



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 10:25 AM JST

PDB ID : 7EU3 / pdb_00007eu3
EMDB ID : EMD-31307
Title : Chloroplast NDH complex
Authors : Wang, W.D.; Shen, L.; Tang, K.; Han, G.Y.; Zhang, X.; Shen, J.R.
Deposited on : 2021-05-15
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

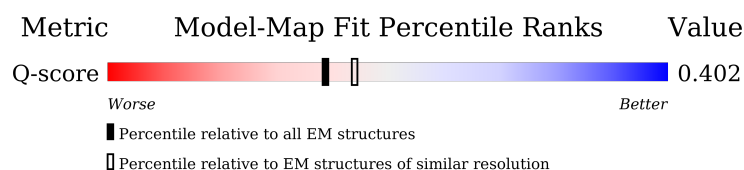
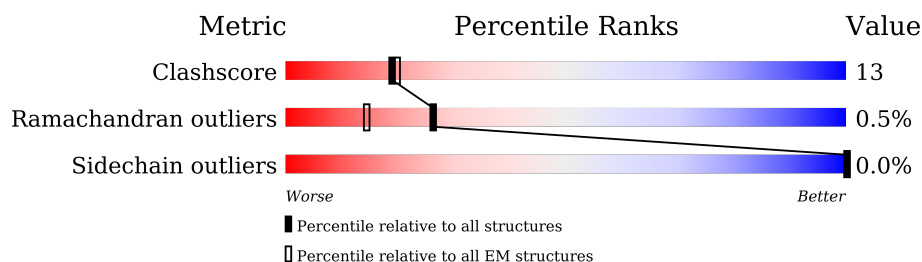
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	346	
2	B	483	
3	C	117	
4	D	499	

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Mol	Chain	Length	Quality of chain
5	E	100	
6	F	777	
7	G	176	
8	H	383	
9	I	165	
10	J	159	
11	K	245	
12	L	192	
13	M	213	
14	N	233	
15	T	61	
16	1	154	
17	2	216	
18	3	227	
19	4	130	
20	5	243	
21	6	469	
22	7	361	
23	8	119	
24	9	83	
25	0	155	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 40775 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 NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	346	Total	C	N	O	S	0	0
			2608	1744	393	463	8		

- Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3646	2400	557	665	24		

- Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	116	Total	C	N	O	S	0	0
			841	575	124	140	2		

- Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	499	Total	C	N	O	S	0	0
			3874	2614	598	639	23		

- Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	100	Total	C	N	O	S	0	0
			750	486	127	135	2		

- Molecule 6 is a protein called NAD(P)H-quinone oxidoreductase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	671	Total	C	N	O	S	0	0
			5124	3425	796	882	21		

- Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	176	Total	C	N	O	S	0	0
			1260	841	194	220	5		

- Molecule 8 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	383	Total	C	N	O	S	0	0
			2991	1944	493	543	11		

- Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1229	772	214	231	12		

- Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	159	Total	C	N	O	S	0	0
			1258	808	213	233	4		

- Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	194	Total	C	N	O	S	0	0
			1474	932	250	282	10		

- Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	69	Total	C	N	O	S	0	0
			572	399	89	81	3		

- Molecule 13 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	112	Total	C	N	O	S	0	0
			876	558	150	162	6		

- Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1154	751	203	198	2		

- Molecule 15 is a protein called Unidentified stromal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	T	61	Total	C	N	O	0	0
			305	183	61	61		

- Molecule 16 is a protein called Photosynthetic NDH subunit of subcomplex L1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	1	150	Total	C	N	O	0	0
			1185	752	206	227		

- Molecule 17 is a protein called Photosynthetic NDH subunit of subcomplex L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	129	Total	C	N	O	S	0	0
			915	580	156	175	4		

- Molecule 18 is a protein called Photosynthetic NDH subunit of subcomplex L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	134	Total	C	N	O	S	0	0
			989	634	164	187	4		

- Molecule 19 is a protein called Photosynthetic NDH subunit of subcomplex L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	4	130	Total	C	N	O	S	0	0
			878	553	153	163	9		

- Molecule 20 is a protein called Photosynthetic NDH subunit of subcomplex L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	5	172	Total	C	N	O	S	0	0
			1289	812	229	241	7		

- Molecule 21 is a protein called Photosynthetic NDH subunit of subcomplex B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	6	343	Total	C	N	O	S	0	0
			2541	1617	435	474	15		

- Molecule 22 is a protein called Photosynthetic NDH subunit of subcomplex B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	7	317	Total	C	N	O	S	0	0
			2311	1444	409	448	10		

- Molecule 23 is a protein called Photosynthetic NDH subunit of subcomplex B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	8	119	Total	C	N	O	S	0	0
			828	523	151	147	7		

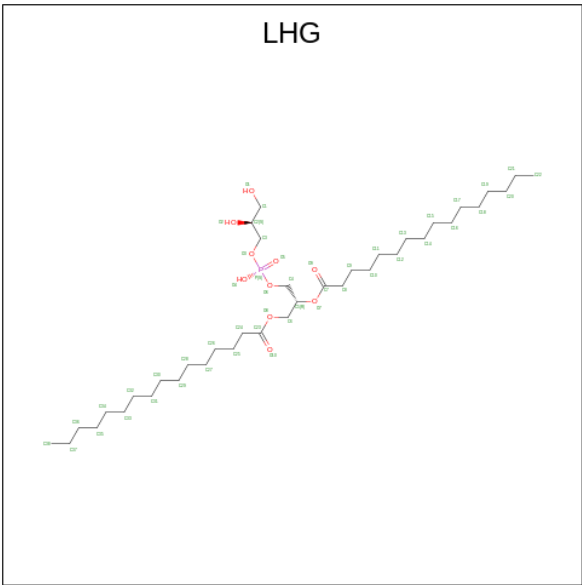
- Molecule 24 is a protein called Photosynthetic NDH subunit of subcomplex B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	9	82	Total	C	N	O	S	0	0
			617	395	101	118	3		

- Molecule 25 is a protein called Photosynthetic NDH subunit of subcomplex B5.

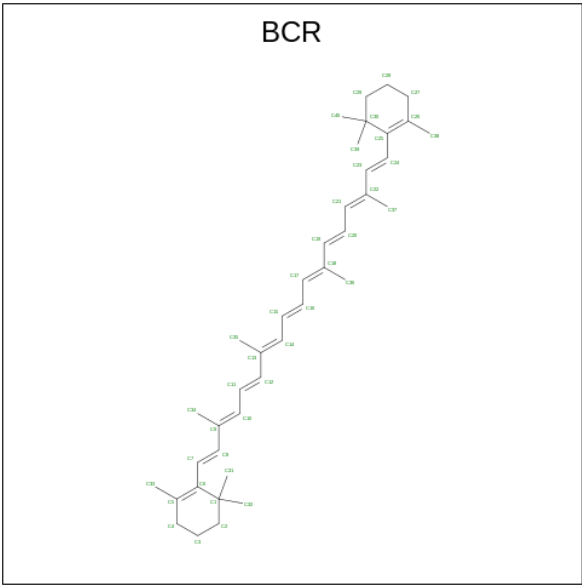
Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	149	Total	C	N	O	S	0	0
			1089	704	175	204	6		

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



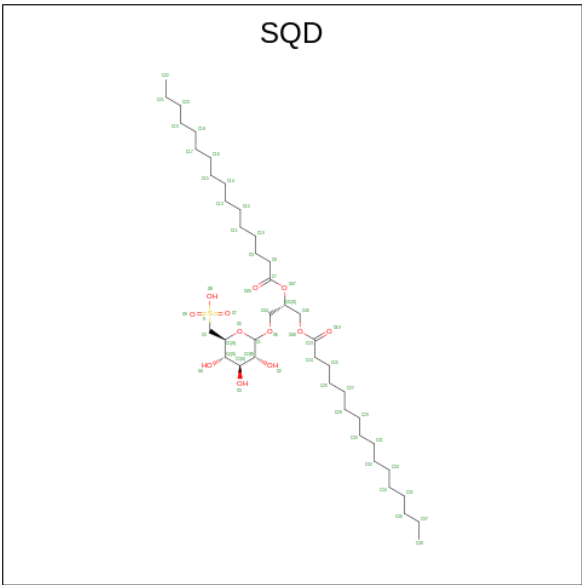
Mol	Chain	Residues	Atoms				AltConf
26	D	1	Total	C	O	P	0
			24	15	8	1	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



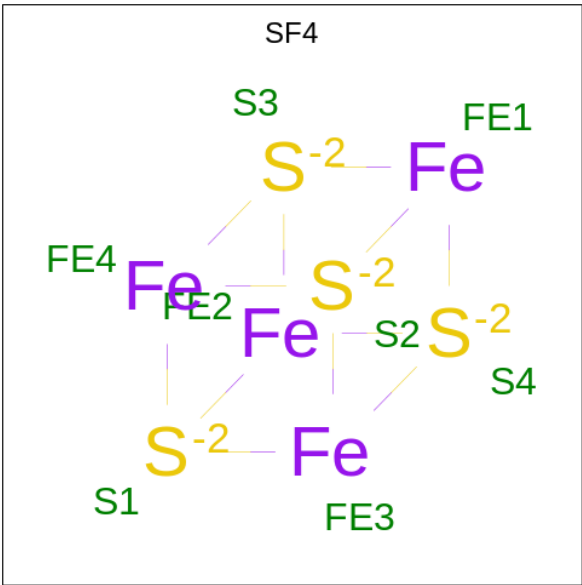
Mol	Chain	Residues	Atoms		AltConf
27	F	1	Total	C	0
			39	39	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms				AltConf
28	F	1	Total	C	O	S	0
			54	41	12	1	
28	F	1	Total	C	O	S	0
			46	33	12	1	

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

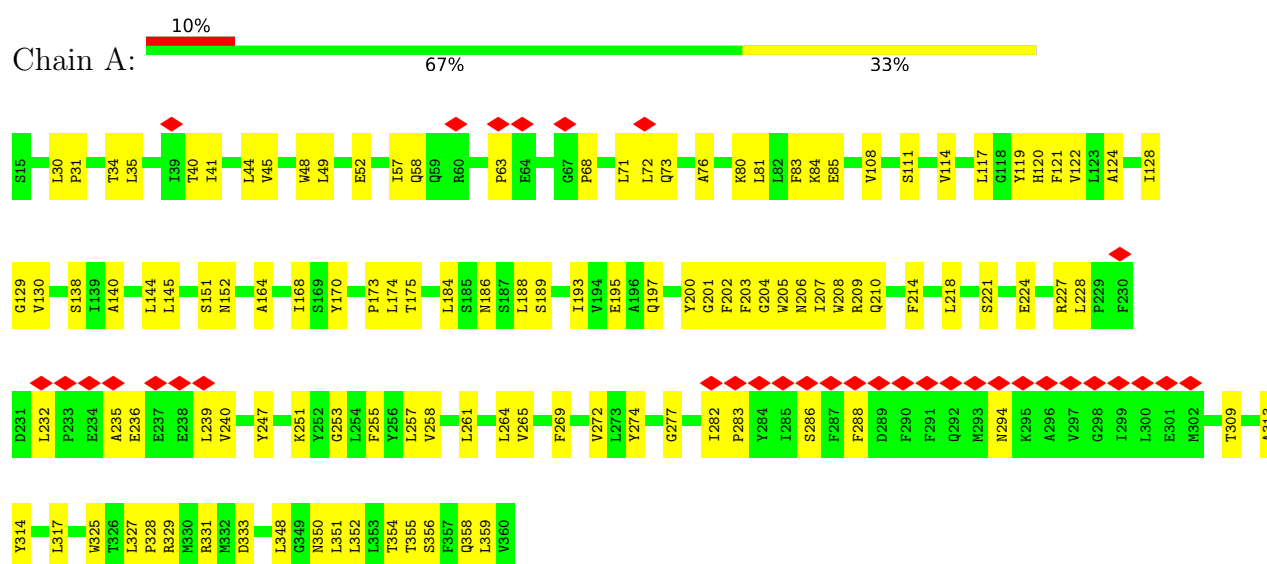


Mol	Chain	Residues	Atoms			AltConf
29	8	1	Total	Fe	S	0
			8	4	4	

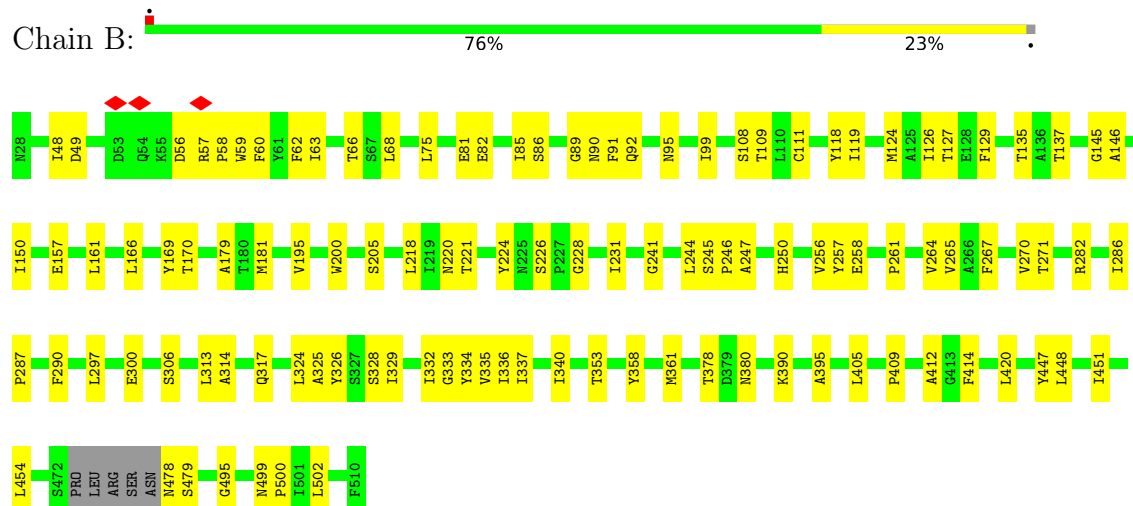
3 Residue-property plots

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.

