



Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 04:35 pm GMT

PDB ID : 4A7H
EMDB ID : EMD-1987
Title : Structure of the Actin-Tropomyosin-Myosin Complex (rigor ATM 2)
Authors : Behrmann, E.; Mueller, M.; Penczek, P.A.; Mannherz, H.G.; Manstein, D.J.;
Raunser, S.
Deposited on : 2011-11-14
Resolution : 7.80 Å (reported)
Based on initial models : 3MFP, 1LKX

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

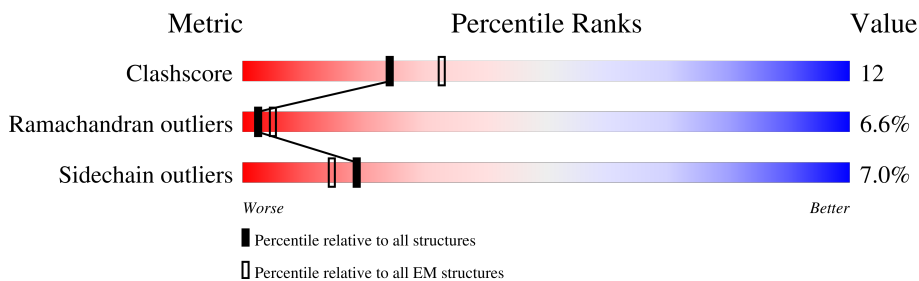
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.80 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
1	D	375	
1	E	375	
1	F	375	
1	G	375	
2	B	136	
2	H	136	
3	C	697	

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Mol	Chain	Length	Quality of chain
3	I	697	 <p>39% 78% 17% . .</p>
3	J	697	 <p>38% 77% 18% . .</p>

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 SKELETAL MUSCLE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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	G	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 2 is a protein called TROPOMYOSIN 1-ALPHA CHAIN.

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

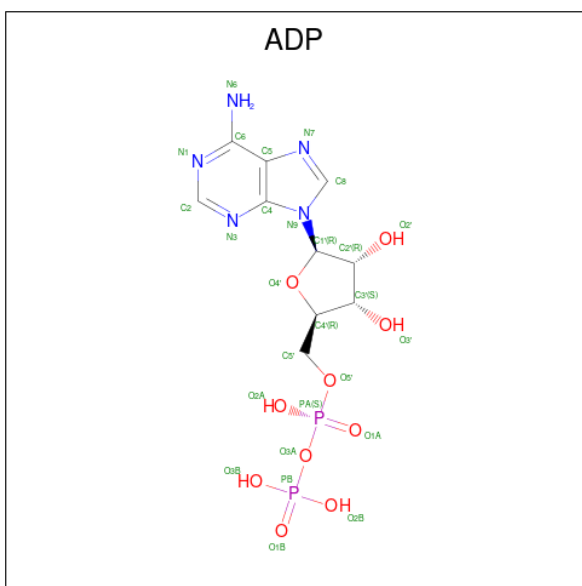
Chain	Residue	Modelled	Actual	Comment	Reference
C	77	MET	ILE	conflict	UNP Q03479

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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
I	77	MET	ILE	conflict	UNP Q03479
I	215	ASP	ASN	conflict	UNP Q03479
I	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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

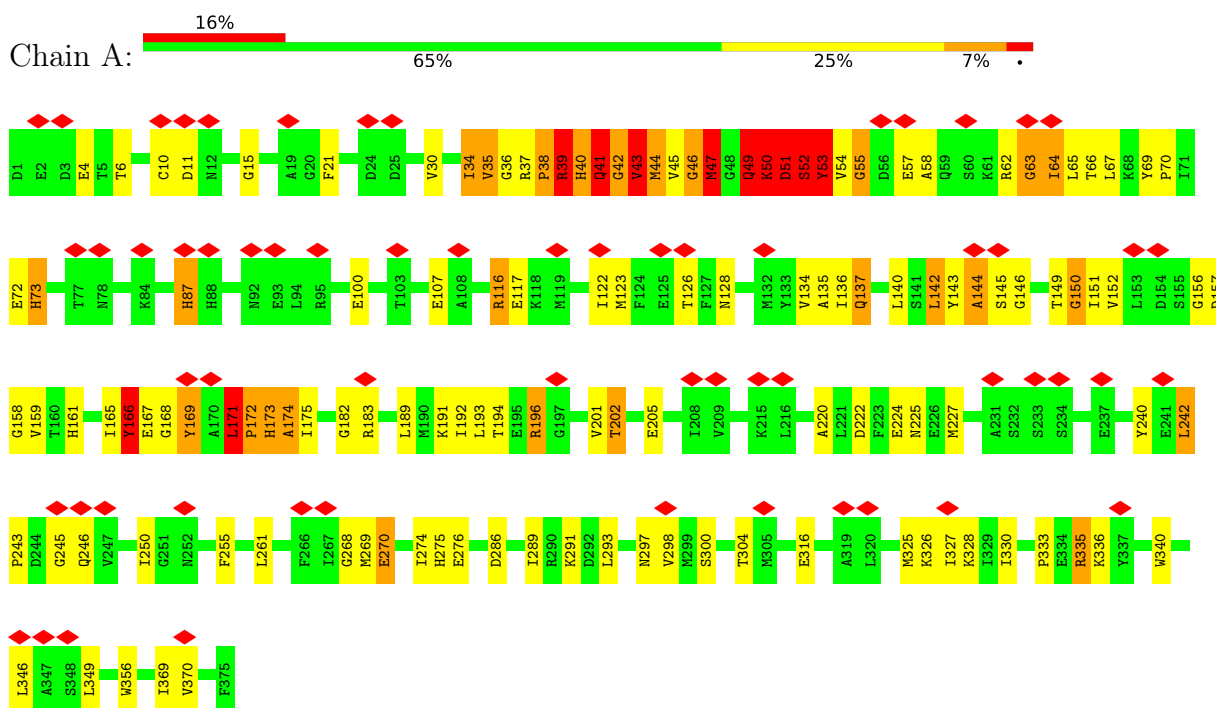
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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	G	1	Total 1	Ca 1	0

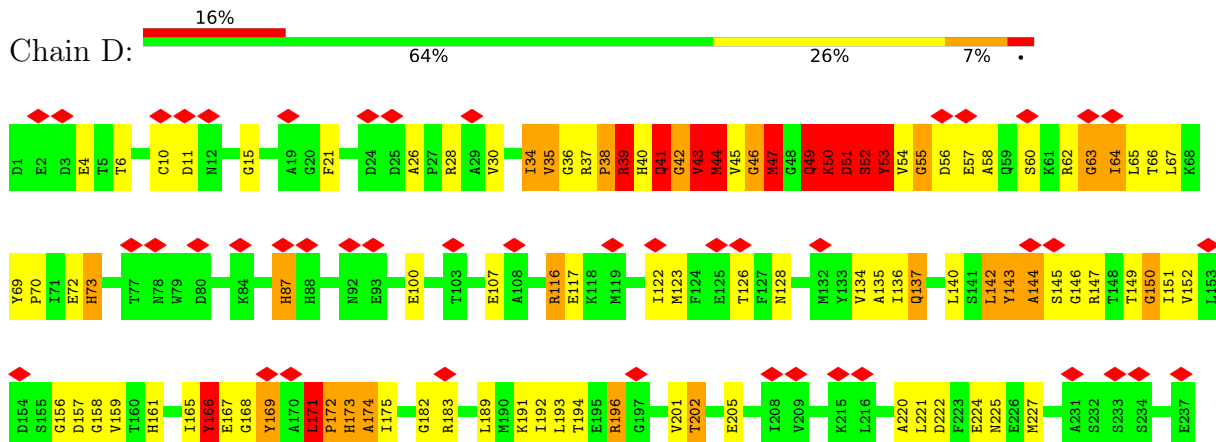
3 Residue-property plots [i](#)

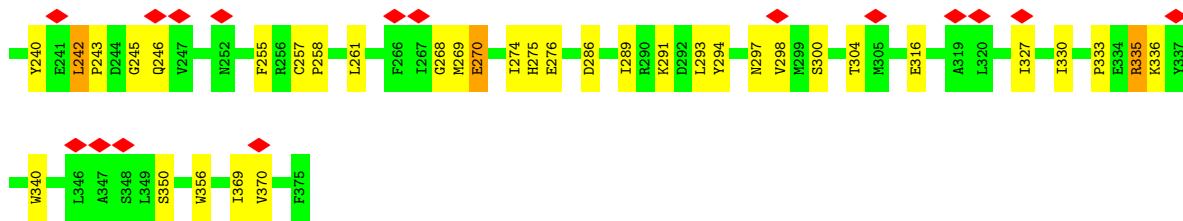
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

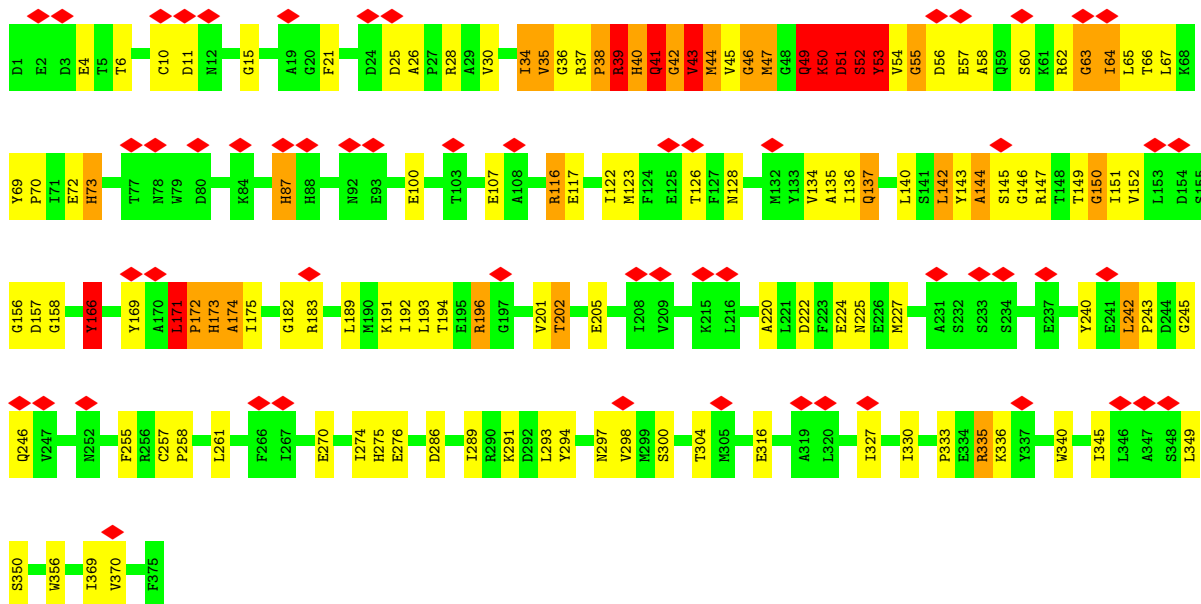


- Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

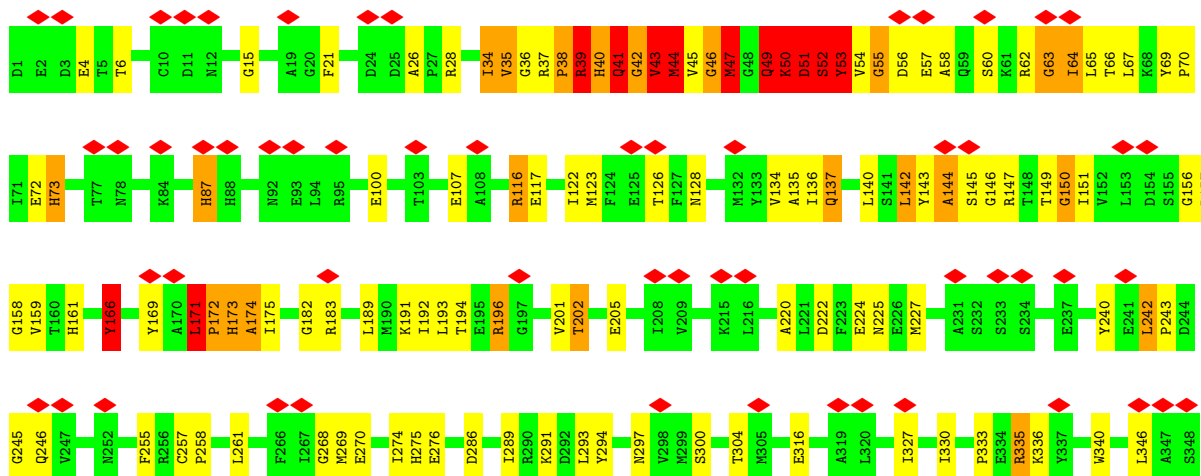


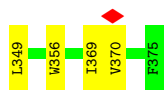


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE

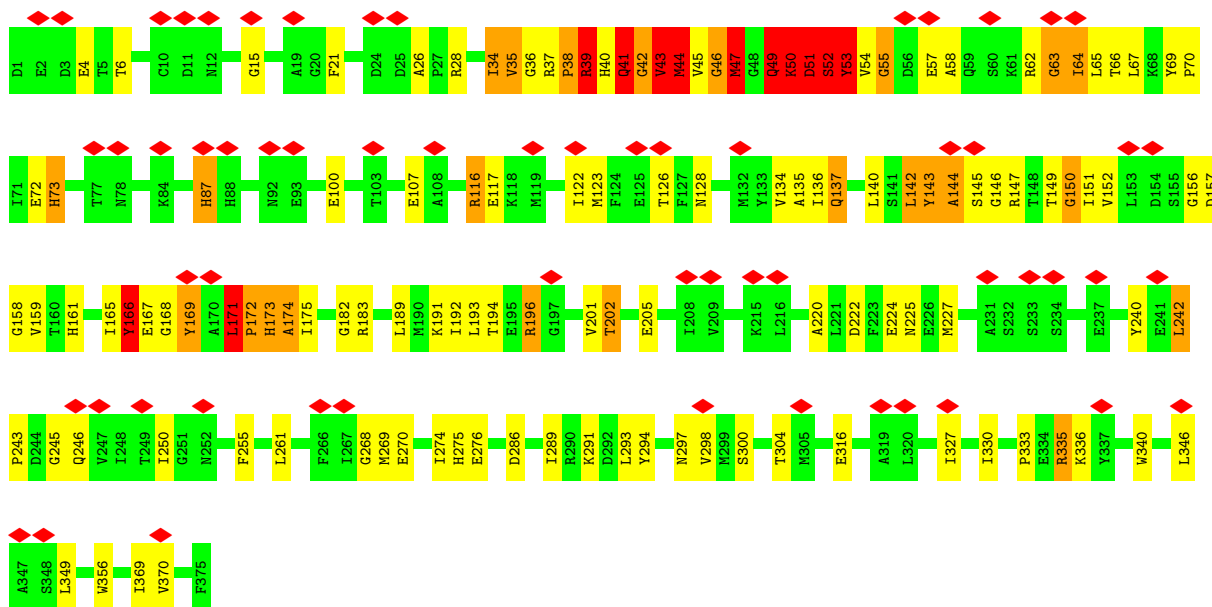


• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE





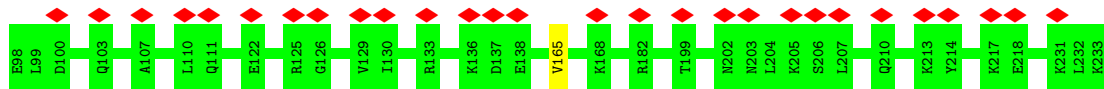
• Molecule 1: ACTIN, ALPHA SKELETAL MUSCLE



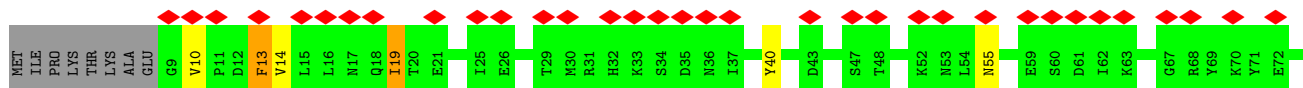
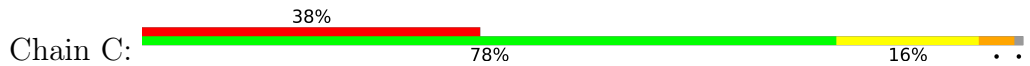
• Molecule 2: TROPOMYOSIN 1-ALPHA CHAIN

