	0.80
1:A:40:HIS:HD2	1:I:167:GLU:HB3	1.46	0.80
1:D:38:PRO:HG3	1:D:49:GLN:CG	2.11	0.80
1:F:38:PRO:HG3	1:F:49:GLN:CG	2.11	0.80
1:A:171:LEU:HB2	1:A:172:PRO:HD2	1.63	0.80
1:E:38:PRO:HG3	1:E:49:GLN:CG	2.11	0.80
1:I:171:LEU:HB2	1:I:172:PRO:HD2	1.63	0.79
1:A:167:GLU:HB3	1:D:40:HIS:HD2	1.45	0.79
1:F:55:GLY:C	1:F:57:GLU:H	1.90	0.79
1:E:55:GLY:C	1:E:57:GLU:H	1.90	0.79
1:D:55:GLY:C	1:D:57:GLU:H	1.90	0.79
1:A:55:GLY:C	1:A:57:GLU:H	1.90	0.78
1:F:55:GLY:CA	1:F:88:HIS:CE1	2.66	0.78
1:E:34:ILE:O	1:E:35:VAL:HG23	1.83	0.78
1:I:34:ILE:O	1:I:35:VAL:HG23	1.83	0.78
1:I:55:GLY:C	1:I:57:GLU:H	1.90	0.78
1:A:168:GLY:O	1:D:40:HIS:CE1	2.37	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:O	1:A:35:VAL:HG23	1.83	0.77
1:E:40:HIS:HD2	1:F:167:GLU:HB3	1.44	0.77
1:F:34:ILE:O	1:F:35:VAL:HG23	1.83	0.77
1:I:55:GLY:CA	1:I:88:HIS:CE1	2.66	0.77
1:D:55:GLY:CA	1:D:88:HIS:CE1	2.66	0.77
1:E:40:HIS:CE1	1:F:168:GLY:H	2.03	0.77
1:E:55:GLY:CA	1:E:88:HIS:CE1	2.66	0.77
1:A:55:GLY:CA	1:A:88:HIS:CE1	2.66	0.77
3:C:560:GLU:HG3	3:C:560:GLU:O	1.83	0.77
3:G:286:GLU:HG3	2:H:145:GLU:OE1	1.84	0.77
1:D:34:ILE:O	1:D:35:VAL:HG23	1.83	0.76
3:J:58:LYS:O	3:J:60:SER:N	2.19	0.76
3:G:58:LYS:O	3:G:60:SER:N	2.19	0.76
1:D:83:GLU:HG2	1:D:87:HIS:CE1	2.21	0.76
1:A:40:HIS:CE1	1:I:168:GLY:O	2.39	0.75
3:C:58:LYS:O	3:C:60:SER:N	2.19	0.75
1:E:53:TYR:HB3	1:E:57:GLU:OE1	1.87	0.74
1:F:42:GLY:C	1:F:44:MET:H	1.94	0.74
1:A:43:VAL:N	1:I:168:GLY:HA2	2.02	0.74
1:I:53:TYR:HB3	1:I:57:GLU:OE1	1.87	0.74
1:A:55:GLY:O	1:A:57:GLU:N	2.21	0.74
1:E:40:HIS:CE1	1:F:168:GLY:O	2.39	0.74
1:F:53:TYR:HB3	1:F:57:GLU:OE1	1.87	0.74
1:A:53:TYR:HB3	1:A:57:GLU:OE1	1.87	0.74
1:F:55:GLY:O	1:F:57:GLU:N	2.21	0.74
3:G:328:GLY:O	3:G:330:GLY:N	2.20	0.74
3:C:328:GLY:O	3:C:330:GLY:N	2.21	0.74
1:D:53:TYR:HB3	1:D:57:GLU:OE1	1.87	0.74
1:D:55:GLY:O	1:D:57:GLU:N	2.21	0.74
1:E:42:GLY:C	1:E:44:MET:H	1.94	0.74
1:E:55:GLY:O	1:E:57:GLU:N	2.21	0.74
1:A:42:GLY:C	1:A:44:MET:H	1.94	0.73
3:J:328:GLY:O	3:J:330:GLY:N	2.21	0.73
1:I:55:GLY:O	1:I:57:GLU:N	2.21	0.73
1:A:168:GLY:H	1:D:40:HIS:CE1	2.05	0.73
1:D:42:GLY:C	1:D:44:MET:H	1.94	0.73
1:I:42:GLY:C	1:I:44:MET:H	1.94	0.73
1:A:168:GLY:O	1:D:40:HIS:HE1	1.72	0.72
1:A:37:ARG:HG3	1:A:38:PRO:HD3	1.71	0.72
1:E:37:ARG:HG3	1:E:38:PRO:HD3	1.71	0.72
1:I:37:ARG:HG3	1:I:38:PRO:HD3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:ARG:HG3	1:F:38:PRO:HD3	1.71	0.72
1:F:43:VAL:HG23	1:F:46:GLY:N	2.05	0.72
3:C:106:GLY:C	3:C:108:THR:N	2.32	0.72
3:G:323:ARG:O	3:G:337:SER:OG	2.06	0.72
1:I:36:GLY:O	1:I:52:SER:HA	1.90	0.72
1:A:36:GLY:O	1:A:52:SER:HA	1.90	0.72
1:D:37:ARG:HG3	1:D:38:PRO:HD3	1.72	0.72
1:E:40:HIS:HE1	1:F:168:GLY:O	1.72	0.72
1:D:36:GLY:O	1:D:52:SER:HA	1.90	0.71
3:G:482:GLU:OE2	3:G:489:SER:OG	2.06	0.71
3:J:323:ARG:O	3:J:337:SER:OG	2.06	0.71
1:A:43:VAL:N	1:I:167:GLU:O	2.22	0.71
1:A:168:GLY:HA2	1:D:43:VAL:N	2.05	0.71
2:H:222:GLU:OE1	3:J:286:GLU:HA	1.91	0.71
1:E:36:GLY:O	1:E:52:SER:HA	1.90	0.71
1:E:36:GLY:O	1:E:52:SER:CA	2.39	0.71
1:E:49:GLN:HG3	1:E:50:LYS:N	2.06	0.71
1:F:36:GLY:O	1:F:52:SER:CA	2.39	0.71
1:F:36:GLY:O	1:F:52:SER:HA	1.90	0.70
1:A:40:HIS:CE1	1:I:168:GLY:H	2.07	0.70
1:D:43:VAL:HG23	1:D:46:GLY:N	2.05	0.70
1:A:43:VAL:HG23	1:A:46:GLY:N	2.05	0.70
1:I:36:GLY:O	1:I:52:SER:CA	2.39	0.70
1:I:49:GLN:HG3	1:I:50:LYS:N	2.06	0.70
1:A:36:GLY:O	1:A:52:SER:CA	2.39	0.70
3:J:482:GLU:OE2	3:J:489:SER:OG	2.06	0.70
1:E:43:VAL:N	1:F:167:GLU:O	2.24	0.70
1:F:49:GLN:HG3	1:F:50:LYS:N	2.06	0.70
3:C:482:GLU:OE2	3:C:489:SER:OG	2.06	0.70
1:D:36:GLY:O	1:D:52:SER:CA	2.39	0.70
1:I:43:VAL:HG23	1:I:46:GLY:N	2.05	0.70
1:A:167:GLU:O	1:D:43:VAL:N	2.25	0.69
1:A:49:GLN:HG3	1:A:50:LYS:N	2.06	0.69
1:D:49:GLN:HG3	1:D:50:LYS:N	2.06	0.69
1:E:53:TYR:C	1:E:58:ALA:HB2	2.18	0.69
1:A:53:TYR:C	1:A:58:ALA:HB2	2.18	0.69
1:D:53:TYR:C	1:D:58:ALA:HB2	2.18	0.69
1:A:43:VAL:H	1:I:168:GLY:HA2	1.58	0.69
1:A:40:HIS:HE1	1:I:168:GLY:O	1.75	0.68
1:F:53:TYR:C	1:F:58:ALA:HB2	2.18	0.68
1:I:53:TYR:C	1:I:58:ALA:HB2	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:VAL:HG23	1:E:46:GLY:N	2.05	0.68
1:D:37:ARG:HG3	1:D:37:ARG:HH11	1.59	0.67
3:G:19:ILE:HG23	3:G:19:ILE:O	1.95	0.67
1:A:37:ARG:HG3	1:A:37:ARG:HH11	1.59	0.67
1:F:54:VAL:CG2	1:F:55:GLY:N	2.43	0.67
1:I:37:ARG:HG3	1:I:37:ARG:HH11	1.60	0.67
1:E:37:ARG:HH11	1:E:37:ARG:CG	2.08	0.67
1:F:37:ARG:CG	1:F:37:ARG:HH11	2.08	0.67
3:G:287:GLN:O	2:H:149:LYS:HE2	1.95	0.67
3:J:19:ILE:O	3:J:19:ILE:HG23	1.95	0.66
3:C:19:ILE:HG23	3:C:19:ILE:O	1.95	0.66
3:J:80:LEU:O	3:J:84:ALA:N	2.29	0.66
3:C:80:LEU:O	3:C:84:ALA:N	2.29	0.66
1:D:37:ARG:HH11	1:D:37:ARG:CG	2.08	0.66
1:E:43:VAL:N	1:F:168:GLY:HA2	2.09	0.66
1:A:37:ARG:HH11	1:A:37:ARG:CG	2.08	0.66
1:A:45:VAL:C	1:A:47:MET:H	2.04	0.66
1:I:37:ARG:HH11	1:I:37:ARG:CG	2.08	0.66
1:F:45:VAL:C	1:F:47:MET:H	2.04	0.66
1:A:168:GLY:HA2	1:D:43:VAL:H	1.61	0.65
3:J:622:ALA:HB3	3:J:678:PHE:CE2	2.31	0.65
3:C:106:GLY:O	3:C:108:THR:N	2.30	0.65
1:E:45:VAL:C	1:E:47:MET:H	2.04	0.65
1:E:37:ARG:HG3	1:E:37:ARG:HH11	1.59	0.65
3:G:80:LEU:O	3:G:84:ALA:N	2.29	0.65
2:H:226:LYS:HG3	3:J:285:ALA:CB	2.22	0.65
3:C:622:ALA:HB3	3:C:678:PHE:CE2	2.31	0.65
1:E:36:GLY:O	1:E:52:SER:HB3	1.98	0.64
1:F:37:ARG:HG3	1:F:37:ARG:HH11	1.59	0.64
1:I:36:GLY:O	1:I:52:SER:HB3	1.98	0.64
1:D:45:VAL:C	1:D:47:MET:H	2.04	0.64
1:I:45:VAL:C	1:I:47:MET:H	2.04	0.64
3:J:625:ALA:O	3:J:627:ARG:NH1	2.30	0.64
1:F:36:GLY:O	1:F:52:SER:HB3	1.98	0.64
3:G:622:ALA:HB3	3:G:678:PHE:CE2	2.31	0.64
1:A:36:GLY:O	1:A:52:SER:HB3	1.98	0.64
3:G:625:ALA:O	3:G:627:ARG:NH1	2.30	0.64
1:I:54:VAL:CG2	1:I:55:GLY:N	2.43	0.64
3:C:625:ALA:O	3:C:627:ARG:NH1	2.30	0.64
1:D:36:GLY:O	1:D:52:SER:HB3	1.98	0.64
1:A:39:ARG:HB3	1:A:66:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ARG:HB3	1:E:66:THR:OG1	1.98	0.64
1:D:349:LEU:HD22	3:J:461:GLU:HA	1.80	0.63
1:F:39:ARG:HB3	1:F:66:THR:OG1	1.98	0.63
1:I:39:ARG:HB3	1:I:66:THR:OG1	1.98	0.62
1:A:54:VAL:CG2	1:A:55:GLY:N	2.43	0.62
1:D:39:ARG:HB3	1:D:66:THR:OG1	1.98	0.62
1:A:43:VAL:HA	1:I:168:GLY:HA2	1.82	0.62
2:H:226:LYS:CG	3:J:285:ALA:HB3	2.26	0.62
1:D:150:GLY:O	1:D:166:TYR:CG	2.53	0.62
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.82	0.62
1:A:150:GLY:O	1:A:166:TYR:CG	2.53	0.62
1:A:55:GLY:C	1:A:57:GLU:N	2.58	0.62
1:E:43:VAL:H	1:F:168:GLY:HA2	1.65	0.61
1:E:150:GLY:O	1:E:166:TYR:CG	2.53	0.61
3:C:334:GLU:O	3:C:335:VAL:HB	2.00	0.61
1:F:26:ALA:O	1:F:28:ARG:NH1	2.34	0.61
3:G:529:GLY:O	3:G:532:ILE:N	2.34	0.61
1:I:55:GLY:C	1:I:57:GLU:N	2.58	0.61
1:D:54:VAL:CG2	1:D:55:GLY:N	2.43	0.61
1:E:43:VAL:HA	1:F:168:GLY:HA2	1.83	0.61
1:I:150:GLY:O	1:I:166:TYR:CG	2.53	0.61
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.82	0.61
2:H:222:GLU:CD	3:J:286:GLU:HA	2.26	0.61
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.82	0.61
3:C:529:GLY:O	3:C:532:ILE:N	2.34	0.61
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.82	0.61
1:F:150:GLY:O	1:F:166:TYR:CG	2.53	0.61
1:I:26:ALA:O	1:I:28:ARG:NH1	2.33	0.61
1:I:107:GLU:HB2	1:I:134:VAL:HG22	1.82	0.61
3:J:529:GLY:O	3:J:532:ILE:N	2.34	0.60
1:A:43:VAL:CA	1:I:168:GLY:HA2	2.31	0.60
1:D:26:ALA:O	1:D:28:ARG:NH1	2.33	0.60
1:E:26:ALA:O	1:E:28:ARG:NH1	2.33	0.60
1:A:168:GLY:HA2	1:D:43:VAL:HA	1.83	0.60
1:E:171:LEU:HB2	1:E:172:PRO:CD	2.31	0.60
3:C:365:VAL:O	3:C:369:ASN:ND2	2.35	0.59
1:A:171:LEU:HB2	1:A:172:PRO:CD	2.31	0.59
1:I:171:LEU:HB2	1:I:172:PRO:CD	2.31	0.59
3:J:645:TRP:O	3:J:647:SER:N	2.35	0.59
3:J:365:VAL:O	3:J:369:ASN:ND2	2.35	0.59
3:C:645:TRP:O	3:C:647:SER:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:LEU:HB2	1:F:172:PRO:CD	2.31	0.59
3:G:645:TRP:O	3:G:647:SER:N	2.35	0.59
3:G:91:SER:O	3:G:92:GLN:HB3	2.02	0.59
1:F:55:GLY:HA3	1:F:88:HIS:NE2	2.17	0.59
3:G:365:VAL:O	3:G:369:ASN:ND2	2.35	0.59
3:J:91:SER:O	3:J:92:GLN:HB3	2.03	0.59
3:C:91:SER:O	3:C:92:GLN:HB3	2.02	0.59
3:G:515:ASP:OD1	3:G:516:VAL:N	2.36	0.58
1:E:55:GLY:HA3	1:E:88:HIS:NE2	2.17	0.58
1:I:38:PRO:CG	1:I:49:GLN:HG2	2.33	0.58
3:J:515:ASP:OD1	3:J:516:VAL:N	2.36	0.58
1:A:41:GLN:CD	1:I:170:ALA:HB3	2.28	0.58
3:C:136:LEU:O	3:C:139:SER:OG	2.19	0.58
1:A:43:VAL:CG2	1:A:46:GLY:HA3	2.34	0.58
3:J:336:ILE:O	3:J:337:SER:OG	2.22	0.58
3:C:515:ASP:OD1	3:C:516:VAL:N	2.36	0.58
2:H:226:LYS:CG	3:J:285:ALA:CB	2.82	0.58
1:I:43:VAL:CG2	1:I:46:GLY:HA3	2.34	0.58
1:D:43:VAL:CG2	1:D:46:GLY:HA3	2.34	0.58
1:F:42:GLY:O	1:F:43:VAL:HG22	2.04	0.58
1:I:38:PRO:HG3	1:I:49:GLN:CD	2.29	0.58
1:E:38:PRO:CG	1:E:49:GLN:HG2	2.33	0.57
1:E:41:GLN:NE2	1:F:169:TYR:C	2.43	0.57
3:G:336:ILE:O	3:G:337:SER:OG	2.22	0.57
1:A:170:ALA:HB3	1:D:41:GLN:CD	2.28	0.57
1:E:40:HIS:NE2	1:F:168:GLY:N	2.50	0.57
3:J:645:TRP:HB3	3:J:646:PRO:HD2	1.86	0.57
1:A:168:GLY:HA2	1:D:43:VAL:CA	2.34	0.57
1:D:38:PRO:HG3	1:D:49:GLN:CD	2.29	0.57
1:I:42:GLY:O	1:I:43:VAL:HG22	2.04	0.57
1:A:42:GLY:O	1:A:43:VAL:HG22	2.04	0.57
1:E:42:GLY:O	1:E:43:VAL:HG22	2.04	0.57
1:D:42:GLY:O	1:D:43:VAL:HG22	2.04	0.57
1:D:55:GLY:HA3	1:D:88:HIS:NE2	2.18	0.57
1:F:43:VAL:CG2	1:F:46:GLY:HA3	2.34	0.57
1:A:38:PRO:HG3	1:A:49:GLN:CD	2.29	0.57
1:A:55:GLY:HA3	1:A:88:HIS:NE2	2.17	0.57
3:C:645:TRP:HB3	3:C:646:PRO:HD2	1.86	0.57
1:E:38:PRO:HG3	1:E:49:GLN:CD	2.29	0.56
3:J:234:CYS:SG	3:J:235:PHE:N	2.78	0.56
3:C:234:CYS:SG	3:C:235:PHE:N	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:LEU:HB2	1:D:172:PRO:CD	2.31	0.56
1:E:43:VAL:CG2	1:E:46:GLY:HA3	2.34	0.56
1:E:43:VAL:CA	1:F:168:GLY:HA2	2.35	0.56
1:F:38:PRO:CG	1:F:49:GLN:HG2	2.33	0.56
3:G:645:TRP:HB3	3:G:646:PRO:HD2	1.86	0.56
1:I:37:ARG:CG	1:I:37:ARG:NH1	2.68	0.56
1:A:38:PRO:CG	1:A:49:GLN:HG2	2.33	0.56
1:F:38:PRO:HG3	1:F:49:GLN:CD	2.29	0.56
3:G:234:CYS:SG	3:G:235:PHE:N	2.78	0.56
1:I:55:GLY:HA3	1:I:88:HIS:NE2	2.17	0.56
1:I:288:ASP:OD1	1:I:291:LYS:NZ	2.39	0.56
1:A:288:ASP:OD1	1:A:291:LYS:NZ	2.39	0.56
3:J:136:LEU:O	3:J:139:SER:OG	2.19	0.56
1:D:288:ASP:OD1	1:D:291:LYS:NZ	2.39	0.55
1:F:288:ASP:OD1	1:F:291:LYS:NZ	2.39	0.55
3:G:462:ALA:O	3:G:468:SER:OG	2.24	0.55
1:A:37:ARG:CG	1:A:37:ARG:NH1	2.68	0.55
1:E:288:ASP:OD1	1:E:291:LYS:NZ	2.39	0.55
1:E:40:HIS:CE1	1:F:168:GLY:N	2.74	0.55
3:G:282:ALA:O	3:G:283:GLU:C	2.50	0.55
3:G:461:GLU:HA	1:I:349:LEU:HD22	1.88	0.55
1:A:42:GLY:O	1:I:167:GLU:O	2.23	0.55
1:A:349:LEU:HD22	3:C:461:GLU:HA	1.88	0.55
3:G:136:LEU:O	3:G:139:SER:OG	2.19	0.55
3:J:462:ALA:O	3:J:468:SER:OG	2.24	0.55
3:G:550:THR:HG22	3:G:551:ARG:HG3	1.88	0.55
3:J:550:THR:HG22	3:J:551:ARG:HG3	1.88	0.55
3:C:282:ALA:O	3:C:283:GLU:C	2.50	0.55
1:E:252:ASN:OD1	1:E:256:ARG:NH2	2.40	0.55
1:I:270:GLU:N	1:I:270:GLU:OE1	2.40	0.55
1:D:270:GLU:N	1:D:270:GLU:OE1	2.40	0.54
1:F:252:ASN:OD1	1:F:256:ARG:NH2	2.40	0.54
3:J:628:ILE:O	3:J:677:VAL:N	2.39	0.54
1:A:252:ASN:OD1	1:A:256:ARG:NH2	2.40	0.54
1:E:43:VAL:HG13	1:F:167:GLU:O	2.07	0.54
3:C:550:THR:HG22	3:C:551:ARG:HG3	1.88	0.54
3:J:282:ALA:O	3:J:283:GLU:C	2.50	0.54
1:A:168:GLY:N	1:D:40:HIS:NE2	2.51	0.54
1:A:270:GLU:N	1:A:270:GLU:OE1	2.40	0.54
1:D:252:ASN:OD1	1:D:256:ARG:NH2	2.40	0.54
1:E:270:GLU:OE1	1:E:270:GLU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:270:GLU:N	1:F:270:GLU:OE1	2.40	0.54
1:I:2:GLU:OE1	1:I:3:ASP:N	2.41	0.54
3:C:494:LYS:HB3	1:D:99:GLU:OE1	2.07	0.54
1:F:2:GLU:OE1	1:F:3:ASP:N	2.41	0.54
1:F:55:GLY:C	1:F:57:GLU:N	2.58	0.54
1:I:35:VAL:HG13	1:I:52:SER:CB	2.38	0.54
1:D:37:ARG:CG	1:D:37:ARG:NH1	2.68	0.54
1:E:37:ARG:CG	1:E:37:ARG:NH1	2.68	0.54
1:I:252:ASN:OD1	1:I:256:ARG:NH2	2.40	0.54
1:E:41:GLN:CD	1:F:170:ALA:HB3	2.32	0.54
3:G:628:ILE:O	3:G:677:VAL:N	2.39	0.54
1:A:35:VAL:HG13	1:A:52:SER:CB	2.38	0.53
1:E:2:GLU:OE1	1:E:3:ASP:N	2.41	0.53
1:F:87:HIS:O	1:F:87:HIS:ND1	2.41	0.53
3:G:106:GLY:C	3:G:108:THR:N	2.63	0.53
3:G:518:GLY:O	3:G:520:LEU:N	2.42	0.53
1:D:83:GLU:O	1:D:87:HIS:CD2	2.61	0.53
1:E:336:LYS:HE3	4:E:376:ADP:O2A	2.09	0.53
1:I:336:LYS:HE3	4:I:376:ADP:O2A	2.09	0.53
1:D:2:GLU:OE1	1:D:3:ASP:N	2.41	0.53
1:D:36:GLY:O	1:D:52:SER:CB	2.57	0.53
1:A:87:HIS:O	1:A:87:HIS:ND1	2.41	0.53
1:A:336:LYS:HE3	4:A:376:ADP:O2A	2.08	0.53
1:D:143:TYR:OH	1:D:169:TYR:OH	2.27	0.53
1:E:87:HIS:O	1:E:87:HIS:ND1	2.41	0.53
1:F:336:LYS:HE3	4:F:376:ADP:O2A	2.09	0.53
2:H:222:GLU:OE2	3:J:286:GLU:CA	2.56	0.53
2:H:222:GLU:OE2	3:J:286:GLU:HA	2.08	0.53
1:A:167:GLU:O	1:D:42:GLY:O	2.26	0.53
1:D:336:LYS:HE3	4:D:376:ADP:O2A	2.09	0.53
1:F:35:VAL:HG13	1:F:52:SER:CB	2.38	0.53
1:I:87:HIS:O	1:I:87:HIS:ND1	2.41	0.53
1:F:107:GLU:N	1:F:135:ALA:O	2.42	0.53
1:A:36:GLY:O	1:A:52:SER:CB	2.57	0.53
3:C:529:GLY:O	3:C:531:LEU:N	2.42	0.53
1:A:43:VAL:H	1:I:168:GLY:CA	2.22	0.53
1:D:35:VAL:HG13	1:D:52:SER:CB	2.38	0.53
1:D:107:GLU:N	1:D:135:ALA:O	2.42	0.53
1:E:36:GLY:O	1:E:52:SER:CB	2.57	0.53
1:I:107:GLU:N	1:I:135:ALA:O	2.42	0.53
3:J:518:GLY:O	3:J:520:LEU:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:518:GLY:O	3:C:520:LEU:N	2.42	0.52
1:D:50:LYS:HG2	1:D:51:ASP:N	2.24	0.52
1:F:36:GLY:O	1:F:52:SER:CB	2.57	0.52
3:J:91:SER:O	3:J:92:GLN:CB	2.57	0.52
1:A:43:VAL:HG21	1:A:46:GLY:HA3	1.92	0.52
3:C:621:ARG:HD2	3:C:627:ARG:HD2	1.92	0.52
1:D:38:PRO:CG	1:D:49:GLN:HG2	2.33	0.52
1:I:36:GLY:O	1:I:52:SER:CB	2.57	0.52
1:A:43:VAL:HG13	1:I:167:GLU:O	2.10	0.52
1:A:170:ALA:HB3	1:D:41:GLN:HE22	1.69	0.52
1:D:43:VAL:HG21	1:D:46:GLY:HA3	1.92	0.52
1:E:35:VAL:HG13	1:E:52:SER:CB	2.38	0.52
1:E:107:GLU:N	1:E:135:ALA:O	2.42	0.52
1:E:202:THR:N	1:E:205:GLU:OE2	2.42	0.52
3:G:529:GLY:O	3:G:531:LEU:N	2.42	0.52
1:I:202:THR:N	1:I:205:GLU:OE2	2.42	0.52
3:C:529:GLY:O	3:C:530:ASP:C	2.52	0.52
3:G:621:ARG:HD2	3:G:627:ARG:HD2	1.92	0.52
3:J:529:GLY:O	3:J:531:LEU:N	2.42	0.52
1:A:202:THR:N	1:A:205:GLU:OE2	2.42	0.52
1:D:42:GLY:C	1:D:44:MET:N	2.66	0.52
3:G:529:GLY:O	3:G:530:ASP:C	2.52	0.52
1:I:43:VAL:HG21	1:I:46:GLY:HA3	1.92	0.52
1:A:107:GLU:N	1:A:135:ALA:O	2.42	0.52
1:A:167:GLU:O	1:D:43:VAL:HG13	2.09	0.52
3:C:91:SER:O	3:C:92:GLN:CB	2.57	0.52
1:E:37:ARG:CB	1:E:38:PRO:CD	2.88	0.52
1:F:42:GLY:C	1:F:44:MET:N	2.66	0.52
3:G:329:VAL:C	3:G:331:LYS:N	2.67	0.52
3:J:621:ARG:HD2	3:J:627:ARG:HD2	1.92	0.52
1:A:37:ARG:CB	1:A:38:PRO:CD	2.88	0.52
1:A:168:GLY:N	1:D:40:HIS:CE1	2.76	0.52
1:A:276:GLU:N	1:A:276:GLU:OE1	2.43	0.52
1:D:37:ARG:CB	1:D:38:PRO:CD	2.88	0.52
1:F:276:GLU:N	1:F:276:GLU:OE1	2.43	0.52
3:J:106:GLY:C	3:J:108:THR:N	2.64	0.52
3:C:329:VAL:C	3:C:331:LYS:N	2.67	0.52
1:E:276:GLU:OE1	1:E:276:GLU:N	2.43	0.52
1:I:276:GLU:N	1:I:276:GLU:OE1	2.43	0.52
3:C:628:ILE:O	3:C:677:VAL:N	2.39	0.52
1:A:41:GLN:HE22	1:I:170:ALA:HB3	1.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:GLU:N	1:D:276:GLU:OE1	2.43	0.51
1:E:41:GLN:HE22	1:F:170:ALA:HB3	1.70	0.51
1:A:40:HIS:NE2	1:I:168:GLY:N	2.54	0.51
3:J:442:LYS:N	3:J:443:PRO:HD3	2.26	0.51
3:J:529:GLY:O	3:J:530:ASP:C	2.52	0.51
1:D:1:ASP:O	1:D:2:GLU:C	2.53	0.51
3:G:91:SER:O	3:G:92:GLN:CB	2.57	0.51
3:G:201:ILE:HG13	3:G:270:LEU:HD11	1.93	0.51
1:I:37:ARG:CB	1:I:38:PRO:CD	2.88	0.51
3:C:442:LYS:N	3:C:443:PRO:HD3	2.26	0.51
1:F:280:ASN:OD1	1:F:284:LYS:NZ	2.43	0.51
1:I:1:ASP:O	1:I:2:GLU:C	2.54	0.51
1:I:173:HIS:CG	1:I:174:ALA:N	2.78	0.51
3:J:201:ILE:HG13	3:J:270:LEU:HD11	1.93	0.51
3:C:201:ILE:HG13	3:C:270:LEU:HD11	1.93	0.51
1:D:349:LEU:HD13	3:J:461:GLU:HG2	1.92	0.51
3:G:442:LYS:N	3:G:443:PRO:HD3	2.26	0.51
1:A:1:ASP:O	1:A:2:GLU:C	2.54	0.51
1:D:53:TYR:CB	1:D:57:GLU:OE1	2.58	0.51
1:F:43:VAL:HG21	1:F:46:GLY:HA3	1.91	0.51
1:F:66:THR:HG23	1:I:270:GLU:HG3	1.93	0.51
1:I:62:ARG:O	1:I:63:GLY:C	2.54	0.51
3:J:329:VAL:C	3:J:331:LYS:N	2.67	0.51
1:D:55:GLY:C	1:D:57:GLU:N	2.58	0.51
1:E:43:VAL:HG21	1:E:46:GLY:HA3	1.92	0.51
1:F:37:ARG:CB	1:F:38:PRO:CD	2.88	0.51
1:I:42:GLY:C	1:I:44:MET:N	2.66	0.51
1:E:34:ILE:O	1:E:35:VAL:CG2	2.57	0.51
1:E:173:HIS:CG	1:E:174:ALA:N	2.78	0.51
1:F:173:HIS:CG	1:F:174:ALA:N	2.78	0.51
1:A:62:ARG:O	1:A:63:GLY:C	2.54	0.50
1:D:173:HIS:CG	1:D:174:ALA:N	2.78	0.50
3:J:463:CYS:HA	3:J:520:LEU:HD22	1.92	0.50
3:G:548:PRO:O	3:G:550:THR:N	2.41	0.50
2:B:221:TYR:OH	3:J:286:GLU:OE2	2.29	0.50
1:E:280:ASN:OD1	1:E:284:LYS:NZ	2.43	0.50
1:I:40:HIS:O	1:I:41:GLN:OE1	2.30	0.50
3:C:41:ILE:HG22	3:C:44:VAL:HB	1.94	0.50
3:C:560:GLU:O	3:C:560:GLU:CG	2.56	0.50
1:E:1:ASP:O	1:E:2:GLU:C	2.53	0.50
1:E:42:GLY:O	1:F:167:GLU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:106:GLY:C	3:J:108:THR:H	2.19	0.50
1:A:173:HIS:CG	1:A:174:ALA:N	2.78	0.50
1:E:40:HIS:O	1:E:41:GLN:OE1	2.30	0.50
1:F:53:TYR:CB	1:F:57:GLU:OE1	2.58	0.50
1:D:202:THR:N	1:D:205:GLU:OE2	2.42	0.50
1:E:42:GLY:C	1:E:44:MET:N	2.66	0.50
1:F:202:THR:N	1:F:205:GLU:OE2	2.42	0.50
3:G:679:ILE:HG21	3:G:684:THR:HG21	1.93	0.50
1:A:40:HIS:O	1:A:41:GLN:OE1	2.30	0.50
1:D:54:VAL:O	1:D:55:GLY:O	2.30	0.50
1:A:54:VAL:O	1:A:55:GLY:O	2.30	0.50
1:F:40:HIS:O	1:F:41:GLN:OE1	2.30	0.50
3:G:463:CYS:HA	3:G:520:LEU:HD22	1.92	0.50
3:J:548:PRO:O	3:J:550:THR:N	2.41	0.50
3:J:601:GLU:OE2	3:J:605:ARG:NH2	2.45	0.50
1:A:40:HIS:CE1	1:I:168:GLY:N	2.78	0.50