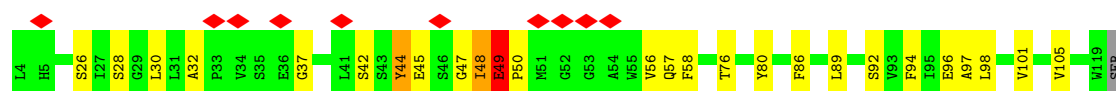
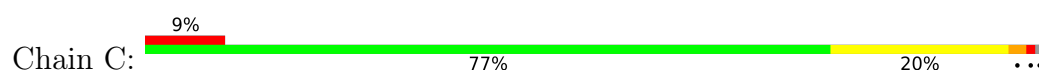
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



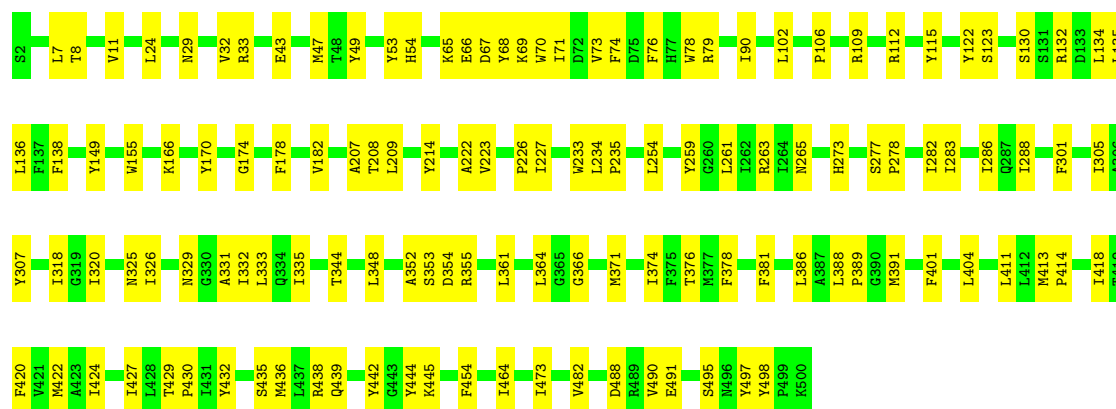
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic



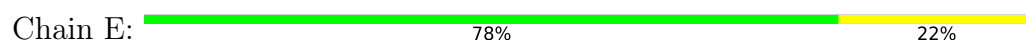
- Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



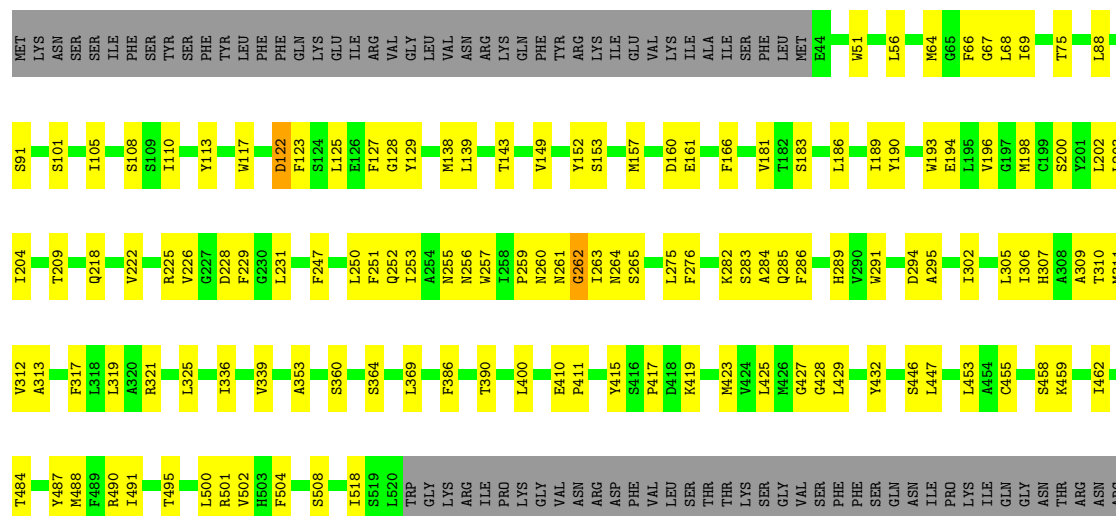
- Molecule 4: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

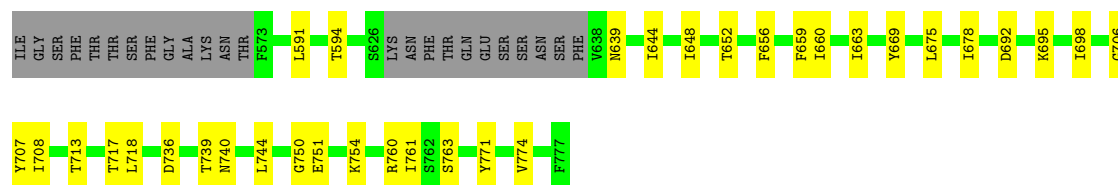


- Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic



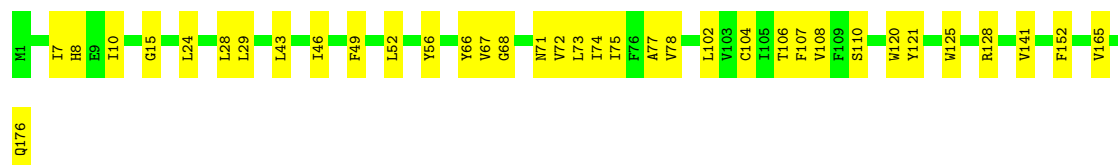
- Molecule 6: NAD(P)H-quinone oxidoreductase subunit F





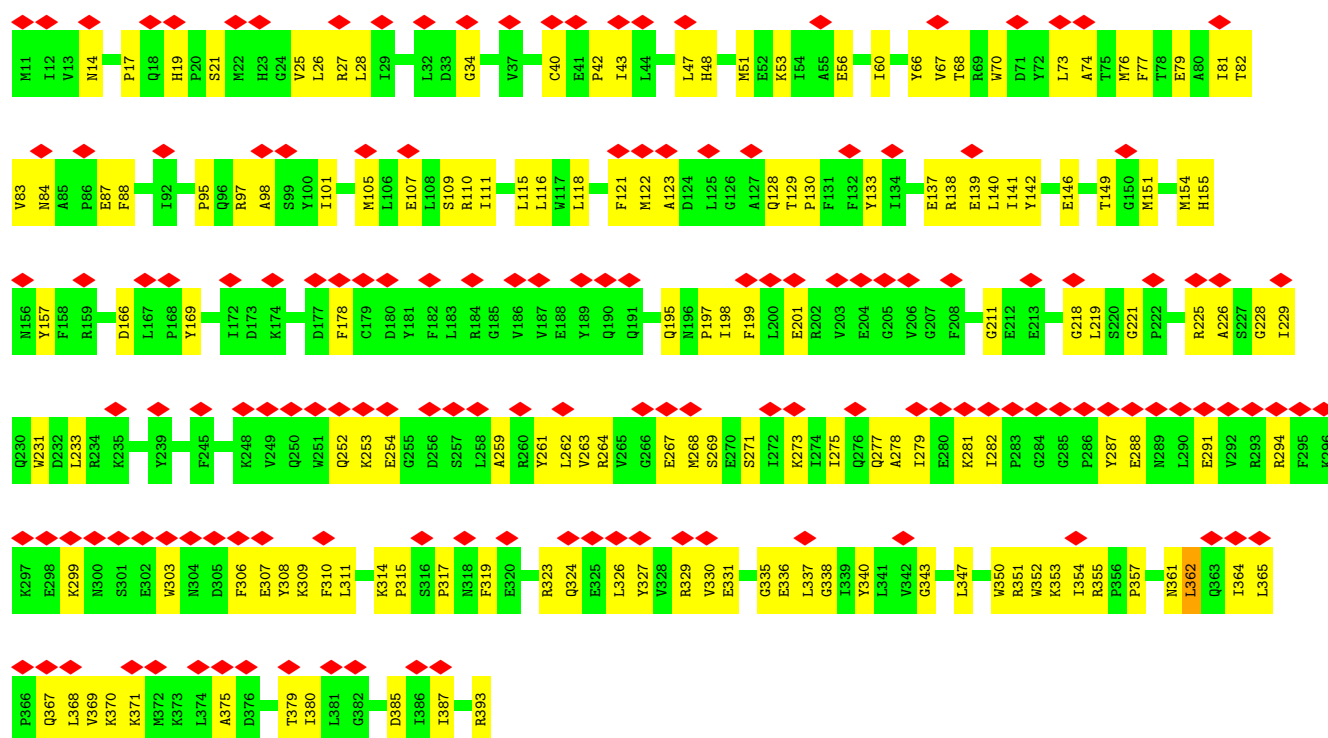
- Molecule 7: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

Chain G: 80% 20%



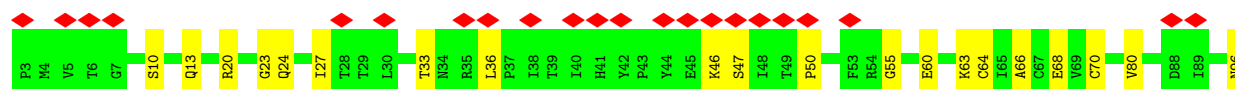
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

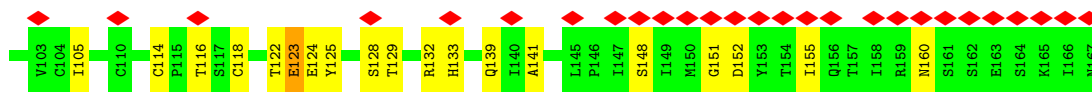
Chain H: 39% 60% 40%



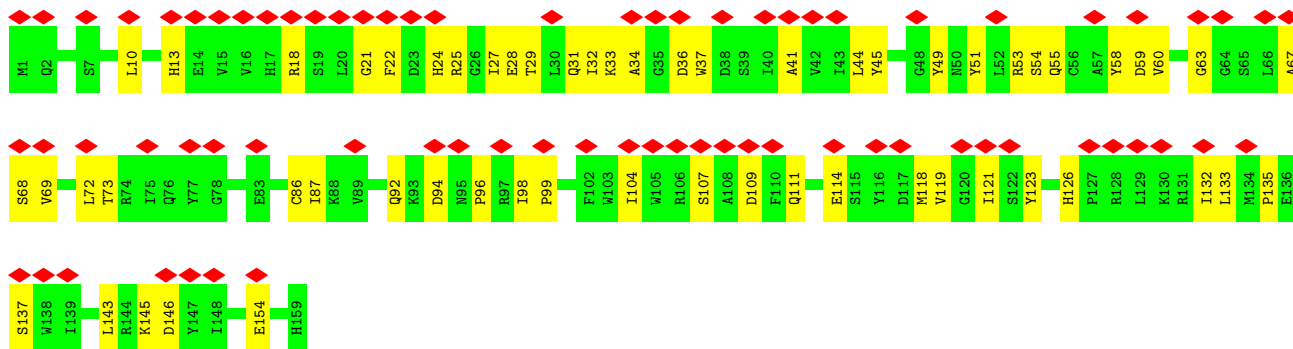
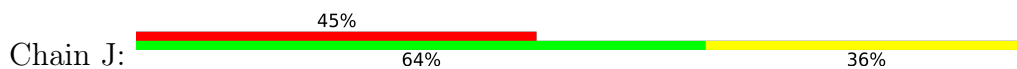
- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

Chain I: 30% 76% 23%

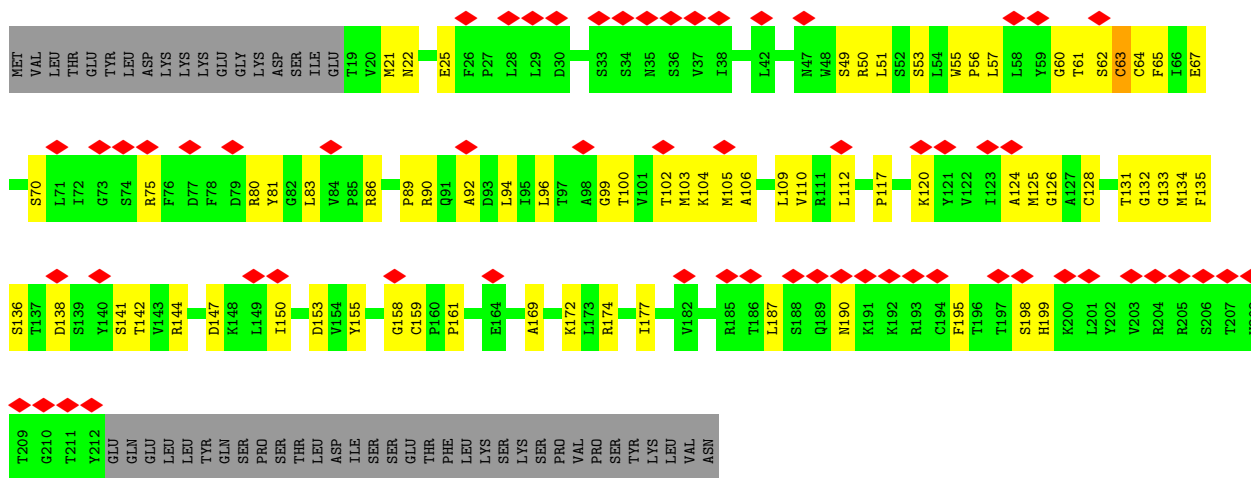




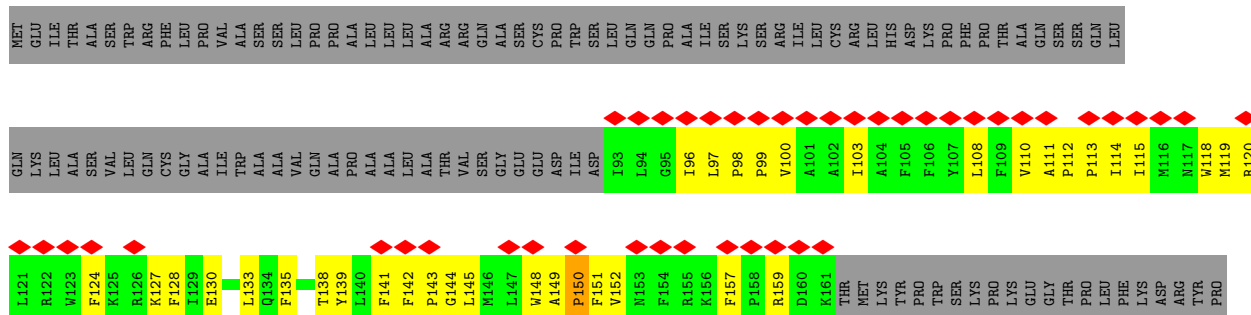
• Molecule 10: NAD(P)H-quinone oxidoreductase subunit J