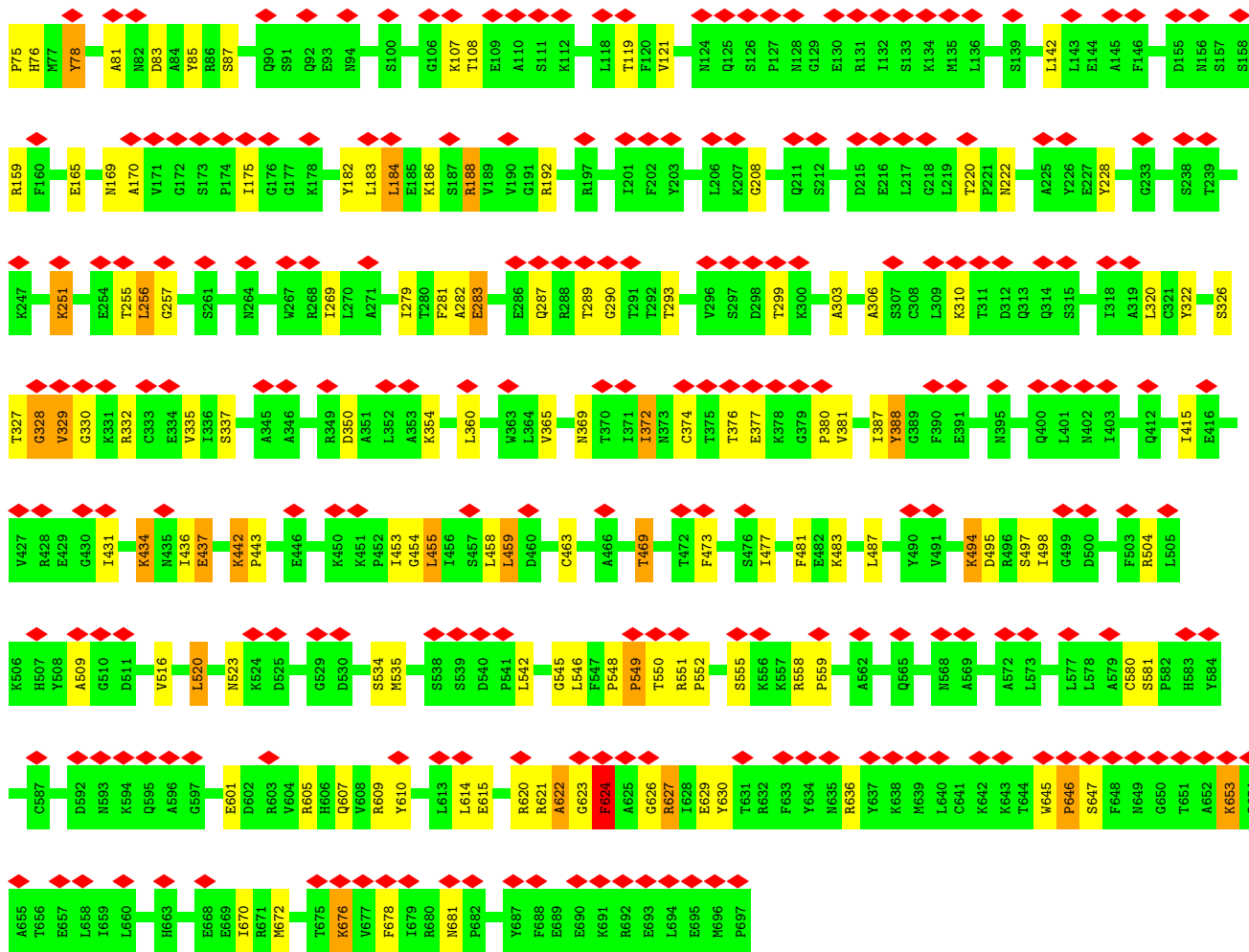


• Molecule 2: TROPOMYOSIN 1-ALPHA CHAIN

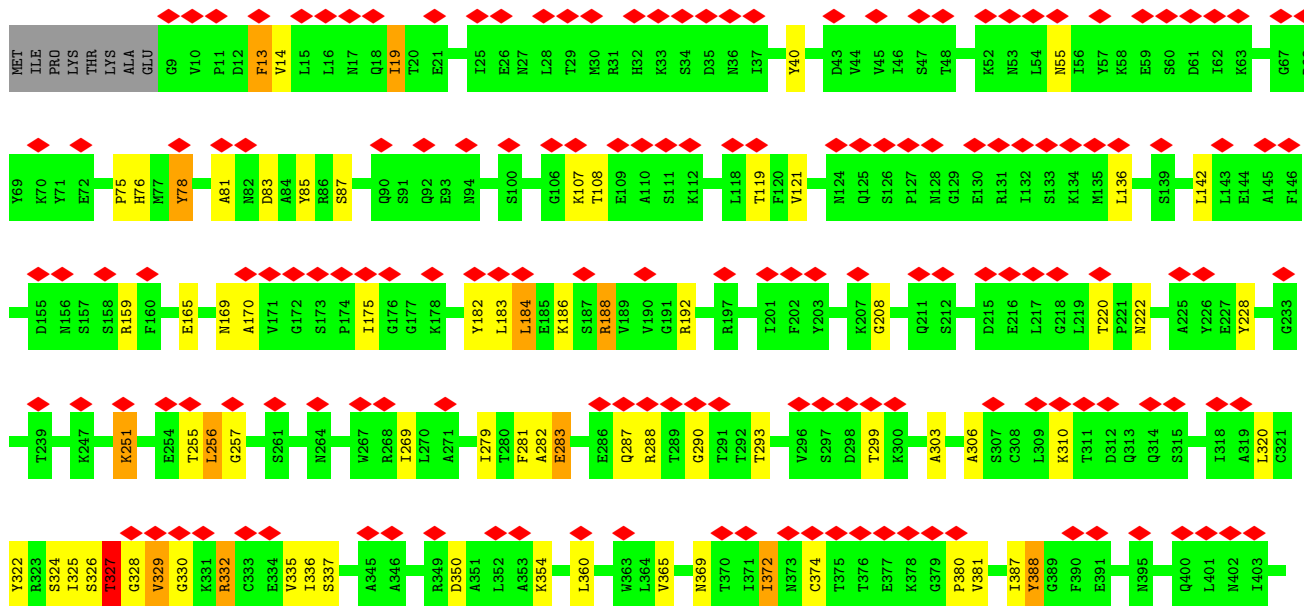
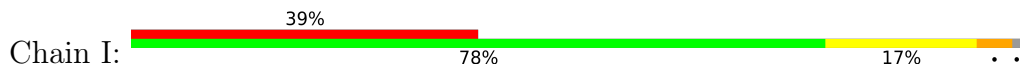


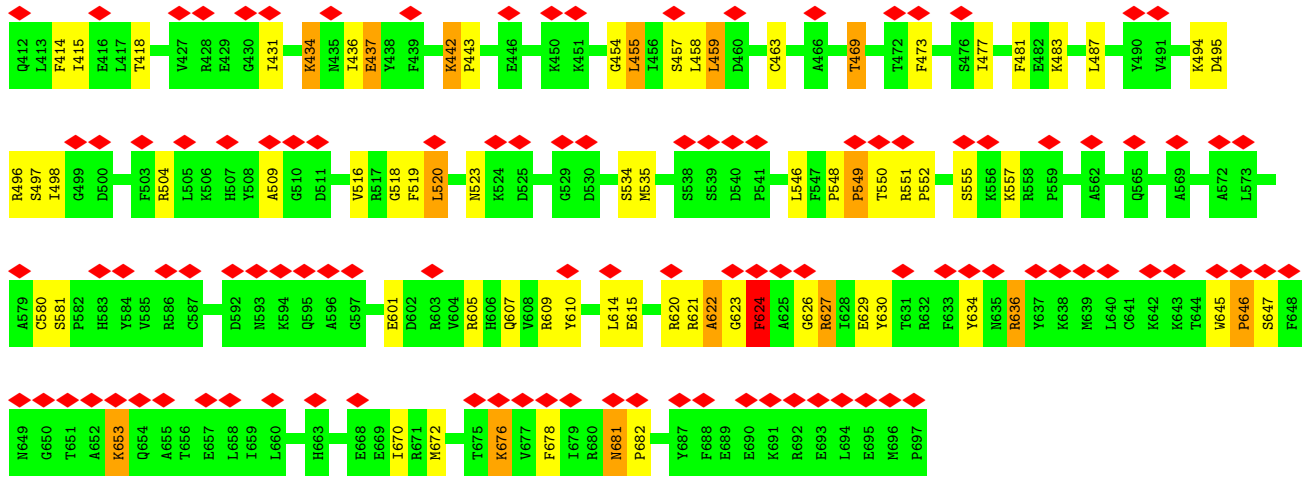
• Molecule 3: MYOSIN IE HEAVY CHAIN



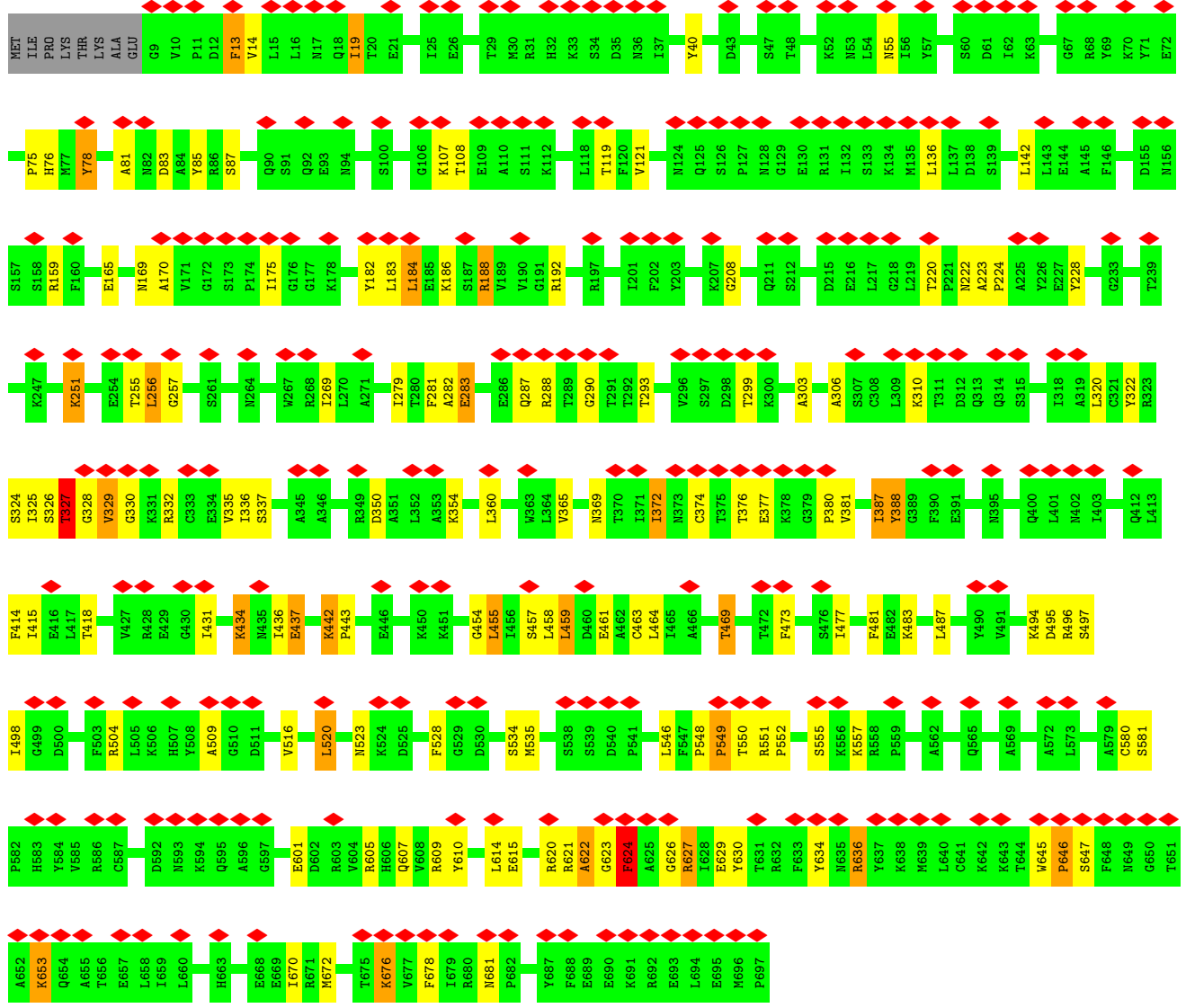
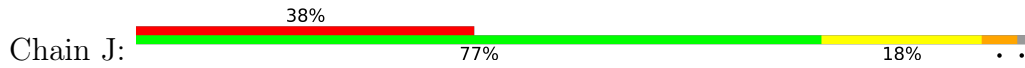


● Molecule 3: MYOSIN IE HEAVY CHAIN





• Molecule 3: MYOSIN IE HEAVY CHAIN



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	9650	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	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	0.070	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	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 [i](#)

5.1 Standard geometry [i](#)

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

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	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	D	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	E	0.92	13/2984 (0.4%)	0.67	10/4040 (0.2%)
1	F	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
1	G	0.91	13/2984 (0.4%)	0.69	11/4040 (0.3%)
2	B	0.20	0/1107	0.31	0/1471
2	H	0.24	0/1107	0.38	0/1471
3	C	0.26	0/5590	0.38	0/7527
3	I	0.22	0/5590	0.37	0/7527
3	J	0.22	0/5590	0.37	0/7527
All	All	0.63	65/33904 (0.2%)	0.53	54/45723 (0.1%)

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	G	0	1
All	All	0	5

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	166	TYR	CD2-CE2	19.25	1.68	1.39
1	D	166	TYR	CD2-CE2	19.25	1.68	1.39
1	A	166	TYR	CD2-CE2	19.24	1.68	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	166	TYR	CD2-CE2	19.24	1.68	1.39
1	E	166	TYR	CD2-CE2	19.18	1.68	1.39
1	G	166	TYR	CD1-CE1	18.68	1.67	1.39
1	F	166	TYR	CD1-CE1	18.67	1.67	1.39
1	D	166	TYR	CD1-CE1	18.67	1.67	1.39
1	E	166	TYR	CD1-CE1	18.67	1.67	1.39
1	A	166	TYR	CD1-CE1	18.66	1.67	1.39
1	F	166	TYR	CE2-CZ	18.48	1.62	1.38
1	D	166	TYR	CE2-CZ	18.47	1.62	1.38
1	A	166	TYR	CE2-CZ	18.45	1.62	1.38
1	E	166	TYR	CE2-CZ	18.45	1.62	1.38
1	G	166	TYR	CE2-CZ	18.44	1.62	1.38
1	E	166	TYR	CE1-CZ	15.37	1.58	1.38
1	F	166	TYR	CE1-CZ	15.35	1.58	1.38
1	A	166	TYR	CE1-CZ	15.34	1.58	1.38
1	G	166	TYR	CE1-CZ	15.34	1.58	1.38
1	D	166	TYR	CE1-CZ	15.33	1.58	1.38
1	F	166	TYR	CG-CD1	12.05	1.54	1.39
1	G	166	TYR	CG-CD1	12.05	1.54	1.39
1	D	166	TYR	CG-CD1	12.04	1.54	1.39
1	E	166	TYR	CG-CD1	12.03	1.54	1.39
1	A	166	TYR	CG-CD1	12.03	1.54	1.39
1	E	166	TYR	CG-CD2	11.29	1.53	1.39
1	A	166	TYR	CG-CD2	11.28	1.53	1.39
1	G	166	TYR	CG-CD2	11.26	1.53	1.39
1	F	166	TYR	CG-CD2	11.23	1.53	1.39
1	D	166	TYR	CG-CD2	11.22	1.53	1.39
1	G	150	GLY	N-CA	9.97	1.61	1.46
1	F	150	GLY	N-CA	9.97	1.61	1.46
1	A	150	GLY	N-CA	9.95	1.60	1.46
1	E	150	GLY	N-CA	9.93	1.60	1.46
1	D	150	GLY	N-CA	9.91	1.60	1.46
1	D	43	VAL	CA-CB	8.42	1.72	1.54
1	E	43	VAL	CA-CB	8.39	1.72	1.54
1	A	43	VAL	CA-CB	8.38	1.72	1.54
1	G	43	VAL	CA-CB	8.37	1.72	1.54
1	F	43	VAL	CA-CB	8.35	1.72	1.54
1	E	149	THR	C-N	6.75	1.45	1.33
1	D	149	THR	C-N	6.74	1.45	1.33
1	F	149	THR	C-N	6.72	1.45	1.33
1	A	149	THR	C-N	6.71	1.45	1.33
1	G	149	THR	C-N	6.69	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	41	GLN	N-CA	6.05	1.58	1.46
1	F	41	GLN	N-CA	6.05	1.58	1.46
1	A	41	GLN	N-CA	6.04	1.58	1.46
1	E	41	GLN	N-CA	6.04	1.58	1.46
1	G	41	GLN	N-CA	6.02	1.58	1.46
1	G	49	GLN	CG-CD	5.83	1.64	1.51
1	F	49	GLN	CG-CD	5.82	1.64	1.51
1	A	49	GLN	CG-CD	5.81	1.64	1.51
1	E	49	GLN	CG-CD	5.81	1.64	1.51
1	D	49	GLN	CG-CD	5.77	1.64	1.51
1	G	53	TYR	CE1-CZ	-5.38	1.31	1.38
1	A	53	TYR	CE1-CZ	-5.36	1.31	1.38
1	D	53	TYR	CE1-CZ	-5.35	1.31	1.38
1	F	53	TYR	CE1-CZ	-5.33	1.31	1.38
1	E	53	TYR	CE1-CZ	-5.32	1.31	1.38
1	G	43	VAL	CA-C	5.11	1.66	1.52
1	F	43	VAL	CA-C	5.11	1.66	1.52
1	E	43	VAL	CA-C	5.10	1.66	1.52
1	A	43	VAL	CA-C	5.10	1.66	1.52
1	D	43	VAL	CA-C	5.09	1.66	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	149	THR	C-N-CA	9.74	142.76	122.30
1	G	149	THR	C-N-CA	9.73	142.74	122.30
1	A	149	THR	C-N-CA	9.73	142.73	122.30
1	E	149	THR	C-N-CA	9.73	142.73	122.30
1	D	149	THR	C-N-CA	9.72	142.72	122.30
1	D	53	TYR	CB-CA-C	9.25	128.90	110.40
1	F	53	TYR	CB-CA-C	9.24	128.89	110.40
1	A	53	TYR	CB-CA-C	9.24	128.88	110.40
1	G	53	TYR	CB-CA-C	9.23	128.86	110.40
1	E	53	TYR	CB-CA-C	9.23	128.85	110.40
1	F	43	VAL	CG1-CB-CG2	-7.15	99.46	110.90
1	G	43	VAL	CG1-CB-CG2	-7.14	99.47	110.90
1	E	43	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	A	43	VAL	CG1-CB-CG2	-7.12	99.51	110.90
1	D	43	VAL	CG1-CB-CG2	-7.11	99.53	110.90
1	G	43	VAL	CA-CB-CG2	6.64	120.86	110.90
1	E	43	VAL	CA-CB-CG2	6.63	120.84	110.90
1	A	43	VAL	CA-CB-CG2	6.62	120.84	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	43	VAL	CA-CB-CG2	6.61	120.81	110.90
1	F	43	VAL	CA-CB-CG2	6.60	120.81	110.90
1	F	47	MET	CB-CA-C	6.04	122.48	110.40
1	G	47	MET	CB-CA-C	6.02	122.44	110.40
1	A	47	MET	CB-CA-C	6.01	122.43	110.40
1	D	47	MET	CB-CA-C	6.01	122.41	110.40
1	D	39	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	G	39	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	E	39	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	F	39	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	39	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	F	46	GLY	C-N-CA	5.84	136.31	121.70
1	D	46	GLY	C-N-CA	5.84	136.30	121.70
1	A	46	GLY	C-N-CA	5.83	136.28	121.70
1	G	46	GLY	C-N-CA	5.83	136.28	121.70
1	E	46	GLY	C-N-CA	5.83	136.26	121.70
1	D	44	MET	CA-CB-CG	5.38	122.45	113.30
1	G	44	MET	CA-CB-CG	5.38	122.45	113.30
1	F	44	MET	CA-CB-CG	5.37	122.43	113.30
1	A	44	MET	CA-CB-CG	5.35	122.40	113.30
1	E	44	MET	CA-CB-CG	5.34	122.39	113.30
1	F	52	SER	C-N-CA	5.34	135.04	121.70
1	D	52	SER	C-N-CA	5.33	135.04	121.70
1	G	52	SER	C-N-CA	5.33	135.03	121.70
1	A	52	SER	C-N-CA	5.33	135.03	121.70
1	E	52	SER	C-N-CA	5.33	135.03	121.70
1	E	46	GLY	CA-C-N	-5.32	105.50	117.20
1	A	46	GLY	CA-C-N	-5.31	105.51	117.20
1	G	46	GLY	CA-C-N	-5.31	105.52	117.20
1	F	46	GLY	CA-C-N	-5.31	105.52	117.20
1	D	46	GLY	CA-C-N	-5.30	105.53	117.20
1	G	52	SER	N-CA-CB	-5.29	102.56	110.50
1	E	52	SER	N-CA-CB	-5.28	102.58	110.50
1	F	52	SER	N-CA-CB	-5.27	102.59	110.50
1	D	52	SER	N-CA-CB	-5.27	102.59	110.50
1	A	52	SER	N-CA-CB	-5.26	102.60	110.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	43	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	D	43	VAL	Mainchain
1	E	43	VAL	Mainchain
1	F	43	VAL	Mainchain
1	G	43	VAL	Mainchain

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	140	0
1	D	2934	0	2895	125	0
1	E	2934	0	2895	124	0
1	F	2934	0	2895	121	0
1	G	2934	0	2894	122	0
2	B	1104	0	1104	3	0
2	H	1104	0	1104	1	0
3	C	5494	0	5488	77	0
3	I	5494	0	5488	82	0
3	J	5494	0	5488	86	0
4	A	27	0	12	3	0
4	D	27	0	12	3	0
4	E	27	0	12	3	0
4	F	27	0	12	3	0
4	G	27	0	12	3	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	G	1	0	0	0	0
All	All	33500	0	33206	795	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 12.