1:F:1:ASP:O	1:F:2:GLU:C	2.54	0.50
1:D:62:ARG:O	1:D:63:GLY:C	2.54	0.49
1:E:62:ARG:O	1:E:63:GLY:C	2.54	0.49
1:D:40:HIS:O	1:D:41:GLN:OE1	2.30	0.49
3:G:286:GLU:HG3	2:H:145:GLU:CD	2.37	0.49
1:I:54:VAL:O	1:I:55:GLY:O	2.30	0.49
3:C:463:CYS:HA	3:C:520:LEU:HD22	1.93	0.49
1:E:35:VAL:HG12	1:E:35:VAL:O	2.12	0.49
1:F:62:ARG:O	1:F:63:GLY:C	2.54	0.49
3:G:106:GLY:C	3:G:108:THR:H	2.19	0.49
3:J:140:ASN:HB2	3:J:141:PRO:HD3	1.94	0.49
1:A:53:TYR:CB	1:A:57:GLU:OE1	2.58	0.49
3:C:679:ILE:HG21	3:C:684:THR:HG21	1.93	0.49
3:G:41:ILE:HG22	3:G:44:VAL:HB	1.94	0.49
3:G:140:ASN:HB2	3:G:141:PRO:HD3	1.94	0.49
1:I:34:ILE:O	1:I:35:VAL:CG2	2.57	0.49
3:J:679:ILE:HG21	3:J:684:THR:HG21	1.93	0.49
1:A:50:LYS:HG3	1:A:51:ASP:H	1.77	0.49
1:A:168:GLY:CA	1:D:43:VAL:H	2.26	0.49
3:G:601:GLU:OE2	3:G:605:ARG:NH2	2.45	0.49
1:I:50:LYS:HG3	1:I:51:ASP:H	1.77	0.49
1:I:336:LYS:HE3	4:I:376:ADP:PA	2.52	0.49
1:A:51:ASP:O	1:A:53:TYR:CA	2.61	0.49
1:F:43:VAL:CG2	1:F:46:GLY:CA	2.90	0.49
1:F:51:ASP:O	1:F:53:TYR:CA	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HE3	4:A:376:ADP:PA	2.52	0.49
3:C:140:ASN:HB2	3:C:141:PRO:HD3	1.94	0.49
1:E:43:VAL:CG2	1:E:46:GLY:CA	2.90	0.49
1:F:34:ILE:O	1:F:35:VAL:CG2	2.57	0.49
1:A:280:ASN:OD1	1:A:284:LYS:NZ	2.43	0.49
1:D:43:VAL:CG2	1:D:46:GLY:CA	2.90	0.49
1:F:54:VAL:O	1:F:55:GLY:O	2.30	0.49
1:I:280:ASN:OD1	1:I:284:LYS:NZ	2.43	0.49
1:A:35:VAL:O	1:A:35:VAL:HG12	2.12	0.49
1:A:43:VAL:CG2	1:A:46:GLY:CA	2.90	0.49
1:D:51:ASP:O	1:D:53:TYR:CA	2.61	0.49
1:E:54:VAL:O	1:E:55:GLY:O	2.30	0.48
1:E:336:LYS:HE3	4:E:376:ADP:PA	2.52	0.48
3:J:41:ILE:HG22	3:J:44:VAL:HB	1.94	0.48
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.95	0.48
1:E:50:LYS:HG3	1:E:51:ASP:H	1.77	0.48
1:I:43:VAL:CG2	1:I:46:GLY:CA	2.90	0.48
1:A:34:ILE:O	1:A:35:VAL:CG2	2.57	0.48
3:C:601:GLU:OE2	3:C:605:ARG:NH2	2.45	0.48
1:D:73:HIC:ND1	1:D:183:ARG:HD3	2.28	0.48
1:I:53:TYR:CB	1:I:57:GLU:OE1	2.58	0.48
1:D:280:ASN:OD1	1:D:284:LYS:NZ	2.43	0.48
1:A:42:GLY:C	1:A:44:MET:N	2.66	0.48
1:D:336:LYS:HE3	4:D:376:ADP:PA	2.52	0.48
1:F:35:VAL:O	1:F:35:VAL:HG12	2.12	0.48
1:F:257:CYS:HB3	1:F:258:PRO:HD3	1.95	0.48
3:J:55:ASN:O	3:J:55:ASN:ND2	2.47	0.48
1:E:51:ASP:O	1:E:53:TYR:CA	2.61	0.48
1:F:50:LYS:HG3	1:F:51:ASP:H	1.77	0.48
1:F:336:LYS:HE3	4:F:376:ADP:PA	2.52	0.48
1:D:35:VAL:HG12	1:D:35:VAL:O	2.12	0.48
1:D:350:SER:HB3	3:J:452:PRO:HA	1.94	0.48
3:G:622:ALA:HB3	3:G:678:PHE:CZ	2.49	0.48
1:I:257:CYS:HB3	1:I:258:PRO:HD3	1.95	0.48
3:C:55:ASN:O	3:C:55:ASN:ND2	2.47	0.48
3:G:327:THR:HG23	3:G:327:THR:O	2.14	0.48
1:A:66:THR:HG23	1:F:270:GLU:HG3	1.95	0.47
3:C:369:ASN:O	3:C:373:ASN:N	2.46	0.47
3:C:622:ALA:HB3	3:C:678:PHE:CZ	2.48	0.47
1:I:35:VAL:O	1:I:35:VAL:HG12	2.12	0.47
3:J:622:ALA:HB3	3:J:678:PHE:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:O	1:D:35:VAL:CG2	2.57	0.47
1:D:257:CYS:HB3	1:D:258:PRO:HD3	1.95	0.47
1:E:64:ILE:HG21	1:F:167:GLU:HG2	1.96	0.47
1:E:257:CYS:HB3	1:E:258:PRO:HD3	1.95	0.47
3:G:639:MET:SD	3:G:639:MET:N	2.87	0.47
3:G:55:ASN:ND2	3:G:55:ASN:O	2.47	0.47
1:A:73:HIC:ND1	1:A:183:ARG:HD3	2.28	0.47
3:C:639:MET:N	3:C:639:MET:SD	2.87	0.47
1:I:51:ASP:O	1:I:53:TYR:CA	2.61	0.47
3:J:530:ASP:N	3:J:530:ASP:OD1	2.48	0.47
1:A:350:SER:HB3	3:C:452:PRO:HA	1.95	0.47
1:A:167:GLU:HG2	1:D:64:ILE:HG21	1.96	0.47
1:E:73:HIC:ND1	1:E:183:ARG:HD3	2.28	0.47
1:E:143:TYR:OH	1:E:169:TYR:OH	2.27	0.47
3:G:369:ASN:O	3:G:373:ASN:N	2.46	0.47
1:I:73:HIC:ND1	1:I:183:ARG:HD3	2.28	0.47
3:J:624:PHE:CD1	3:J:624:PHE:C	2.92	0.47
3:J:639:MET:SD	3:J:639:MET:N	2.87	0.47
1:A:41:GLN:NE2	1:I:170:ALA:CB	2.68	0.47
1:F:73:HIC:ND1	1:F:183:ARG:HD3	2.28	0.47
3:J:369:ASN:O	3:J:373:ASN:N	2.46	0.47
1:E:47:MET:SD	1:E:49:GLN:HA	2.55	0.47
1:E:53:TYR:CB	1:E:57:GLU:OE1	2.58	0.47
3:G:467:LYS:HE3	3:G:467:LYS:HA	1.97	0.47
3:J:558:ARG:HB2	3:J:559:PRO:HD3	1.96	0.47
3:C:530:ASP:OD1	3:C:530:ASP:N	2.48	0.47
3:G:452:PRO:HA	1:I:350:SER:HB3	1.96	0.47
2:H:222:GLU:OE1	3:J:286:GLU:CG	2.57	0.47
3:G:624:PHE:CG	3:G:625:ALA:N	2.83	0.46
3:J:674:LYS:HG3	3:J:675:THR:HG23	1.97	0.46
1:A:43:VAL:HG13	1:I:167:GLU:C	2.40	0.46
1:A:47:MET:SD	1:A:49:GLN:HA	2.55	0.46
3:C:558:ARG:HB2	3:C:559:PRO:HD3	1.96	0.46
1:E:43:VAL:H	1:F:168:GLY:CA	2.29	0.46
3:C:322:TYR:HB3	3:C:337:SER:HB3	1.96	0.46
3:C:629:GLU:O	3:C:633:PHE:N	2.48	0.46
1:D:157:ASP:CB	4:D:376:ADP:O3B	2.60	0.46
1:E:203:THR:HA	1:E:206:ARG:HB3	1.97	0.46
3:G:558:ARG:HB2	3:G:559:PRO:HD3	1.96	0.46
3:J:629:GLU:O	3:J:633:PHE:N	2.48	0.46
3:C:183:LEU:HD13	3:C:184:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:VAL:CG2	1:E:55:GLY:N	2.43	0.46
1:F:47:MET:SD	1:F:49:GLN:HA	2.55	0.46
3:G:183:LEU:HD13	3:G:184:LEU:O	2.16	0.46
3:J:327:THR:HG23	3:J:327:THR:O	2.14	0.46
1:A:41:GLN:OE1	1:I:170:ALA:O	2.32	0.46
1:A:170:ALA:O	1:D:41:GLN:OE1	2.33	0.46
3:C:624:PHE:CG	3:C:625:ALA:N	2.83	0.46
3:C:674:LYS:HG3	3:C:675:THR:HG23	1.97	0.46
1:F:173:HIS:CG	1:F:174:ALA:H	2.34	0.46
3:G:629:GLU:O	3:G:633:PHE:N	2.48	0.46
3:J:634:TYR:O	3:J:636:ARG:N	2.48	0.46
1:F:37:ARG:CG	1:F:37:ARG:NH1	2.68	0.46
1:F:203:THR:HA	1:F:206:ARG:HB3	1.97	0.46
3:G:530:ASP:N	3:G:530:ASP:OD1	2.48	0.46
3:J:107:LYS:O	3:J:111:SER:HB2	2.16	0.46
1:A:173:HIS:CG	1:A:174:ALA:H	2.34	0.46
1:D:173:HIS:CG	1:D:174:ALA:H	2.34	0.46
1:F:189:LEU:HG	1:F:193:LEU:HD13	1.98	0.46
3:J:107:LYS:H	3:J:107:LYS:CD	2.20	0.46
3:C:467:LYS:HA	3:C:467:LYS:HE3	1.97	0.46
1:E:189:LEU:HG	1:E:193:LEU:HD13	1.98	0.46
3:G:674:LYS:HG3	3:G:675:THR:HG23	1.97	0.46
1:E:136:ILE:O	1:E:137:GLN:C	2.59	0.46
1:E:173:HIS:CG	1:E:174:ALA:H	2.34	0.46
1:I:203:THR:HA	1:I:206:ARG:HB3	1.97	0.46
3:J:624:PHE:CG	3:J:625:ALA:N	2.83	0.46
1:A:50:LYS:NZ	1:A:51:ASP:HA	2.31	0.46
1:F:50:LYS:NZ	1:F:51:ASP:HA	2.31	0.46
1:I:173:HIS:CG	1:I:174:ALA:H	2.34	0.46
3:J:467:LYS:HE3	3:J:467:LYS:HA	1.97	0.46
1:A:41:GLN:O	1:A:43:VAL:N	2.49	0.45
1:A:203:THR:HA	1:A:206:ARG:HB3	1.97	0.45
3:C:573:LEU:HD22	3:C:573:LEU:O	2.16	0.45
1:E:50:LYS:NZ	1:E:51:ASP:HA	2.31	0.45
1:F:136:ILE:O	1:F:137:GLN:C	2.59	0.45
3:G:107:LYS:O	3:G:111:SER:HB2	2.16	0.45
1:I:47:MET:SD	1:I:49:GLN:HA	2.55	0.45
1:I:157:ASP:CB	4:I:376:ADP:O3B	2.60	0.45
3:J:183:LEU:HD13	3:J:184:LEU:O	2.16	0.45
1:A:167:GLU:C	1:D:43:VAL:HG13	2.41	0.45
3:G:573:LEU:O	3:G:573:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:LEU:HG	1:D:193:LEU:HD13	1.98	0.45
1:A:64:ILE:HG21	1:I:167:GLU:HG2	1.97	0.45
1:A:349:LEU:HD13	3:C:461:GLU:HG2	1.98	0.45
1:D:37:ARG:HB3	1:D:38:PRO:CD	2.47	0.45
1:D:203:THR:HA	1:D:206:ARG:HB3	1.97	0.45
1:F:41:GLN:O	1:F:43:VAL:N	2.49	0.45
3:G:634:TYR:O	3:G:636:ARG:N	2.48	0.45
1:E:41:GLN:O	1:E:43:VAL:N	2.49	0.45
3:G:78:TYR:CZ	3:G:81:ALA:HB2	2.52	0.45
1:I:41:GLN:O	1:I:43:VAL:N	2.49	0.45
1:A:136:ILE:O	1:A:137:GLN:C	2.59	0.45
1:A:189:LEU:HG	1:A:193:LEU:HD13	1.98	0.45
1:E:230:ALA:HA	1:E:236:LEU:HD22	1.99	0.45
3:G:470:ASP:HB3	3:G:516:VAL:HG22	1.99	0.45
1:I:37:ARG:HB3	1:I:38:PRO:CD	2.47	0.45
3:J:78:TYR:CZ	3:J:81:ALA:HB2	2.52	0.45
1:I:50:LYS:NZ	1:I:51:ASP:HA	2.31	0.45
3:J:329:VAL:O	3:J:331:LYS:N	2.50	0.45
1:A:37:ARG:HB3	1:A:38:PRO:CD	2.47	0.45
1:D:136:ILE:O	1:D:137:GLN:C	2.59	0.45
1:E:22:ALA:N	1:E:24:ASP:OD1	2.50	0.45
1:F:230:ALA:HA	1:F:236:LEU:HD22	1.99	0.45
3:C:470:ASP:HB3	3:C:516:VAL:HG22	1.99	0.45
1:D:72:GLU:O	1:D:73:HIC:C	2.65	0.45
3:J:108:THR:OG1	3:J:109:GLU:N	2.50	0.45
3:J:470:ASP:HB3	3:J:516:VAL:HG22	1.99	0.45
1:E:72:GLU:O	1:E:73:HIC:C	2.65	0.45
1:A:72:GLU:O	1:A:73:HIC:C	2.65	0.44
3:C:78:TYR:CZ	3:C:81:ALA:HB2	2.52	0.44
1:E:37:ARG:HB3	1:E:38:PRO:CD	2.47	0.44
1:F:136:ILE:N	1:F:136:ILE:HD12	2.32	0.44
3:C:58:LYS:O	3:C:59:GLU:C	2.61	0.44
1:E:43:VAL:HG13	1:F:167:GLU:C	2.41	0.44
1:I:72:GLU:O	1:I:73:HIC:C	2.65	0.44
3:J:58:LYS:O	3:J:59:GLU:C	2.61	0.44
3:C:456:ILE:HA	3:C:459:LEU:HB3	2.00	0.44
1:D:136:ILE:N	1:D:136:ILE:HD12	2.32	0.44
1:F:22:ALA:N	1:F:24:ASP:OD1	2.50	0.44
3:G:58:LYS:O	3:G:59:GLU:C	2.61	0.44
3:G:108:THR:OG1	3:G:109:GLU:N	2.50	0.44
1:I:136:ILE:N	1:I:136:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:ILE:O	1:I:137:GLN:C	2.59	0.44
3:C:329:VAL:O	3:C:331:LYS:N	2.50	0.44
3:C:548:PRO:O	3:C:550:THR:N	2.41	0.44
3:G:19:ILE:O	3:G:19:ILE:CG2	2.65	0.44
3:G:329:VAL:O	3:G:331:LYS:N	2.50	0.44
2:H:226:LYS:HG2	3:J:285:ALA:HB1	2.00	0.44
1:I:22:ALA:N	1:I:24:ASP:OD1	2.50	0.44
3:J:456:ILE:HA	3:J:459:LEU:HB3	2.00	0.44
3:J:573:LEU:HD22	3:J:573:LEU:O	2.16	0.44
1:F:37:ARG:HB3	1:F:38:PRO:CD	2.47	0.44
3:J:645:TRP:C	3:J:647:SER:N	2.76	0.44
1:F:72:GLU:O	1:F:73:HIC:C	2.65	0.44
3:G:456:ILE:HA	3:G:459:LEU:HB3	2.00	0.44
1:I:12:ASN:OD1	1:I:13:GLY:N	2.51	0.44
3:C:635:ASN:HA	3:C:638:LYS:HD2	2.00	0.44
1:D:12:ASN:OD1	1:D:13:GLY:N	2.51	0.44
1:D:41:GLN:O	1:D:43:VAL:N	2.49	0.44
1:D:286:ASP:O	1:D:289:ILE:HG22	2.18	0.44
3:G:288:ARG:HG3	2:H:152:LYS:NZ	2.33	0.44
1:I:230:ALA:HA	1:I:236:LEU:HD22	1.99	0.44
3:J:635:ASN:HA	3:J:638:LYS:HD2	2.00	0.44
1:A:136:ILE:N	1:A:136:ILE:HD12	2.32	0.44
1:A:286:ASP:O	1:A:289:ILE:HG22	2.18	0.44
3:C:645:TRP:C	3:C:647:SER:N	2.76	0.44
1:E:12:ASN:OD1	1:E:13:GLY:N	2.51	0.44
1:E:286:ASP:O	1:E:289:ILE:HG22	2.18	0.44
1:I:189:LEU:HG	1:I:193:LEU:HD13	1.98	0.44
3:G:635:ASN:HA	3:G:638:LYS:HD2	2.00	0.44
3:G:645:TRP:C	3:G:647:SER:N	2.76	0.44
1:A:230:ALA:HA	1:A:236:LEU:HD22	1.99	0.43
1:D:230:ALA:HA	1:D:236:LEU:HD22	1.99	0.43
1:F:12:ASN:OD1	1:F:13:GLY:N	2.51	0.43
1:F:286:ASP:O	1:F:289:ILE:HG22	2.18	0.43
2:B:199:THR:O	2:B:203:ASN:ND2	2.48	0.43
1:D:22:ALA:N	1:D:24:ASP:OD1	2.50	0.43
1:I:286:ASP:O	1:I:289:ILE:HG22	2.18	0.43
3:C:10:VAL:N	3:C:11:PRO:HD3	2.33	0.43
1:E:136:ILE:HD12	1:E:136:ILE:N	2.32	0.43
3:J:623:GLY:O	3:J:624:PHE:HB3	2.19	0.43
1:A:43:VAL:N	1:I:168:GLY:CA	2.78	0.43
3:C:623:GLY:O	3:C:624:PHE:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:634:TYR:O	3:C:636:ARG:N	2.48	0.43
3:G:10:VAL:N	3:G:11:PRO:HD3	2.33	0.43
1:A:35:VAL:HG13	1:A:52:SER:OG	2.19	0.43
1:F:35:VAL:HG13	1:F:52:SER:OG	2.19	0.43
3:J:81:ALA:O	3:J:85:TYR:N	2.52	0.43
1:D:83:GLU:O	1:D:87:HIS:CG	2.71	0.43
1:D:148:THR:HG23	3:J:467:LYS:HB3	2.00	0.43
3:G:624:PHE:C	3:G:624:PHE:CD1	2.92	0.43
1:A:12:ASN:OD1	1:A:13:GLY:N	2.51	0.43
3:C:81:ALA:O	3:C:85:TYR:N	2.52	0.43
3:C:624:PHE:CD1	3:C:624:PHE:C	2.92	0.43
3:J:10:VAL:N	3:J:11:PRO:HD3	2.33	0.43
1:E:41:GLN:OE1	1:F:170:ALA:O	2.36	0.43
3:G:81:ALA:O	3:G:85:TYR:N	2.52	0.43
3:C:183:LEU:HD13	3:C:183:LEU:C	2.44	0.43
1:D:35:VAL:HG13	1:D:52:SER:OG	2.19	0.43
3:G:183:LEU:HD13	3:G:183:LEU:C	2.44	0.43
3:G:461:GLU:HG2	1:I:349:LEU:HD13	2.00	0.43
1:A:270:GLU:HG3	1:E:66:THR:HG23	2.01	0.42
1:D:325:MET:SD	1:D:325:MET:N	2.92	0.42
3:J:334:GLU:O	3:J:335:VAL:HB	2.20	0.42
3:C:334:GLU:O	3:C:335:VAL:CB	2.66	0.42
3:C:607:GLN:HA	3:C:610:TYR:CE2	2.54	0.42
3:G:607:GLN:HA	3:G:610:TYR:CE2	2.55	0.42
3:J:183:LEU:HD13	3:J:183:LEU:C	2.44	0.42
1:F:37:ARG:CG	1:F:38:PRO:HD3	2.47	0.42
3:J:620:ARG:CZ	3:J:620:ARG:O	2.67	0.42
1:A:157:ASP:CB	4:A:376:ADP:O3B	2.60	0.42
3:C:620:ARG:CZ	3:C:620:ARG:O	2.67	0.42
3:G:136:LEU:C	3:G:139:SER:HG	2.20	0.42
1:E:35:VAL:HG13	1:E:52:SER:OG	2.19	0.42
1:E:296:ASN:OD1	1:E:328:LYS:NZ	2.50	0.42
1:F:62:ARG:O	1:F:64:ILE:N	2.53	0.42
3:G:149:ALA:HA	3:G:200:HIS:CE1	2.55	0.42
3:G:334:GLU:O	3:G:335:VAL:HB	2.20	0.42
3:G:557:LYS:HE2	1:I:22:ALA:HB3	2.02	0.42
3:G:620:ARG:CZ	3:G:620:ARG:O	2.67	0.42
3:G:630:TYR:CD2	3:G:677:VAL:HG22	2.55	0.42
1:A:168:GLY:CA	1:D:43:VAL:N	2.81	0.42
1:F:296:ASN:OD1	1:F:328:LYS:NZ	2.50	0.42
1:A:325:MET:SD	1:A:325:MET:N	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:ALA:HA	3:C:200:HIS:CE1	2.54	0.42
3:C:630:TYR:CD2	3:C:677:VAL:HG22	2.55	0.42
1:D:202:THR:OG1	1:D:205:GLU:OE1	2.37	0.42
1:F:325:MET:SD	1:F:325:MET:N	2.92	0.42
1:A:166:TYR:HD1	1:A:166:TYR:HA	1.82	0.42
1:A:202:THR:OG1	1:A:205:GLU:OE1	2.37	0.42
3:C:417:LEU:O	3:C:421:SER:OG	2.33	0.42
1:D:375:PHE:N	1:D:375:PHE:CD1	2.88	0.42
1:E:37:ARG:HG3	1:E:38:PRO:CD	2.47	0.42
1:E:202:THR:OG1	1:E:205:GLU:OE1	2.37	0.42
1:I:35:VAL:HG13	1:I:52:SER:OG	2.19	0.42
3:J:149:ALA:HA	3:J:200:HIS:CE1	2.54	0.42
3:J:607:GLN:HA	3:J:610:TYR:CE2	2.55	0.42
1:E:375:PHE:CD1	1:E:375:PHE:N	2.88	0.42
3:G:329:VAL:HG23	3:G:330:GLY:H	1.85	0.42
3:G:645:TRP:O	3:G:646:PRO:C	2.63	0.42
1:I:171:LEU:O	1:I:172:PRO:C	2.62	0.42
3:J:329:VAL:HG23	3:J:330:GLY:H	1.85	0.42
3:J:494:LYS:HE2	3:J:494:LYS:HA	2.02	0.42
1:A:375:PHE:N	1:A:375:PHE:CD1	2.87	0.41
1:D:37:ARG:CG	1:D:38:PRO:HD3	2.47	0.41
1:F:287:ILE:HA	1:F:290:ARG:NH1	2.35	0.41
3:G:623:GLY:O	3:G:624:PHE:HB3	2.19	0.41
1:I:202:THR:OG1	1:I:205:GLU:OE1	2.37	0.41
1:E:62:ARG:O	1:E:64:ILE:N	2.53	0.41
1:D:171:LEU:O	1:D:172:PRO:C	2.62	0.41
1:F:38:PRO:HD3	1:F:49:GLN:OE1	2.21	0.41
3:J:630:TYR:CD2	3:J:677:VAL:HG22	2.55	0.41
3:J:645:TRP:O	3:J:646:PRO:C	2.63	0.41
1:E:38:PRO:HD3	1:E:49:GLN:OE1	2.21	0.41
1:E:157:ASP:CB	4:E:376:ADP:O3B	2.60	0.41
1:F:135:ALA:HB1	1:F:140:LEU:HD11	2.02	0.41
1:A:117:GLU:OE1	1:A:117:GLU:N	2.54	0.41
1:A:171:LEU:O	1:A:172:PRO:C	2.62	0.41
3:C:414:PHE:O	3:C:418:THR:N	2.51	0.41
1:E:135:ALA:HB1	1:E:140:LEU:HD11	2.02	0.41
1:F:157:ASP:CB	4:F:376:ADP:O3B	2.60	0.41
1:F:202:THR:OG1	1:F:205:GLU:OE1	2.37	0.41
1:F:375:PHE:CD1	1:F:375:PHE:N	2.88	0.41
3:G:414:PHE:O	3:G:418:THR:N	2.51	0.41
3:C:645:TRP:O	3:C:646:PRO:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:GLU:OE1	1:F:117:GLU:N	2.54	0.41
2:H:222:GLU:OE1	3:J:286:GLU:CB	2.68	0.41
1:I:171:LEU:CB	1:I:172:PRO:HD2	2.44	0.41
1:I:325:MET:SD	1:I:325:MET:N	2.92	0.41
1:I:375:PHE:N	1:I:375:PHE:CD1	2.88	0.41
3:J:142:LEU:HD13	3:J:142:LEU:C	2.46	0.41
1:A:54:VAL:O	1:A:57:GLU:HB3	2.21	0.41
1:D:54:VAL:O	1:D:57:GLU:HB3	2.21	0.41
1:D:62:ARG:O	1:D:64:ILE:N	2.53	0.41
1:E:345:ILE:O	1:E:349:LEU:HG	2.20	0.41
3:G:223:ALA:N	3:G:224:PRO:CD	2.84	0.41
3:G:494:LYS:HE2	3:G:494:LYS:HA	2.02	0.41
1:I:62:ARG:O	1:I:64:ILE:N	2.53	0.41
1:A:6:THR:HG23	1:A:22:ALA:HB2	2.02	0.41
1:A:170:ALA:CB	1:D:41:GLN:NE2	2.70	0.41
3:C:142:LEU:HD13	3:C:142:LEU:C	2.46	0.41
1:D:287:ILE:HA	1:D:290:ARG:NH1	2.36	0.41
1:E:287:ILE:HA	1:E:290:ARG:NH1	2.36	0.41
3:G:181:ASN:OD1	3:G:362:ASN:ND2	2.54	0.41
3:G:417:LEU:O	3:G:421:SER:OG	2.33	0.41
3:J:79:ALA:O	3:J:83:ASP:N	2.53	0.41
1:A:62:ARG:O	1:A:64:ILE:N	2.53	0.41
3:C:79:ALA:O	3:C:83:ASP:N	2.53	0.41
3:C:181:ASN:OD1	3:C:362:ASN:ND2	2.54	0.41
3:C:498:ILE:HD12	3:C:504:ARG:HB2	2.03	0.41
3:C:532:ILE:HG23	3:C:547:PHE:CE2	2.56	0.41
1:D:22:ALA:HB3	3:J:557:LYS:HE2	2.02	0.41
1:D:135:ALA:HB1	1:D:140:LEU:HD11	2.02	0.41
1:D:171:LEU:CB	1:D:172:PRO:HD2	2.44	0.41
1:E:325:MET:SD	1:E:325:MET:N	2.92	0.41
3:G:142:LEU:HD13	3:G:142:LEU:C	2.46	0.41
3:G:532:ILE:HG23	3:G:547:PHE:CE2	2.56	0.41
2:H:222:GLU:OE1	3:J:286:GLU:CA	2.64	0.41
1:I:135:ALA:HB1	1:I:140:LEU:HD11	2.02	0.41
3:J:181:ASN:OD1	3:J:362:ASN:ND2	2.54	0.41
1:A:345:ILE:O	1:A:349:LEU:HG	2.20	0.41
1:F:50:LYS:O	1:F:52:SER:N	2.54	0.41
1:F:163:VAL:HA	1:F:175:ILE:HG22	2.03	0.41
1:I:50:LYS:O	1:I:52:SER:N	2.54	0.41
3:J:532:ILE:HG23	3:J:547:PHE:CE2	2.56	0.41
1:A:41:GLN:HE22	1:I:170:ALA:CB	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ALA:HB1	1:A:140:LEU:HD11	2.02	0.40
3:C:621:ARG:O	3:C:622:ALA:HB2	2.21	0.40
1:D:37:ARG:HG3	1:D:38:PRO:CD	2.48	0.40
1:D:38:PRO:HD3	1:D:49:GLN:OE1	2.21	0.40
1:E:50:LYS:O	1:E:52:SER:N	2.54	0.40
3:G:79:ALA:O	3:G:83:ASP:N	2.53	0.40
1:I:287:ILE:HA	1:I:290:ARG:NH1	2.35	0.40
1:A:50:LYS:O	1:A:52:SER:N	2.54	0.40
1:A:163:VAL:HA	1:A:175:ILE:HG22	2.03	0.40
2:B:169:LEU:HD22	2:H:165:VAL:HG13	2.04	0.40
1:D:163:VAL:HA	1:D:175:ILE:HG22	2.03	0.40
1:D:345:ILE:O	1:D:349:LEU:HG	2.20	0.40
3:G:390:PHE:CZ	3:G:392:VAL:HG23	2.57	0.40
1:I:38:PRO:HD3	1:I:49:GLN:OE1	2.21	0.40
1:A:372:ARG:CZ	1:A:372:ARG:HA	2.51	0.40
1:D:372:ARG:HA	1:D:372:ARG:CZ	2.51	0.40
1:E:163:VAL:HA	1:E:175:ILE:HG22	2.03	0.40
1:E:372:ARG:CZ	1:E:372:ARG:HA	2.51	0.40
1:I:117:GLU:OE1	1:I:117:GLU:N	2.54	0.40
1:A:287:ILE:HA	1:A:290:ARG:NH1	2.36	0.40
3:C:390:PHE:CZ	3:C:392:VAL:HG23	2.57	0.40
1:E:123:MET:SD	1:E:123:MET:N	2.95	0.40
1:I:123:MET:N	1:I:123:MET:SD	2.95	0.40
3:J:223:ALA:N	3:J:224:PRO:CD	2.84	0.40
3:J:390:PHE:CZ	3:J:392:VAL:HG23	2.57	0.40
3:J:498:ILE:HD12	3:J:504:ARG:HB2	2.03	0.40
3:C:615:GLU:OE1	3:C:615:GLU:N	2.54	0.40
1:D:50:LYS:O	1:D:52:SER:N	2.55	0.40
1:E:54:VAL:O	1:E:57:GLU:HB3	2.21	0.40
1:F:345:ILE:O	1:F:349:LEU:HG	2.20	0.40
3:G:621:ARG:O	3:G:622:ALA:HB2	2.22	0.40
1:I:54:VAL:O	1:I:57:GLU:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	10
1	D	372/375 (99%)	288 (77%)	56 (15%)	28 (8%)	1	10
1	E	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	10
1	F	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	10
1	I	372/375 (99%)	289 (78%)	55 (15%)	28 (8%)	1	10
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	687/697 (99%)	574 (84%)	78 (11%)	35 (5%)	1	15
3	G	687/697 (99%)	573 (83%)	80 (12%)	34 (5%)	1	16
3	J	687/697 (99%)	574 (84%)	79 (12%)	34 (5%)	1	16
All	All	4189/4238 (99%)	3433 (82%)	513 (12%)	243 (6%)	2	14