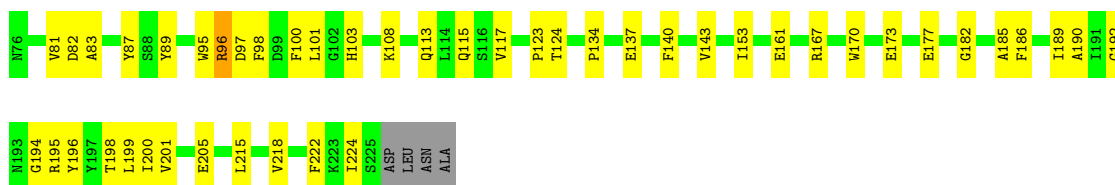


• Molecule 11: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic

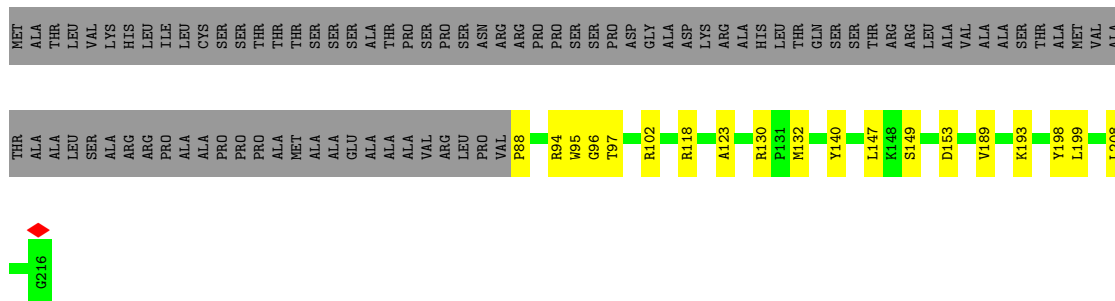


• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

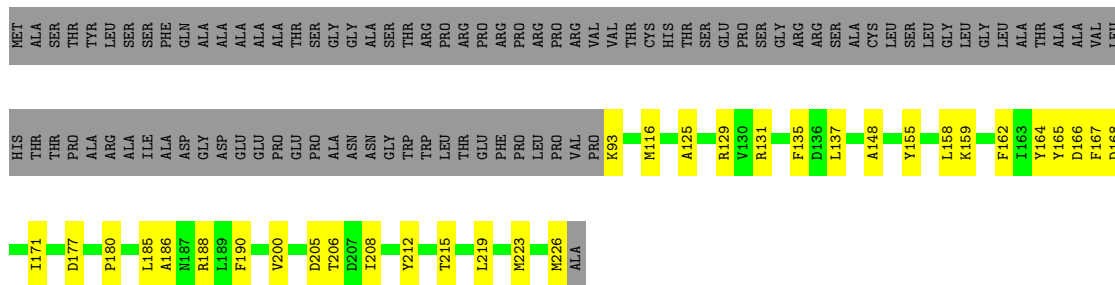




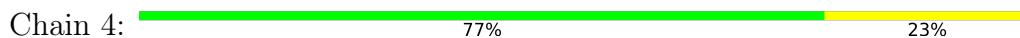
- Molecule 17: Photosynthetic NDH subunit of subcomplex L2



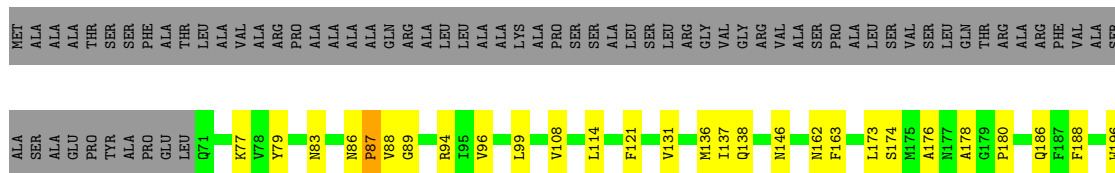
- Molecule 18: Photosynthetic NDH subunit of subcomplex L3



- Molecule 19: Photosynthetic NDH subunit of subcomplex L4

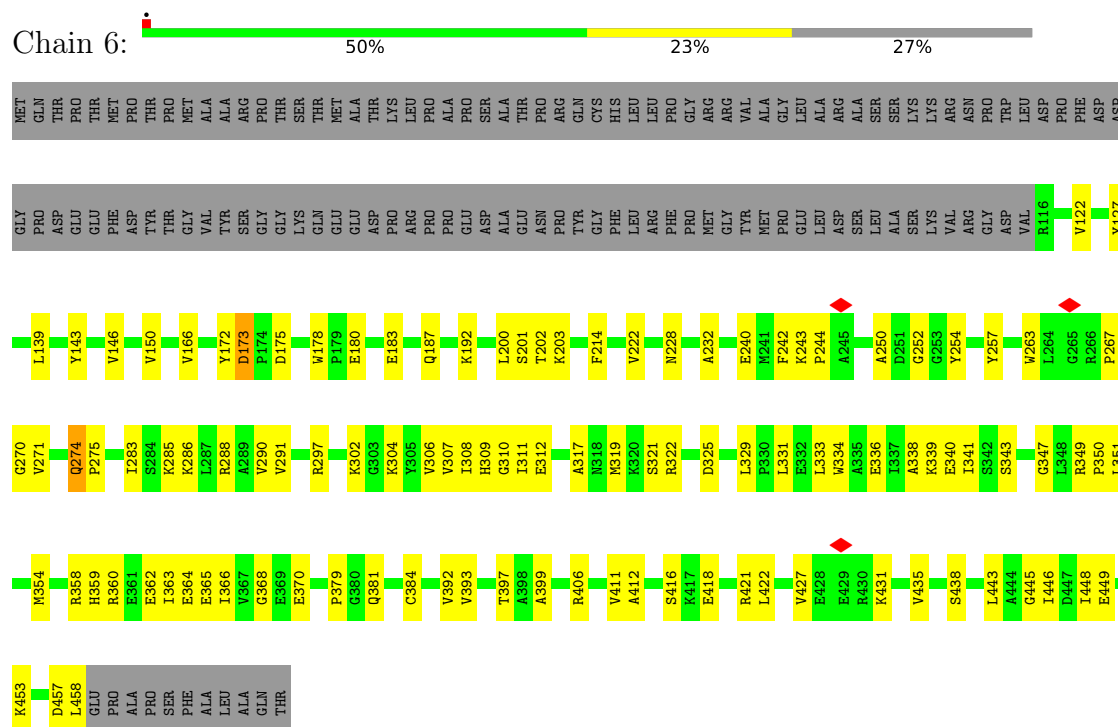


- Molecule 20: Photosynthetic NDH subunit of subcomplex L5

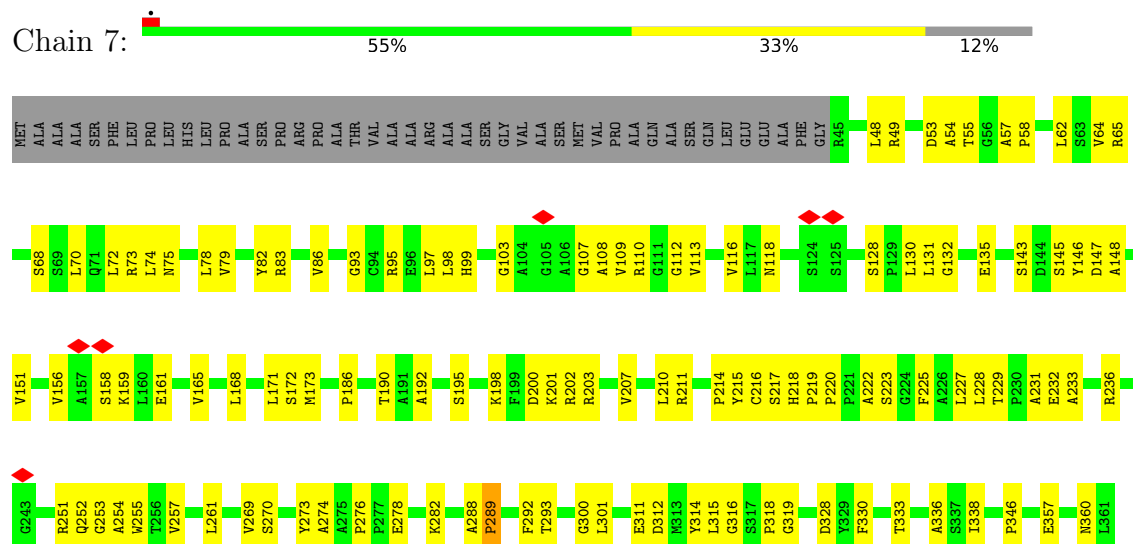




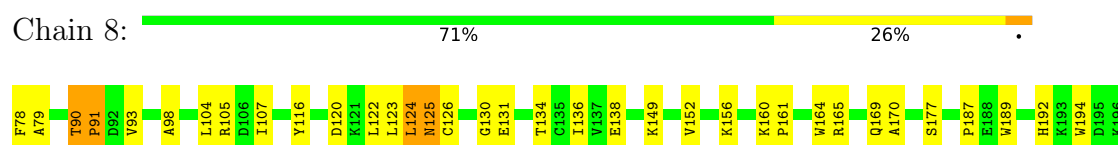
• Molecule 21: Photosynthetic NDH subunit of subcomplex B1



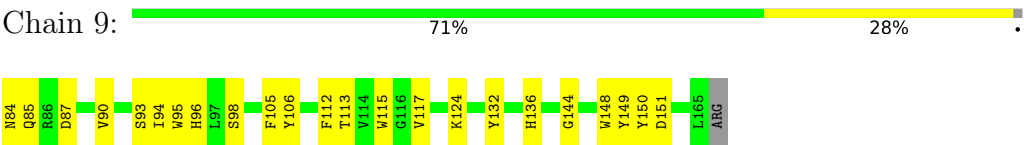
• Molecule 22: Photosynthetic NDH subunit of subcomplex B2



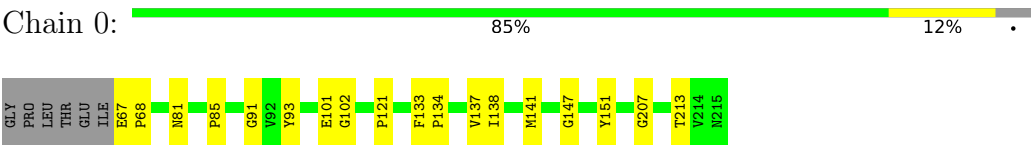
• Molecule 23: Photosynthetic NDH subunit of subcomplex B3



- Molecule 24: Photosynthetic NDH subunit of subcomplex B4



- Molecule 25: Photosynthetic NDH subunit of subcomplex B5



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103844	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	38.925	Depositor
Minimum map value	-17.534	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.3	Depositor
Map size ($\text{\AA}$)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.307, 1.307, 1.307	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, SQD, LHG, BCR

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	0.13	0/2670	0.38	0/3644
2	B	0.15	0/3730	0.39	0/5082
3	C	0.22	0/865	0.83	3/1188 (0.3%)
4	D	0.16	0/3987	0.43	3/5427 (0.1%)
5	E	0.14	0/759	0.32	0/1028
6	F	0.15	0/5270	0.41	1/7186 (0.0%)
7	G	0.15	0/1288	0.45	1/1765 (0.1%)
8	H	0.13	0/3070	0.39	0/4173
9	I	0.22	0/1254	0.54	3/1702 (0.2%)
10	J	0.12	0/1297	0.37	0/1771
11	K	0.13	0/1505	0.40	0/2048
12	L	0.18	0/597	0.46	0/816
13	M	0.12	0/896	0.41	0/1218
14	N	0.32	1/1189 (0.1%)	0.70	6/1617 (0.4%)
16	1	0.17	0/1213	0.54	0/1651
17	2	0.13	0/935	0.45	1/1276 (0.1%)
18	3	0.14	0/1006	0.36	0/1365
19	4	0.15	0/894	0.49	0/1216
20	5	0.13	0/1314	0.38	0/1771
21	6	0.19	0/2589	0.58	2/3513 (0.1%)
22	7	0.18	0/2358	0.53	0/3200
23	8	0.29	0/844	0.62	0/1145
24	9	0.14	0/636	0.46	0/868
25	0	0.22	0/1122	0.69	0/1536
All	All	0.17	1/41288 (0.0%)	0.47	20/56206 (0.0%)

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
4	D	0	1
6	F	0	2
9	I	0	1
14	N	0	1
16	1	0	1
17	2	0	1
20	5	0	1
21	6	0	4
22	7	0	1
23	8	0	2
25	0	0	3
All	All	0	18

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	158	VAL	N-CA	5.78	1.53	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	157	LYS	N-CA-C	17.48	131.24	108.34
3	C	49	GLU	CA-C-N	-16.76	102.80	119.90
3	C	49	GLU	C-N-CA	-16.76	102.80	119.90
21	6	274	GLN	CA-C-N	12.68	135.69	119.84
21	6	274	GLN	C-N-CA	12.68	135.69	119.84
7	G	141	VAL	N-CA-C	-7.71	106.39	113.71
6	F	262	GLY	N-CA-C	-6.90	100.81	111.64
9	I	125	TYR	N-CA-C	6.69	122.57	113.21
9	I	123	GLU	N-CA-C	6.18	123.97	110.80
14	N	158	VAL	CA-C-N	-6.12	110.68	121.70
14	N	158	VAL	C-N-CA	-6.12	110.68	121.70
17	2	189	VAL	N-CA-C	-6.06	107.59	113.53
3	C	44	TYR	N-CA-C	5.58	122.68	110.80
4	D	490	VAL	N-CA-C	-5.50	108.14	113.53
14	N	157	LYS	CA-C-N	5.42	131.73	121.97
14	N	157	LYS	C-N-CA	5.42	131.73	121.97
14	N	156	ALA	O-C-N	-5.36	115.27	122.19
4	D	497	TYR	CA-C-N	-5.25	108.99	121.80
4	D	497	TYR	C-N-CA	-5.25	108.99	121.80
9	I	124	GLU	N-CA-C	5.05	117.32	110.35

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	0	121	PRO	Peptide
25	0	207	GLY	Peptide
25	0	91	GLY	Peptide
16	1	115	GLN	Peptide
17	2	96	GLY	Peptide
20	5	86	ASN	Peptide
21	6	173	ASP	Peptide
21	6	178	TRP	Peptide
21	6	274	GLN	Mainchain
21	6	368	GLY	Peptide
22	7	254	ALA	Peptide
23	8	160	LYS	Peptide
23	8	90	THR	Peptide
4	D	495	SER	Peptide
6	F	122	ASP	Peptide
6	F	261	ASN	Peptide
9	I	122	THR	Mainchain
14	N	125	PRO	Peptide