All (795) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:VAL:O	1:G:169:TYR:OH	1.53	1.21
1:A:169:TYR:OH	1:E:43:VAL:O	1.62	1.14
1:D:157:ASP:N	4:D:376:ADP:O3B	1.82	1.13
1:E:157:ASP:N	4:E:376:ADP:O3B	1.82	1.13
1:A:43:VAL:O	1:D:169:TYR:OH	1.63	1.12
1:A:157:ASP:N	4:A:376:ADP:O3B	1.82	1.12
1:F:157:ASP:N	4:F:376:ADP:O3B	1.82	1.11
1:G:157:ASP:N	4:G:376:ADP:O3B	1.82	1.11
1:D:30:VAL:HG22	3:I:327:THR:CG2	1.84	1.08
1:G:36:GLY:O	1:G:52:SER:CA	2.03	1.07
1:A:42:GLY:C	1:D:167:GLU:O	1.92	1.07
1:F:36:GLY:O	1:F:52:SER:CA	2.03	1.06
1:A:36:GLY:O	1:A:52:SER:CA	2.03	1.06
1:D:36:GLY:O	1:D:52:SER:CA	2.03	1.05
1:E:30:VAL:HG22	3:J:327:THR:CG2	1.85	1.05
1:E:36:GLY:O	1:E:52:SER:CA	2.03	1.05
1:A:36:GLY:O	1:A:52:SER:HA	1.59	1.02
1:A:42:GLY:O	1:D:167:GLU:O	1.77	1.02
1:A:41:GLN:NE2	1:D:169:TYR:HD1	1.56	1.02
1:D:36:GLY:O	1:D:52:SER:HA	1.59	1.02
1:F:42:GLY:O	1:G:167:GLU:O	1.78	1.01
1:E:36:GLY:O	1:E:52:SER:HA	1.59	1.01
1:A:167:GLU:O	1:E:42:GLY:C	2.00	1.00
1:F:36:GLY:O	1:F:52:SER:HA	1.59	0.99
1:G:36:GLY:O	1:G:52:SER:HA	1.59	0.99
1:F:42:GLY:C	1:G:167:GLU:O	2.03	0.97
1:A:169:TYR:HD1	1:E:41:GLN:NE2	1.60	0.97
1:A:53:TYR:OH	1:D:167:GLU:OE2	1.82	0.95
1:A:167:GLU:O	1:E:42:GLY:O	1.83	0.95
1:F:53:TYR:OH	1:G:167:GLU:OE2	1.85	0.94
1:A:41:GLN:NE2	1:D:169:TYR:CD1	2.36	0.93
1:D:30:VAL:HG22	3:I:327:THR:HG21	1.50	0.92
1:E:38:PRO:HG3	1:E:49:GLN:HG2	1.52	0.92
1:A:38:PRO:HG3	1:A:49:GLN:HG2	1.52	0.92
1:A:167:GLU:OE2	1:E:53:TYR:OH	1.85	0.92
1:E:54:VAL:HG22	1:E:55:GLY:H	1.35	0.92
1:D:38:PRO:HG3	1:D:49:GLN:HG2	1.52	0.91
1:E:350:SER:HG	3:J:457:SER:HG	1.00	0.91
1:E:30:VAL:HG22	3:J:327:THR:HG21	1.48	0.91
1:F:54:VAL:HG22	1:F:55:GLY:H	1.35	0.91
1:A:54:VAL:HG22	1:A:55:GLY:H	1.34	0.90
1:D:350:SER:HG	3:I:457:SER:HG	1.07	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:TYR:CD1	1:E:41:GLN:NE2	2.39	0.90
1:G:54:VAL:HG22	1:G:55:GLY:H	1.35	0.89
1:G:38:PRO:HG3	1:G:49:GLN:HG2	1.52	0.89
1:D:54:VAL:HG22	1:D:55:GLY:H	1.35	0.89
1:F:38:PRO:HG3	1:F:49:GLN:HG2	1.52	0.89
1:A:38:PRO:HG3	1:A:49:GLN:CG	2.05	0.87
1:D:38:PRO:HG3	1:D:49:GLN:CG	2.05	0.87
1:E:38:PRO:HG3	1:E:49:GLN:CG	2.05	0.86
1:E:30:VAL:CG2	3:J:327:THR:HG22	2.06	0.86
1:F:38:PRO:HG3	1:F:49:GLN:CG	2.05	0.86
1:G:38:PRO:HG3	1:G:49:GLN:CG	2.05	0.86
1:F:41:GLN:NE2	1:G:169:TYR:HD1	1.73	0.85
1:A:51:ASP:O	1:A:53:TYR:N	2.10	0.85
1:D:30:VAL:CG2	3:I:327:THR:HG22	2.06	0.85
1:F:36:GLY:O	1:F:52:SER:CB	2.26	0.84
1:F:51:ASP:O	1:F:53:TYR:N	2.10	0.84
1:G:36:GLY:O	1:G:52:SER:CB	2.26	0.84
1:G:51:ASP:C	1:G:53:TYR:H	1.80	0.84
1:G:51:ASP:O	1:G:53:TYR:N	2.10	0.84
1:D:51:ASP:O	1:D:53:TYR:N	2.10	0.84
1:E:51:ASP:O	1:E:53:TYR:N	2.10	0.83
1:A:35:VAL:HG13	1:A:52:SER:CB	2.08	0.83
1:D:35:VAL:HG13	1:D:52:SER:CB	2.08	0.83
1:E:35:VAL:HG13	1:E:52:SER:CB	2.08	0.83
1:F:35:VAL:HG13	1:F:52:SER:CB	2.08	0.83
1:G:35:VAL:HG13	1:G:52:SER:CB	2.08	0.83
1:E:36:GLY:O	1:E:52:SER:CB	2.26	0.83
1:D:36:GLY:O	1:D:52:SER:CB	2.26	0.83
1:F:51:ASP:C	1:F:53:TYR:H	1.80	0.83
1:A:36:GLY:O	1:A:52:SER:CB	2.26	0.82
1:D:30:VAL:CG2	3:I:327:THR:CG2	2.59	0.81
3:C:188:ARG:O	3:C:192:ARG:NH1	2.14	0.81
3:I:188:ARG:O	3:I:192:ARG:NH1	2.14	0.81
3:J:188:ARG:O	3:J:192:ARG:NH1	2.14	0.81
1:G:36:GLY:O	1:G:52:SER:HB3	1.82	0.80
1:D:51:ASP:C	1:D:53:TYR:H	1.80	0.80
1:A:36:GLY:O	1:A:52:SER:HB3	1.82	0.80
1:F:42:GLY:O	1:F:43:VAL:HG22	1.82	0.80
1:D:36:GLY:O	1:D:52:SER:HB3	1.82	0.80
1:G:42:GLY:O	1:G:43:VAL:HG22	1.82	0.79
1:E:30:VAL:CG2	3:J:327:THR:CG2	2.59	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLY:O	1:E:52:SER:HB3	1.82	0.79
1:A:42:GLY:O	1:A:43:VAL:HG22	1.82	0.79
1:A:51:ASP:C	1:A:53:TYR:H	1.80	0.79
1:E:49:GLN:HG3	1:E:50:LYS:N	1.98	0.79
1:D:42:GLY:O	1:D:43:VAL:HG22	1.82	0.79
1:A:49:GLN:HG3	1:A:50:LYS:N	1.98	0.78
1:F:36:GLY:O	1:F:52:SER:HB3	1.82	0.78
3:I:630:TYR:OH	3:I:672:MET:SD	2.40	0.78
3:J:630:TYR:OH	3:J:672:MET:SD	2.40	0.78
3:C:630:TYR:OH	3:C:672:MET:SD	2.40	0.78
1:E:42:GLY:O	1:E:43:VAL:HG22	1.82	0.78
1:G:49:GLN:HG3	1:G:50:LYS:N	1.98	0.78
1:F:49:GLN:HG3	1:F:50:LYS:N	1.98	0.77
1:E:51:ASP:C	1:E:53:TYR:H	1.80	0.77
1:D:49:GLN:HG3	1:D:50:LYS:N	1.98	0.77
1:F:41:GLN:NE2	1:G:169:TYR:CD1	2.53	0.75
1:A:54:VAL:HG22	1:A:55:GLY:N	2.02	0.75
1:F:54:VAL:HG22	1:F:55:GLY:N	2.02	0.75
1:E:54:VAL:HG22	1:E:55:GLY:N	2.02	0.74
1:D:54:VAL:HG22	1:D:55:GLY:N	2.02	0.73
1:G:54:VAL:HG22	1:G:55:GLY:N	2.02	0.73
1:A:168:GLY:C	1:E:40:HIS:CE1	2.62	0.73
1:D:142:LEU:O	1:D:144:ALA:N	2.22	0.73
1:F:142:LEU:O	1:F:144:ALA:N	2.22	0.73
1:E:142:LEU:O	1:E:144:ALA:N	2.22	0.72
1:G:142:LEU:O	1:G:144:ALA:N	2.22	0.72
1:A:142:LEU:O	1:A:144:ALA:N	2.22	0.72
1:A:173:HIS:O	1:A:175:ILE:N	2.23	0.72
1:D:173:HIS:O	1:D:175:ILE:N	2.23	0.72
1:E:30:VAL:HG22	3:J:327:THR:HG22	1.65	0.71
1:F:173:HIS:O	1:F:175:ILE:N	2.23	0.71
1:D:196:ARG:O	1:D:196:ARG:NE	2.23	0.71
1:G:173:HIS:O	1:G:175:ILE:N	2.23	0.71
1:E:173:HIS:O	1:E:175:ILE:N	2.23	0.71
1:E:196:ARG:NE	1:E:196:ARG:O	2.23	0.70
1:G:196:ARG:NE	1:G:196:ARG:O	2.23	0.70
1:A:196:ARG:O	1:A:196:ARG:NE	2.23	0.70
1:D:172:PRO:O	1:G:191:LYS:NZ	2.22	0.70
1:F:196:ARG:O	1:F:196:ARG:NE	2.23	0.70
1:E:171:LEU:HB2	1:E:172:PRO:HD3	1.74	0.70
1:D:171:LEU:HB2	1:D:172:PRO:HD3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:OE1	1:D:169:TYR:O	2.10	0.69
1:G:171:LEU:HB2	1:G:172:PRO:HD3	1.74	0.69
1:A:171:LEU:HB2	1:A:172:PRO:HD3	1.74	0.68
1:F:43:VAL:O	1:G:169:TYR:CZ	2.46	0.68
1:D:35:VAL:HG13	1:D:52:SER:OG	1.94	0.68
1:F:171:LEU:HB2	1:F:172:PRO:HD3	1.74	0.68
1:A:35:VAL:HG13	1:A:52:SER:OG	1.94	0.68
1:G:35:VAL:HG13	1:G:52:SER:OG	1.94	0.68
1:A:40:HIS:CE1	1:D:168:GLY:C	2.67	0.68
1:F:35:VAL:HG13	1:F:52:SER:OG	1.94	0.67
1:F:35:VAL:HG13	1:F:52:SER:HB2	1.75	0.67
1:E:35:VAL:HG13	1:E:52:SER:HB2	1.75	0.67
1:E:35:VAL:HG13	1:E:52:SER:OG	1.94	0.67
1:F:336:LYS:HE3	4:F:376:ADP:PA	2.35	0.67
1:G:35:VAL:HG13	1:G:52:SER:HB2	1.75	0.67
1:E:336:LYS:HE3	4:E:376:ADP:PA	2.35	0.67
1:G:336:LYS:HE3	4:G:376:ADP:PA	2.35	0.67
1:G:53:TYR:C	1:G:58:ALA:HB2	2.15	0.67
1:A:336:LYS:HE3	4:A:376:ADP:PA	2.35	0.67
3:C:494:LYS:HG3	3:C:494:LYS:O	1.94	0.67
1:A:53:TYR:C	1:A:58:ALA:HB2	2.16	0.66
1:E:53:TYR:C	1:E:58:ALA:HB2	2.16	0.66
1:F:53:TYR:C	1:F:58:ALA:HB2	2.15	0.66
1:A:35:VAL:HG13	1:A:52:SER:HB2	1.75	0.66
1:D:53:TYR:C	1:D:58:ALA:HB2	2.16	0.66
1:D:336:LYS:HE3	4:D:376:ADP:PA	2.35	0.66
1:D:35:VAL:HG13	1:D:52:SER:HB2	1.75	0.66
3:C:269:ILE:HD12	3:C:546:LEU:HD11	1.78	0.64
3:C:558:ARG:HB2	3:C:559:PRO:HD3	1.80	0.64
3:I:269:ILE:HD12	3:I:546:LEU:HD11	1.79	0.64
3:J:19:ILE:O	3:J:19:ILE:HG23	1.97	0.64
3:J:269:ILE:HD12	3:J:546:LEU:HD11	1.79	0.64
1:G:117:GLU:N	1:G:117:GLU:OE1	2.31	0.64
1:F:117:GLU:N	1:F:117:GLU:OE1	2.31	0.63
3:J:365:VAL:O	3:J:369:ASN:ND2	2.31	0.63
1:A:169:TYR:O	1:E:41:GLN:OE1	2.16	0.63
1:D:37:ARG:HB3	1:D:38:PRO:CD	2.29	0.63
1:D:117:GLU:N	1:D:117:GLU:OE1	2.31	0.63
1:A:37:ARG:HB3	1:A:38:PRO:CD	2.29	0.63
1:F:40:HIS:CE1	1:G:168:GLY:C	2.72	0.63
1:G:333:PRO:O	1:G:335:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:VAL:O	3:C:369:ASN:ND2	2.31	0.63
1:F:37:ARG:HB3	1:F:38:PRO:CD	2.29	0.63
1:D:122:ILE:O	1:D:126:THR:OG1	2.17	0.63
1:E:117:GLU:N	1:E:117:GLU:OE1	2.31	0.63
3:I:365:VAL:O	3:I:369:ASN:ND2	2.31	0.63
1:E:37:ARG:HB3	1:E:38:PRO:CD	2.29	0.63
1:E:122:ILE:O	1:E:126:THR:OG1	2.17	0.63
3:I:19:ILE:HG23	3:I:19:ILE:O	1.97	0.63
1:G:122:ILE:O	1:G:126:THR:OG1	2.17	0.63
3:C:19:ILE:HG23	3:C:19:ILE:O	1.97	0.62
1:G:37:ARG:HB3	1:G:38:PRO:CD	2.29	0.62
1:F:333:PRO:O	1:F:335:ARG:NH2	2.32	0.62
1:A:333:PRO:O	1:A:335:ARG:NH2	2.32	0.62
1:E:191:LYS:NZ	1:F:172:PRO:O	2.28	0.62
1:A:117:GLU:OE1	1:A:117:GLU:N	2.31	0.62
1:E:333:PRO:O	1:E:335:ARG:NH2	2.32	0.62
1:A:168:GLY:O	1:E:40:HIS:CE1	2.52	0.62
1:F:122:ILE:O	1:F:126:THR:OG1	2.17	0.62
1:D:269:MET:N	1:G:39:ARG:HH21	1.98	0.62
1:A:122:ILE:O	1:A:126:THR:OG1	2.17	0.61
1:D:333:PRO:O	1:D:335:ARG:NH2	2.32	0.61
1:A:172:PRO:O	1:F:191:LYS:NZ	2.22	0.61
1:A:43:VAL:O	1:D:169:TYR:CZ	2.52	0.61
3:I:495:ASP:OD2	3:I:497:SER:OG	2.19	0.60
3:J:495:ASP:OD2	3:J:497:SER:OG	2.19	0.60
3:C:495:ASP:OD2	3:C:497:SER:OG	2.19	0.60
1:G:54:VAL:CG2	1:G:55:GLY:H	2.13	0.60
3:C:494:LYS:O	3:C:494:LYS:CG	2.49	0.60
1:D:43:VAL:HG23	1:D:46:GLY:HA3	1.83	0.60
1:A:43:VAL:HG23	1:A:46:GLY:HA3	1.83	0.60
1:E:43:VAL:HG23	1:E:46:GLY:HA3	1.82	0.60
1:D:38:PRO:HG3	1:D:49:GLN:CD	2.22	0.60
1:A:40:HIS:CE1	1:D:168:GLY:O	2.55	0.59
1:F:43:VAL:HG23	1:F:46:GLY:HA3	1.83	0.59
1:E:38:PRO:HG3	1:E:49:GLN:CD	2.22	0.59
1:G:43:VAL:HG23	1:G:46:GLY:HA3	1.83	0.59
3:C:463:CYS:SG	3:C:523:ASN:ND2	2.76	0.59
3:I:463:CYS:SG	3:I:523:ASN:ND2	2.76	0.59
1:F:43:VAL:HG12	1:G:165:ILE:HD11	1.85	0.59
1:D:26:ALA:O	1:D:28:ARG:NH1	2.36	0.59
1:A:38:PRO:CG	1:A:49:GLN:HG2	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:VAL:CG2	1:E:55:GLY:H	2.13	0.58
1:G:26:ALA:O	1:G:28:ARG:NH1	2.36	0.58
3:J:376:THR:OG1	3:J:377:GLU:OE1	2.11	0.58
1:A:38:PRO:HG3	1:A:49:GLN:CD	2.23	0.58
1:D:45:VAL:C	1:D:47:MET:H	2.06	0.58
1:E:45:VAL:C	1:E:47:MET:H	2.06	0.58
3:J:107:LYS:O	3:J:108:THR:N	2.36	0.58
3:J:463:CYS:SG	3:J:523:ASN:ND2	2.76	0.58
1:A:54:VAL:CG2	1:A:55:GLY:H	2.13	0.58
1:E:26:ALA:O	1:E:28:ARG:NH1	2.36	0.58
1:E:42:GLY:O	1:E:43:VAL:CG2	2.52	0.58
1:F:38:PRO:HG3	1:F:49:GLN:CD	2.23	0.58
1:A:45:VAL:C	1:A:47:MET:H	2.06	0.58
1:F:26:ALA:O	1:F:28:ARG:NH1	2.36	0.58
1:D:38:PRO:CG	1:D:49:GLN:HG2	2.31	0.57
3:I:107:LYS:O	3:I:108:THR:N	2.36	0.57
1:A:43:VAL:N	1:D:168:GLY:HA2	2.19	0.57
3:C:107:LYS:O	3:C:108:THR:N	2.36	0.57
1:F:45:VAL:C	1:F:47:MET:H	2.06	0.57
1:G:38:PRO:HG3	1:G:49:GLN:CD	2.23	0.57
1:F:171:LEU:HD12	1:F:171:LEU:N	2.19	0.57
1:G:42:GLY:O	1:G:43:VAL:CG2	2.52	0.57
1:A:42:GLY:O	1:A:43:VAL:CG2	2.52	0.57
1:D:242:LEU:HD23	1:D:243:PRO:HD2	1.86	0.57
1:G:202:THR:N	1:G:205:GLU:OE2	2.38	0.57
1:D:54:VAL:CG2	1:D:55:GLY:H	2.13	0.57
1:G:171:LEU:N	1:G:171:LEU:HD12	2.19	0.57
1:D:171:LEU:N	1:D:171:LEU:HD12	2.19	0.57
1:E:171:LEU:N	1:E:171:LEU:HD12	2.19	0.57
1:E:242:LEU:HD23	1:E:243:PRO:HD2	1.86	0.57
1:F:38:PRO:CG	1:F:49:GLN:HG2	2.31	0.57
1:G:45:VAL:C	1:G:47:MET:H	2.06	0.57
1:A:202:THR:N	1:A:205:GLU:OE2	2.38	0.57
1:A:169:TYR:CZ	1:E:43:VAL:O	2.55	0.56
1:A:242:LEU:HD23	1:A:243:PRO:HD2	1.86	0.56
1:E:150:GLY:O	1:E:166:TYR:CG	2.59	0.56
1:E:202:THR:N	1:E:205:GLU:OE2	2.38	0.56
1:F:150:GLY:O	1:F:166:TYR:CG	2.59	0.56
1:F:242:LEU:HD23	1:F:243:PRO:HD2	1.85	0.56
1:G:242:LEU:HD23	1:G:243:PRO:HD2	1.86	0.56
1:D:202:THR:N	1:D:205:GLU:OE2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD12	1:A:171:LEU:N	2.19	0.56
1:A:150:GLY:O	1:A:166:TYR:CG	2.59	0.56
1:A:269:MET:N	1:F:39:ARG:HH21	2.04	0.56
3:C:376:THR:OG1	3:C:377:GLU:OE1	2.11	0.56
1:G:150:GLY:O	1:G:166:TYR:CG	2.59	0.56
1:A:275:HIS:ND1	1:A:316:GLU:OE1	2.39	0.56
1:D:150:GLY:O	1:D:166:TYR:CG	2.59	0.55
1:G:275:HIS:ND1	1:G:316:GLU:OE1	2.39	0.55
1:F:304:THR:O	1:F:335:ARG:NH1	2.40	0.55
1:G:304:THR:O	1:G:335:ARG:NH1	2.40	0.55
1:D:42:GLY:O	1:D:43:VAL:CG2	2.52	0.55
1:E:275:HIS:ND1	1:E:316:GLU:OE1	2.40	0.55
1:F:43:VAL:N	1:G:168:GLY:HA2	2.20	0.55
1:F:49:GLN:CG	1:F:50:LYS:N	2.69	0.55
1:F:202:THR:N	1:F:205:GLU:OE2	2.38	0.55
1:F:191:LYS:O	1:F:194:THR:OG1	2.24	0.55
1:E:304:THR:O	1:E:335:ARG:NH1	2.40	0.55
1:G:38:PRO:CG	1:G:49:GLN:HG2	2.31	0.55
3:J:326:SER:O	3:J:327:THR:HB	2.05	0.55
1:A:304:THR:O	1:A:335:ARG:NH1	2.40	0.55
1:D:38:PRO:HD3	1:D:49:GLN:OE1	2.07	0.55
1:F:38:PRO:HD3	1:F:49:GLN:OE1	2.07	0.55
3:I:622:ALA:HB3	3:I:678:PHE:CE2	2.41	0.55
1:E:38:PRO:HD3	1:E:49:GLN:OE1	2.07	0.55
1:F:42:GLY:O	1:F:43:VAL:CG2	2.52	0.55
1:G:191:LYS:O	1:G:194:THR:OG1	2.24	0.55
3:C:322:TYR:HB3	3:C:337:SER:HA	1.89	0.55
3:C:622:ALA:HB3	3:C:678:PHE:CE2	2.41	0.55
1:D:304:THR:O	1:D:335:ARG:NH1	2.40	0.55
1:A:38:PRO:HD3	1:A:49:GLN:OE1	2.07	0.55
1:D:49:GLN:CG	1:D:50:LYS:N	2.69	0.55
3:I:326:SER:O	3:I:327:THR:HB	2.06	0.54
1:D:275:HIS:ND1	1:D:316:GLU:OE1	2.39	0.54
1:F:275:HIS:ND1	1:F:316:GLU:OE1	2.39	0.54
3:J:622:ALA:HB3	3:J:678:PHE:CE2	2.41	0.54
1:G:38:PRO:HD3	1:G:49:GLN:OE1	2.07	0.54
3:I:580:CYS:SG	3:I:581:SER:N	2.81	0.54
1:G:171:LEU:HD13	1:G:172:PRO:HD3	1.90	0.54
1:F:41:GLN:OE1	1:G:169:TYR:O	2.26	0.54
1:F:171:LEU:HD13	1:F:172:PRO:HD3	1.90	0.54
3:C:282:ALA:O	3:C:283:GLU:C	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:509:ALA:HB1	3:C:610:TYR:HB2	1.90	0.54
3:I:142:LEU:HG	3:I:256:LEU:HD12	1.90	0.54
3:I:509:ALA:HB1	3:I:610:TYR:HB2	1.90	0.54
3:J:580:CYS:SG	3:J:581:SER:N	2.81	0.54
1:E:49:GLN:CG	1:E:50:LYS:N	2.69	0.53
1:A:30:VAL:O	1:A:30:VAL:HG23	2.08	0.53
3:C:142:LEU:HG	3:C:256:LEU:HD12	1.90	0.53
1:E:336:LYS:HE3	4:E:376:ADP:O2A	2.09	0.53
1:G:336:LYS:HE3	4:G:376:ADP:O2A	2.09	0.53
3:J:142:LEU:HG	3:J:256:LEU:HD12	1.90	0.53
3:J:322:TYR:HB3	3:J:337:SER:HA	1.91	0.53
3:J:509:ALA:HB1	3:J:610:TYR:HB2	1.90	0.53
1:A:34:ILE:O	1:A:35:VAL:HG23	2.09	0.53
1:A:39:ARG:HH21	1:G:269:MET:N	2.06	0.53
1:A:72:GLU:O	1:A:73:HIC:C	2.57	0.53
1:A:336:LYS:HE3	4:A:376:ADP:O2A	2.09	0.53
3:I:322:TYR:HB3	3:I:337:SER:HA	1.91	0.53
1:E:171:LEU:HD13	1:E:172:PRO:HD3	1.90	0.53
1:E:191:LYS:O	1:E:194:THR:OG1	2.24	0.53
1:A:49:GLN:CG	1:A:50:LYS:N	2.69	0.53
3:J:282:ALA:O	3:J:283:GLU:C	2.46	0.53
1:A:37:ARG:HB3	1:A:38:PRO:HD2	1.91	0.53
1:E:37:ARG:HB3	1:E:38:PRO:HD2	1.91	0.53
1:A:171:LEU:HD13	1:A:172:PRO:HD3	1.90	0.53
1:D:171:LEU:HD13	1:D:172:PRO:HD3	1.90	0.53
1:D:336:LYS:HE3	4:D:376:ADP:O2A	2.09	0.53
1:G:72:GLU:O	1:G:73:HIC:C	2.57	0.53
1:A:43:VAL:HG12	1:D:165:ILE:HD11	1.92	0.53
1:D:72:GLU:O	1:D:73:HIC:C	2.57	0.53
1:F:336:LYS:HE3	4:F:376:ADP:O2A	2.09	0.53
1:D:191:LYS:O	1:D:194:THR:OG1	2.24	0.52
1:E:34:ILE:O	1:E:35:VAL:HG23	2.09	0.52
3:C:580:CYS:SG	3:C:581:SER:N	2.81	0.52
3:I:282:ALA:O	3:I:283:GLU:C	2.46	0.52
1:F:107:GLU:HB2	1:F:134:VAL:HG22	1.92	0.52
1:G:49:GLN:CG	1:G:50:LYS:N	2.69	0.52
1:F:40:HIS:CD2	1:G:171:LEU:HD21	2.44	0.52
1:F:54:VAL:CG2	1:F:55:GLY:H	2.13	0.52
1:F:72:GLU:O	1:F:73:HIC:C	2.57	0.52
1:D:34:ILE:O	1:D:35:VAL:HG23	2.09	0.52
1:D:37:ARG:HB3	1:D:38:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLU:O	1:E:73:HIC:C	2.57	0.52
1:G:107:GLU:HB2	1:G:134:VAL:HG22	1.92	0.52
1:F:34:ILE:O	1:F:35:VAL:HG23	2.09	0.52
1:G:107:GLU:N	1:G:135:ALA:O	2.43	0.52
1:D:107:GLU:HB2	1:D:134:VAL:HG22	1.92	0.52
1:A:191:LYS:O	1:A:194:THR:OG1	2.24	0.52
1:F:304:THR:HB	1:F:335:ARG:HD2	1.92	0.52
3:J:455:LEU:O	3:J:459:LEU:N	2.43	0.52
1:F:107:GLU:N	1:F:135:ALA:O	2.43	0.51
1:E:107:GLU:HB2	1:E:134:VAL:HG22	1.92	0.51
1:G:34:ILE:O	1:G:35:VAL:HG23	2.09	0.51
1:A:107:GLU:N	1:A:135:ALA:O	2.43	0.51
3:C:455:LEU:O	3:C:459:LEU:N	2.43	0.51
1:G:34:ILE:HD13	1:G:34:ILE:H	1.76	0.51
1:A:34:ILE:HD13	1:A:34:ILE:H	1.76	0.51
1:A:168:GLY:HA2	1:E:43:VAL:N	2.26	0.51
3:J:473:PHE:CZ	3:J:477:ILE:HD11	2.45	0.51
1:A:107:GLU:HB2	1:A:134:VAL:HG22	1.92	0.51
1:E:34:ILE:HD13	1:E:34:ILE:H	1.76	0.51
1:G:304:THR:HB	1:G:335:ARG:HD2	1.92	0.51
1:D:41:GLN:O	1:D:43:VAL:N	2.44	0.51
1:E:304:THR:HB	1:E:335:ARG:HD2	1.92	0.51
1:F:37:ARG:HB3	1:F:38:PRO:HD2	1.91	0.51
1:G:37:ARG:HB3	1:G:38:PRO:HD2	1.91	0.51
3:C:454:GLY:O	3:C:458:LEU:N	2.44	0.51
1:D:107:GLU:N	1:D:135:ALA:O	2.43	0.51
1:A:304:THR:HB	1:A:335:ARG:HD2	1.92	0.51
1:E:107:GLU:N	1:E:135:ALA:O	2.43	0.51
1:F:34:ILE:HD13	1:F:34:ILE:H	1.76	0.51
3:I:81:ALA:O	3:I:85:TYR:N	2.44	0.51
3:I:455:LEU:O	3:I:459:LEU:N	2.43	0.51
3:I:473:PHE:CZ	3:I:477:ILE:HD11	2.45	0.51
3:J:454:GLY:O	3:J:458:LEU:N	2.44	0.51
1:E:39:ARG:HH21	1:F:269:MET:N	2.08	0.51
3:I:454:GLY:O	3:I:458:LEU:N	2.44	0.51
3:J:621:ARG:HB3	3:J:678:PHE:HZ	1.76	0.51
3:C:473:PHE:CZ	3:C:477:ILE:HD11	2.45	0.51
1:E:38:PRO:CG	1:E:49:GLN:HG2	2.31	0.51
1:F:300:SER:HA	1:F:335:ARG:HB2	1.93	0.51
1:D:304:THR:HB	1:D:335:ARG:HD2	1.92	0.50
1:E:300:SER:HA	1:E:335:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HA	1:A:335:ARG:HB2	1.93	0.50
1:D:34:ILE:HD13	1:D:34:ILE:H	1.76	0.50
3:I:621:ARG:HB3	3:I:678:PHE:HZ	1.76	0.50
3:C:621:ARG:HB3	3:C:678:PHE:HZ	1.76	0.50
1:G:300:SER:HA	1:G:335:ARG:HB2	1.93	0.50
3:C:81:ALA:O	3:C:85:TYR:N	2.44	0.50
1:E:41:GLN:O	1:E:43:VAL:N	2.44	0.50
1:F:41:GLN:O	1:F:43:VAL:N	2.44	0.50
1:D:222:ASP:OD2	1:D:225:ASN:ND2	2.45	0.50
1:D:300:SER:HA	1:D:335:ARG:HB2	1.93	0.50
1:E:222:ASP:OD2	1:E:225:ASN:ND2	2.45	0.50
1:G:222:ASP:OD2	1:G:225:ASN:ND2	2.45	0.50
1:F:222:ASP:OD2	1:F:225:ASN:ND2	2.45	0.50
3:C:550:THR:HG22	3:C:551:ARG:HG3	1.94	0.50
3:I:550:THR:HG22	3:I:551:ARG:HG3	1.94	0.50
1:A:43:VAL:HB	1:D:143:TYR:OH	2.11	0.49
1:A:165:ILE:HD11	1:E:43:VAL:HG12	1.94	0.49
1:E:224:GLU:OE1	1:E:224:GLU:N	2.45	0.49
3:I:436:ILE:O	3:I:437:GLU:C	2.50	0.49
3:C:320:LEU:HD21	3:C:534:SER:HB2	1.94	0.49
1:F:40:HIS:CE1	1:G:168:GLY:O	2.65	0.49
3:C:436:ILE:O	3:C:437:GLU:C	2.50	0.49
1:F:224:GLU:N	1:F:224:GLU:OE1	2.45	0.49
3:I:320:LEU:HD21	3:I:534:SER:HB2	1.94	0.49
3:J:436:ILE:O	3:J:437:GLU:C	2.50	0.49
1:A:224:GLU:N	1:A:224:GLU:OE1	2.45	0.49
3:J:306:ALA:O	3:J:310:LYS:N	2.45	0.49
3:C:306:ALA:O	3:C:310:LYS:N	2.45	0.49
3:J:81:ALA:O	3:J:85:TYR:N	2.44	0.49
3:J:320:LEU:HD21	3:J:534:SER:HB2	1.94	0.49
3:J:550:THR:HG22	3:J:551:ARG:HG3	1.94	0.49
1:E:51:ASP:C	1:E:53:TYR:N	2.60	0.49
1:E:349:LEU:HA	3:J:461:GLU:HB2	1.95	0.49
3:I:306:ALA:O	3:I:310:LYS:N	2.45	0.49
3:C:645:TRP:O	3:C:647:SER:N	2.46	0.49
3:I:326:SER:O	3:I:327:THR:CB	2.60	0.49
1:A:222:ASP:OD2	1:A:225:ASN:ND2	2.45	0.49