All (243) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	GLY
1	A	43	VAL
1	A	47	MET
1	A	49	GLN
1	A	51	ASP
1	A	52	SER
1	A	56	ASP
1	A	63	GLY
1	A	137	GLN
3	C	59	GLU
3	C	326	SER
3	C	329	VAL
3	C	331	LYS
3	C	335	VAL
3	C	519	PHE
3	C	530	ASP
1	D	42	GLY
1	D	43	VAL
1	D	47	MET
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	51	ASP
1	D	52	SER
1	D	56	ASP
1	D	63	GLY
1	D	137	GLN
1	E	42	GLY
1	E	43	VAL
1	E	47	MET
1	E	49	GLN
1	E	51	ASP
1	E	52	SER
1	E	56	ASP
1	E	63	GLY
1	E	137	GLN
1	F	42	GLY
1	F	43	VAL
1	F	47	MET
1	F	49	GLN
1	F	51	ASP
1	F	52	SER
1	F	56	ASP
1	F	63	GLY
1	F	137	GLN
3	G	59	GLU
3	G	326	SER
3	G	329	VAL
3	G	331	LYS
3	G	335	VAL
3	G	519	PHE
3	G	530	ASP
1	I	42	GLY
1	I	43	VAL
1	I	47	MET
1	I	49	GLN
1	I	51	ASP
1	I	52	SER
1	I	56	ASP
1	I	63	GLY
1	I	137	GLN
3	J	59	GLU
3	J	326	SER
3	J	329	VAL