5.2 Too-close contacts

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	2608	0	2609	83	0
2	B	3646	0	3652	83	0
3	C	841	0	761	26	0
4	D	3874	0	3923	92	0
5	E	750	0	760	20	0
6	F	5124	0	4962	128	0
7	G	1260	0	1197	28	0
8	H	2991	0	2849	136	0
9	I	1229	0	1109	27	0
10	J	1258	0	1151	52	0
11	K	1474	0	1442	56	0
12	L	572	0	559	28	0
13	M	876	0	801	29	0
14	N	1154	0	1117	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	T	305	0	69	3	0
16	1	1185	0	1086	30	0
17	2	915	0	764	14	0
18	3	989	0	927	22	0
19	4	878	0	823	20	0
20	5	1289	0	1247	21	0
21	6	2541	0	2461	72	0
22	7	2311	0	2232	91	0
23	8	828	0	742	26	0
24	9	617	0	520	17	0
25	0	1089	0	901	13	0
26	D	24	0	19	1	0
27	F	39	0	53	6	0
28	F	100	0	137	6	0
29	8	8	0	0	1	0
All	All	40775	0	38873	1019	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 (1019) 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)
3:C:47:GLY:HA3	8:H:14:ASN:ND2	1.45	1.30
3:C:47:GLY:CA	8:H:14:ASN:HD21	1.48	1.26
3:C:47:GLY:HA3	8:H:14:ASN:HD21	1.02	1.00
23:8:123:LEU:O	23:8:124:LEU:O	1.82	0.96
3:C:47:GLY:N	8:H:14:ASN:HD21	1.67	0.92
3:C:47:GLY:CA	8:H:14:ASN:ND2	2.17	0.91
3:C:49:GLU:O	3:C:50:PRO:C	2.08	0.90
23:8:123:LEU:C	23:8:124:LEU:O	2.15	0.89
18:3:148:ALA:HB3	24:9:105:PHE:HB2	1.67	0.76
3:C:47:GLY:O	3:C:48:ILE:C	2.28	0.75
22:7:68:SER:HA	22:7:83:ARG:O	1.87	0.75
3:C:47:GLY:HA3	8:H:14:ASN:HD22	1.51	0.74
23:8:152:VAL:HG21	23:8:169:GLN:OE1	1.88	0.74
23:8:123:LEU:O	23:8:124:LEU:C	2.31	0.73
3:C:47:GLY:O	3:C:50:PRO:N	2.22	0.72
6:F:669:TYR:HB3	22:7:300:GLY:HA2	1.74	0.69
4:D:109:ARG:HB3	4:D:155:TRP:HE1	1.58	0.68
18:3:185:LEU:HA	18:3:188:ARG:HH11	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:488:ASP:HA	4:D:491:GLU:HB3	1.76	0.67
17:2:94:ARG:O	17:2:118:ARG:NH2	2.27	0.67
20:5:131:VAL:HG13	20:5:137:ILE:HG22	1.76	0.67
16:1:134:PRO:HG2	16:1:137:GLU:HB2	1.77	0.67
2:B:247:ALA:O	2:B:250:HIS:ND1	2.28	0.66
21:6:310:GLY:O	21:6:334:TRP:NE1	2.28	0.66
21:6:285:LYS:HA	21:6:288:ARG:HB3	1.77	0.66
16:1:140:PHE:HA	16:1:143:VAL:HG12	1.78	0.66
16:1:82:ASP:HB2	16:1:87:TYR:HE1	1.61	0.65
3:C:58:PHE:HB2	8:H:34:GLY:HA3	1.78	0.65
23:8:130:GLY:N	29:8:201:SF4:S3	2.70	0.65
22:7:58:PRO:HB2	22:7:74:LEU:HB2	1.79	0.65
23:8:120:ASP:H	23:8:124:LEU:HD12	1.63	0.64
8:H:324:GLN:H	8:H:343:GLY:HA3	1.62	0.64
21:6:250:ALA:HB3	21:6:422:LEU:HA	1.78	0.63
6:F:291:TRP:O	6:F:295:ALA:HB2	1.99	0.63
24:9:93:SER:HG	24:9:95:TRP:CD1	2.17	0.63
1:A:201:GLY:O	1:A:205:TRP:NE1	2.32	0.63
21:6:397:THR:HG23	21:6:399:ALA:H	1.63	0.63
11:K:62:SER:OG	11:K:100:THR:N	2.32	0.62
16:1:173:GLU:HA	16:1:185:ALA:O	1.98	0.62
11:K:110:VAL:HA	11:K:150:ILE:HD11	1.82	0.61
11:K:103:MET:N	11:K:141:SER:O	2.34	0.61
4:D:438:ARG:HA	4:D:442:TYR:HD2	1.66	0.61
6:F:706:GLY:O	6:F:708:ILE:N	2.34	0.60
14:N:194:MET:O	14:N:198:LEU:N	2.34	0.60
23:8:152:VAL:CG2	23:8:169:GLN:OE1	2.50	0.60
6:F:262:GLY:O	6:F:264:ASN:N	2.35	0.60
1:A:57:ILE:HG13	1:A:58:GLN:H	1.66	0.60
23:8:105:ARG:NE	23:8:116:TYR:OH	2.32	0.60
23:8:125:ASN:CB	23:8:134:THR:HG21	2.32	0.59
3:C:101:VAL:O	3:C:105:VAL:HG23	2.03	0.59
2:B:150:ILE:HG12	5:E:62:PHE:CD1	2.38	0.59
6:F:313:ALA:O	6:F:317:PHE:HB3	2.03	0.59
2:B:81:GLU:HG3	2:B:82:GLU:H	1.67	0.59
8:H:275:ILE:O	8:H:279:ILE:HG13	2.03	0.59
20:5:173:LEU:N	20:5:205:GLY:O	2.35	0.59
5:E:43:LEU:HB2	7:G:46:ILE:HD11	1.85	0.59
22:7:99:HIS:NE2	22:7:110:ARG:HD3	2.17	0.59
6:F:459:LYS:HA	6:F:462:ILE:HG12	1.85	0.59
22:7:217:SER:O	22:7:219:PRO:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:68:TYR:O	4:D:69:LYS:NZ	2.36	0.58
2:B:86:SER:HB2	2:B:90:ASN:H	1.68	0.58
6:F:88:LEU:O	6:F:91:SER:HB3	2.02	0.58
10:J:107:SER:O	10:J:111:GLN:NE2	2.36	0.58
16:1:215:LEU:O	16:1:218:VAL:HB	2.03	0.58
8:H:67:VAL:HG11	8:H:82:THR:HG21	1.85	0.58
8:H:277:GLN:O	8:H:281:LYS:HB2	2.04	0.58
11:K:21:MET:HE3	11:K:22:ASN:H	1.68	0.58
19:4:152:GLN:NE2	19:4:153:VAL:O	2.36	0.58
21:6:288:ARG:HA	21:6:384:CYS:SG	2.43	0.58
24:9:85:GLN:HG3	24:9:98:SER:HB3	1.85	0.58
2:B:119:ILE:HD11	2:B:126:ILE:HG23	1.85	0.58
13:M:93:TRP:CD1	13:M:95:SER:HG	2.22	0.58
14:N:108:SER:O	14:N:114:HIS:ND1	2.37	0.58
6:F:260:ASN:O	6:F:262:GLY:N	2.34	0.58
1:A:288:PHE:HB3	1:A:294:ASN:HD21	1.68	0.58
6:F:250:LEU:HD21	6:F:325:LEU:HD11	1.86	0.58
8:H:140:LEU:HD13	8:H:178:PHE:HB2	1.85	0.58
8:H:362:LEU:HG	8:H:365:LEU:HD22	1.86	0.58
10:J:118:MET:HE2	10:J:143:LEU:HD13	1.86	0.58
11:K:57:LEU:N	11:K:94:LEU:O	2.36	0.58
22:7:116:VAL:HG13	22:7:192:ALA:HB3	1.86	0.58
1:A:128:ILE:HD13	7:G:56:TYR:HB3	1.86	0.57
3:C:47:GLY:H	8:H:14:ASN:HD21	1.45	0.57
3:C:86:PHE:HE1	3:C:94:PHE:HB2	1.69	0.57
8:H:138:ARG:NH1	8:H:142:TYR:OH	2.37	0.57
9:I:132:ARG:HD2	11:K:131:THR:HG22	1.85	0.57
10:J:31:GLN:HA	10:J:87:ILE:HG23	1.86	0.57
11:K:169:ALA:HA	11:K:172:LYS:HD2	1.86	0.57
16:1:100:PHE:HB2	16:1:108:LYS:NZ	2.17	0.57
1:A:49:LEU:HD21	1:A:314:TYR:CE2	2.39	0.57
2:B:378:THR:OG1	2:B:380:ASN:OD1	2.22	0.57
8:H:51:MET:HE1	8:H:66:TYR:HD1	1.68	0.57
20:5:87:PRO:HG2	20:5:88:VAL:HG22	1.86	0.57
23:8:149:LYS:HG2	23:8:165:ARG:HE	1.69	0.57
2:B:62:PHE:O	2:B:66:THR:HG23	2.04	0.57
2:B:361:MET:HE2	2:B:405:LEU:HD23	1.85	0.57
22:7:251:ARG:HG2	22:7:276:PRO:HB3	1.85	0.57
23:8:131:GLU:O	23:8:156:LYS:NZ	2.37	0.57
16:1:186:PHE:HB2	16:1:201:VAL:HG22	1.87	0.57
2:B:195:VAL:HG13	5:E:41:ILE:HG21	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1:100:PHE:HB2	16:1:108:LYS:HZ3	1.69	0.57
22:7:220:PRO:HD2	22:7:225:PHE:CZ	2.40	0.57
8:H:19:HIS:CE1	8:H:26:LEU:HB2	2.40	0.57
21:6:283:ILE:HG12	21:6:406:ARG:HH11	1.68	0.57
2:B:161:LEU:HD12	5:E:76:ILE:HD12	1.85	0.57
8:H:83:VAL:O	8:H:87:GLU:HG2	2.05	0.57
10:J:118:MET:HE3	10:J:118:MET:HA	1.86	0.57
11:K:50:ARG:HH21	11:K:177:ILE:HG23	1.69	0.57
18:3:131:ARG:HD2	18:3:226:MET:HE3	1.85	0.57
22:7:112:GLY:O	22:7:195:SER:HA	2.03	0.57
6:F:291:TRP:O	6:F:295:ALA:CB	2.53	0.56
8:H:326:LEU:HA	10:J:25:ARG:HE	1.70	0.56
10:J:10:LEU:HA	10:J:13:HIS:HD2	1.70	0.56
12:L:135:PHE:O	12:L:138:THR:HB	2.05	0.56
22:7:72:LEU:HD12	22:7:79:VAL:HG22	1.87	0.56
7:G:74:ILE:O	7:G:78:VAL:HG23	2.04	0.56
8:H:354:ILE:O	8:H:393:ARG:NH1	2.39	0.56
2:B:85:ILE:HG22	2:B:89:GLY:HA2	1.86	0.56
5:E:33:CYS:O	5:E:37:ILE:HG13	2.04	0.56
6:F:123:PHE:HE2	6:F:125:LEU:HG	1.71	0.56
6:F:203:LEU:HD13	6:F:302:ILE:HD12	1.86	0.56
11:K:147:ASP:O	13:M:99:ARG:NH1	2.37	0.56
21:6:139:LEU:HD11	21:6:200:LEU:HD21	1.85	0.56
25:0:67:GLU:N	25:0:68:PRO:HD2	2.21	0.56
4:D:386:LEU:O	6:F:225:ARG:NH2	2.38	0.56
21:6:338:ALA:HA	21:6:341:ILE:HG12	1.87	0.56
21:6:359:HIS:O	21:6:363:ILE:N	2.30	0.56
21:6:366:ILE:HB	21:6:370:GLU:HG3	1.86	0.56
4:D:333:LEU:HD13	4:D:482:VAL:HG21	1.88	0.56
8:H:277:GLN:O	8:H:281:LYS:CB	2.53	0.56
10:J:68:SER:OG	10:J:123:TYR:OH	2.21	0.56
23:8:192:HIS:C	23:8:194:TRP:H	2.14	0.56
10:J:132:ILE:HG13	10:J:133:LEU:HD12	1.87	0.56
4:D:376:THR:OG1	28:F:803:SQD:O47	2.24	0.56
10:J:18:ARG:HB3	10:J:31:GLN:HB3	1.88	0.56
1:A:41:ILE:O	1:A:45:VAL:HG23	2.05	0.56
3:C:42:SER:O	11:K:90:ARG:NH2	2.39	0.56
8:H:353:LYS:NZ	8:H:354:ILE:O	2.36	0.56
16:1:100:PHE:O	16:1:101:LEU:HD22	2.06	0.56
2:B:129:PHE:HD2	2:B:169:TYR:HD2	1.54	0.55
4:D:283:ILE:HD13	4:D:286:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:195:GLN:HE22	9:I:24:GLN:HB3	1.71	0.55
21:6:243:LYS:HB2	21:6:244:PRO:HD2	1.87	0.55
22:7:65:ARG:N	22:7:146:TYR:O	2.37	0.55
6:F:251:PHE:O	6:F:255:ASN:ND2	2.39	0.55
8:H:319:PHE:H	8:H:347:LEU:HD12	1.71	0.55
9:I:80:VAL:HG21	9:I:96:ASN:ND2	2.20	0.55
21:6:333:LEU:HD22	21:6:448:ILE:HG21	1.89	0.55
11:K:187:LEU:HD13	13:M:190:SER:HB2	1.88	0.55
4:D:32:VAL:HG12	4:D:115:TYR:HD2	1.72	0.55
10:J:135:PRO:HG3	11:K:104:LYS:HD3	1.89	0.55
19:4:155:ASP:O	19:4:220:GLY:HA2	2.06	0.55
4:D:178:PHE:O	4:D:182:VAL:HG23	2.07	0.55
14:N:63:ASP:OD2	14:N:216:TRP:NE1	2.39	0.55
22:7:301:LEU:HA	22:7:360:ASN:ND2	2.21	0.55
6:F:306:ILE:HA	6:F:310:THR:HG22	1.89	0.55
4:D:438:ARG:HH12	25:0:81:ASN:HA	1.71	0.55
6:F:183:SER:HB2	6:F:189:ILE:HG22	1.88	0.55
8:H:310:PHE:HD2	8:H:311:LEU:HD13	1.71	0.55
1:A:151:SER:OG	1:A:152:ASN:N	2.40	0.54
8:H:268:MET:O	8:H:271:SER:OG	2.24	0.54