3:C:299:THR:O	3:C:303:ALA:N	2.42	0.49
3:J:326:SER:O	3:J:327:THR:CB	2.60	0.49
1:A:43:VAL:HG23	1:A:46:GLY:CA	2.43	0.49
3:C:119:THR:O	3:C:121:VAL:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:CA	1:D:167:GLU:O	2.59	0.48
1:D:43:VAL:HG23	1:D:46:GLY:CA	2.43	0.48
1:D:224:GLU:OE1	1:D:224:GLU:N	2.45	0.48
1:E:43:VAL:HG23	1:E:46:GLY:CA	2.43	0.48
1:A:41:GLN:O	1:A:43:VAL:N	2.44	0.48
1:F:43:VAL:HB	1:G:143:TYR:OH	2.14	0.48
1:G:41:GLN:O	1:G:43:VAL:N	2.44	0.48
3:I:119:THR:O	3:I:121:VAL:N	2.44	0.48
3:I:645:TRP:O	3:I:647:SER:N	2.46	0.48
3:C:55:ASN:O	3:C:55:ASN:ND2	2.47	0.48
3:C:607:GLN:HA	3:C:610:TYR:CE2	2.49	0.48
3:J:607:GLN:HA	3:J:610:TYR:CE2	2.49	0.48
3:J:645:TRP:O	3:J:647:SER:N	2.46	0.48
3:I:607:GLN:HA	3:I:610:TYR:CE2	2.49	0.48
1:A:107:GLU:OE2	1:A:116:ARG:NH1	2.47	0.48
1:A:191:LYS:NZ	1:G:172:PRO:O	2.33	0.48
1:E:107:GLU:OE2	1:E:116:ARG:NH1	2.47	0.48
1:F:107:GLU:OE2	1:F:116:ARG:NH1	2.47	0.48
1:G:224:GLU:OE1	1:G:224:GLU:N	2.45	0.48
3:J:55:ASN:O	3:J:55:ASN:ND2	2.47	0.48
3:J:119:THR:O	3:J:121:VAL:N	2.44	0.48
3:J:442:LYS:N	3:J:443:PRO:HD3	2.29	0.48
3:C:350:ASP:HB3	3:C:354:LYS:HE3	1.96	0.48
1:G:107:GLU:OE2	1:G:116:ARG:NH1	2.47	0.48
3:I:324:SER:HA	3:I:336:ILE:HG22	1.95	0.48
3:J:324:SER:HA	3:J:336:ILE:HG22	1.95	0.48
3:I:350:ASP:HB3	3:I:354:LYS:HE3	1.96	0.47
3:I:621:ARG:HG2	3:I:676:LYS:HG3	1.96	0.47
3:J:621:ARG:HG2	3:J:676:LYS:HG3	1.96	0.47
1:F:43:VAL:HG23	1:F:46:GLY:CA	2.43	0.47
3:C:453:ILE:HG22	3:C:453:ILE:O	2.14	0.47
1:F:286:ASP:O	1:F:289:ILE:HG22	2.15	0.47
1:F:56:ASP:O	1:F:60:SER:OG	2.22	0.47
1:G:43:VAL:HG23	1:G:46:GLY:CA	2.43	0.47
1:G:286:ASP:O	1:G:289:ILE:HG22	2.15	0.47
3:J:350:ASP:HB3	3:J:354:LYS:HE3	1.96	0.47
3:J:624:PHE:O	3:J:627:ARG:NH1	2.47	0.47
3:C:621:ARG:HG2	3:C:676:LYS:HG3	1.96	0.47
1:F:73:HIC:CG	1:F:73:HIC:O	2.63	0.47
3:I:624:PHE:O	3:I:627:ARG:NH1	2.47	0.47
1:A:286:ASP:O	1:A:289:ILE:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:GLU:OE2	1:D:116:ARG:NH1	2.47	0.47
1:E:73:HIC:O	1:E:73:HIC:CG	2.63	0.47
3:I:55:ASN:O	3:I:55:ASN:ND2	2.47	0.47
3:I:442:LYS:N	3:I:443:PRO:HD3	2.29	0.47
1:A:43:VAL:H	1:D:168:GLY:HA2	1.80	0.47
3:J:299:THR:O	3:J:303:ALA:N	2.42	0.47
1:D:73:HIC:O	1:D:73:HIC:CG	2.63	0.46
1:D:286:ASP:O	1:D:289:ILE:HG22	2.15	0.46
1:G:220:ALA:HB2	1:G:255:PHE:HB2	1.97	0.46
3:C:431:ILE:HG23	3:C:653:LYS:HB3	1.98	0.46
3:C:459:LEU:HD22	3:C:523:ASN:ND2	2.31	0.46
1:D:171:LEU:CB	1:D:172:PRO:HD3	2.44	0.46
3:J:431:ILE:HG23	3:J:653:LYS:HB3	1.97	0.46
3:J:459:LEU:HD22	3:J:523:ASN:ND2	2.31	0.46
1:E:286:ASP:O	1:E:289:ILE:HG22	2.15	0.46
3:I:431:ILE:HG23	3:I:653:LYS:HB3	1.97	0.46
3:J:287:GLN:HG3	3:J:293:THR:HG23	1.97	0.46
3:C:442:LYS:N	3:C:443:PRO:HD3	2.29	0.46
3:I:459:LEU:HD22	3:I:523:ASN:ND2	2.31	0.46
1:A:171:LEU:CB	1:A:172:PRO:HD3	2.44	0.46
3:C:182:TYR:O	3:C:184:LEU:N	2.48	0.46
1:F:220:ALA:HB2	1:F:255:PHE:HB2	1.97	0.46
3:I:615:GLU:N	3:I:615:GLU:OE1	2.49	0.46
3:C:287:GLN:HG3	3:C:293:THR:HG23	1.97	0.46
1:A:220:ALA:HB2	1:A:255:PHE:HB2	1.97	0.46
3:C:186:LYS:HD2	3:C:354:LYS:HD3	1.98	0.46
3:C:326:SER:O	3:C:327:THR:HB	2.15	0.46
3:C:601:GLU:OE2	3:C:605:ARG:NH2	2.49	0.46
3:I:299:THR:O	3:I:303:ALA:N	2.42	0.46
3:J:186:LYS:HD2	3:J:354:LYS:HD3	1.98	0.46
3:J:645:TRP:HB3	3:J:646:PRO:HD2	1.97	0.46
1:A:39:ARG:HH21	1:G:268:GLY:C	2.19	0.46
1:E:54:VAL:N	1:E:58:ALA:HB2	2.31	0.46
1:F:54:VAL:N	1:F:58:ALA:HB2	2.31	0.46
3:I:469:THR:HA	3:I:520:LEU:HD11	1.98	0.46
3:J:388:TYR:N	3:J:388:TYR:CD1	2.84	0.46
3:J:469:THR:HA	3:J:520:LEU:HD11	1.98	0.46
1:A:73:HIC:O	1:A:73:HIC:CG	2.63	0.46
1:A:64:ILE:C	1:A:65:LEU:HD12	2.37	0.45
3:C:551:ARG:HB3	3:C:555:SER:OG	2.17	0.45
3:C:615:GLU:OE1	3:C:615:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ASP:HB3	3:J:528:PHE:CE1	2.51	0.45
1:E:62:ARG:O	1:E:63:GLY:C	2.55	0.45
1:E:171:LEU:CB	1:E:172:PRO:HD3	2.44	0.45
1:F:274:ILE:HD12	1:F:275:HIS:N	2.31	0.45
1:G:49:GLN:HG3	1:G:50:LYS:H	1.79	0.45
1:G:62:ARG:O	1:G:63:GLY:C	2.55	0.45
3:I:83:ASP:O	3:I:87:SER:N	2.49	0.45
3:I:186:LYS:HD2	3:I:354:LYS:HD3	1.98	0.45
3:I:287:GLN:HG3	3:I:293:THR:HG23	1.97	0.45
3:J:615:GLU:N	3:J:615:GLU:OE1	2.49	0.45
1:A:135:ALA:HB1	1:A:140:LEU:HD11	1.99	0.45
3:C:83:ASP:O	3:C:87:SER:N	2.49	0.45
1:E:135:ALA:HB1	1:E:140:LEU:HD11	1.99	0.45
1:F:171:LEU:CB	1:F:172:PRO:HD3	2.44	0.45
1:G:54:VAL:N	1:G:58:ALA:HB2	2.31	0.45
3:C:645:TRP:HB3	3:C:646:PRO:HD2	1.97	0.45
1:D:268:GLY:C	1:G:39:ARG:NH2	2.69	0.45
1:D:274:ILE:HD12	1:D:275:HIS:N	2.31	0.45
1:E:274:ILE:HD12	1:E:275:HIS:N	2.31	0.45
1:G:289:ILE:O	1:G:293:LEU:HG	2.17	0.45
3:J:551:ARG:HB3	3:J:555:SER:OG	2.17	0.45
1:A:40:HIS:CD2	1:D:171:LEU:HD21	2.50	0.45
1:A:43:VAL:CG1	1:D:166:TYR:O	2.64	0.45
1:A:270:GLU:HG2	1:F:202:THR:HG22	1.97	0.45
3:C:624:PHE:O	3:C:627:ARG:NH1	2.47	0.45
1:D:62:ARG:O	1:D:63:GLY:C	2.55	0.45
1:D:136:ILE:N	1:D:136:ILE:HD12	2.31	0.45
1:G:73:HIC:CG	1:G:73:HIC:O	2.63	0.45
3:J:83:ASP:O	3:J:87:SER:N	2.49	0.45
1:D:270:GLU:HG2	1:G:202:THR:HG22	1.97	0.45
1:E:64:ILE:C	1:E:65:LEU:HD12	2.37	0.45
1:F:62:ARG:O	1:F:63:GLY:C	2.55	0.45
1:F:135:ALA:HB1	1:F:140:LEU:HD11	1.98	0.45
1:G:135:ALA:HB1	1:G:140:LEU:HD11	1.99	0.45
3:I:78:TYR:CZ	3:I:81:ALA:HB2	2.52	0.45
3:I:601:GLU:OE2	3:I:605:ARG:NH2	2.49	0.45
1:F:289:ILE:O	1:F:293:LEU:HG	2.17	0.45
1:G:43:VAL:CG2	1:G:46:GLY:HA3	2.47	0.45
1:G:51:ASP:C	1:G:53:TYR:N	2.60	0.45
2:B:139:GLU:OE2	1:D:221:LEU:HD22	2.17	0.45
1:D:135:ALA:HB1	1:D:140:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ILE:HD12	1:E:136:ILE:N	2.31	0.45
1:F:49:GLN:HG3	1:F:50:LYS:H	1.79	0.45
1:G:274:ILE:HD12	1:G:275:HIS:N	2.31	0.45
1:A:173:HIS:O	1:A:174:ALA:C	2.55	0.45
1:A:297:ASN:O	1:A:330:ILE:N	2.50	0.45
1:A:328:LYS:HG3	3:C:289:THR:HB	1.99	0.45
1:E:220:ALA:HB2	1:E:255:PHE:HB2	1.97	0.45
1:F:43:VAL:CG2	1:F:46:GLY:HA3	2.47	0.45
1:F:173:HIS:O	1:F:174:ALA:C	2.55	0.45
1:G:136:ILE:N	1:G:136:ILE:HD12	2.31	0.45
1:G:171:LEU:CB	1:G:172:PRO:HD3	2.44	0.45
3:I:645:TRP:HB3	3:I:646:PRO:HD2	1.97	0.45
1:A:54:VAL:N	1:A:58:ALA:HB2	2.31	0.45
3:C:360:LEU:HD13	3:C:546:LEU:HD22	1.99	0.45
1:D:268:GLY:C	1:G:39:ARG:HH21	2.19	0.45
3:J:601:GLU:OE2	3:J:605:ARG:NH2	2.49	0.45
1:A:274:ILE:HD12	1:A:275:HIS:N	2.31	0.45
1:A:289:ILE:O	1:A:293:LEU:HG	2.17	0.45
1:D:54:VAL:N	1:D:58:ALA:HB2	2.31	0.45
1:D:173:HIS:O	1:D:174:ALA:C	2.55	0.45
1:D:220:ALA:HB2	1:D:255:PHE:HB2	1.97	0.45
1:F:51:ASP:C	1:F:53:TYR:N	2.60	0.45
1:F:297:ASN:O	1:F:330:ILE:N	2.50	0.45
1:G:64:ILE:C	1:G:65:LEU:HD12	2.37	0.45
1:A:136:ILE:N	1:A:136:ILE:HD12	2.31	0.44
1:D:64:ILE:C	1:D:65:LEU:HD12	2.37	0.44
1:F:136:ILE:N	1:F:136:ILE:HD12	2.31	0.44
3:I:360:LEU:HD13	3:I:546:LEU:HD22	2.00	0.44
3:J:78:TYR:CZ	3:J:81:ALA:HB2	2.52	0.44
3:J:629:GLU:HA	3:J:676:LYS:HA	2.00	0.44
1:D:43:VAL:CG2	1:D:46:GLY:HA3	2.47	0.44
1:D:289:ILE:O	1:D:293:LEU:HG	2.17	0.44
1:D:297:ASN:O	1:D:330:ILE:N	2.50	0.44
1:F:64:ILE:C	1:F:65:LEU:HD12	2.37	0.44
3:I:551:ARG:HB3	3:I:555:SER:OG	2.17	0.44
3:I:629:GLU:HA	3:I:676:LYS:HA	2.00	0.44
3:J:360:LEU:HD13	3:J:546:LEU:HD22	2.00	0.44
1:A:169:TYR:N	1:E:40:HIS:CE1	2.85	0.44
3:C:78:TYR:CZ	3:C:81:ALA:HB2	2.52	0.44
1:D:49:GLN:HG3	1:D:50:LYS:H	1.80	0.44
1:E:297:ASN:O	1:E:330:ILE:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:629:GLU:HA	3:C:676:LYS:HA	2.00	0.44
1:E:173:HIS:O	1:E:174:ALA:C	2.55	0.44
1:E:289:ILE:O	1:E:293:LEU:HG	2.17	0.44
1:A:171:LEU:HB2	1:A:172:PRO:CD	2.46	0.44
1:G:171:LEU:HD13	1:G:172:PRO:CD	2.48	0.44
1:G:173:HIS:O	1:G:174:ALA:C	2.55	0.44
3:I:388:TYR:N	3:I:388:TYR:CD1	2.84	0.44
3:J:182:TYR:O	3:J:184:LEU:N	2.49	0.44
1:A:62:ARG:O	1:A:63:GLY:C	2.55	0.44
1:E:87:HIS:O	1:E:87:HIS:ND1	2.51	0.44
1:G:297:ASN:O	1:G:330:ILE:N	2.50	0.44
3:I:19:ILE:O	3:I:19:ILE:CG2	2.66	0.44
1:A:87:HIS:O	1:A:87:HIS:ND1	2.51	0.44
3:C:388:TYR:CD1	3:C:388:TYR:N	2.84	0.44
1:D:171:LEU:HD13	1:D:172:PRO:CD	2.48	0.44
1:E:171:LEU:HD13	1:E:172:PRO:CD	2.48	0.44
1:F:171:LEU:HD13	1:F:172:PRO:CD	2.48	0.44
3:J:19:ILE:O	3:J:19:ILE:CG2	2.66	0.44
3:J:251:LYS:O	3:J:255:THR:OG1	2.30	0.44
3:C:469:THR:HA	3:C:520:LEU:HD11	1.99	0.44
1:F:87:HIS:O	1:F:87:HIS:ND1	2.51	0.44
2:B:199:THR:O	2:B:203:ASN:ND2	2.48	0.43
1:D:56:ASP:O	1:D:60:SER:OG	2.22	0.43
1:E:275:HIS:NE2	1:E:276:GLU:OE2	2.51	0.43
1:G:34:ILE:HB	1:G:67:LEU:HD22	2.00	0.43
1:A:275:HIS:NE2	1:A:276:GLU:OE2	2.52	0.43
1:D:35:VAL:O	1:D:35:VAL:HG12	2.18	0.43
1:D:87:HIS:O	1:D:87:HIS:ND1	2.51	0.43
1:G:275:HIS:NE2	1:G:276:GLU:OE2	2.51	0.43
1:A:43:VAL:CG2	1:A:46:GLY:HA3	2.47	0.43
3:C:328:GLY:O	3:C:329:VAL:HB	2.19	0.43
1:F:34:ILE:HB	1:F:67:LEU:HD22	2.00	0.43
1:F:275:HIS:NE2	1:F:276:GLU:OE2	2.52	0.43
1:G:87:HIS:O	1:G:87:HIS:ND1	2.51	0.43
3:I:182:TYR:O	3:I:184:LEU:N	2.48	0.43
3:J:624:PHE:CZ	3:J:626:GLY:O	2.71	0.43
1:A:169:TYR:HA	1:E:40:HIS:HE1	1.83	0.43
1:D:275:HIS:NE2	1:D:276:GLU:OE2	2.52	0.43
1:E:136:ILE:O	1:E:140:LEU:HD13	2.19	0.43
1:D:34:ILE:HB	1:D:67:LEU:HD22	2.00	0.43
1:F:35:VAL:O	1:F:35:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:LEU:HB2	1:G:172:PRO:CD	2.46	0.43
1:A:50:LYS:O	1:A:52:SER:N	2.48	0.43
1:A:136:ILE:O	1:A:140:LEU:HD13	2.19	0.43
1:A:171:LEU:HD13	1:A:172:PRO:CD	2.48	0.43
1:E:34:ILE:HB	1:E:67:LEU:HD22	2.00	0.43
3:J:19:ILE:HD13	3:J:19:ILE:C	2.39	0.43
3:J:220:THR:O	3:J:222:ASN:N	2.51	0.43
1:A:34:ILE:HB	1:A:67:LEU:HD22	1.99	0.43
3:C:624:PHE:CZ	3:C:626:GLY:O	2.71	0.43
1:D:136:ILE:O	1:D:140:LEU:HD13	2.19	0.43
1:D:171:LEU:HB2	1:D:172:PRO:CD	2.46	0.43
1:E:35:VAL:O	1:E:35:VAL:HG12	2.18	0.43
3:I:481:PHE:HB3	3:I:487:LEU:HD23	2.01	0.43
1:A:325:MET:SD	1:A:327:ILE:HD11	2.59	0.43
3:C:19:ILE:HD13	3:C:19:ILE:C	2.39	0.43
3:I:19:ILE:HD13	3:I:19:ILE:C	2.39	0.43
3:J:548:PRO:O	3:J:549:PRO:C	2.57	0.43
1:F:39:ARG:HG2	1:F:66:THR:OG1	2.19	0.43
1:F:55:GLY:C	1:F:57:GLU:N	2.73	0.43
1:G:39:ARG:HG2	1:G:66:THR:OG1	2.19	0.43
3:C:175:ILE:HB	3:C:374:CYS:HB3	2.01	0.43
3:C:481:PHE:HB3	3:C:487:LEU:HD23	2.01	0.43
1:E:50:LYS:O	1:E:52:SER:N	2.48	0.43
1:F:136:ILE:O	1:F:140:LEU:HD13	2.19	0.43
1:G:136:ILE:O	1:G:140:LEU:HD13	2.19	0.43
3:I:220:THR:O	3:I:222:ASN:N	2.51	0.43
3:I:634:TYR:O	3:I:636:ARG:N	2.50	0.43
1:A:167:GLU:O	1:E:42:GLY:CA	2.65	0.42
1:G:50:LYS:O	1:G:52:SER:N	2.48	0.42
1:G:55:GLY:C	1:G:57:GLU:N	2.73	0.42
3:I:175:ILE:HB	3:I:374:CYS:HB3	2.01	0.42
3:J:481:PHE:HB3	3:J:487:LEU:HD23	2.01	0.42
3:C:220:THR:O	3:C:222:ASN:N	2.51	0.42
1:D:50:LYS:O	1:D:52:SER:N	2.48	0.42
3:I:624:PHE:CZ	3:I:626:GLY:O	2.71	0.42
3:J:175:ILE:HB	3:J:374:CYS:HB3	2.01	0.42
1:A:35:VAL:O	1:A:35:VAL:HG12	2.18	0.42
1:A:49:GLN:HG3	1:A:50:LYS:H	1.79	0.42
1:E:55:GLY:C	1:E:57:GLU:N	2.73	0.42
1:E:276:GLU:OE1	1:E:276:GLU:N	2.53	0.42
1:G:35:VAL:O	1:G:35:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:498:ILE:HD11	3:I:504:ARG:HE	1.84	0.42
3:I:548:PRO:O	3:I:549:PRO:C	2.57	0.42
3:J:169:ASN:OD1	3:J:170:ALA:N	2.52	0.42
1:A:276:GLU:N	1:A:276:GLU:OE1	2.53	0.42
3:C:169:ASN:OD1	3:C:170:ALA:N	2.53	0.42
3:C:548:PRO:O	3:C:549:PRO:C	2.57	0.42
1:E:43:VAL:CG2	1:E:46:GLY:HA3	2.46	0.42
1:F:202:THR:OG1	1:F:205:GLU:OE2	2.38	0.42
3:I:251:LYS:O	3:I:255:THR:OG1	2.30	0.42
3:I:431:ILE:HG12	3:I:653:LYS:HD2	2.01	0.42
3:I:623:GLY:O	3:I:624:PHE:HB3	2.20	0.42
3:C:183:LEU:O	3:C:184:LEU:HB3	2.19	0.42
3:C:498:ILE:HD11	3:C:504:ARG:HE	1.84	0.42
3:C:623:GLY:O	3:C:624:PHE:HB3	2.20	0.42
1:D:276:GLU:N	1:D:276:GLU:OE1	2.53	0.42
1:F:276:GLU:N	1:F:276:GLU:OE1	2.53	0.42
1:G:276:GLU:OE1	1:G:276:GLU:N	2.53	0.42
3:C:251:LYS:O	3:C:255:THR:OG1	2.30	0.42
1:E:39:ARG:HH21	1:F:268:GLY:C	2.21	0.42
1:G:42:GLY:C	1:G:44:MET:H	2.21	0.42
3:I:183:LEU:O	3:I:184:LEU:HB3	2.19	0.42
3:J:498:ILE:HD11	3:J:504:ARG:HE	1.84	0.42
1:G:202:THR:OG1	1:G:205:GLU:OE2	2.38	0.42
3:J:622:ALA:HB3	3:J:678:PHE:CZ	2.55	0.42
1:A:55:GLY:C	1:A:57:GLU:N	2.73	0.42
3:C:431:ILE:HG12	3:C:653:LYS:HD2	2.01	0.42
1:E:56:ASP:O	1:E:60:SER:OG	2.22	0.42
3:I:434:LYS:HD3	3:I:434:LYS:N	2.35	0.42
3:J:623:GLY:O	3:J:624:PHE:HB3	2.20	0.42
1:D:42:GLY:C	1:D:44:MET:H	2.22	0.42
1:D:53:TYR:N	1:D:53:TYR:CD1	2.88	0.42
3:I:622:ALA:HB3	3:I:678:PHE:CZ	2.54	0.42
1:A:53:TYR:N	1:A:53:TYR:CD1	2.88	0.42
3:C:19:ILE:O	3:C:19:ILE:CG2	2.66	0.42
3:C:622:ALA:HB3	3:C:678:PHE:CZ	2.54	0.42
1:D:269:MET:CA	1:G:39:ARG:HH21	2.33	0.42
1:E:53:TYR:N	1:E:53:TYR:CD1	2.88	0.42
1:E:202:THR:OG1	1:E:205:GLU:OE2	2.38	0.42
3:I:169:ASN:OD1	3:I:170:ALA:N	2.53	0.42
3:I:369:ASN:HA	3:I:372:ILE:HB	2.02	0.42
3:J:165:GLU:HB3	3:J:381:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:434:LYS:HD3	3:J:434:LYS:N	2.35	0.42
1:A:39:ARG:HG2	1:A:66:THR:OG1	2.19	0.41
1:A:39:ARG:NH2	1:G:268:GLY:C	2.73	0.41
3:C:369:ASN:HA	3:C:372:ILE:HB	2.02	0.41
1:D:189:LEU:HG	1:D:193:LEU:HD13	2.02	0.41
1:G:53:TYR:N	1:G:53:TYR:CD1	2.88	0.41
3:J:183:LEU:O	3:J:184:LEU:HB3	2.19	0.41
1:A:43:VAL:HG13	1:D:166:TYR:O	2.19	0.41
3:C:165:GLU:HB3	3:C:381:VAL:HG13	2.02	0.41
3:C:434:LYS:HD3	3:C:434:LYS:N	2.35	0.41
1:E:39:ARG:HG2	1:E:66:THR:OG1	2.19	0.41
1:E:49:GLN:HG3	1:E:50:LYS:H	1.79	0.41
1:G:47:MET:O	1:G:49:GLN:N	2.51	0.41
3:I:165:GLU:HB3	3:I:381:VAL:HG13	2.02	0.41
3:J:369:ASN:HA	3:J:372:ILE:HB	2.02	0.41
1:A:202:THR:OG1	1:A:205:GLU:OE2	2.38	0.41
1:A:326:LYS:HD3	1:A:328:LYS:HE3	2.00	0.41
1:F:171:LEU:HB2	1:F:172:PRO:CD	2.46	0.41
1:D:202:THR:OG1	1:D:205:GLU:OE2	2.38	0.41
1:F:42:GLY:C	1:F:44:MET:H	2.22	0.41
1:A:62:ARG:O	1:A:65:LEU:N	2.53	0.41
1:A:159:VAL:HG23	1:A:161:HIS:CE1	2.56	0.41
3:C:415:ILE:HD12	3:C:442:LYS:HD2	2.03	0.41
1:F:257:CYS:HB3	1:F:258:PRO:HD3	2.02	0.41
3:I:415:ILE:HD12	3:I:442:LYS:HD2	2.03	0.41
1:D:39:ARG:HG2	1:D:66:THR:OG1	2.19	0.41
1:D:257:CYS:HB3	1:D:258:PRO:HD3	2.02	0.41
1:G:189:LEU:HG	1:G:193:LEU:HD13	2.02	0.41
1:G:346:LEU:HD23	1:G:349:LEU:HD12	2.03	0.41
3:I:621:ARG:O	3:I:622:ALA:HB2	2.21	0.41
3:I:681:ASN:HA	3:I:682:PRO:HD3	1.97	0.41
1:D:55:GLY:C	1:D:57:GLU:N	2.73	0.41
1:D:152:VAL:HA	1:D:298:VAL:HB	2.02	0.41
1:E:62:ARG:O	1:E:65:LEU:N	2.53	0.41
1:F:40:HIS:CE1	1:G:169:TYR:N	2.89	0.41
1:G:62:ARG:O	1:G:65:LEU:N	2.53	0.41
3:I:142:LEU:HD13	3:I:142:LEU:C	2.41	0.41
3:J:415:ILE:HD12	3:J:442:LYS:HD2	2.03	0.41
1:A:171:LEU:HD21	1:E:40:HIS:CD2	2.55	0.41
1:A:268:GLY:C	1:F:39:ARG:HH21	2.23	0.41
3:C:40:TYR:CZ	3:C:75:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:621:ARG:O	3:C:622:ALA:HB2	2.21	0.41
1:D:294:TYR:HB3	1:D:327:ILE:HD13	2.03	0.41
1:E:34:ILE:HD13	1:E:34:ILE:N	2.36	0.41
1:E:189:LEU:HG	1:E:193:LEU:HD13	2.02	0.41
1:E:294:TYR:HB3	1:E:327:ILE:HD13	2.03	0.41
1:F:53:TYR:N	1:F:53:TYR:CD1	2.88	0.41
1:F:294:TYR:HB3	1:F:327:ILE:HD13	2.03	0.41
1:F:346:LEU:HD23	1:F:349:LEU:HD12	2.03	0.41
1:G:51:ASP:O	1:G:53:TYR:CA	2.69	0.41
1:G:250:ILE:O	1:G:250:ILE:HG13	2.21	0.41
1:G:294:TYR:HB3	1:G:327:ILE:HD13	2.03	0.41
3:J:40:TYR:CZ	3:J:75:PRO:HA	2.56	0.41
3:J:136:LEU:HD21	3:J:372:ILE:HG23	2.03	0.41
3:J:142:LEU:HD13	3:J:142:LEU:C	2.41	0.41
3:J:414:PHE:O	3:J:418:THR:N	2.51	0.41
3:J:431:ILE:HG12	3:J:653:LYS:HD2	2.01	0.41
3:J:634:TYR:O	3:J:636:ARG:N	2.50	0.41
1:A:189:LEU:HG	1:A:193:LEU:HD13	2.02	0.41
1:F:47:MET:O	1:F:49:GLN:N	2.51	0.41
1:F:189:LEU:HG	1:F:193:LEU:HD13	2.02	0.41
3:I:40:TYR:CZ	3:I:75:PRO:HA	2.56	0.41
3:I:136:LEU:HD21	3:I:372:ILE:HG23	2.03	0.41
1:A:152:VAL:HA	1:A:298:VAL:HB	2.02	0.40
1:A:346:LEU:HD23	1:A:349:LEU:HD12	2.03	0.40
1:D:159:VAL:HG23	1:D:161:HIS:CE1	2.56	0.40
1:E:47:MET:O	1:E:49:GLN:N	2.51	0.40
1:F:34:ILE:HD13	1:F:34:ILE:N	2.36	0.40
1:F:159:VAL:HG23	1:F:161:HIS:CE1	2.56	0.40
1:G:152:VAL:HA	1:G:298:VAL:HB	2.02	0.40
1:A:169:TYR:CA	1:E:40:HIS:CE1	3.04	0.40
1:D:52:SER:C	1:D:53:TYR:HD1	2.24	0.40
1:D:62:ARG:O	1:D:65:LEU:N	2.53	0.40
1:E:345:ILE:HG12	3:J:464:LEU:HB3	2.03	0.40
1:F:62:ARG:O	1:F:65:LEU:N	2.53	0.40
1:A:10:CYS:SG	1:A:11:ASP:N	2.95	0.40
1:A:268:GLY:C	1:F:39:ARG:NH2	2.75	0.40
2:B:169:LEU:HD22	2:H:165:VAL:HG13	2.03	0.40
3:C:10:VAL:O	3:C:10:VAL:HG12	2.21	0.40
1:D:10:CYS:SG	1:D:11:ASP:N	2.95	0.40
1:E:10:CYS:SG	1:E:11:ASP:N	2.95	0.40
1:E:52:SER:C	1:E:53:TYR:HD1	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:HIS:HE1	1:G:169:TYR:HA	1.87	0.40
1:G:159:VAL:HG23	1:G:161:HIS:CE1	2.56	0.40
3:J:223:ALA:N	3:J:224:PRO:CD	2.85	0.40
1:A:250:ILE:O	1:A:250:ILE:HG13	2.21	0.40
1:E:152:VAL:HA	1:E:298:VAL:HB	2.03	0.40
1:E:257:CYS:HB3	1:E:258:PRO:HD3	2.02	0.40
1:F:50:LYS:O	1:F:52:SER:N	2.48	0.40
3:I:326:SER:H	3:I:332:ARG:HB2	1.86	0.40
3:I:414:PHE:O	3:I:418:THR:N	2.51	0.40
3:I:518:GLY:O	3:I:519:PHE:C	2.60	0.40
3:J:621:ARG:O	3:J:622:ALA:HB2	2.21	0.40
1:A:52:SER:C	1:A:53:TYR:HD1	2.24	0.40
3:C:542:LEU:O	3:C:545:GLY:N	2.55	0.40
1:F:52:SER:C	1:F:53:TYR:HD1	2.24	0.40
3:J:387:ILE:HD13	3:J:387:ILE:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	0	9
1	D	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	0	9
1	E	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	0	9
1	F	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	0	9
1	G	372/375 (99%)	284 (76%)	51 (14%)	37 (10%)	0	9
2	B	134/136 (98%)	134 (100%)	0	0	100	100
2	H	134/136 (98%)	134 (100%)	0	0	100	100
3	C	680/697 (98%)	551 (81%)	99 (15%)	30 (4%)	2	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	680/697 (98%)	551 (81%)	98 (14%)	31 (5%)	2	21
3	J	680/697 (98%)	551 (81%)	98 (14%)	31 (5%)	2	21
All	All	4168/4238 (98%)	3341 (80%)	550 (13%)	277 (7%)	2	16