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Mol	Chain	Res	Type
3	J	331	LYS
3	J	335	VAL
3	J	519	PHE
3	J	530	ASP
1	A	2	GLU
1	A	35	VAL
1	A	41	GLN
1	A	44	MET
1	A	48	GLY
1	A	55	GLY
1	A	167	GLU
1	A	171	LEU
1	A	173	HIS
1	A	245	GLY
3	C	42	GLY
3	C	76	HIS
3	C	92	GLN
3	C	107	LYS
3	C	283	GLU
3	C	560	GLU
3	C	622	ALA
3	C	624	PHE
1	D	2	GLU
1	D	35	VAL
1	D	41	GLN
1	D	44	MET
1	D	48	GLY
1	D	55	GLY
1	D	167	GLU
1	D	171	LEU
1	D	173	HIS
1	D	245	GLY
1	E	2	GLU
1	E	35	VAL
1	E	41	GLN
1	E	44	MET
1	E	48	GLY
1	E	55	GLY
1	E	167	GLU
1	E	171	LEU
1	E	245	GLY
1	F	2	GLU

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Mol	Chain	Res	Type
1	F	35	VAL
1	F	41	GLN
1	F	44	MET
1	F	48	GLY
1	F	55	GLY
1	F	167	GLU
1	F	171	LEU
1	F	173	HIS
1	F	245	GLY
3	G	42	GLY
3	G	76	HIS
3	G	92	GLN
3	G	283	GLU
3	G	560	GLU
3	G	622	ALA
3	G	624	PHE
1	I	2	GLU
1	I	35	VAL
1	I	41	GLN
1	I	44	MET
1	I	48	GLY
1	I	55	GLY
1	I	167	GLU
1	I	171	LEU
1	I	173	HIS
1	I	245	GLY
3	J	42	GLY
3	J	76	HIS
3	J	92	GLN
3	J	283	GLU
3	J	560	GLU
3	J	622	ALA
3	J	624	PHE
1	A	6	THR
1	A	38	PRO
3	C	12	ASP
3	C	380	PRO
3	C	468	SER
3	C	636	ARG
3	C	646	PRO
1	D	6	THR
1	D	38	PRO