11:K:153:ASP:HA	13:M:192:VAL:HG21	1.89	0.54
19:4:133:GLU:HG3	19:4:134:LEU:H	1.72	0.54
8:H:351:ARG:NH1	8:H:352:TRP:O	2.40	0.54
10:J:119:VAL:HG23	10:J:121:ILE:HG22	1.89	0.54
16:1:177:GLU:HA	16:1:182:GLY:HA2	1.89	0.54
1:A:247:TYR:HD2	1:A:251:LYS:HB3	1.71	0.54
6:F:252:GLN:OE1	6:F:256:ASN:ND2	2.38	0.54
8:H:169:TYR:HA	8:H:287:TYR:HB3	1.89	0.54
8:H:365:LEU:HA	8:H:368:LEU:HD12	1.89	0.54
4:D:53:TYR:CE2	25:0:147:GLY:HA3	2.43	0.54
4:D:79:ARG:HG3	4:D:132:ARG:HB3	1.89	0.54
4:D:420:PHE:O	4:D:424:ILE:HG12	2.08	0.54
7:G:43:LEU:HG	7:G:66:TYR:CE1	2.42	0.54
9:I:46:LYS:NZ	9:I:47:SER:O	2.40	0.54
14:N:72:ILE:HG22	14:N:74:PRO:HD3	1.90	0.54
18:3:167:PHE:CE2	18:3:186:ALA:HB2	2.42	0.54
21:6:308:ILE:O	21:6:354:MET:HB3	2.07	0.54
10:J:41:ALA:HB1	10:J:104:ILE:HG21	1.87	0.54
18:3:131:ARG:HG3	18:3:223:MET:HG3	1.89	0.54
18:3:137:LEU:HB2	18:3:219:LEU:HD21	1.90	0.54
4:D:444:TYR:HB2	6:F:209:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:LEU:HD23	28:F:803:SQD:H91	1.88	0.54
19:4:162:SER:OG	19:4:163:MET:N	2.41	0.54
21:6:416:SER:OG	21:6:438:SER:O	2.24	0.54
22:7:215:TYR:HE2	22:7:252:GLN:HE21	1.53	0.54
22:7:269:VAL:O	22:7:316:GLY:HA2	2.08	0.54
2:B:267:PHE:O	2:B:271:THR:HG22	2.07	0.54
10:J:72:LEU:HD23	10:J:73:THR:N	2.23	0.54
24:9:151:ASP:N	24:9:151:ASP:OD1	2.39	0.54
2:B:261:PRO:O	2:B:265:VAL:HG23	2.08	0.54
2:B:325:ALA:HA	2:B:329:ILE:HD13	1.89	0.54
4:D:326:ILE:HG21	6:F:123:PHE:CE1	2.43	0.54
8:H:76:MET:HG3	8:H:157:TYR:OH	2.08	0.54
22:7:223:SER:HB3	22:7:227:LEU:HD12	1.90	0.54
1:A:236:GLU:HG3	1:A:239:LEU:C	2.33	0.54
6:F:740:ASN:O	6:F:744:LEU:N	2.41	0.54
13:M:99:ARG:HH22	13:M:194:ASN:HD21	1.55	0.54
1:A:352:LEU:O	1:A:355:THR:OG1	2.26	0.54
6:F:423:MET:HB2	6:F:495:THR:HB	1.89	0.54
11:K:142:THR:O	11:K:144:ARG:NH2	2.41	0.54
21:6:172:TYR:CG	21:6:187:GLN:HG2	2.42	0.54
8:H:169:TYR:HB2	8:H:288:GLU:HB3	1.90	0.53
13:M:106:ALA:HA	13:M:120:THR:HA	1.91	0.53
21:6:127:TYR:HB3	21:6:319:MET:HA	1.90	0.53
1:A:31:PRO:O	1:A:35:LEU:HG	2.07	0.53
1:A:184:LEU:HA	1:A:358:GLN:HE21	1.74	0.53
6:F:675:LEU:HA	6:F:678:ILE:HB	1.89	0.53
11:K:51:LEU:HD13	11:K:174:ARG:HG2	1.91	0.53
12:L:149:ALA:O	12:L:152:VAL:HG23	2.08	0.53
14:N:92:GLY:HA3	14:N:147:LYS:H	1.73	0.53
21:6:393:VAL:HG22	21:6:411:VAL:HB	1.90	0.53
1:A:145:LEU:HD13	7:G:75:ILE:HG21	1.89	0.53
1:A:197:GLN:NE2	1:A:206:ASN:H	2.07	0.53
6:F:276:PHE:HZ	6:F:339:VAL:HG11	1.72	0.53
27:F:801:BCR:H271	28:F:803:SQD:H121	1.90	0.53
13:M:136:THR:O	13:M:139:THR:OG1	2.26	0.53
6:F:203:LEU:HB3	6:F:302:ILE:HG21	1.90	0.53
21:6:427:VAL:HG13	21:6:431:LYS:H	1.72	0.53
1:A:164:ALA:O	1:A:168:ILE:HG12	2.09	0.53
4:D:170:TYR:CE2	4:D:223:VAL:HG13	2.44	0.53
22:7:82:TYR:OH	22:7:171:LEU:O	2.27	0.53
22:7:214:PRO:O	22:7:253:GLY:HA3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:692:ASP:O	6:F:695:LYS:HB2	2.07	0.53
6:F:760:ARG:O	6:F:763:SER:N	2.40	0.53
7:G:15:GLY:HA3	7:G:49:PHE:HE1	1.73	0.53
8:H:195:GLN:NE2	9:I:24:GLN:HB3	2.24	0.53
21:6:362:GLU:O	21:6:365:GLU:HG3	2.08	0.53
2:B:409:PRO:HA	2:B:414:PHE:CG	2.44	0.53
16:1:161:GLU:HG2	16:1:170:TRP:CD1	2.44	0.53
4:D:388:LEU:HD21	6:F:198:MET:HE2	1.89	0.53
9:I:160:ASN:HD22	11:K:75:ARG:HH12	1.57	0.53
10:J:37:TRP:HB3	10:J:99:PRO:HB2	1.90	0.53
23:8:161:PRO:HD2	23:8:164:TRP:CZ2	2.44	0.52
1:A:175:THR:HG21	3:C:76:THR:HB	1.90	0.52
2:B:226:SER:HB2	19:4:239:CYS:HB2	1.92	0.52
10:J:22:PHE:HA	10:J:28:GLU:HA	1.91	0.52
12:L:115:ILE:HD13	12:L:145:LEU:HD22	1.90	0.52
14:N:151:VAL:HB	14:N:204:VAL:HG12	1.90	0.52
19:4:177:GLY:HA3	20:5:180:PRO:HD2	1.91	0.52
4:D:438:ARG:NH1	25:0:81:ASN:O	2.41	0.52
6:F:415:TYR:O	25:0:93:TYR:HB2	2.09	0.52
8:H:151:MET:SD	8:H:151:MET:N	2.82	0.52
6:F:484:THR:HA	6:F:487:TYR:CE2	2.44	0.52
10:J:55:GLN:HG3	10:J:111:GLN:HB3	1.92	0.52
11:K:132:GLY:O	11:K:136:SER:OG	2.25	0.52
21:6:412:ALA:HB3	21:6:435:VAL:HG22	1.92	0.52
11:K:100:THR:HG21	11:K:135:PHE:HD2	1.75	0.52
20:5:138:GLN:NE2	20:5:186:GLN:OE1	2.42	0.52
1:A:30:LEU:O	1:A:34:THR:HG23	2.08	0.52
4:D:438:ARG:HA	4:D:442:TYR:CD2	2.44	0.52
6:F:736:ASP:HA	6:F:739:THR:HG22	1.91	0.52
13:M:149:ASP:O	13:M:153:HIS:HB2	2.09	0.52
24:9:115:TRP:C	24:9:117:VAL:H	2.17	0.52
1:A:114:VAL:HG11	1:A:129:GLY:HA2	1.92	0.52
4:D:207:ALA:O	4:D:208:THR:HG22	2.09	0.52
6:F:312:VAL:HG12	6:F:369:LEU:HD21	1.90	0.52
7:G:102:LEU:O	7:G:106:THR:HG23	2.09	0.52
14:N:114:HIS:HE1	14:N:133:PRO:HA	1.75	0.52
2:B:135:THR:HG21	7:G:165:VAL:HG21	1.92	0.52
16:1:98:PHE:HB2	16:1:108:LYS:HD3	1.91	0.52
1:A:72:LEU:HB2	12:L:150:PRO:HG2	1.92	0.52
7:G:7:ILE:HA	7:G:10:ILE:HD12	1.92	0.52
8:H:291:GLU:HA	8:H:294:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:80:ARG:NH2	11:K:81:TYR:OH	2.43	0.52
12:L:130:GLU:HA	12:L:133:LEU:HD13	1.91	0.52
1:A:108:VAL:O	1:A:111:SER:OG	2.28	0.52
4:D:49:TYR:HB2	25:O:151:TYR:HD2	1.74	0.52
4:D:388:LEU:HG	4:D:389:PRO:HD2	1.92	0.52
10:J:33:LYS:HB3	10:J:36:ASP:HB2	1.92	0.52
11:K:89:PRO:HG3	11:K:112:LEU:HD22	1.91	0.52
19:4:137:SER:HB2	19:4:173:ARG:HH12	1.75	0.52
21:6:322:ARG:O	21:6:322:ARG:NH2	2.43	0.52
2:B:57:ARG:HB2	2:B:58:PRO:HD3	1.92	0.51
6:F:123:PHE:CE2	6:F:125:LEU:HG	2.45	0.51
6:F:193:TRP:CZ2	6:F:282:LYS:HB2	2.45	0.51
8:H:375:ALA:O	8:H:379:THR:HG23	2.09	0.51
11:K:25:GLU:HG3	13:M:185:LYS:HB2	1.92	0.51
22:7:314:TYR:OH	22:7:336:ALA:HB3	2.10	0.51
1:A:232:LEU:HB2	1:A:235:ALA:HB3	1.92	0.51
20:5:136:MET:HE1	20:5:138:GLN:HB2	1.91	0.51
22:7:145:SER:OG	22:7:146:TYR:N	2.43	0.51
10:J:59:ASP:OD1	10:J:60:VAL:N	2.44	0.51
21:6:379:PRO:C	21:6:381:GLN:H	2.18	0.51
19:4:200:LEU:HD12	19:4:231:ALA:HA	1.92	0.51
22:7:270:SER:HA	22:7:315:LEU:O	2.10	0.51
1:A:348:LEU:O	1:A:352:LEU:HG	2.10	0.51
8:H:231:TRP:CE2	8:H:233:LEU:HD21	2.46	0.51
8:H:314:LYS:NZ	8:H:315:PRO:O	2.43	0.51
21:6:175:ASP:HB3	21:6:203:LYS:HE3	1.92	0.51
21:6:311:ILE:HG23	21:6:331:LEU:HD13	1.93	0.51
1:A:174:LEU:HD11	1:A:224:GLU:HG3	1.92	0.51
6:F:190:TYR:OH	6:F:194:GLU:OE2	2.23	0.51
8:H:324:GLN:HG3	10:J:25:ARG:HA	1.92	0.51
14:N:70:LEU:HD21	14:N:216:TRP:HB2	1.93	0.51
14:N:115:PRO:HA	14:N:130:TYR:HA	1.93	0.51
22:7:278:GLU:HG3	22:7:282:LYS:HB2	1.91	0.51
4:D:67:ASP:OD1	4:D:67:ASP:N	2.44	0.51
6:F:51:TRP:HB3	6:F:129:TYR:CE1	2.46	0.51
11:K:124:ALA:HB3	11:K:155:TYR:HA	1.93	0.51
22:7:65:ARG:HB3	22:7:146:TYR:CD2	2.45	0.51
1:A:283:PRO:O	1:A:286:SER:OG	2.27	0.51
4:D:331:ALA:O	4:D:335:ILE:HG23	2.10	0.51
11:K:67:GLU:O	11:K:70:SER:OG	2.24	0.51
22:7:73:ARG:HH22	22:7:108:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:98:LEU:HD22	22:7:330:PHE:CD1	2.46	0.51
1:A:117:LEU:HB2	1:A:121:PHE:HD2	1.75	0.51
3:C:37:GLY:HA3	11:K:190:ASN:HD21	1.75	0.51
7:G:43:LEU:HG	7:G:66:TYR:CD1	2.45	0.51
24:9:136:HIS:O	24:9:136:HIS:ND1	2.44	0.51
2:B:337:ILE:HD13	2:B:340:ILE:HD12	1.93	0.51
4:D:102:LEU:HG	4:D:464:ILE:HD11	1.93	0.51
6:F:386:PHE:O	6:F:390:THR:HG23	2.11	0.51
11:K:103:MET:HG3	11:K:104:LYS:HD2	1.92	0.51
4:D:43:GLU:HG2	4:D:122:TYR:CE1	2.46	0.50
12:L:114:ILE:HG13	12:L:118:TRP:CD1	2.45	0.50
12:L:149:ALA:HB1	12:L:150:PRO:HD2	1.93	0.50
13:M:137:ASP:O	13:M:141:GLN:HG2	2.09	0.50
1:A:277:GLY:O	1:A:309:THR:OG1	2.22	0.50
6:F:423:MET:O	6:F:423:MET:HG2	2.10	0.50
8:H:73:LEU:HB2	8:H:387:ILE:HD13	1.92	0.50
8:H:76:MET:SD	8:H:105:MET:HB3	2.52	0.50
22:7:222:ALA:HB2	22:7:236:ARG:HH21	1.75	0.50
4:D:386:LEU:HD22	4:D:430:PRO:HG3	1.92	0.50
4:D:427:ILE:HD13	6:F:226:VAL:HG22	1.93	0.50
9:I:60:GLU:HB2	9:I:118:CYS:SG	2.51	0.50
4:D:353:SER:O	4:D:354:ASP:HB3	2.11	0.50
6:F:663:ILE:HG23	6:F:678:ILE:HD11	1.94	0.50
12:L:149:ALA:O	12:L:151:PHE:N	2.45	0.50
14:N:105:ASP:OD1	14:N:105:ASP:N	2.44	0.50
16:1:103:HIS:CD2	17:2:193:LYS:HA	2.46	0.50
21:6:302:LYS:HD3	21:6:304:LYS:HE3	1.92	0.50
2:B:91:PHE:O	2:B:92:GLN:HB2	2.12	0.50
22:7:314:TYR:O	22:7:333:THR:HA	2.11	0.50
8:H:111:ILE:O	8:H:115:LEU:HG	2.11	0.50
18:3:215:THR:O	18:3:219:LEU:HB2	2.12	0.50
10:J:34:ALA:HB1	10:J:98:ILE:HD12	1.94	0.50
12:L:127:LYS:HG2	12:L:128:PHE:H	1.77	0.50
1:A:327:LEU:HD22	8:H:198:ILE:HD12	1.93	0.50
8:H:107:GLU:HA	8:H:110:ARG:HG3	1.92	0.50
12:L:108:LEU:HB2	12:L:144:GLY:HA3	1.93	0.50
19:4:164:VAL:HG22	19:4:165:VAL:H	1.76	0.50