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
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	63	GLY
1	A	143	TYR
1	A	172	PRO
1	A	174	ALA
3	C	78	TYR
3	C	469	THR
1	D	41	GLN
1	D	42	GLY
1	D	43	VAL
1	D	47	MET
1	D	49	GLN
1	D	51	ASP
1	D	52	SER
1	D	63	GLY
1	D	143	TYR
1	D	172	PRO
1	D	174	ALA
1	E	41	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	63	GLY
1	E	143	TYR
1	E	172	PRO

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Mol	Chain	Res	Type
1	E	174	ALA
1	F	41	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	63	GLY
1	F	143	TYR
1	F	172	PRO
1	F	174	ALA
1	G	41	GLN
1	G	42	GLY
1	G	43	VAL
1	G	47	MET
1	G	49	GLN
1	G	51	ASP
1	G	52	SER
1	G	63	GLY
1	G	143	TYR
1	G	172	PRO
1	G	174	ALA
3	I	78	TYR
3	I	469	THR
3	J	78	TYR
3	J	469	THR
1	A	50	LYS
1	A	245	GLY
3	C	76	HIS
3	C	283	GLU
3	C	290	GLY
3	C	335	VAL
3	C	437	GLU
3	C	622	ALA
1	D	15	GLY
1	D	50	LYS
1	D	245	GLY
1	E	50	LYS
1	E	245	GLY
1	F	50	LYS
1	F	245	GLY