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Mol	Chain	Res	Type
1	E	6	THR
1	E	38	PRO
1	E	173	HIS
1	F	6	THR
1	F	38	PRO
3	G	12	ASP
3	G	380	PRO
3	G	468	SER
3	G	636	ARG
1	I	6	THR
1	I	38	PRO
3	J	12	ASP
3	J	380	PRO
3	J	468	SER
3	J	636	ARG
1	A	53	TYR
3	C	257	GLY
3	C	282	ALA
3	C	290	GLY
3	C	455	LEU
3	C	486	HIS
3	C	550	THR
3	C	551	ARG
1	D	53	TYR
1	E	53	TYR
1	F	53	TYR
3	G	257	GLY
3	G	282	ALA
3	G	290	GLY
3	G	455	LEU
3	G	486	HIS
3	G	550	THR
3	G	551	ARG
3	G	646	PRO
1	I	53	TYR
3	J	257	GLY
3	J	282	ALA
3	J	290	GLY
3	J	455	LEU
3	J	486	HIS
3	J	550	THR
3	J	551	ARG

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Mol	Chain	Res	Type
3	J	646	PRO
1	A	158	GLY
1	A	172	PRO
3	C	330	GLY
3	C	524	LYS
1	D	158	GLY
1	D	172	PRO
1	E	158	GLY
1	E	172	PRO
1	F	158	GLY
1	F	172	PRO
3	G	330	GLY
3	G	524	LYS
1	I	158	GLY
1	I	172	PRO
3	J	330	GLY
3	J	524	LYS
1	A	15	GLY
1	A	70	PRO
3	C	549	PRO
3	C	635	ASN
1	D	15	GLY
1	D	70	PRO
1	E	15	GLY
1	E	70	PRO
1	F	15	GLY
1	F	70	PRO
3	G	549	PRO
3	G	635	ASN
1	I	15	GLY
1	I	70	PRO
3	J	549	PRO
3	J	635	ASN
3	C	126	SER
3	C	208	GLY
3	G	126	SER
3	G	208	GLY
3	J	126	SER
3	J	208	GLY
3	C	453	ILE
3	C	681	ASN
3	G	453	ILE

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Mol	Chain	Res	Type
3	G	681	ASN
3	J	453	ILE
3	J	681	ASN
1	A	102	PRO
1	A	251	GLY
1	D	102	PRO
1	D	251	GLY
1	E	102	PRO
1	E	251	GLY
1	F	102	PRO
1	F	251	GLY
1	I	102	PRO
1	I	251	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/317 (100%)	292 (92%)	25 (8%)	11	32
1	D	317/317 (100%)	291 (92%)	26 (8%)	10	31
1	E	317/317 (100%)	288 (91%)	29 (9%)	9	27
1	F	317/317 (100%)	288 (91%)	29 (9%)	9	27
1	I	317/317 (100%)	288 (91%)	29 (9%)	9	27
2	B	118/118 (100%)	118 (100%)	0	100	100
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	576 (95%)	33 (5%)	20	41
3	G	609/616 (99%)	573 (94%)	36 (6%)	18	39
3	J	609/616 (99%)	573 (94%)	36 (6%)	18	39
All	All	3648/3669 (99%)	3405 (93%)	243 (7%)	17	36

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	39	ARG
1	A	41	GLN
1	A	47	MET
1	A	49	GLN
1	A	50	LYS
1	A	52	SER
1	A	53	TYR
1	A	87	HIS
1	A	113	LYS
1	A	151	ILE
1	A	165	ILE
1	A	166	TYR
1	A	171	LEU
1	A	183	ARG
1	A	192	ILE
1	A	193	LEU
1	A	196	ARG
1	A	236	LEU
1	A	238	LYS
1	A	246	GLN
1	A	261	LEU
1	A	291	LYS
1	A	340	TRP
1	A	375	PHE
3	C	19	ILE
3	C	39	THR
3	C	41	ILE
3	C	54	LEU
3	C	58	LYS
3	C	90	GLN
3	C	91	SER
3	C	94	ASN
3	C	107	LYS
3	C	143	LEU
3	C	152	LEU
3	C	178	LYS
3	C	184	LEU
3	C	325	ILE
3	C	331	LYS
3	C	338	VAL
3	C	356	LEU
3	C	373	ASN

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Mol	Chain	Res	Type
3	C	395	ASN
3	C	410	LEU
3	C	434	LYS
3	C	439	PHE
3	C	442	LYS
3	C	459	LEU
3	C	467	LYS
3	C	508	TYR
3	C	550	THR
3	C	551	ARG
3	C	573	LEU
3	C	624	PHE
3	C	636	ARG
3	C	653	LYS
3	C	667	LYS
1	D	2	GLU
1	D	37	ARG
1	D	39	ARG
1	D	41	GLN
1	D	49	GLN
1	D	52	SER
1	D	53	TYR
1	D	113	LYS
1	D	148	THR
1	D	151	ILE
1	D	165	ILE
1	D	166	TYR
1	D	171	LEU
1	D	183	ARG
1	D	192	ILE
1	D	193	LEU
1	D	196	ARG
1	D	236	LEU
1	D	238	LYS
1	D	246	GLN
1	D	261	LEU
1	D	291	LYS
1	D	326	LYS
1	D	328	LYS
1	D	340	TRP
1	D	375	PHE
1	E	2	GLU