21:6:329:LEU:HB2	21:6:334:TRP:NE1	2.26	0.50
7:G:125:TRP:HZ2	17:2:147:LEU:HD23	1.77	0.50
11:K:25:GLU:HB2	13:M:188:MET:HG3	1.93	0.50
14:N:113:ILE:HA	14:N:133:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:168:ASP:HA	18:3:171:ILE:HG22	1.94	0.50
21:6:143:TYR:HB2	21:6:146:VAL:HG21	1.95	0.49
2:B:335:VAL:HG22	2:B:420:LEU:HD13	1.95	0.49
4:D:318:ILE:HD13	4:D:422:MET:HE2	1.94	0.49
8:H:81:ILE:HD12	8:H:337:LEU:HG	1.94	0.49
10:J:96:PRO:HB2	10:J:121:ILE:HA	1.94	0.49
10:J:137:SER:OG	13:M:161:GLU:OE1	2.26	0.49
23:8:138:GLU:HA	23:8:164:TRP:HB3	1.93	0.49
8:H:73:LEU:HG	8:H:387:ILE:HG21	1.93	0.49
11:K:126:GLY:HA2	11:K:161:PRO:HG3	1.95	0.49
8:H:329:ARG:HD3	10:J:53:ARG:HH12	1.77	0.49
1:A:209:ARG:O	1:A:210:GLN:NE2	2.39	0.49
6:F:257:TRP:CG	18:3:125:ALA:HB2	2.46	0.49
8:H:225:ARG:HH21	8:H:263:VAL:HG22	1.77	0.49
11:K:67:GLU:OE1	11:K:70:SER:OG	2.31	0.49
17:2:95:TRP:O	17:2:118:ARG:NH2	2.44	0.49
1:A:269:PHE:HA	1:A:272:VAL:HG12	1.93	0.49
2:B:68:LEU:HB3	2:B:109:THR:HG22	1.95	0.49
4:D:376:THR:HG21	6:F:69:ILE:HD11	1.95	0.49
4:D:404:LEU:HD22	4:D:422:MET:HE1	1.94	0.49
26:D:601:LHG:H241	24:9:124:LYS:HD3	1.94	0.49
8:H:19:HIS:NE2	8:H:21:SER:HB2	2.27	0.49
22:7:274:ALA:HB2	22:7:312:ASP:HA	1.95	0.49
2:B:205:SER:HA	2:B:218:LEU:HD13	1.93	0.49
6:F:200:SER:O	6:F:204:ILE:HG12	2.12	0.49
6:F:487:TYR:HA	6:F:490:ARG:HB3	1.95	0.49
8:H:19:HIS:CD2	8:H:21:SER:HB2	2.48	0.49
10:J:49:TYR:HB3	10:J:72:LEU:HD21	1.94	0.49
16:1:153:ILE:HG13	16:1:177:GLU:HB2	1.95	0.49
20:5:176:ALA:HB2	20:5:188:PHE:HD1	1.78	0.49
21:6:290:VAL:HG23	21:6:291:VAL:HG23	1.95	0.49
1:A:83:PHE:O	1:A:85:GLU:N	2.46	0.49
6:F:446:SER:HB2	6:F:453:LEU:HD23	1.94	0.49
10:J:44:LEU:HB3	10:J:49:TYR:HB2	1.93	0.49
3:C:57:GLN:OE1	3:C:57:GLN:N	2.46	0.49
6:F:247:PHE:CE2	6:F:321:ARG:HD3	2.47	0.49
22:7:86:VAL:H	22:7:93:GLY:HA3	1.77	0.49
2:B:150:ILE:HD12	7:G:152:PHE:CE1	2.47	0.49
2:B:412:ALA:HA	2:B:495:GLY:HA3	1.94	0.49
4:D:8:THR:HG23	4:D:78:TRP:HE1	1.78	0.49
4:D:371:MET:HE3	4:D:454:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:427:ILE:HD11	6:F:229:PHE:CD2	2.48	0.49
16:1:182:GLY:O	16:1:205:GLU:HB2	2.12	0.49
19:4:238:GLY:HA2	19:4:242:GLU:HA	1.95	0.49
10:J:111:GLN:O	10:J:114:GLU:HG3	2.13	0.48
20:5:162:ASN:OD1	20:5:163:PHE:N	2.46	0.48
5:E:29:ARG:NH2	7:G:29:LEU:O	2.46	0.48
6:F:491:ILE:O	6:F:495:THR:HG22	2.13	0.48
10:J:58:TYR:HD2	10:J:67:ALA:HB3	1.77	0.48
23:8:136:ILE:HB	23:8:187:PRO:HD2	1.95	0.48
1:A:205:TRP:HB2	1:A:208:TRP:CD1	2.48	0.48
2:B:241:GLY:O	2:B:245:SER:N	2.45	0.48
4:D:326:ILE:HG21	6:F:123:PHE:HE1	1.76	0.48
8:H:60:ILE:HD13	8:H:319:PHE:CE1	2.49	0.48
8:H:264:ARG:NE	8:H:385:ASP:OD2	2.45	0.48
8:H:306:PHE:HA	8:H:309:LYS:HE2	1.94	0.48
21:6:350:PRO:O	21:6:351:LEU:HD23	2.13	0.48
22:7:252:GLN:HG3	22:7:253:GLY:H	1.76	0.48
8:H:326:LEU:HG	10:J:25:ARG:HE	1.78	0.48
11:K:195:PHE:HB3	13:M:144:TYR:HE1	1.78	0.48
1:A:72:LEU:HD22	12:L:150:PRO:HB2	1.96	0.48
8:H:76:MET:HG3	8:H:157:TYR:HH	1.78	0.48
8:H:299:LYS:HD3	8:H:299:LYS:N	2.29	0.48
1:A:197:GLN:HE22	1:A:274:TYR:C	2.21	0.48
1:A:218:LEU:O	1:A:221:SER:OG	2.30	0.48
8:H:48:HIS:HE1	10:J:133:LEU:HD23	1.78	0.48
8:H:133:TYR:O	8:H:137:GLU:HG2	2.14	0.48
8:H:367:GLN:HA	8:H:370:LYS:HD3	1.95	0.48
16:1:124:THR:H	16:1:195:ARG:CB	2.26	0.48
22:7:318:PRO:HG3	22:7:330:PHE:CZ	2.49	0.48
6:F:518:ILE:HA	22:7:165:VAL:HG11	1.94	0.48
8:H:337:LEU:HD12	8:H:338:GLY:H	1.79	0.48
10:J:96:PRO:HB2	10:J:121:ILE:HG13	1.95	0.48
11:K:64:CYS:H	11:K:99:GLY:HA2	1.79	0.48
13:M:147:PHE:O	13:M:151:VAL:HG12	2.14	0.48
14:N:107:GLU:O	14:N:111:THR:HG22	2.14	0.48
16:1:199:LEU:HD22	16:1:222:PHE:HD2	1.78	0.48
18:3:212:TYR:HA	18:3:215:THR:HG22	1.96	0.48
21:6:339:LYS:O	21:6:343:SER:OG	2.32	0.48
22:7:82:TYR:CE1	22:7:173:MET:HB3	2.48	0.48
4:D:325:ASN:O	4:D:329:ASN:HB2	2.14	0.48
9:I:64:CYS:C	9:I:66:ALA:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:79:VAL:H	22:7:113:VAL:HG12	1.78	0.48
5:E:78:LEU:HD12	7:G:73:LEU:HG	1.96	0.48
20:5:146:ASN:HA	20:5:227:ARG:HH11	1.78	0.48
21:6:306:VAL:N	21:6:350:PRO:HB3	2.29	0.48
25:0:134:PRO:O	25:0:138:ILE:HG22	2.13	0.48
8:H:42:PRO:HG3	8:H:365:LEU:HD23	1.96	0.48
8:H:149:THR:OG1	8:H:157:TYR:HB3	2.14	0.48
18:3:200:VAL:HG22	18:3:208:ILE:HG23	1.95	0.48
19:4:139:CYS:H	20:5:196:TRP:CD1	2.32	0.48
1:A:40:THR:O	1:A:44:LEU:HG	2.13	0.47
1:A:351:LEU:HA	1:A:354:THR:HG22	1.96	0.47
4:D:413:MET:HB3	4:D:414:PRO:HD3	1.95	0.47
6:F:659:PHE:CZ	6:F:663:ILE:HD11	2.49	0.47
8:H:97:ARG:O	8:H:101:ILE:HG13	2.14	0.47
20:5:83:ASN:HB3	20:5:89:GLY:HA3	1.96	0.47
2:B:502:LEU:HD13	4:D:73:VAL:HG21	1.96	0.47
4:D:429:THR:HA	4:D:432:TYR:CE2	2.50	0.47
6:F:305:LEU:O	6:F:309:ALA:HB3	2.14	0.47
8:H:278:ALA:O	8:H:282:ILE:HG13	2.14	0.47
9:I:133:HIS:ND1	14:N:119:PRO:HD2	2.29	0.47
20:5:99:LEU:HB3	20:5:108:VAL:HG13	1.95	0.47
22:7:227:LEU:O	22:7:228:LEU:HB2	2.14	0.47
2:B:247:ALA:HB2	2:B:306:SER:HA	1.95	0.47
4:D:332:ILE:O	4:D:335:ILE:HG12	2.14	0.47
6:F:692:ASP:HA	6:F:695:LYS:HD2	1.94	0.47
8:H:226:ALA:HB1	8:H:259:ALA:HB1	1.97	0.47
10:J:21:GLY:O	10:J:29:THR:OG1	2.26	0.47
18:3:116:MET:HE1	18:3:165:TYR:HB2	1.96	0.47
1:A:140:ALA:O	1:A:144:LEU:HG	2.14	0.47
1:A:227:ARG:HA	1:A:228:LEU:HA	1.59	0.47
8:H:53:LYS:HZ3	10:J:143:LEU:HA	1.79	0.47
8:H:364:ILE:HD12	8:H:367:GLN:HB3	1.96	0.47
21:6:201:SER:OG	21:6:202:THR:N	2.47	0.47
22:7:195:SER:OG	22:7:333:THR:O	2.33	0.47
1:A:175:THR:HG23	3:C:80:TYR:OH	2.14	0.47
1:A:257:LEU:O	1:A:261:LEU:HG	2.14	0.47
6:F:117:TRP:HB3	6:F:127:PHE:CD2	2.49	0.47
6:F:508:SER:HB2	23:8:189:TRP:HE3	1.78	0.47
11:K:104:LYS:C	11:K:106:ALA:H	2.22	0.47
14:N:61:LEU:HA	14:N:64:VAL:HG12	1.97	0.47
22:7:73:ARG:HH22	22:7:108:ALA:CB	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:231:LEU:HD12	6:F:275:LEU:HD22	1.97	0.47
6:F:264:ASN:OD1	6:F:265:SER:N	2.48	0.47
8:H:116:LEU:HD21	8:H:138:ARG:NH1	2.29	0.47
8:H:141:ILE:H	8:H:141:ILE:HD12	1.78	0.47
11:K:62:SER:H	11:K:99:GLY:HA3	1.80	0.47
13:M:151:VAL:HG13	13:M:152:ASP:OD1	2.14	0.47
1:A:130:VAL:HG22	1:A:188:LEU:O	2.14	0.47
1:A:200:TYR:HB2	1:A:204:GLY:H	1.79	0.47
1:A:356:SER:HA	1:A:359:LEU:HB2	1.96	0.47
2:B:181:MET:SD	5:E:84:ILE:HD12	2.55	0.47
2:B:317:GLN:HE22	6:F:754:LYS:HE3	1.80	0.47
6:F:294:ASP:OD1	6:F:294:ASP:N	2.44	0.47
11:K:56:PRO:HG3	11:K:83:LEU:HD12	1.96	0.47
22:7:48:LEU:O	22:7:49:ARG:HD2	2.15	0.47
23:8:79:ALA:N	23:8:98:ALA:O	2.47	0.47
2:B:124:MET:HE2	2:B:170:THR:HA	1.95	0.47
5:E:14:PHE:O	5:E:18:ILE:HG12	2.14	0.47
5:E:27:MET:HG2	5:E:81:LEU:HD13	1.96	0.47
6:F:639:ASN:HB3	6:F:644:ILE:HD11	1.96	0.47
7:G:43:LEU:HA	7:G:46:ILE:HG22	1.97	0.47
21:6:359:HIS:HA	21:6:362:GLU:HG3	1.97	0.47
1:A:80:LYS:HD3	11:K:53:SER:HB2	1.96	0.47
4:D:24:LEU:O	4:D:112:ARG:NH2	2.48	0.47
4:D:444:TYR:O	25:0:85:PRO:HD3	2.14	0.47
6:F:319:LEU:HD21	6:F:336:ILE:HD13	1.96	0.47
8:H:233:LEU:HB2	8:H:331:GLU:HB2	1.97	0.47
17:2:123:ALA:HA	17:2:208:LEU:HD23	1.96	0.47
4:D:70:TRP:HD1	4:D:71:ILE:HG12	1.79	0.47
6:F:750:GLY:O	6:F:754:LYS:HB2	2.15	0.47
7:G:67:VAL:HA	7:G:71:ASN:HD22	1.80	0.47
8:H:27:ARG:HB3	8:H:43:ILE:HB	1.97	0.47
18:3:164:TYR:HA	18:3:190:PHE:CZ	2.50	0.47
22:7:95:ARG:NH1	22:7:198:LYS:HG2	2.30	0.47
3:C:94:PHE:O	3:C:98:LEU:HD23	2.15	0.46
2:B:60:PHE:HA	2:B:63:ILE:HB	1.96	0.46
2:B:111:CYS:SG	2:B:267:PHE:HB2	2.55	0.46
4:D:7:LEU:HD22	4:D:130:SER:HB2	1.97	0.46
6:F:644:ILE:O	6:F:648:ILE:HG12	2.16	0.46
6:F:713:THR:HA	6:F:717:THR:HG22	1.97	0.46
8:H:97:ARG:N	8:H:307:GLU:OE1	2.48	0.46
8:H:211:GLY:HA3	8:H:229:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:226:ALA:O	8:H:254:GLU:N	2.47	0.46
1:A:81:LEU:HD21	11:K:55:TRP:CH2	2.50	0.46
4:D:355:ARG:HD2	4:D:371:MET:HE1	1.97	0.46
1:A:80:LYS:HG3	11:K:50:ARG:HA	1.97	0.46
2:B:91:PHE:HB2	2:B:146:ALA:H	1.80	0.46
4:D:47:MET:HE3	4:D:90:ILE:HG22	1.98	0.46
6:F:458:SER:O	6:F:462:ILE:HG23	2.15	0.46
8:H:68:THR:OG1	8:H:155:HIS:ND1	2.43	0.46
12:L:96:ILE:O	12:L:100:VAL:HG22	2.14	0.46
22:7:130:LEU:HB2	22:7:132:GLY:H	1.80	0.46
22:7:255:TRP:C	22:7:257:VAL:H	2.23	0.46
2:B:118:TYR:OH	15:T:65:UNK:O	2.32	0.46
2:B:324:LEU:O	2:B:328:SER:OG	2.23	0.46