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Mol	Chain	Res	Type
1	G	50	LYS
1	G	245	GLY
3	I	76	HIS
3	I	283	GLU
3	I	290	GLY
3	I	335	VAL
3	I	437	GLU
3	I	622	ALA
3	J	76	HIS
3	J	283	GLU
3	J	290	GLY
3	J	335	VAL
3	J	437	GLU
3	J	622	ALA
1	A	15	GLY
1	A	21	PHE
1	A	38	PRO
1	A	44	MET
1	A	53	TYR
1	A	100	GLU
1	A	128	ASN
1	A	137	GLN
1	A	144	ALA
1	A	145	SER
1	A	158	GLY
1	A	171	LEU
1	A	182	GLY
1	A	370	VAL
3	C	184	LEU
3	C	257	GLY
3	C	624	PHE
3	C	636	ARG
1	D	6	THR
1	D	21	PHE
1	D	38	PRO
1	D	44	MET
1	D	53	TYR
1	D	100	GLU
1	D	128	ASN
1	D	137	GLN
1	D	144	ALA
1	D	145	SER

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Mol	Chain	Res	Type
1	D	158	GLY
1	D	171	LEU
1	D	182	GLY
1	D	370	VAL
1	E	15	GLY
1	E	21	PHE
1	E	38	PRO
1	E	44	MET
1	E	53	TYR
1	E	100	GLU
1	E	128	ASN
1	E	137	GLN
1	E	144	ALA
1	E	145	SER
1	E	158	GLY
1	E	171	LEU
1	E	182	GLY
1	E	370	VAL
1	F	6	THR
1	F	15	GLY
1	F	21	PHE
1	F	38	PRO
1	F	44	MET
1	F	53	TYR
1	F	100	GLU
1	F	128	ASN
1	F	137	GLN
1	F	144	ALA
1	F	145	SER
1	F	158	GLY
1	F	171	LEU
1	F	182	GLY
1	F	370	VAL
1	G	15	GLY
1	G	21	PHE
1	G	38	PRO
1	G	44	MET
1	G	53	TYR
1	G	100	GLU
1	G	128	ASN
1	G	137	GLN
1	G	144	ALA

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Mol	Chain	Res	Type
1	G	145	SER
1	G	158	GLY
1	G	171	LEU
1	G	182	GLY
1	G	370	VAL
3	I	184	LEU
3	I	257	GLY
3	I	624	PHE
3	I	636	ARG
3	J	184	LEU
3	J	257	GLY
3	J	624	PHE
3	J	636	ARG
1	A	4	GLU
1	A	6	THR
3	C	328	GLY
3	C	455	LEU
3	C	494	LYS
3	C	520	LEU
3	C	676	LYS
1	D	4	GLU
1	E	4	GLU
1	E	6	THR
1	F	4	GLU
1	G	4	GLU
1	G	6	THR
3	I	328	GLY
3	I	455	LEU
3	I	494	LYS
3	I	520	LEU
3	I	676	LYS
3	J	327	THR
3	J	328	GLY
3	J	455	LEU
3	J	494	LYS
3	J	520	LEU
3	J	676	LYS
1	A	146	GLY
3	C	13	PHE
3	C	330	GLY
3	C	380	PRO
3	C	483	LYS

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Mol	Chain	Res	Type
3	C	549	PRO
1	D	142	LEU
1	D	146	GLY
1	E	146	GLY
1	F	146	GLY
1	G	146	GLY
3	I	13	PHE
3	I	327	THR
3	I	330	GLY
3	I	380	PRO
3	I	483	LYS
3	I	549	PRO
3	J	13	PHE
3	J	330	GLY
3	J	380	PRO
3	J	483	LYS
3	J	549	PRO
1	A	142	LEU
3	C	279	ILE
3	C	552	PRO
3	C	646	PRO
1	E	142	LEU
1	F	142	LEU
1	G	142	LEU
3	I	279	ILE
3	I	552	PRO
3	I	646	PRO
3	J	279	ILE
3	J	552	PRO
3	J	646	PRO
1	A	369	ILE
3	C	329	VAL
1	D	369	ILE
1	E	369	ILE
1	F	369	ILE
1	G	369	ILE
3	I	329	VAL
3	J	329	VAL
1	A	35	VAL
1	A	156	GLY
3	C	14	VAL
3	C	208	GLY

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Mol	Chain	Res	Type
1	D	35	VAL
1	D	70	PRO
1	D	156	GLY
1	E	35	VAL
1	E	156	GLY
1	F	35	VAL
1	F	70	PRO
1	F	156	GLY
1	G	35	VAL
1	G	156	GLY
3	I	14	VAL
3	I	208	GLY
3	J	14	VAL
3	J	208	GLY
1	A	55	GLY
1	A	70	PRO
3	C	372	ILE
3	C	681	ASN
1	D	55	GLY
1	E	55	GLY
1	E	70	PRO
1	F	55	GLY
1	G	55	GLY
1	G	70	PRO
3	I	372	ILE
3	I	681	ASN
3	J	372	ILE
3	J	681	ASN
1	A	201	VAL
1	D	201	VAL
1	E	201	VAL
1	F	201	VAL
1	G	201	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/317 (100%)	283 (89%)	34 (11%)	6	23
1	D	317/317 (100%)	282 (89%)	35 (11%)	6	22
1	E	317/317 (100%)	283 (89%)	34 (11%)	6	23
1	F	317/317 (100%)	282 (89%)	35 (11%)	6	22
1	G	317/317 (100%)	282 (89%)	35 (11%)	6	22
2	B	118/118 (100%)	117 (99%)	1 (1%)	81	89
2	H	118/118 (100%)	118 (100%)	0	100	100
3	C	609/616 (99%)	586 (96%)	23 (4%)	33	57
3	I	609/616 (99%)	580 (95%)	29 (5%)	25	51
3	J	609/616 (99%)	580 (95%)	29 (5%)	25	51
All	All	3648/3669 (99%)	3393 (93%)	255 (7%)	19	40

All (255) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	39	ARG
1	A	40	HIS
1	A	47	MET
1	A	49	GLN
1	A	50	LYS
1	A	51	ASP
1	A	52	SER
1	A	53	TYR
1	A	64	ILE
1	A	69	TYR
1	A	87	HIS
1	A	116	ARG
1	A	123	MET
1	A	137	GLN
1	A	151	ILE
1	A	166	TYR
1	A	169	TYR
1	A	171	LEU
1	A	173	HIS
1	A	183	ARG
1	A	192	ILE
1	A	196	ARG
1	A	202	THR

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Mol	Chain	Res	Type
1	A	227	MET
1	A	240	TYR
1	A	242	LEU
1	A	246	GLN
1	A	261	LEU
1	A	270	GLU
1	A	291	LYS
1	A	335	ARG
1	A	340	TRP
1	A	356	TRP
2	B	154	ILE
3	C	13	PHE
3	C	19	ILE
3	C	159	ARG
3	C	188	ARG
3	C	228	TYR
3	C	251	LYS
3	C	256	LEU
3	C	281	PHE
3	C	332	ARG
3	C	387	ILE
3	C	388	TYR
3	C	434	LYS
3	C	442	LYS
3	C	459	LEU
3	C	516	VAL
3	C	535	MET
3	C	609	ARG
3	C	614	LEU
3	C	620	ARG
3	C	624	PHE
3	C	627	ARG
3	C	653	LYS
3	C	670	ILE
1	D	34	ILE
1	D	39	ARG
1	D	40	HIS
1	D	47	MET
1	D	49	GLN
1	D	50	LYS
1	D	51	ASP
1	D	52	SER

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Mol	Chain	Res	Type
1	D	53	TYR
1	D	64	ILE
1	D	69	TYR
1	D	87	HIS
1	D	116	ARG
1	D	123	MET
1	D	137	GLN
1	D	147	ARG
1	D	151	ILE
1	D	166	TYR
1	D	169	TYR
1	D	171	LEU
1	D	173	HIS
1	D	183	ARG
1	D	192	ILE
1	D	196	ARG
1	D	202	THR
1	D	227	MET
1	D	240	TYR
1	D	242	LEU
1	D	246	GLN
1	D	261	LEU
1	D	270	GLU
1	D	291	LYS
1	D	335	ARG
1	D	340	TRP
1	D	356	TRP
1	E	34	ILE
1	E	39	ARG
1	E	40	HIS
1	E	49	GLN
1	E	50	LYS
1	E	51	ASP
1	E	52	SER
1	E	53	TYR
1	E	64	ILE
1	E	69	TYR
1	E	87	HIS
1	E	116	ARG
1	E	123	MET
1	E	137	GLN
1	E	147	ARG

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Mol	Chain	Res	Type
1	E	151	ILE
1	E	166	TYR
1	E	169	TYR
1	E	171	LEU
1	E	173	HIS
1	E	183	ARG
1	E	192	ILE
1	E	196	ARG
1	E	202	THR
1	E	227	MET
1	E	240	TYR
1	E	242	LEU
1	E	246	GLN
1	E	261	LEU
1	E	270	GLU
1	E	291	LYS
1	E	335	ARG
1	E	340	TRP
1	E	356	TRP
1	F	34	ILE
1	F	39	ARG
1	F	40	HIS
1	F	47	MET
1	F	49	GLN
1	F	50	LYS
1	F	51	ASP
1	F	52	SER
1	F	53	TYR
1	F	64	ILE
1	F	69	TYR
1	F	87	HIS
1	F	116	ARG
1	F	123	MET
1	F	137	GLN
1	F	147	ARG
1	F	151	ILE
1	F	166	TYR
1	F	169	TYR
1	F	171	LEU
1	F	173	HIS
1	F	183	ARG
1	F	192	ILE

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Mol	Chain	Res	Type
1	F	196	ARG
1	F	202	THR
1	F	227	MET
1	F	240	TYR
1	F	242	LEU
1	F	246	GLN
1	F	261	LEU
1	F	270	GLU
1	F	291	LYS
1	F	335	ARG
1	F	340	TRP
1	F	356	TRP
1	G	34	ILE
1	G	39	ARG
1	G	40	HIS
1	G	47	MET
1	G	49	GLN
1	G	50	LYS
1	G	51	ASP
1	G	52	SER
1	G	53	TYR
1	G	64	ILE
1	G	69	TYR
1	G	87	HIS
1	G	116	ARG
1	G	123	MET
1	G	137	GLN
1	G	147	ARG
1	G	151	ILE
1	G	166	TYR
1	G	169	TYR
1	G	171	LEU
1	G	173	HIS
1	G	183	ARG
1	G	192	ILE
1	G	196	ARG
1	G	202	THR
1	G	227	MET
1	G	240	TYR
1	G	242	LEU
1	G	246	GLN
1	G	261	LEU

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Mol	Chain	Res	Type
1	G	270	GLU
1	G	291	LYS
1	G	335	ARG
1	G	340	TRP
1	G	356	TRP
3	I	13	PHE
3	I	19	ILE
3	I	159	ARG
3	I	188	ARG
3	I	228	TYR
3	I	251	LYS
3	I	256	LEU
3	I	281	PHE
3	I	288	ARG
3	I	325	ILE
3	I	327	THR
3	I	329	VAL
3	I	332	ARG
3	I	387	ILE
3	I	388	TYR
3	I	434	LYS
3	I	442	LYS
3	I	459	LEU
3	I	496	ARG
3	I	516	VAL
3	I	535	MET
3	I	557	LYS
3	I	609	ARG
3	I	614	LEU
3	I	620	ARG
3	I	624	PHE
3	I	627	ARG
3	I	653	LYS
3	I	670	ILE
3	J	13	PHE
3	J	19	ILE
3	J	159	ARG
3	J	188	ARG
3	J	228	TYR
3	J	251	LYS
3	J	256	LEU
3	J	281	PHE

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Mol	Chain	Res	Type
3	J	288	ARG
3	J	325	ILE
3	J	327	THR
3	J	329	VAL
3	J	332	ARG
3	J	387	ILE
3	J	388	TYR
3	J	434	LYS
3	J	442	LYS
3	J	459	LEU
3	J	496	ARG
3	J	516	VAL
3	J	535	MET
3	J	557	LYS
3	J	609	ARG
3	J	614	LEU
3	J	620	ARG
3	J	624	PHE
3	J	627	ARG
3	J	653	LYS
3	J	670	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	88	HIS
1	A	137	GLN
1	A	161	HIS
1	A	252	ASN
2	B	216	GLN
3	C	95	GLN
3	C	125	GLN
3	C	154	ASN
3	C	167	GLN
3	C	313	GLN
3	C	402	ASN
3	C	523	ASN
3	C	536	GLN
1	D	88	HIS
1	D	137	GLN
1	D	161	HIS