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Mol	Chain	Res	Type
1	E	37	ARG
1	E	39	ARG
1	E	41	GLN
1	E	47	MET
1	E	49	GLN
1	E	50	LYS
1	E	52	SER
1	E	53	TYR
1	E	87	HIS
1	E	113	LYS
1	E	148	THR
1	E	151	ILE
1	E	165	ILE
1	E	166	TYR
1	E	171	LEU
1	E	183	ARG
1	E	192	ILE
1	E	193	LEU
1	E	196	ARG
1	E	236	LEU
1	E	238	LYS
1	E	246	GLN
1	E	261	LEU
1	E	291	LYS
1	E	326	LYS
1	E	328	LYS
1	E	340	TRP
1	E	375	PHE
1	F	2	GLU
1	F	37	ARG
1	F	39	ARG
1	F	41	GLN
1	F	47	MET
1	F	49	GLN
1	F	50	LYS
1	F	52	SER
1	F	53	TYR
1	F	87	HIS
1	F	113	LYS
1	F	148	THR
1	F	151	ILE
1	F	165	ILE

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Mol	Chain	Res	Type
1	F	166	TYR
1	F	171	LEU
1	F	183	ARG
1	F	192	ILE
1	F	193	LEU
1	F	196	ARG
1	F	236	LEU
1	F	238	LYS
1	F	246	GLN
1	F	261	LEU
1	F	291	LYS
1	F	326	LYS
1	F	328	LYS
1	F	340	TRP
1	F	375	PHE
3	G	19	ILE
3	G	39	THR
3	G	41	ILE
3	G	54	LEU
3	G	58	LYS
3	G	90	GLN
3	G	91	SER
3	G	94	ASN
3	G	143	LEU
3	G	152	LEU
3	G	178	LYS
3	G	184	LEU
3	G	325	ILE
3	G	331	LYS
3	G	335	VAL
3	G	336	ILE
3	G	338	VAL
3	G	356	LEU
3	G	373	ASN
3	G	395	ASN
3	G	410	LEU
3	G	434	LYS
3	G	439	PHE
3	G	442	LYS
3	G	459	LEU
3	G	467	LYS
3	G	496	ARG

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Mol	Chain	Res	Type
3	G	508	TYR
3	G	550	THR
3	G	551	ARG
3	G	560	GLU
3	G	573	LEU
3	G	624	PHE
3	G	636	ARG
3	G	653	LYS
3	G	667	LYS
1	I	2	GLU
1	I	37	ARG
1	I	39	ARG
1	I	41	GLN
1	I	47	MET
1	I	49	GLN
1	I	50	LYS
1	I	52	SER
1	I	53	TYR
1	I	87	HIS
1	I	113	LYS
1	I	148	THR
1	I	151	ILE
1	I	165	ILE
1	I	166	TYR
1	I	171	LEU
1	I	183	ARG
1	I	192	ILE
1	I	193	LEU
1	I	196	ARG
1	I	236	LEU
1	I	238	LYS
1	I	246	GLN
1	I	261	LEU
1	I	291	LYS
1	I	326	LYS
1	I	328	LYS
1	I	340	TRP
1	I	375	PHE
3	J	19	ILE
3	J	39	THR
3	J	41	ILE
3	J	54	LEU

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Mol	Chain	Res	Type
3	J	58	LYS
3	J	90	GLN
3	J	91	SER
3	J	94	ASN
3	J	143	LEU
3	J	152	LEU
3	J	178	LYS
3	J	184	LEU
3	J	325	ILE
3	J	331	LYS
3	J	335	VAL
3	J	336	ILE
3	J	338	VAL
3	J	356	LEU
3	J	373	ASN
3	J	395	ASN
3	J	410	LEU
3	J	434	LYS
3	J	439	PHE
3	J	442	LYS
3	J	459	LEU
3	J	467	LYS
3	J	496	ARG
3	J	508	TYR
3	J	550	THR
3	J	551	ARG
3	J	560	GLU
3	J	573	LEU
3	J	624	PHE
3	J	636	ARG
3	J	653	LYS
3	J	667	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	88	HIS
1	A	137	GLN
1	A	246	GLN
2	B	103	GLN
2	B	153	HIS

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Mol	Chain	Res	Type
3	C	18	GLN
3	C	36	ASN
3	C	66	ASN
3	C	76	HIS
3	C	167	GLN
3	C	200	HIS
3	C	204	GLN
3	C	275	HIS
3	C	313	GLN
3	C	344	GLN
3	C	362	ASN
3	C	395	ASN
3	C	396	ASN
3	C	402	ASN
1	D	41	GLN
1	D	87	HIS
1	D	88	HIS
1	D	137	GLN
1	D	246	GLN
1	D	354	GLN
1	E	41	GLN
1	E	88	HIS
1	E	137	GLN
1	E	246	GLN
1	E	354	GLN
1	F	88	HIS
1	F	137	GLN
1	F	246	GLN
1	F	354	GLN
3	G	18	GLN
3	G	36	ASN
3	G	66	ASN
3	G	76	HIS
3	G	167	GLN
3	G	200	HIS
3	G	275	HIS
3	G	313	GLN
3	G	362	ASN
3	G	395	ASN
3	G	396	ASN
3	G	402	ASN
3	G	568	ASN

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Mol	Chain	Res	Type
2	H	210	GLN
1	I	88	HIS
1	I	137	GLN
1	I	246	GLN
1	I	354	GLN
3	J	18	GLN
3	J	27	ASN
3	J	36	ASN
3	J	66	ASN
3	J	76	HIS
3	J	167	GLN
3	J	200	HIS
3	J	275	HIS
3	J	313	GLN
3	J	362	ASN
3	J	395	ASN
3	J	396	ASN
3	J	402	ASN
3	J	568	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	HIC	E	73	1	10,11,12	1.63	1 (10%)	9,14,16	2.86	3 (33%)
1	HIC	A	73	1	10,11,12	1.63	1 (10%)	9,14,16	2.86	3 (33%)
1	HIC	F	73	1	10,11,12	1.63	2 (20%)	9,14,16	2.88	3 (33%)
1	HIC	I	73	1	10,11,12	1.63	2 (20%)	9,14,16	2.87	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HIC	D	73	1	10,11,12	1.62	1 (10%)	9,14,16	2.85	3 (33%)

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
1	HIC	E	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	2/5/6/8	0/1/1/1
1	HIC	F	73	1	-	2/5/6/8	0/1/1/1
1	HIC	I	73	1	-	2/5/6/8	0/1/1/1
1	HIC	D	73	1	-	2/5/6/8	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	HIC	CA-N	3.05	1.56	1.48
1	I	73	HIC	CA-N	3.04	1.56	1.48
1	F	73	HIC	CA-N	3.04	1.56	1.48
1	A	73	HIC	CA-N	3.04	1.56	1.48
1	D	73	HIC	CA-N	3.03	1.56	1.48
1	I	73	HIC	CE1-NE2	2.01	1.41	1.35
1	F	73	HIC	CE1-NE2	2.01	1.41	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	HIC	NE2-CE1-ND1	-7.31	109.86	112.66
1	I	73	HIC	NE2-CE1-ND1	-7.29	109.87	112.66
1	A	73	HIC	NE2-CE1-ND1	-7.25	109.89	112.66
1	D	73	HIC	NE2-CE1-ND1	-7.23	109.89	112.66
1	E	73	HIC	NE2-CE1-ND1	-7.23	109.89	112.66
1	E	73	HIC	CD2-NE2-CE1	3.41	108.06	106.71
1	F	73	HIC	CD2-NE2-CE1	3.37	108.04	106.71
1	I	73	HIC	CD2-NE2-CE1	3.33	108.03	106.71
1	D	73	HIC	CD2-NE2-CE1	3.33	108.03	106.71
1	A	73	HIC	CD2-NE2-CE1	3.32	108.02	106.71
1	I	73	HIC	CA-CB-CG	-2.20	108.33	113.77
1	D	73	HIC	CA-CB-CG	-2.19	108.37	113.77
1	F	73	HIC	CA-CB-CG	-2.19	108.37	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	HIC	CA-CB-CG	-2.19	108.37	113.77
1	E	73	HIC	CA-CB-CG	-2.17	108.41	113.77

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	N-CA-CB-CG
1	A	73	HIC	C-CA-CB-CG
1	D	73	HIC	N-CA-CB-CG
1	D	73	HIC	C-CA-CB-CG
1	E	73	HIC	N-CA-CB-CG
1	E	73	HIC	C-CA-CB-CG
1	F	73	HIC	N-CA-CB-CG
1	F	73	HIC	C-CA-CB-CG
1	I	73	HIC	N-CA-CB-CG
1	I	73	HIC	C-CA-CB-CG

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	73	HIC	2	0
1	A	73	HIC	2	0
1	F	73	HIC	2	0
1	I	73	HIC	2	0
1	D	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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
4	ADP	E	376	-	28,29,29	1.12	2 (7%)	43,45,45	1.24	6 (13%)
4	ADP	D	376	-	28,29,29	1.13	2 (7%)	43,45,45	1.24	6 (13%)
4	ADP	F	376	-	28,29,29	1.12	2 (7%)	43,45,45	1.25	6 (13%)
4	ADP	I	376	-	28,29,29	1.12	2 (7%)	43,45,45	1.25	6 (13%)
4	ADP	A	376	-	28,29,29	1.13	2 (7%)	43,45,45	1.24	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	E	376	-	-	0/16/32/32	0/3/3/3
4	ADP	D	376	-	-	0/16/32/32	0/3/3/3
4	ADP	F	376	-	-	0/16/32/32	0/3/3/3
4	ADP	I	376	-	-	0/16/32/32	0/3/3/3
4	ADP	A	376	-	-	0/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	376	ADP	C5-N7	-3.26	1.33	1.39
4	E	376	ADP	C5-N7	-3.26	1.33	1.39
4	A	376	ADP	C5-N7	-3.24	1.33	1.39
4	F	376	ADP	C5-N7	-3.22	1.33	1.39
4	I	376	ADP	C5-N7	-3.22	1.33	1.39
4	A	376	ADP	C2-N1	3.15	1.39	1.33
4	D	376	ADP	C2-N1	3.13	1.39	1.33
4	I	376	ADP	C2-N1	3.12	1.39	1.33
4	F	376	ADP	C2-N1	3.11	1.39	1.33
4	E	376	ADP	C2-N1	3.07	1.39	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	376	ADP	C4-C5-N7	2.57	113.52	110.58
4	I	376	ADP	C4-C5-N7	2.55	113.50	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	376	ADP	C5-C4-N3	2.55	130.22	126.72
4	F	376	ADP	C4-C5-N7	2.54	113.49	110.58
4	E	376	ADP	C5-C4-N3	2.53	130.20	126.72
4	F	376	ADP	C5-C4-N3	2.52	130.19	126.72
4	A	376	ADP	C4-C5-N7	2.51	113.45	110.58
4	A	376	ADP	C5-C4-N3	2.49	130.15	126.72
4	D	376	ADP	C4-C5-N7	2.49	113.43	110.58
4	D	376	ADP	C5-C4-N3	2.49	130.14	126.72
4	A	376	ADP	C4-N9-C8	-2.32	103.30	105.74
4	I	376	ADP	C2-N1-C6	2.31	122.52	118.73
4	F	376	ADP	C4-N9-C8	-2.30	103.32	105.74
4	D	376	ADP	C4-N9-C8	-2.30	103.33	105.74
4	A	376	ADP	C2-N1-C6	2.29	122.50	118.73
4	E	376	ADP	C4-N9-C8	-2.29	103.33	105.74
4	F	376	ADP	C2-N1-C6	2.28	122.48	118.73
4	I	376	ADP	C4-N9-C8	-2.28	103.34	105.74
4	E	376	ADP	C2-N1-C6	2.28	122.47	118.73
4	D	376	ADP	C2-N1-C6	2.26	122.45	118.73
4	A	376	ADP	N3-C2-N1	-2.22	125.23	128.58
4	I	376	ADP	N3-C2-N1	-2.20	125.25	128.58
4	F	376	ADP	N3-C2-N1	-2.19	125.26	128.58
4	D	376	ADP	N3-C2-N1	-2.19	125.26	128.58
4	E	376	ADP	N3-C2-N1	-2.17	125.30	128.58
4	A	376	ADP	O3B-PB-O2B	2.11	115.71	107.80
4	F	376	ADP	O3B-PB-O2B	2.10	115.67	107.80
4	D	376	ADP	O3B-PB-O2B	2.10	115.66	107.80
4	E	376	ADP	O3B-PB-O2B	2.09	115.66	107.80
4	I	376	ADP	O3B-PB-O2B	2.08	115.61	107.80

There are no chirality outliers.

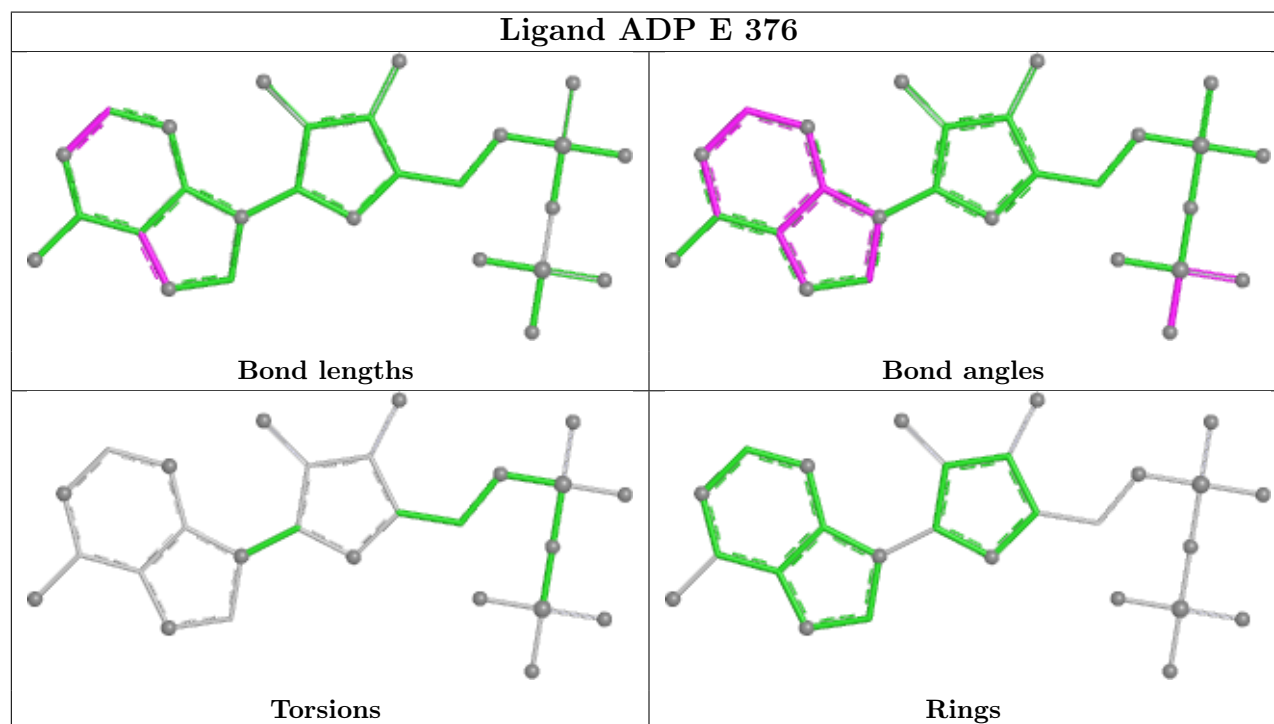
There are no torsion outliers.