5:E:86:ARG:O	5:E:89:LYS:NZ	2.48	0.46
6:F:101:SER:O	6:F:105:ILE:HG12	2.15	0.46
6:F:122:ASP:HA	18:3:158:LEU:HD13	1.97	0.46
6:F:591:LEU:HA	6:F:594:THR:HG22	1.96	0.46
21:6:457:ASP:OD1	21:6:458:LEU:N	2.49	0.46
4:D:134:LEU:HD21	4:D:182:VAL:HG22	1.98	0.46
4:D:277:SER:N	4:D:278:PRO:HD2	2.31	0.46
6:F:656:PHE:O	6:F:660:ILE:HG12	2.16	0.46
9:I:148:SER:O	9:I:151:GLY:N	2.47	0.46
13:M:201:ARG:HD3	14:N:129:TRP:CG	2.51	0.46
8:H:97:ARG:HH12	8:H:166:ASP:CG	2.24	0.46
8:H:326:LEU:HG	10:J:25:ARG:HH11	1.80	0.46
12:L:141:PHE:C	12:L:145:LEU:HG	2.41	0.46
16:1:190:ALA:O	16:1:196:TYR:HA	2.15	0.46
19:4:151:LEU:HD22	19:4:213:VAL:HG22	1.97	0.46
21:6:347:GLY:C	21:6:349:ARG:H	2.23	0.46
6:F:186:LEU:O	6:F:189:ILE:HG12	2.15	0.46
11:K:128:CYS:SG	11:K:134:MET:HG3	2.56	0.46
18:3:129:ARG:HD2	18:3:166:ASP:OD2	2.15	0.46
22:7:156:VAL:HG12	22:7:161:GLU:HA	1.97	0.46
1:A:76:ALA:O	11:K:49:SER:OG	2.34	0.46
4:D:259:TYR:OH	4:D:263:ARG:NE	2.48	0.46
6:F:66:PHE:CZ	27:F:801:BCR:H21C	2.51	0.46
6:F:283:SER:OG	6:F:284:ALA:N	2.49	0.46
11:K:198:SER:OG	11:K:199:HIS:N	2.49	0.46
13:M:108:ILE:H	13:M:124:THR:HG21	1.80	0.46
21:6:358:ARG:O	21:6:360:ARG:N	2.48	0.46
1:A:313:ALA:O	1:A:317:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:139:LEU:O	6:F:143:THR:HG22	2.16	0.46
6:F:695:LYS:HA	6:F:698:ILE:HG22	1.98	0.46
8:H:28:LEU:HD12	8:H:40:CYS:SG	2.56	0.46
22:7:202:ARG:NH1	22:7:319:GLY:O	2.39	0.46
5:E:27:MET:HB2	5:E:93:ILE:HD11	1.98	0.45
6:F:110:ILE:HD11	24:9:95:TRP:CD2	2.51	0.45
6:F:648:ILE:O	6:F:652:THR:OG1	2.24	0.45
6:F:771:TYR:HA	6:F:774:VAL:HG12	1.98	0.45
22:7:225:PHE:HD2	22:7:338:ILE:HG21	1.81	0.45
1:A:328:PRO:HD3	8:H:199:PHE:CE1	2.51	0.45
2:B:258:GLU:HB3	5:E:99:LEU:HD11	1.98	0.45
6:F:108:SER:O	24:9:94:ILE:HD12	2.16	0.45
6:F:306:ILE:O	6:F:311:MET:HB2	2.17	0.45
9:I:36:LEU:HA	12:L:124:PHE:O	2.16	0.45
18:3:177:ASP:O	18:3:180:PRO:HD2	2.16	0.45
20:5:83:ASN:HB3	20:5:89:GLY:C	2.41	0.45
6:F:117:TRP:HE1	6:F:125:LEU:HB3	1.82	0.45
6:F:153:SER:HB2	6:F:166:PHE:HE2	1.81	0.45
6:F:259:PRO:HG2	6:F:264:ASN:HD21	1.81	0.45
7:G:128:ARG:HA	17:2:140:TYR:HE2	1.82	0.45
8:H:154:MET:O	8:H:157:TYR:HD1	2.00	0.45
12:L:111:ALA:HA	12:L:114:ILE:HG22	1.98	0.45
13:M:124:THR:C	13:M:125:LEU:HD12	2.42	0.45
14:N:108:SER:HA	14:N:112:LYS:HB2	1.97	0.45
21:6:445:GLY:C	21:6:446:ILE:HG13	2.42	0.45
22:7:219:PRO:HA	22:7:225:PHE:CE1	2.52	0.45
4:D:214:TYR:OH	4:D:273:HIS:ND1	2.37	0.45
5:E:81:LEU:HA	5:E:84:ILE:HG22	1.97	0.45
8:H:228:GLY:N	8:H:252:GLN:O	2.43	0.45
9:I:105:ILE:HG23	11:K:159:CYS:HB3	1.99	0.45
13:M:150:LEU:HD13	13:M:167:ILE:HD12	1.97	0.45
22:7:118:ASN:ND2	22:7:227:LEU:O	2.46	0.45
4:D:344:THR:HG21	4:D:381:PHE:CZ	2.52	0.45
4:D:411:LEU:HD12	4:D:411:LEU:O	2.16	0.45
8:H:254:GLU:HB2	8:H:259:ALA:HB2	1.97	0.45
8:H:371:LYS:HD3	8:H:371:LYS:N	2.32	0.45
9:I:128:SER:O	9:I:128:SER:OG	2.30	0.45
11:K:102:THR:HA	11:K:142:THR:HA	1.98	0.45
1:A:228:LEU:H	1:A:329:ARG:HD3	1.81	0.45
2:B:49:ASP:HB2	2:B:127:THR:HG21	1.99	0.45
4:D:106:PRO:HG3	24:9:132:TYR:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:259:PRO:HG2	6:F:264:ASN:ND2	2.31	0.45
8:H:81:ILE:HD11	8:H:330:VAL:HB	1.99	0.45
20:5:77:LYS:HB2	20:5:240:LEU:O	2.16	0.45
20:5:174:SER:HB2	20:5:188:PHE:CE1	2.51	0.45
21:6:449:GLU:O	21:6:453:LYS:HG2	2.16	0.45
22:7:190:THR:HG22	22:7:338:ILE:HG13	1.99	0.45
2:B:161:LEU:HD11	5:E:73:GLU:HG3	1.97	0.45
2:B:358:TYR:HA	2:B:361:MET:HG2	1.97	0.45
4:D:391:MET:HE3	28:F:803:SQD:H332	1.99	0.45
6:F:410:GLU:N	6:F:411:PRO:HD2	2.32	0.45
6:F:751:GLU:HB3	21:6:214:PHE:CZ	2.51	0.45
6:F:761:ILE:HD12	6:F:761:ILE:H	1.81	0.45
27:F:801:BCR:HC8	24:9:112:PHE:CE1	2.52	0.45
12:L:142:PHE:N	12:L:143:PRO:HD2	2.32	0.45
13:M:102:ARG:HB3	13:M:104:TYR:CE1	2.52	0.45
13:M:148:GLN:HA	13:M:151:VAL:HG12	1.98	0.45
14:N:129:TRP:HB2	14:N:131:PHE:CE1	2.52	0.45
21:6:364:GLU:OE1	21:6:364:GLU:N	2.49	0.45
24:9:90:VAL:HG13	24:9:93:SER:H	1.82	0.45
1:A:119:TYR:CE2	1:A:120:HIS:HD2	2.34	0.45
2:B:91:PHE:CG	2:B:92:GLN:N	2.84	0.45
2:B:353:THR:HG21	2:B:502:LEU:HD23	1.98	0.45
4:D:29:ASN:HD21	4:D:33:ARG:HD3	1.82	0.45
4:D:235:PRO:HG3	4:D:307:TYR:CE1	2.52	0.45
13:M:147:PHE:HA	13:M:150:LEU:HG	1.99	0.45
17:2:102:ARG:HD2	17:2:102:ARG:HA	1.75	0.45
21:6:307:VAL:HB	21:6:392:VAL:HG23	1.99	0.45
22:7:62:LEU:HD21	22:7:151:VAL:HG23	1.99	0.45
22:7:216:CYS:O	22:7:218:HIS:N	2.49	0.45
1:A:170:TYR:O	1:A:173:PRO:HD2	2.16	0.45
6:F:276:PHE:CZ	6:F:339:VAL:HG11	2.50	0.45
1:A:57:ILE:HG22	9:I:33:THR:HA	1.99	0.45
1:A:200:TYR:HB3	1:A:203:PHE:HD2	1.82	0.45
2:B:91:PHE:HA	2:B:146:ALA:HA	1.99	0.45
4:D:473:ILE:HD13	27:F:801:BCR:H372	1.99	0.45
5:E:86:ARG:NH1	7:G:176:GLN:HB3	2.32	0.45
6:F:113:TYR:O	6:F:128:GLY:HA3	2.17	0.45
6:F:225:ARG:HA	6:F:228:ASP:OD2	2.17	0.45
8:H:303:TRP:HA	8:H:308:TYR:HB2	1.99	0.45
10:J:154:GLU:OE1	13:M:165:ARG:NH2	2.50	0.45
11:K:60:GLY:HA3	11:K:65:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:187:LEU:O	13:M:191:ARG:NH1	2.44	0.45
14:N:100:ALA:HB2	14:N:153:VAL:HG13	1.98	0.45
18:3:93:LYS:HB2	18:3:93:LYS:HE3	1.83	0.45
22:7:200:ASP:O	22:7:328:ASP:HB3	2.17	0.45
4:D:11:VAL:O	4:D:123:SER:OG	2.34	0.44
4:D:366:GLY:H	4:D:445:LYS:CB	2.29	0.44
6:F:67:GLY:HA3	6:F:75:THR:HG21	1.99	0.44
6:F:193:TRP:O	6:F:196:VAL:HG22	2.17	0.44
6:F:447:LEU:HD23	6:F:488:MET:HE2	1.98	0.44
8:H:17:PRO:O	8:H:25:VAL:HG23	2.16	0.44
8:H:98:ALA:HA	8:H:101:ILE:HD12	2.00	0.44
8:H:146:GLU:OE1	9:I:50:PRO:HG2	2.16	0.44
21:6:317:ALA:C	21:6:319:MET:H	2.25	0.44
22:7:236:ARG:HA	22:7:236:ARG:NH2	2.31	0.44
1:A:138:SER:O	1:A:138:SER:OG	2.28	0.44
1:A:253:GLY:O	1:A:257:LEU:HD23	2.17	0.44
2:B:92:GLN:HG2	2:B:282:ARG:HH12	1.82	0.44
4:D:261:LEU:HD22	4:D:320:ILE:HG21	2.00	0.44
6:F:66:PHE:CD1	27:F:801:BCR:H403	2.52	0.44
8:H:118:LEU:O	8:H:122:MET:N	2.44	0.44
14:N:103:LEU:HD13	14:N:109:THR:HB	1.99	0.44
1:A:255:PHE:HA	1:A:258:VAL:HG12	1.98	0.44
1:A:325:TRP:HE3	8:H:128:GLN:HG3	1.82	0.44
9:I:139:GLN:OE1	14:N:180:ARG:NH2	2.50	0.44
11:K:128:CYS:HA	11:K:133:GLY:H	1.82	0.44
24:9:87:ASP:HA	24:9:96:HIS:HB2	2.00	0.44
1:A:207:ILE:HB	1:A:274:TYR:HB3	2.00	0.44
1:A:232:LEU:HD23	8:H:128:GLN:HA	2.00	0.44
2:B:499:ASN:HB3	2:B:500:PRO:HD3	1.99	0.44
3:C:97:ALA:O	3:C:101:VAL:HG22	2.17	0.44
4:D:53:TYR:O	4:D:54:HIS:ND1	2.50	0.44
9:I:68:GLU:C	9:I:70:CYS:H	2.25	0.44
17:2:130:ARG:NE	17:2:198:TYR:OH	2.50	0.44
19:4:128:ALA:N	19:4:241:SER:HB3	2.32	0.44
21:6:270:GLY:O	21:6:271:VAL:C	2.61	0.44
21:6:359:HIS:C	21:6:362:GLU:H	2.24	0.44
22:7:192:ALA:HA	22:7:336:ALA:HB2	1.98	0.44
22:7:255:TRP:NE1	22:7:257:VAL:HB	2.32	0.44
1:A:350:ASN:OD1	1:A:351:LEU:N	2.50	0.44
2:B:256:VAL:HG13	2:B:257:TYR:HD1	1.83	0.44
4:D:166:LYS:HD3	4:D:233:TRP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:18:ILE:HD13	5:E:37:ILE:HD13	1.98	0.44
10:J:114:GLU:HB2	10:J:133:LEU:HD11	2.00	0.44
18:3:215:THR:O	18:3:219:LEU:CB	2.65	0.44
21:6:359:HIS:O	21:6:362:GLU:N	2.41	0.44
4:D:353:SER:C	4:D:355:ARG:H	2.24	0.44
6:F:253:ILE:HD13	6:F:257:TRP:HE3	1.82	0.44
6:F:317:PHE:HZ	6:F:321:ARG:HH21	1.66	0.44
8:H:218:GLY:HA2	10:J:51:TYR:HE1	1.83	0.44
8:H:278:ALA:O	8:H:281:LYS:N	2.51	0.44
8:H:335:GLY:HA3	8:H:357:PRO:HB3	1.99	0.44
19:4:172:ALA:HB3	19:4:181:ASP:OD1	2.18	0.44
22:7:86:VAL:HG11	22:7:301:LEU:HD22	1.98	0.44
22:7:131:LEU:O	22:7:159:LYS:NZ	2.36	0.44
22:7:222:ALA:HB2	22:7:236:ARG:NH2	2.33	0.44
1:A:232:LEU:HD13	8:H:123:ALA:O	2.17	0.44
2:B:63:ILE:O	2:B:66:THR:OG1	2.30	0.44
2:B:314:ALA:HB2	2:B:326:TYR:HB3	1.99	0.44
6:F:446:SER:O	6:F:455:CYS:HB3	2.18	0.44
6:F:501:ARG:HA	6:F:504:PHE:CD1	2.53	0.44
8:H:323:ARG:O	10:J:24:HIS:HB3	2.18	0.44
10:J:29:THR:HG22	10:J:86:CYS:HB2	2.00	0.44
21:6:254:TYR:O	21:6:257:TYR:N	2.44	0.44
5:E:78:LEU:HD13	7:G:77:ALA:HB2	2.00	0.44
9:I:23:GLY:O	9:I:27:ILE:HG13	2.18	0.44
9:I:66:ALA:O	9:I:68:GLU:HG2	2.18	0.44
23:8:165:ARG:HH12	23:8:170:ALA:HB1	1.81	0.44
1:A:186:ASN:O	16:1:113:GLN:NE2	2.51	0.44
2:B:395:ALA:HB1	2:B:454:LEU:HD23	2.00	0.44
6:F:285:GLN:O	6:F:289:HIS:HB3	2.18	0.44
7:G:104:CYS:O	7:G:108:VAL:HG23	2.18	0.44
19:4:160:SER:OG	19:4:161:VAL:N	2.50	0.44