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Mol	Chain	Res	Type
1	D	252	ASN
1	E	40	HIS
1	E	88	HIS
1	E	92	ASN
1	E	137	GLN
1	E	161	HIS
1	E	252	ASN
1	F	40	HIS
1	F	137	GLN
1	F	161	HIS
1	F	252	ASN
1	G	88	HIS
1	G	137	GLN
1	G	161	HIS
1	G	252	ASN
3	I	95	GLN
3	I	125	GLN
3	I	154	ASN
3	I	167	GLN
3	I	313	GLN
3	I	402	ASN
3	I	523	ASN
3	I	536	GLN
3	J	95	GLN
3	J	125	GLN
3	J	154	ASN
3	J	167	GLN
3	J	313	GLN
3	J	402	ASN
3	J	523	ASN
3	J	536	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	8,11,12	1.71	3 (37%)	6,14,16	1.64	2 (33%)
1	HIC	A	73	1	8,11,12	1.70	3 (37%)	6,14,16	1.64	2 (33%)
1	HIC	F	73	1	8,11,12	1.70	3 (37%)	6,14,16	1.64	2 (33%)
1	HIC	D	73	1	8,11,12	1.71	3 (37%)	6,14,16	1.64	2 (33%)
1	HIC	G	73	1	8,11,12	1.71	3 (37%)	6,14,16	1.65	2 (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	-	1/5/6/8	0/1/1/1
1	HIC	A	73	1	-	1/5/6/8	0/1/1/1
1	HIC	F	73	1	-	1/5/6/8	0/1/1/1
1	HIC	D	73	1	-	1/5/6/8	0/1/1/1
1	HIC	G	73	1	-	1/5/6/8	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	73	HIC	CA-N	2.86	1.56	1.48
1	A	73	HIC	CA-N	2.86	1.56	1.48
1	D	73	HIC	CA-N	2.86	1.56	1.48
1	G	73	HIC	CA-N	2.85	1.56	1.48
1	F	73	HIC	CA-N	2.85	1.56	1.48
1	G	73	HIC	CD2-CG	2.27	1.39	1.36
1	F	73	HIC	CD2-CG	2.26	1.39	1.36
1	A	73	HIC	CD2-CG	2.22	1.39	1.36
1	D	73	HIC	CD2-CG	2.21	1.39	1.36
1	E	73	HIC	CD2-CG	2.20	1.39	1.36
1	E	73	HIC	CB-CA	2.14	1.58	1.53
1	F	73	HIC	CB-CA	2.11	1.58	1.53
1	A	73	HIC	CB-CA	2.10	1.58	1.53
1	D	73	HIC	CB-CA	2.10	1.58	1.53
1	G	73	HIC	CB-CA	2.09	1.58	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	HIC	CB-CA-C	-3.16	105.55	111.47
1	G	73	HIC	CB-CA-C	-3.16	105.55	111.47
1	E	73	HIC	CB-CA-C	-3.15	105.56	111.47
1	A	73	HIC	CB-CA-C	-3.14	105.58	111.47
1	D	73	HIC	CB-CA-C	-3.14	105.59	111.47
1	G	73	HIC	CG-CD2-NE2	-2.37	105.21	107.78
1	A	73	HIC	CG-CD2-NE2	-2.37	105.21	107.78
1	D	73	HIC	CG-CD2-NE2	-2.36	105.22	107.78
1	F	73	HIC	CG-CD2-NE2	-2.36	105.22	107.78
1	E	73	HIC	CG-CD2-NE2	-2.35	105.23	107.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	D	73	HIC	O-C-CA-CB
1	E	73	HIC	O-C-CA-CB
1	F	73	HIC	O-C-CA-CB
1	G	73	HIC	O-C-CA-CB

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	D	73	HIC	2	0
1	G	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	-	24,29,29	1.20	1 (4%)	29,45,45	1.41	4 (13%)
4	ADP	A	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (13%)
4	ADP	F	376	-	24,29,29	1.19	1 (4%)	29,45,45	1.41	4 (13%)
4	ADP	D	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (13%)
4	ADP	G	376	-	24,29,29	1.20	2 (8%)	29,45,45	1.41	4 (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	-	-	0/12/32/32	0/3/3/3
4	ADP	A	376	-	-	0/12/32/32	0/3/3/3
4	ADP	F	376	-	-	0/12/32/32	0/3/3/3
4	ADP	D	376	-	-	0/12/32/32	0/3/3/3
4	ADP	G	376	-	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	376	ADP	C2-N1	3.01	1.39	1.33
4	E	376	ADP	C2-N1	3.01	1.39	1.33
4	D	376	ADP	C2-N1	2.99	1.39	1.33
4	F	376	ADP	C2-N1	2.97	1.39	1.33
4	G	376	ADP	C2-N1	2.96	1.39	1.33
4	A	376	ADP	C2'-C1'	-2.04	1.50	1.53
4	D	376	ADP	C2'-C1'	-2.01	1.50	1.53
4	G	376	ADP	C8-N7	-2.01	1.31	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	376	ADP	C4-C5-N7	3.95	113.51	109.40
4	E	376	ADP	C4-C5-N7	3.94	113.50	109.40
4	A	376	ADP	C4-C5-N7	3.93	113.50	109.40
4	D	376	ADP	C4-C5-N7	3.93	113.50	109.40
4	G	376	ADP	C4-C5-N7	3.92	113.49	109.40
4	E	376	ADP	N3-C2-N1	-2.21	125.22	128.68
4	D	376	ADP	N3-C2-N1	-2.20	125.23	128.68
4	F	376	ADP	C2-N1-C6	2.20	122.51	118.75
4	F	376	ADP	N3-C2-N1	-2.19	125.25	128.68
4	A	376	ADP	N3-C2-N1	-2.19	125.26	128.68
4	D	376	ADP	C2-N1-C6	2.18	122.49	118.75
4	E	376	ADP	C2-N1-C6	2.18	122.49	118.75
4	G	376	ADP	N3-C2-N1	-2.17	125.29	128.68
4	G	376	ADP	C2-N1-C6	2.17	122.46	118.75
4	A	376	ADP	C2-N1-C6	2.16	122.45	118.75
4	A	376	ADP	O3B-PB-O2B	2.10	115.67	107.64
4	G	376	ADP	O3B-PB-O2B	2.10	115.67	107.64
4	F	376	ADP	O3B-PB-O2B	2.10	115.66	107.64
4	E	376	ADP	O3B-PB-O2B	2.09	115.62	107.64
4	D	376	ADP	O3B-PB-O2B	2.09	115.62	107.64

There are no chirality outliers.

There are no torsion outliers.

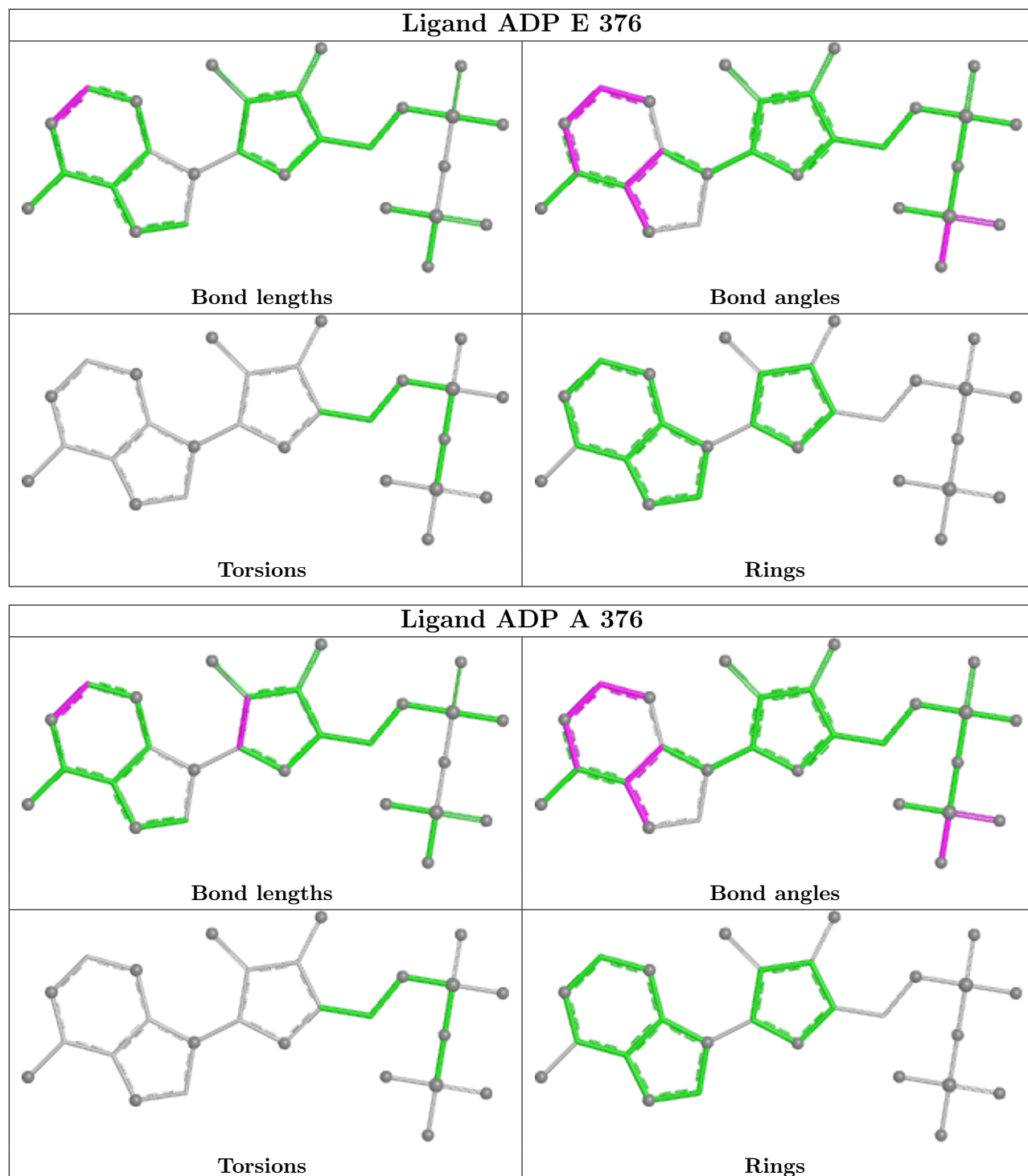
There are no ring outliers.

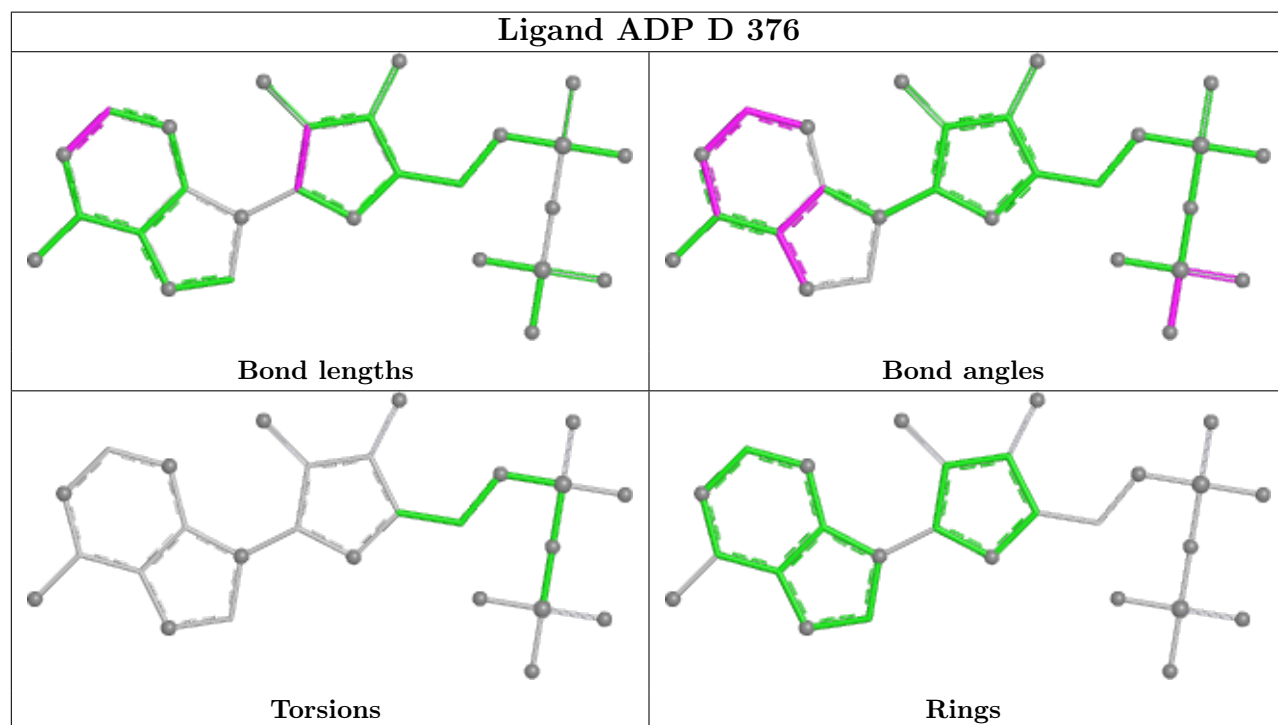
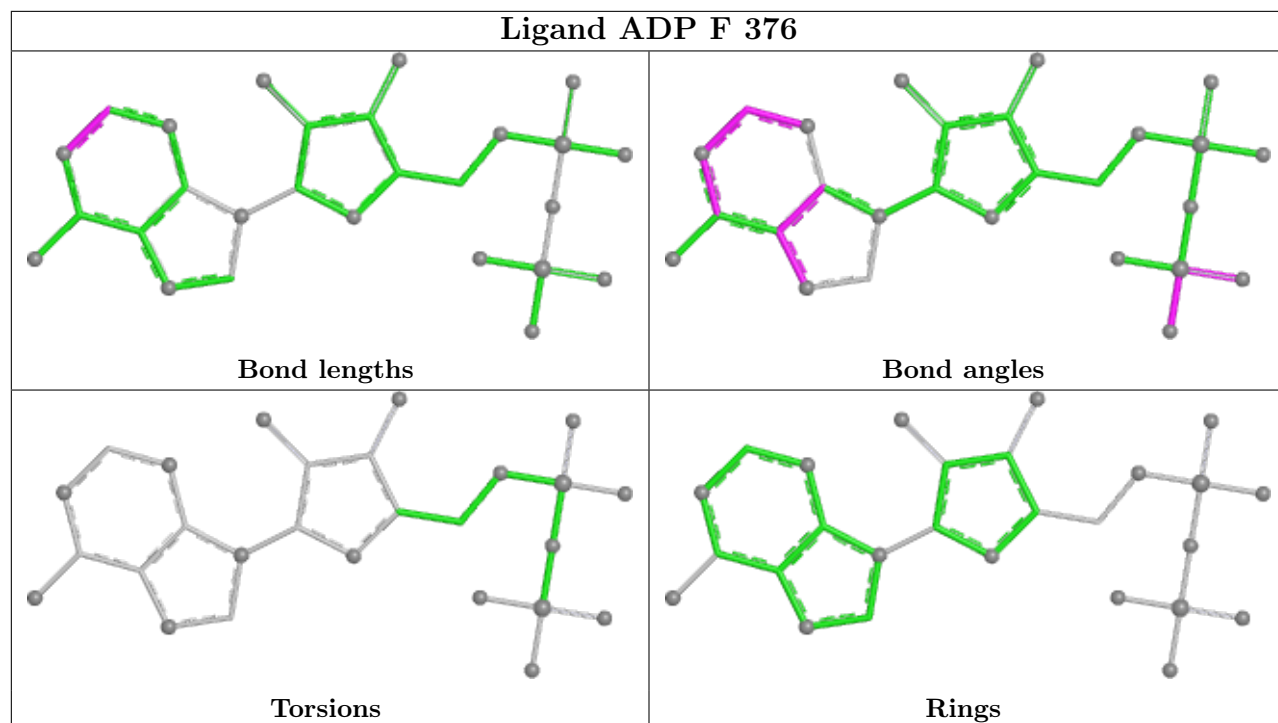
5 monomers are involved in 15 short contacts:

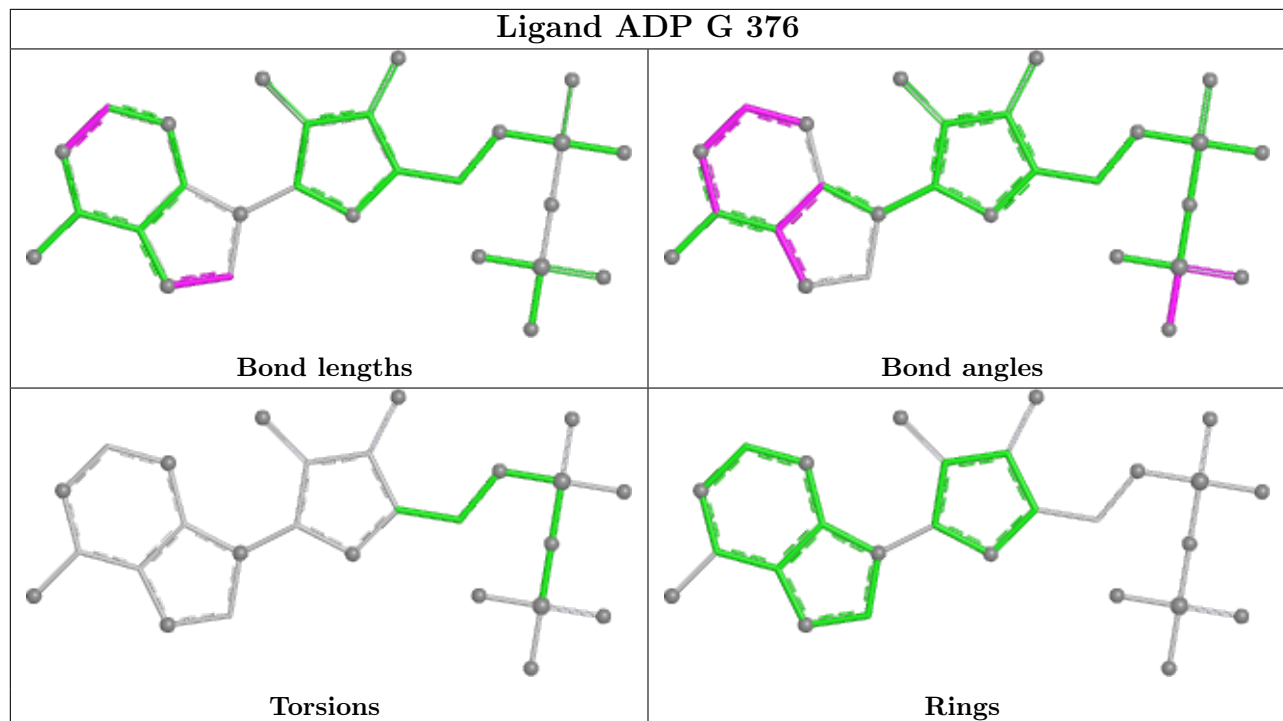
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	376	ADP	3	0
4	A	376	ADP	3	0
4	F	376	ADP	3	0
4	D	376	ADP	3	0
4	G	376	ADP	3	0

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

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	4
3	I	4
3	J	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	123:SER	C	124:ASN	N	5.40
1	I	123:SER	C	124:ASN	N	5.40
1	J	123:SER	C	124:ASN	N	5.40
1	C	124:ASN	C	125:GLN	N	3.43
1	I	124:ASN	C	125:GLN	N	3.43
1	J	124:ASN	C	125:GLN	N	3.43
1	C	90:GLN	C	91:SER	N	3.17
1	I	90:GLN	C	91:SER	N	3.17

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	90:GLN	C	91:SER	N	3.17
1	C	107:LYS	C	108:THR	N	3.04
1	I	107:LYS	C	108:THR	N	3.04
1	J	107:LYS	C	108:THR	N	3.04

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1987. These allow visual inspection of the internal detail of the map and identification of artifacts.