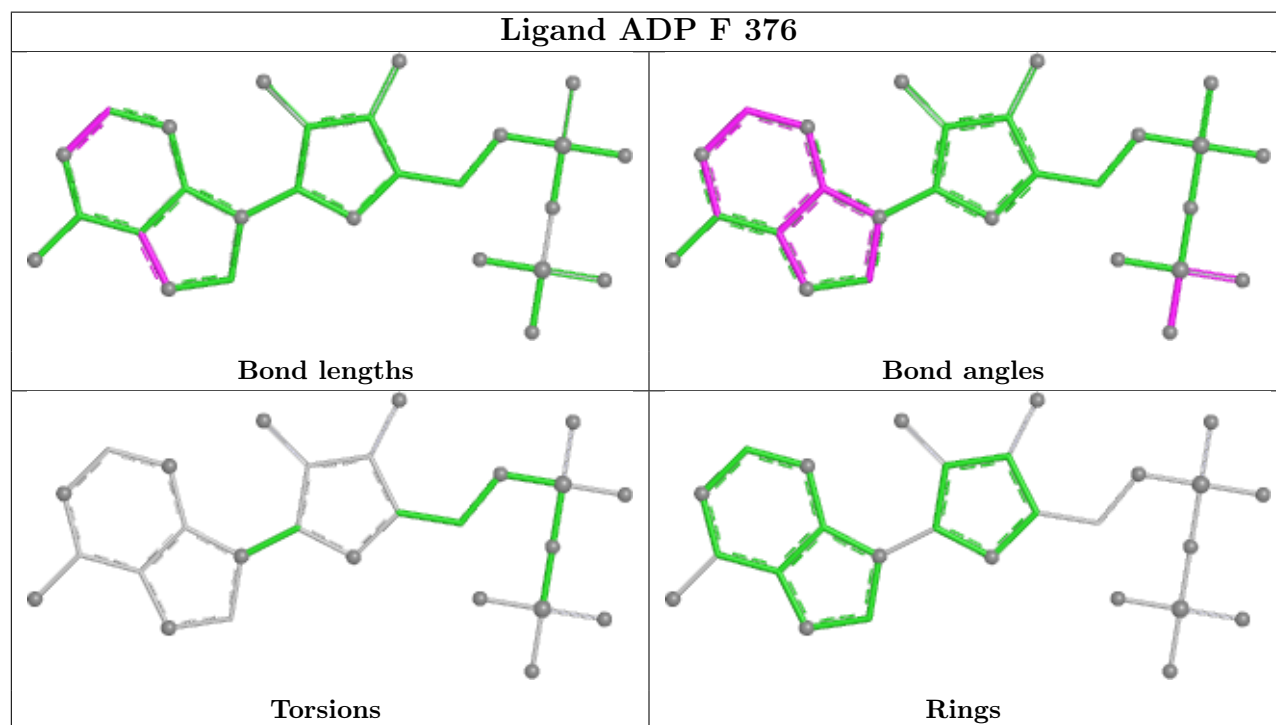
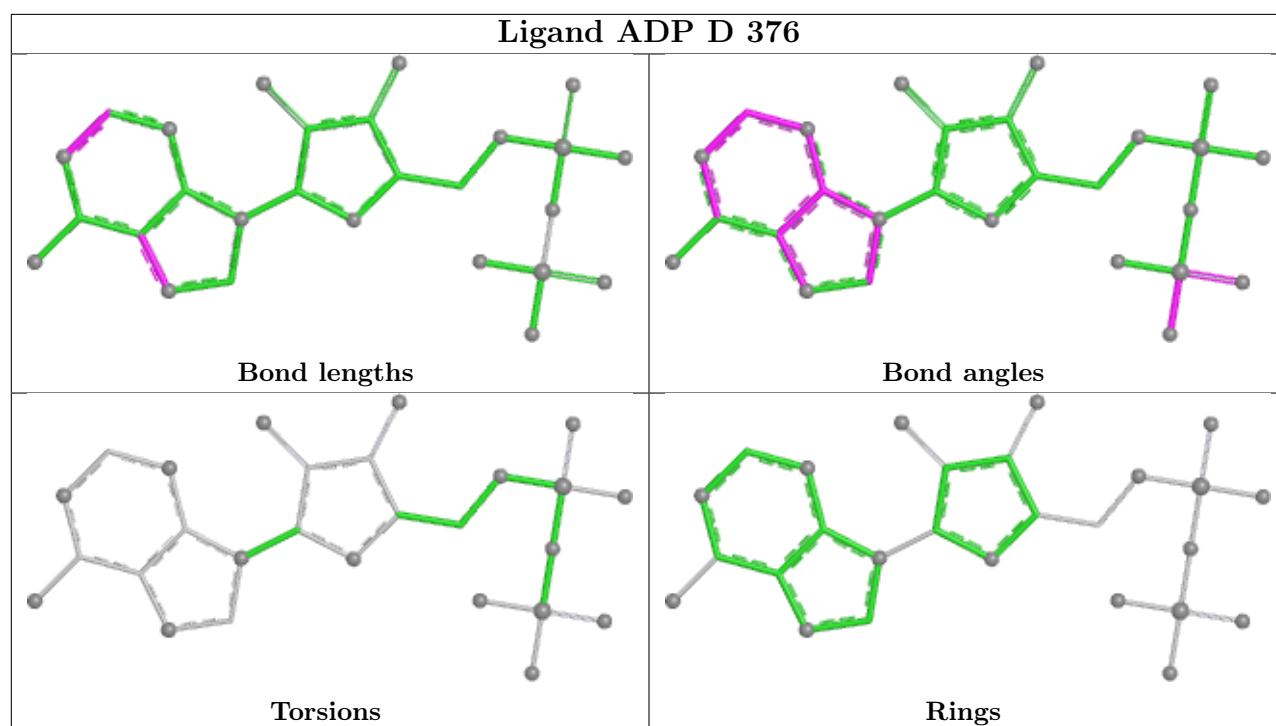
There are no ring outliers.

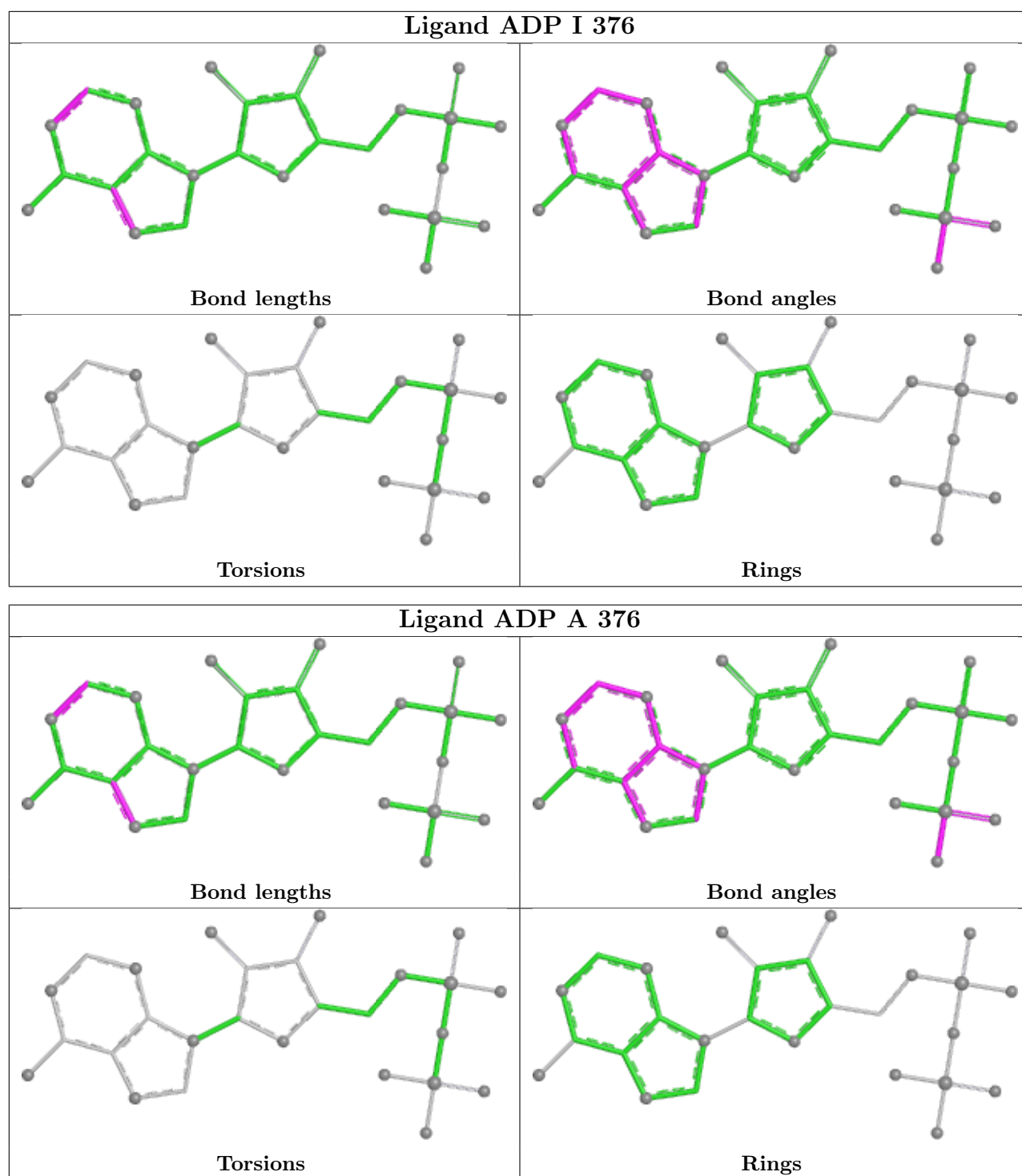
5 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	376	ADP	4	0
4	D	376	ADP	4	0
4	F	376	ADP	4	0
4	I	376	ADP	4	0
4	A	376	ADP	4	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 than 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.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1989. These allow visual inspection of the internal detail of the map and identification of artifacts.

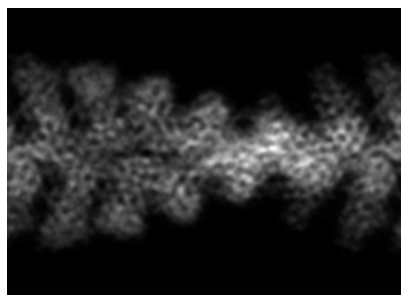
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

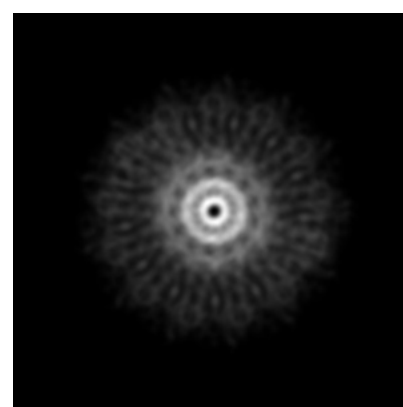
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 80



Y Index: 80



Z Index: 110

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

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 83



Y Index: 77

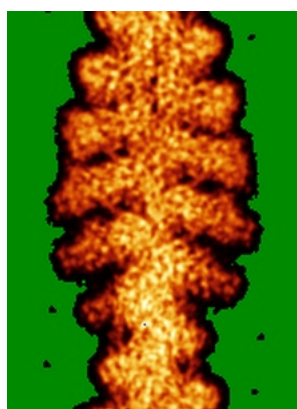


Z Index: 56

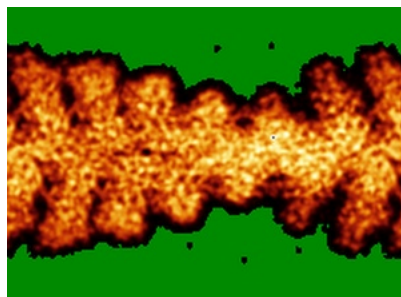
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

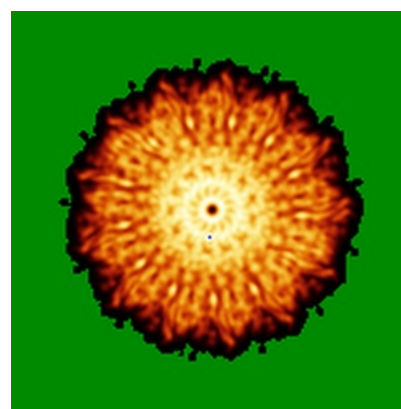
6.4.1 Primary map



X



Y

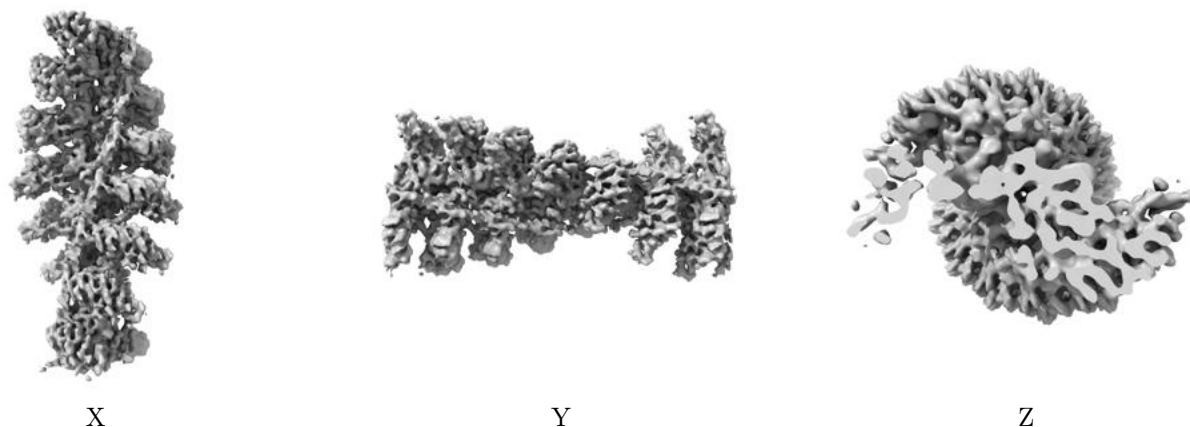


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

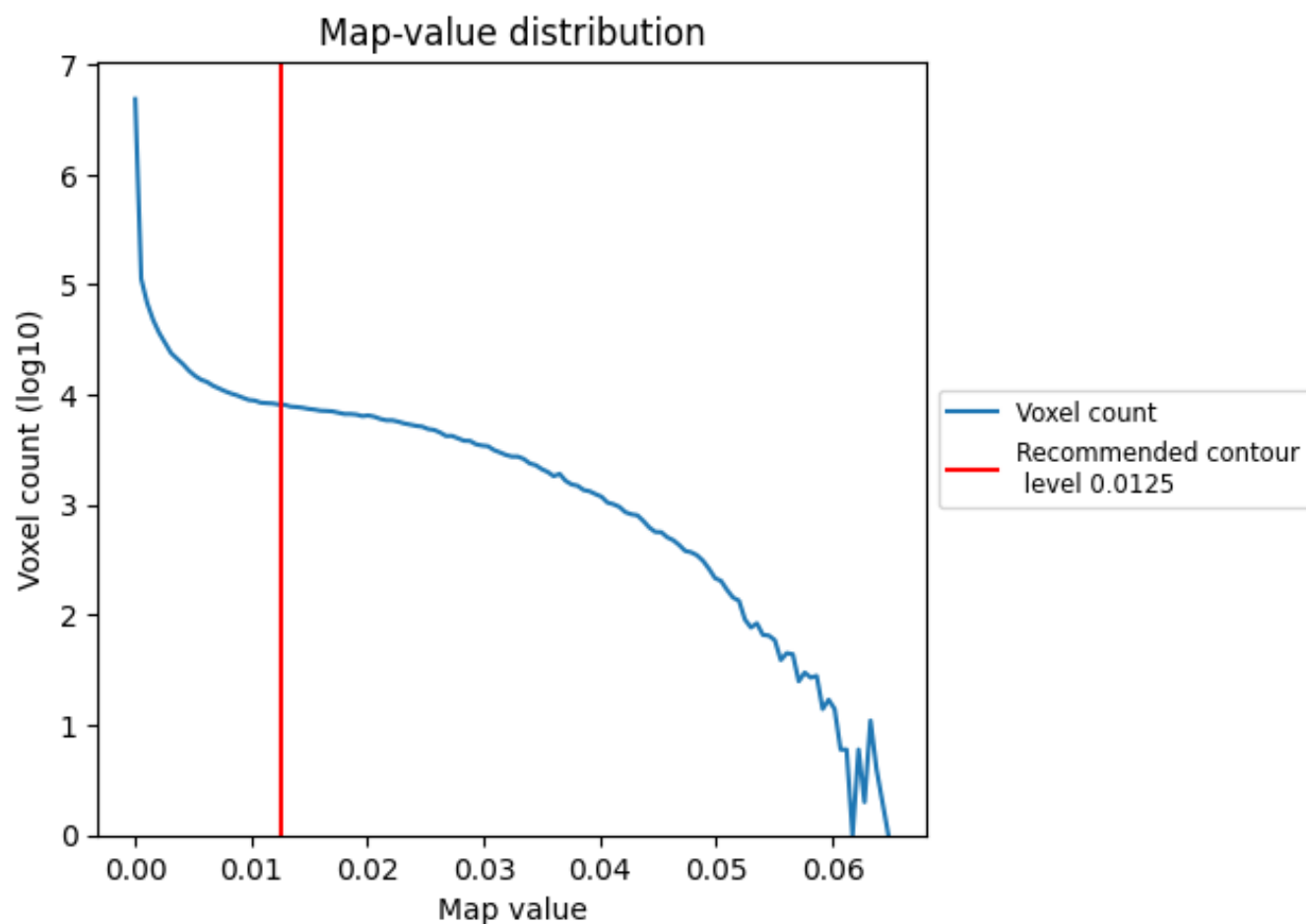
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

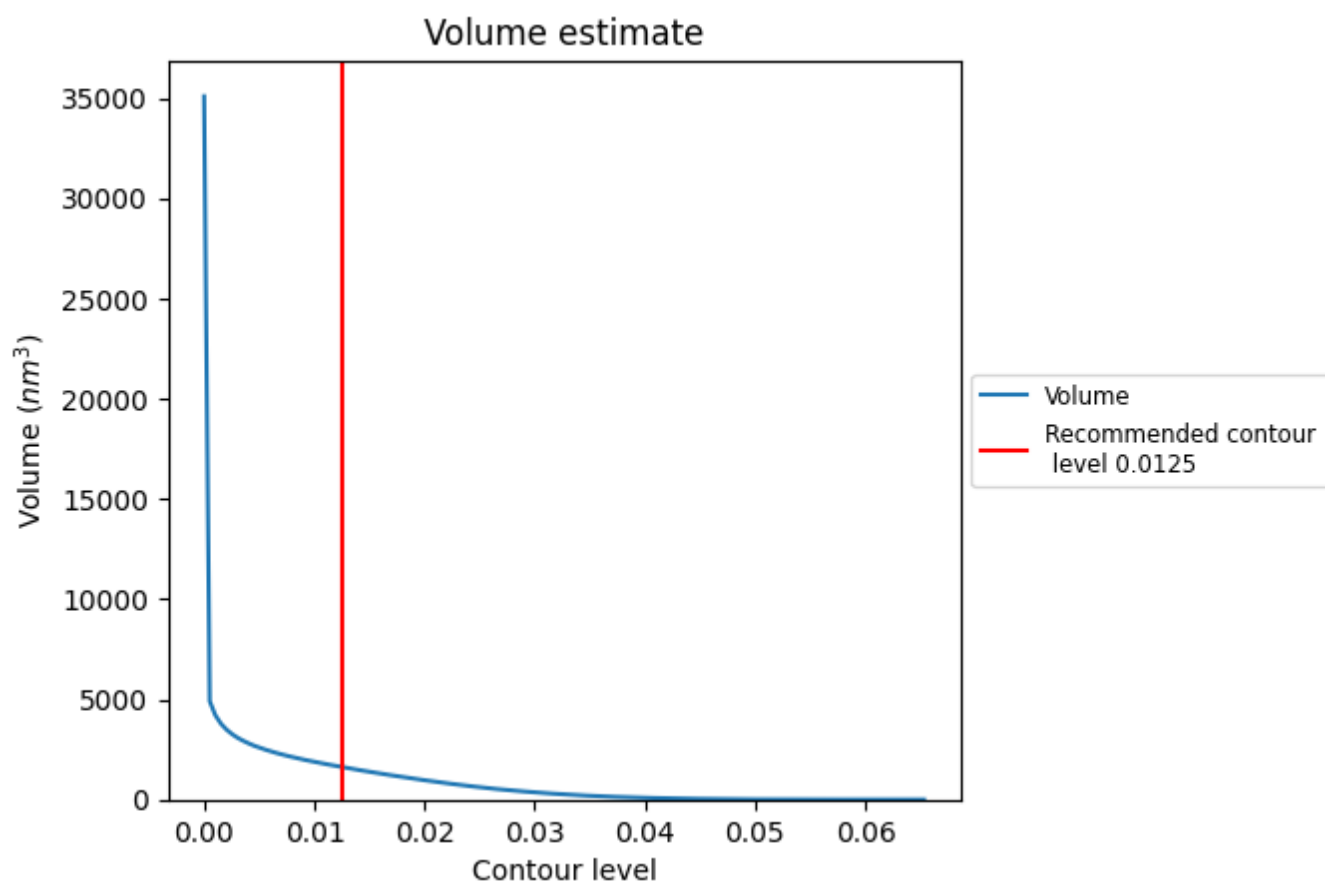
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1624 nm³; this corresponds to an approximate mass of 1467 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

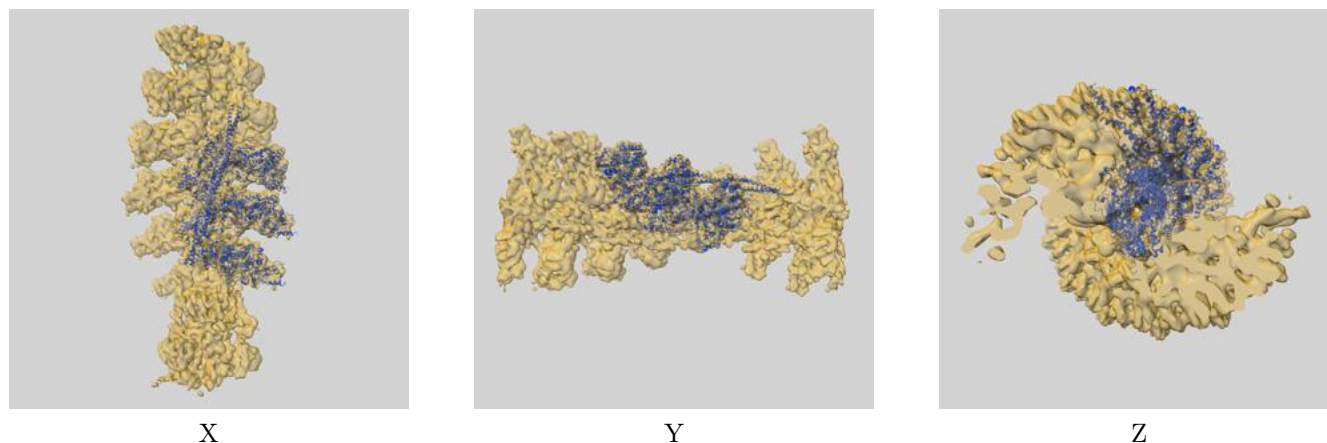
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1989 and PDB model 4A7L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

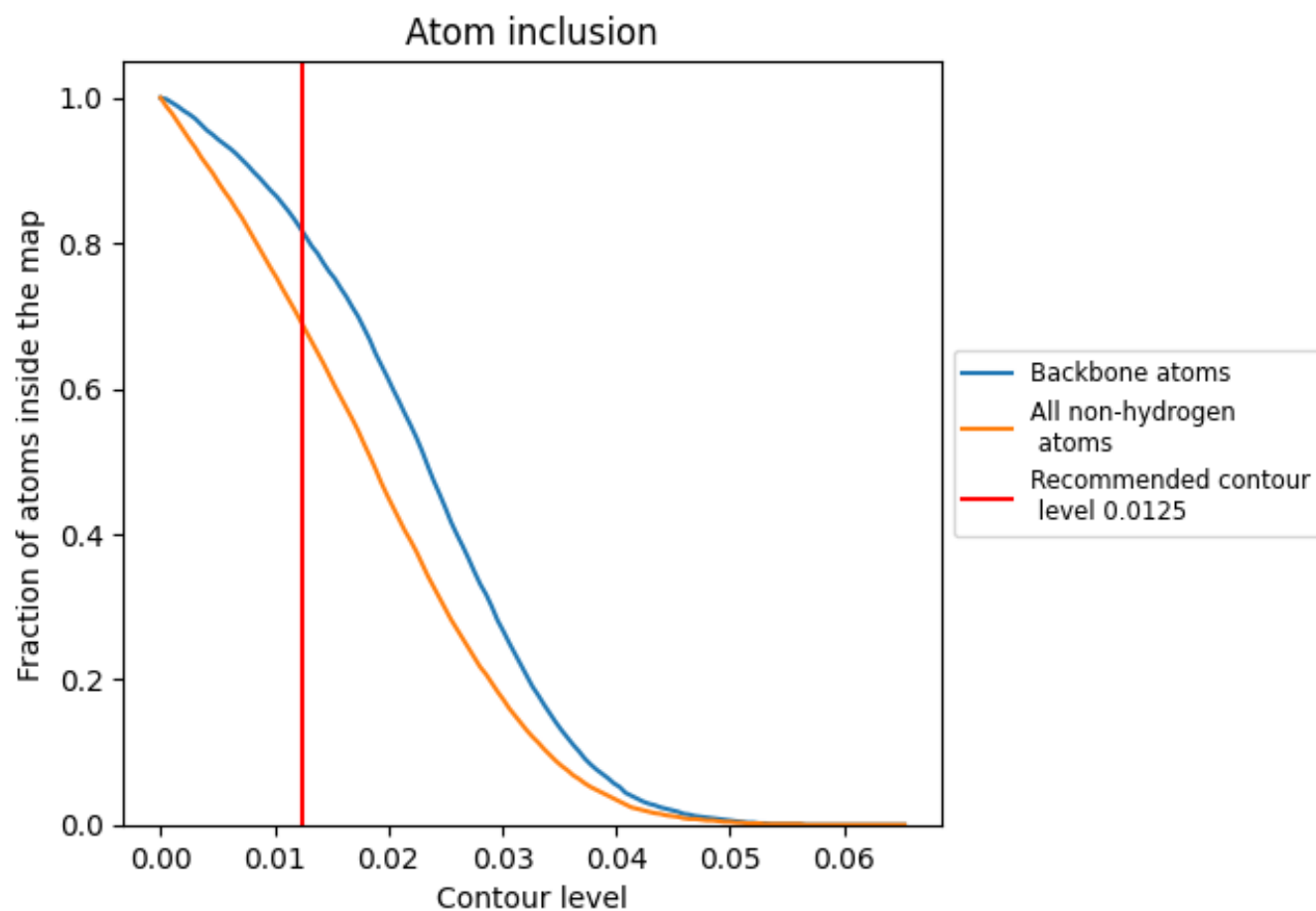


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 69% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6870	0.0880
A	0.8080	0.1160
B	0.6260	0.1070
C	0.5850	0.0650
D	0.8070	0.1120
E	0.8060	0.1130
F	0.8100	0.1120
G	0.5900	0.0650
H	0.6050	0.0780
I	0.8080	0.1130
J	0.5900	0.0650

1.0

0.0

<0.0