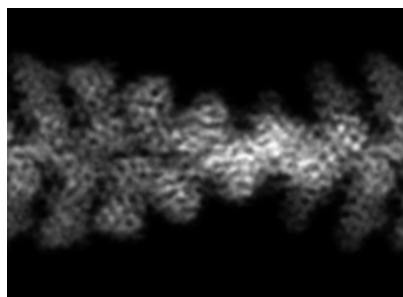
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

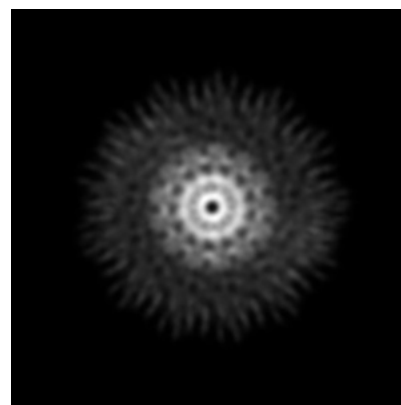
6.1.1 Primary map



X



Y



Z

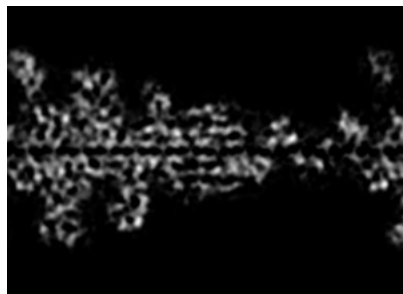
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 80



Y Index: 80

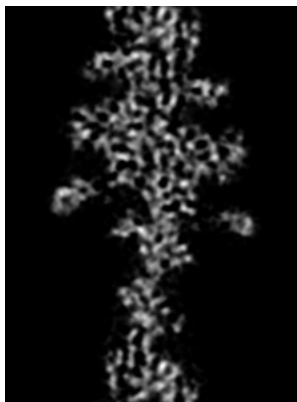


Z Index: 110

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: 76



Z Index: 57

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

6.4 Orthogonal surface views [i](#)

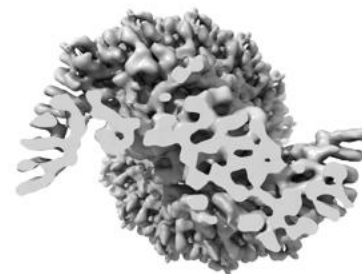
6.4.1 Primary map



X



Y



Z

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.

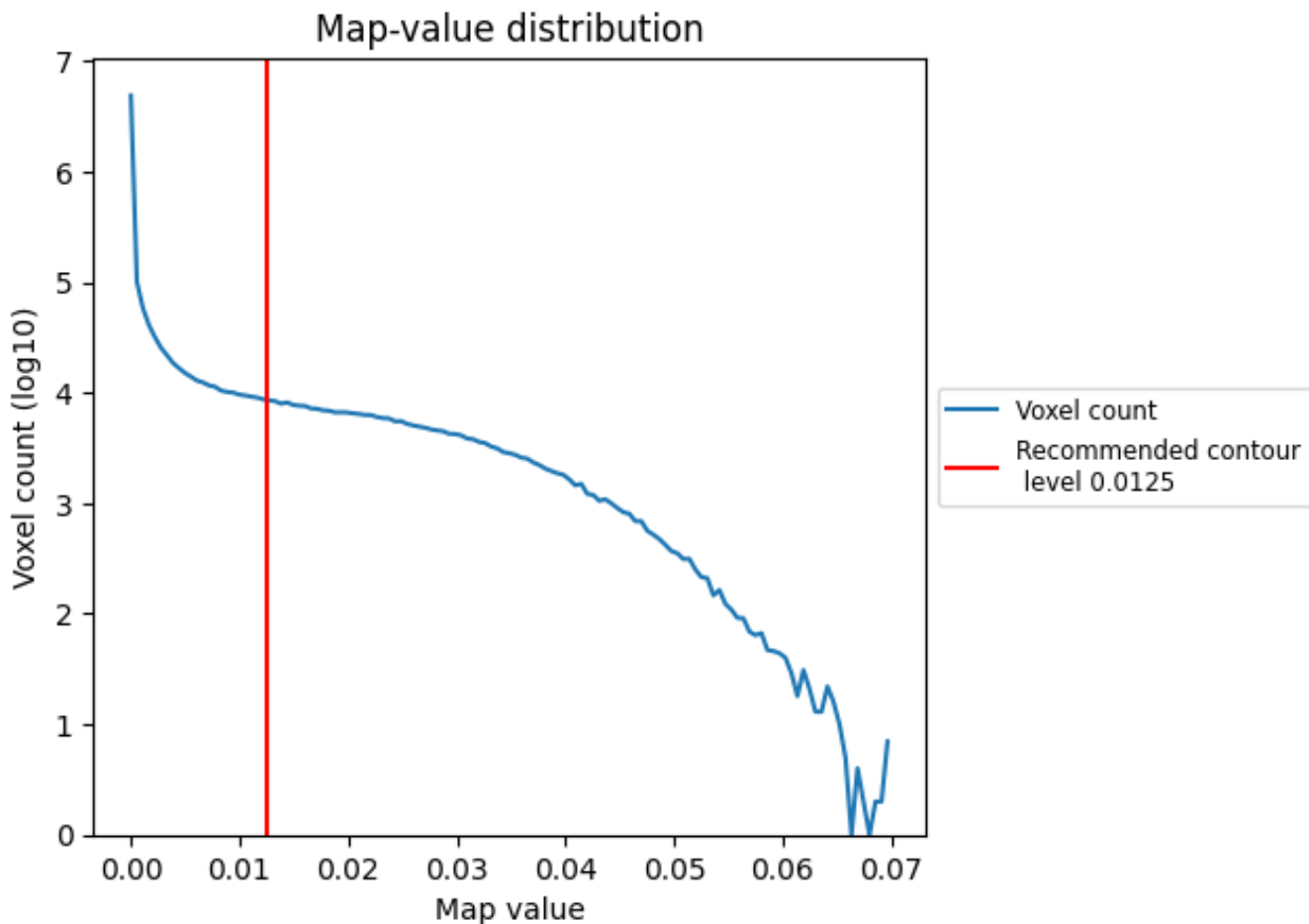
6.5 Mask visualisation

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

7 Map analysis [i](#)

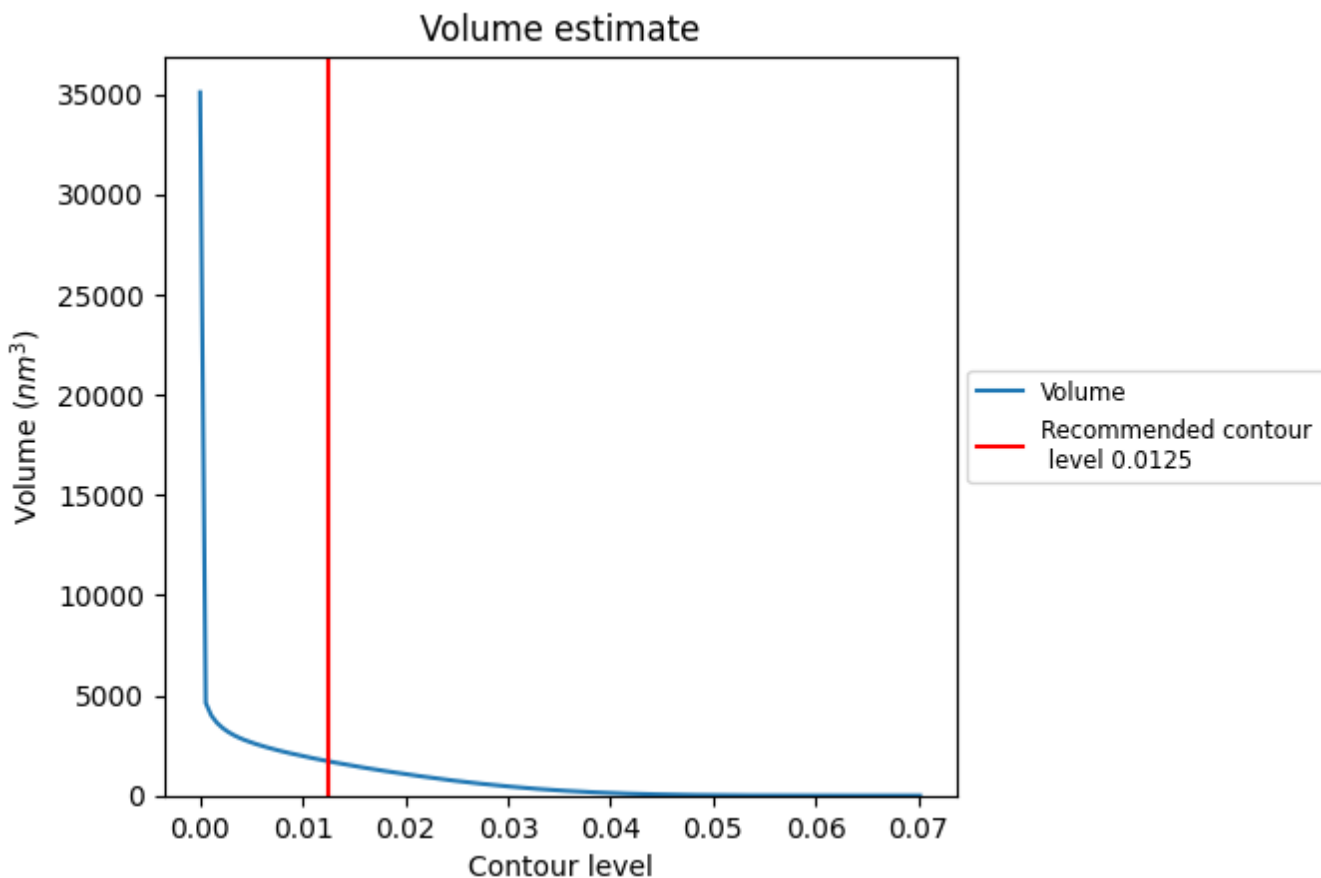
This section contains the results of statistical analysis of the map.

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 1711 nm³; this corresponds to an approximate mass of 1546 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.

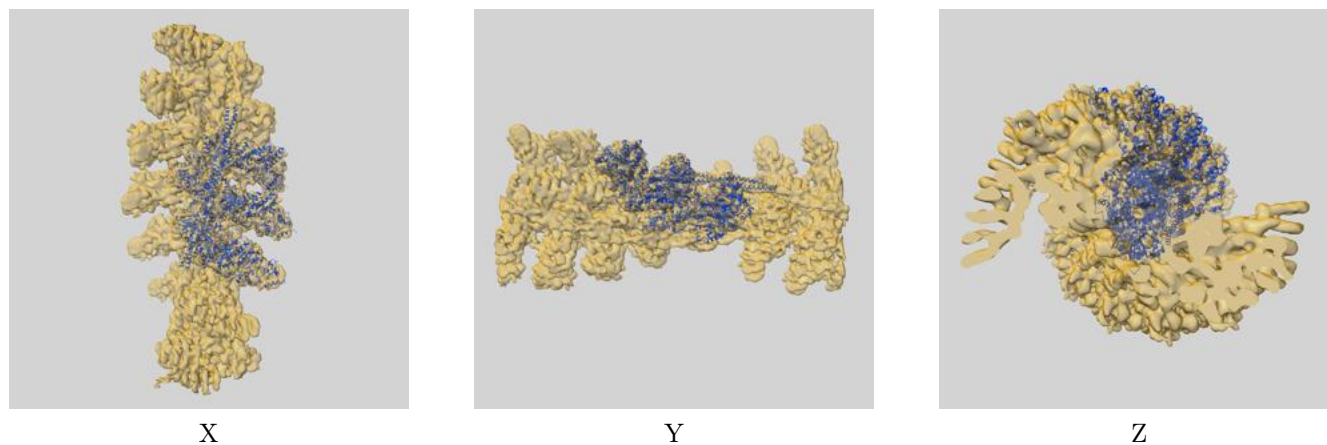
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

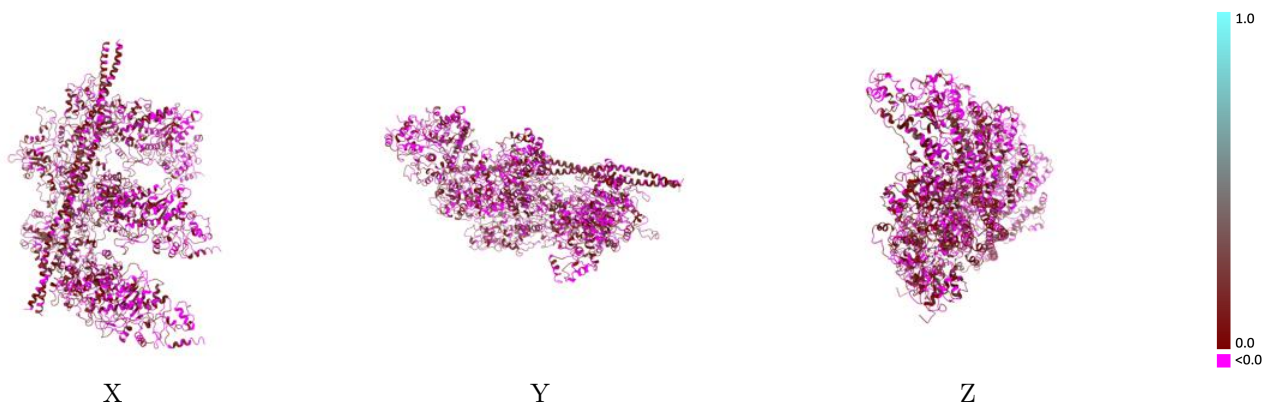
This section contains information regarding the fit between EMDB map EMD-1987 and PDB model 4A7H. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



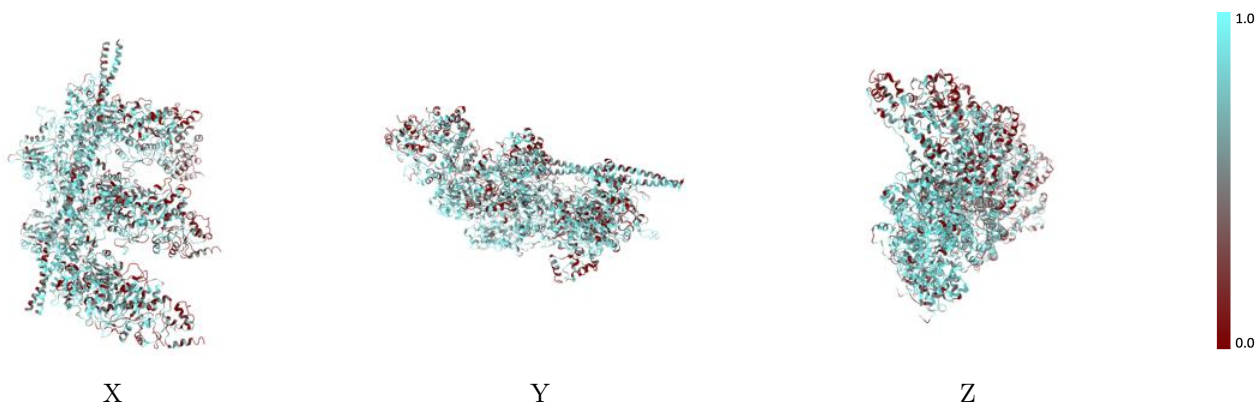
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



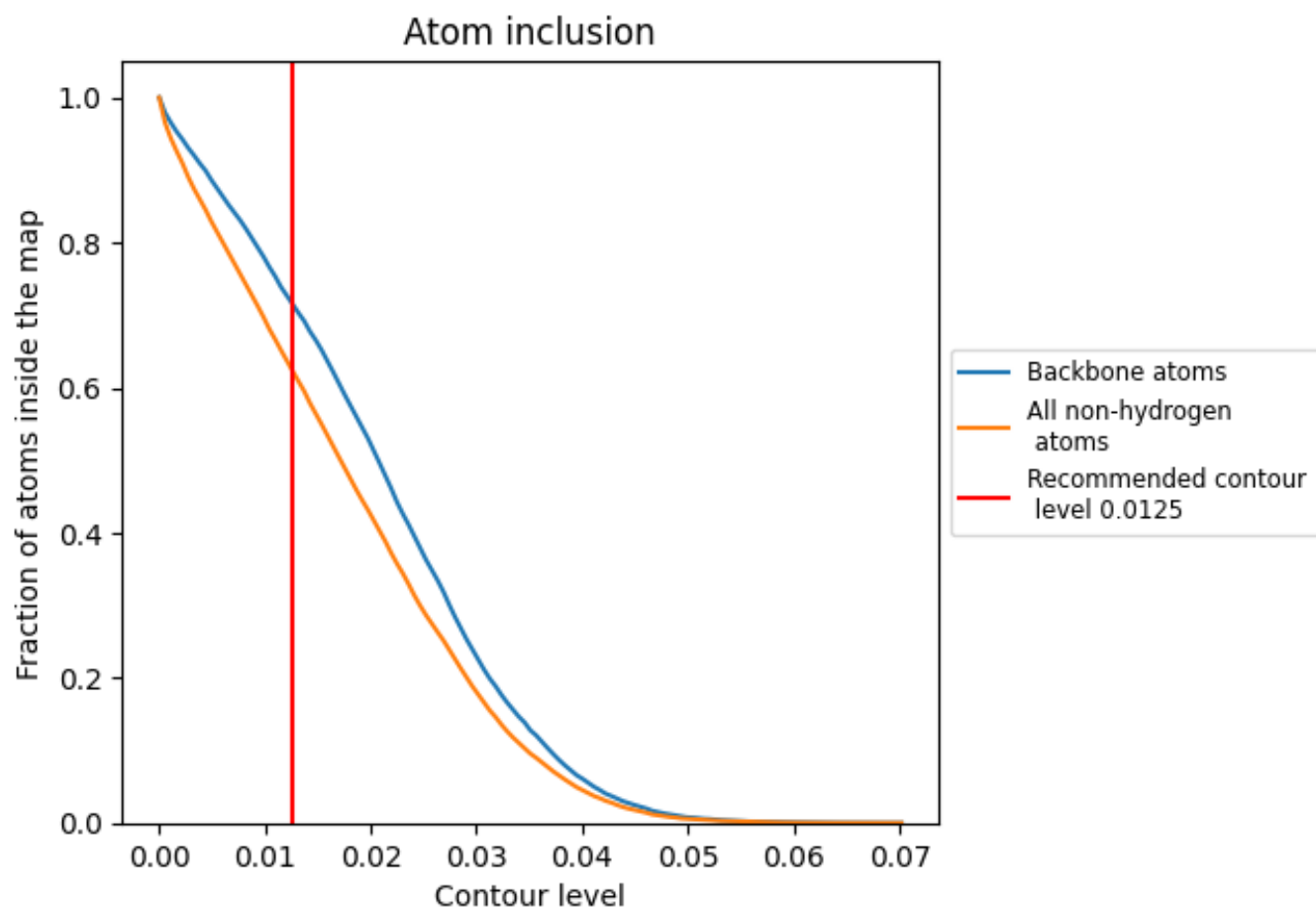
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).























9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 63% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

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

Chain	Atom inclusion	Q-score
All	 0.6259	 0.0450
A	 0.7319	 0.0730
B	 0.6387	 0.1010
C	 0.5273	 0.0150
D	 0.7343	 0.0690
E	 0.7357	 0.0710
F	 0.7337	 0.0730
G	 0.7333	 0.0700
H	 0.6166	 0.0860
I	 0.5286	 0.0160
J	 0.5302	 0.0160