22:7:195:SER:OG	22:7:195:SER:O	2.36	0.44
22:7:229:THR:OG1	22:7:233:ALA:N	2.51	0.44
2:B:59:TRP:O	2:B:63:ILE:HG12	2.18	0.43
2:B:200:TRP:HZ3	7:G:120:TRP:HH2	1.65	0.43
2:B:270:VAL:HG23	2:B:271:THR:N	2.33	0.43
7:G:67:VAL:HA	7:G:71:ASN:ND2	2.33	0.43
9:I:63:LYS:HB3	9:I:116:THR:O	2.18	0.43
12:L:99:PRO:O	12:L:103:ILE:HG22	2.18	0.43
22:7:210:LEU:HD23	22:7:210:LEU:HA	1.84	0.43
22:7:211:ARG:HA	22:7:255:TRP:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ILE:HG21	2:B:59:TRP:CZ3	2.53	0.43
2:B:333:GLY:HA2	2:B:336:ILE:HD12	2.01	0.43
4:D:138:PHE:HB2	4:D:178:PHE:HE1	1.82	0.43
8:H:350:TRP:NE1	10:J:145:LYS:HE3	2.33	0.43
9:I:129:THR:OG1	11:K:155:TYR:HB2	2.18	0.43
12:L:112:PRO:HB3	12:L:148:TRP:HB2	2.00	0.43
16:1:81:VAL:HG13	16:1:83:ALA:H	1.83	0.43
17:2:88:PRO:HB2	19:4:175:PRO:HB2	2.01	0.43
22:7:99:HIS:HE2	22:7:110:ARG:HD3	1.83	0.43
1:A:184:LEU:HD13	1:A:358:GLN:NE2	2.34	0.43
2:B:129:PHE:HD2	2:B:169:TYR:CD2	2.34	0.43
3:C:26:SER:O	3:C:30:LEU:HG	2.18	0.43
4:D:371:MET:SD	4:D:374:ILE:HD12	2.58	0.43
8:H:261:TYR:HD2	8:H:262:LEU:HD22	1.84	0.43
9:I:152:ASP:HB3	9:I:155:ILE:HD12	2.00	0.43
12:L:139:TYR:O	12:L:142:PHE:CB	2.66	0.43
14:N:138:ARG:N	14:N:138:ARG:HD2	2.33	0.43
22:7:223:SER:HG	22:7:225:PHE:C	2.26	0.43
1:A:247:TYR:CD2	1:A:251:LYS:HB3	2.53	0.43
3:C:92:SER:O	3:C:96:GLU:HG3	2.19	0.43
5:E:10:SER:OG	5:E:44:ASN:HB2	2.18	0.43
8:H:19:HIS:O	8:H:21:SER:N	2.48	0.43
8:H:116:LEU:HD11	8:H:138:ARG:NH2	2.33	0.43
8:H:329:ARG:HD3	10:J:53:ARG:NH1	2.33	0.43
10:J:63:GLY:H	10:J:146:ASP:HB2	1.83	0.43
21:6:222:VAL:HG12	21:6:240:GLU:HB2	2.01	0.43
1:A:261:LEU:HA	1:A:264:LEU:HD12	2.01	0.43
2:B:166:LEU:HB3	2:B:264:VAL:HG21	2.01	0.43
2:B:290:PHE:HB3	19:4:186:ARG:HD3	1.99	0.43
4:D:226:PRO:HD3	4:D:254:LEU:HD22	1.99	0.43
6:F:56:LEU:HD12	6:F:56:LEU:HA	1.87	0.43
8:H:317:PRO:O	8:H:347:LEU:HD11	2.19	0.43
17:2:97:THR:HG23	19:4:240:PHE:HA	1.99	0.43
21:6:122:VAL:HA	21:6:202:THR:OG1	2.17	0.43
22:7:135:GLU:H	22:7:135:GLU:CD	2.25	0.43
2:B:129:PHE:HB2	2:B:169:TYR:HE2	1.83	0.43
3:C:28:SER:O	3:C:32:ALA:HB2	2.18	0.43
6:F:66:PHE:HZ	27:F:801:BCR:H21C	1.83	0.43
6:F:360:SER:OG	6:F:491:ILE:HD11	2.18	0.43
8:H:74:ALA:HB1	8:H:77:PHE:HD2	1.84	0.43
8:H:118:LEU:HA	8:H:121:PHE:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:20:ARG:O	9:I:24:GLN:HB2	2.19	0.43
21:6:242:PHE:HB3	21:6:243:LYS:H	1.69	0.43
22:7:64:VAL:HB	22:7:147:ASP:HA	1.99	0.43
22:7:128:SER:OG	22:7:227:LEU:HB3	2.18	0.43
23:8:104:LEU:HA	23:8:107:ILE:HG22	2.00	0.43
2:B:108:SER:OG	2:B:137:THR:OG1	2.29	0.43
2:B:157:GLU:HB3	2:B:161:LEU:HD23	1.99	0.43
4:D:261:LEU:HD22	4:D:320:ILE:HD13	2.01	0.43
6:F:218:GLN:O	6:F:222:VAL:HG23	2.19	0.43
6:F:432:TYR:HE2	6:F:500:LEU:HD22	1.83	0.43
8:H:291:GLU:HA	8:H:294:ARG:NE	2.34	0.43
8:H:369:VAL:HG12	8:H:380:ILE:HD12	2.01	0.43
10:J:133:LEU:HD12	10:J:133:LEU:H	1.83	0.43
16:1:95:TRP:O	16:1:97:ASP:N	2.51	0.43
22:7:143:SER:C	22:7:145:SER:H	2.27	0.43
2:B:145:GLY:HA2	2:B:282:ARG:NH2	2.34	0.43
4:D:361:LEU:HD21	4:D:436:MET:HA	2.00	0.43
6:F:202:LEU:HD11	28:F:803:SQD:H291	1.99	0.43
6:F:500:LEU:O	6:F:502:VAL:N	2.52	0.43
8:H:67:VAL:HG21	8:H:79:GLU:HG2	2.00	0.43
16:1:89:TYR:HE2	16:1:117:VAL:HG21	1.83	0.43
18:3:116:MET:HE3	18:3:162:PHE:HA	2.01	0.43
22:7:148:ALA:HA	22:7:168:LEU:O	2.19	0.43
23:8:124:LEU:HA	23:8:124:LEU:HD23	1.76	0.43
2:B:56:ASP:HB3	2:B:60:PHE:CD2	2.54	0.43
2:B:297:LEU:O	2:B:300:GLU:HB3	2.19	0.43
4:D:207:ALA:C	4:D:209:LEU:H	2.27	0.43
4:D:301:PHE:O	4:D:305:ILE:HG12	2.18	0.43
11:K:158:GLY:HA3	11:K:161:PRO:HA	2.00	0.43
14:N:101:ARG:H	14:N:155:GLU:HB2	1.83	0.43
16:1:123:PRO:HG3	17:2:199:LEU:HA	2.01	0.43
21:6:302:LYS:HB2	21:6:349:ARG:HE	1.83	0.43
22:7:255:TRP:HZ2	22:7:261:LEU:HD22	1.84	0.43
1:A:122:VAL:HG22	1:A:124:ALA:H	1.84	0.43
4:D:435:SER:O	4:D:439:GLN:HG3	2.18	0.43
6:F:760:ARG:O	6:F:763:SER:OG	2.34	0.43
8:H:51:MET:HE2	8:H:70:TRP:CD1	2.54	0.43
8:H:76:MET:HB3	8:H:109:SER:HB3	2.01	0.43
8:H:327:TYR:CD2	8:H:340:TYR:HB2	2.54	0.43
9:I:10:SER:HA	9:I:13:GLN:HG2	1.99	0.43
13:M:108:ILE:H	13:M:124:THR:CG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:150:VAL:HG12	21:6:166:VAL:HG11	2.01	0.43
21:6:339:LYS:HG3	21:6:340:GLU:OE1	2.19	0.43
22:7:207:VAL:HG11	22:7:292:PHE:CZ	2.53	0.43
22:7:210:LEU:HD13	22:7:273:TYR:CD2	2.54	0.43
2:B:328:SER:HA	2:B:332:ILE:HD12	2.01	0.42
4:D:8:THR:OG1	4:D:66:GLU:OE2	2.37	0.42
4:D:352:ALA:O	4:D:355:ARG:HB2	2.19	0.42
6:F:428:GLY:O	6:F:429:LEU:HD12	2.18	0.42
8:H:51:MET:HG3	8:H:70:TRP:CD1	2.54	0.42
11:K:86:ARG:HB2	11:K:92:ALA:HB2	2.00	0.42
19:4:133:GLU:O	20:5:178:ALA:HB2	2.18	0.42
21:6:250:ALA:N	21:6:421:ARG:O	2.36	0.42
22:7:49:ARG:HB3	22:7:146:TYR:CE1	2.53	0.42
22:7:216:CYS:C	22:7:218:HIS:H	2.26	0.42
1:A:48:TRP:CE2	1:A:52:GLU:HG3	2.54	0.42
4:D:67:ASP:HB3	4:D:79:ARG:HD2	2.00	0.42
6:F:64:MET:O	6:F:68:LEU:N	2.46	0.42
6:F:427:GLY:HA2	6:F:495:THR:HA	2.02	0.42
12:L:112:PRO:HG3	12:L:145:LEU:HD23	2.00	0.42
13:M:103:ILE:HA	13:M:125:LEU:HG	2.00	0.42
14:N:115:PRO:HB3	14:N:130:TYR:CD1	2.54	0.42
21:6:180:GLU:OE2	21:6:183:GLU:N	2.50	0.42
21:6:286:LYS:O	21:6:290:VAL:HG22	2.19	0.42
21:6:297:ARG:N	21:6:297:ARG:HD2	2.34	0.42
22:7:116:VAL:HA	22:7:131:LEU:HD21	2.01	0.42
23:8:78:PHE:N	23:8:177:SER:O	2.52	0.42
2:B:380:ASN:OD1	2:B:380:ASN:N	2.51	0.42
8:H:331:GLU:HA	8:H:336:GLU:HA	2.00	0.42
9:I:55:GLY:HA3	9:I:123:GLU:HA	2.01	0.42
10:J:109:ASP:O	10:J:126:HIS:NE2	2.52	0.42
22:7:172:SER:OG	22:7:357:GLU:HA	2.20	0.42
25:0:133:PHE:HB3	25:0:134:PRO:HD3	2.01	0.42
1:A:282:ILE:HG22	1:A:286:SER:OG	2.19	0.42
1:A:331:ARG:C	1:A:333:ASP:H	2.27	0.42
4:D:361:LEU:HA	4:D:364:LEU:HD23	2.00	0.42
8:H:53:LYS:O	8:H:56:GLU:HG2	2.19	0.42
8:H:252:GLN:CD	8:H:253:LYS:H	2.26	0.42
1:A:214:PHE:HB2	1:A:274:TYR:CD2	2.54	0.42
4:D:74:PHE:HE2	4:D:135:LEU:HD22	1.84	0.42
7:G:121:TYR:O	7:G:125:TRP:NE1	2.52	0.42
8:H:53:LYS:NZ	10:J:143:LEU:HA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:95:PRO:HG2	8:H:309:LYS:O	2.18	0.42
13:M:99:ARG:NH2	13:M:194:ASN:HD21	2.17	0.42
4:D:222:ALA:HB2	4:D:227:ILE:HD12	2.01	0.42
7:G:24:LEU:O	7:G:28:LEU:HB2	2.19	0.42
10:J:54:SER:O	10:J:69:VAL:HG13	2.19	0.42
21:6:443:LEU:HD12	21:6:446:ILE:HD11	2.01	0.42
1:A:48:TRP:CD2	1:A:52:GLU:HG3	2.54	0.42
2:B:95:ASN:O	2:B:99:ILE:HG13	2.20	0.42
6:F:183:SER:CB	6:F:189:ILE:HG22	2.48	0.42
8:H:139:GLU:HA	8:H:142:TYR:CD2	2.55	0.42
16:1:167:ARG:CZ	16:1:224:ILE:HD11	2.50	0.42
16:1:192:GLY:C	16:1:194:GLY:H	2.27	0.42
1:A:189:SER:O	1:A:193:ILE:HG12	2.20	0.42
2:B:448:LEU:HD12	4:D:149:TYR:CE2	2.55	0.42
6:F:122:ASP:O	6:F:123:PHE:HB3	2.19	0.42
11:K:96:LEU:HD12	11:K:125:MET:HB2	2.01	0.42
22:7:53:ASP:OD1	22:7:54:ALA:N	2.43	0.42
22:7:97:LEU:HD13	22:7:112:GLY:O	2.20	0.42
23:8:91:PRO:HB2	23:8:93:VAL:HG13	2.01	0.42
23:8:125:ASN:O	23:8:126:CYS:HB3	2.20	0.42
1:A:81:LEU:HD21	11:K:55:TRP:HH2	1.85	0.42
1:A:240:VAL:HG11	3:C:45:GLU:CB	2.50	0.42
2:B:228:GLY:O	2:B:231:ILE:N	2.44	0.42
4:D:411:LEU:O	4:D:413:MET:N	2.53	0.42
28:F:802:SQD:H322	28:F:802:SQD:H291	1.83	0.42
7:G:68:GLY:O	7:G:72:VAL:HG22	2.20	0.42
8:H:314:LYS:HD2	8:H:315:PRO:HD2	2.02	0.42
8:H:364:ILE:O	8:H:368:LEU:HG	2.20	0.42
10:J:25:ARG:HH21	10:J:27:ILE:HD13	1.85	0.42
10:J:92:GLN:HG3	10:J:94:ASP:H	1.84	0.42
1:A:52:GLU:HG2	1:A:63:PRO:HD2	2.02	0.42
1:A:202:PHE:HA	1:A:205:TRP:CD1	2.55	0.42
2:B:286:ILE:HB	2:B:287:PRO:HD3	2.02	0.42
6:F:157:MET:HG3	6:F:160:ASP:CB	2.50	0.42
6:F:425:LEU:O	6:F:502:VAL:HG23	2.20	0.42
8:H:47:LEU:HD11	11:K:61:THR:HB	2.02	0.42
21:6:263:TRP:O	21:6:263:TRP:CG	2.73	0.42
22:7:215:TYR:O	22:7:216:CYS:C	2.63	0.42
2:B:179:ALA:HB1	2:B:256:VAL:HA	2.01	0.41
2:B:220:ASN:OD1	2:B:221:THR:N	2.53	0.41
2:B:313:LEU:HD22	6:F:754:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:6:VAL:HG11	5:E:47:THR:HG21	2.01	0.41
6:F:138:MET:HB2	6:F:181:VAL:HG11	2.02	0.41
6:F:417:PRO:C	6:F:419:LYS:H	2.28	0.41
6:F:718:LEU:HD23	6:F:718:LEU:HA	1.85	0.41
8:H:138:ARG:CZ	8:H:142:TYR:HE1	2.33	0.41
18:3:205:ASP:OD1	18:3:206:THR:N	2.51	0.41
20:5:96:VAL:HB	20:5:209:GLU:HB2	2.02	0.41
23:8:149:LYS:HE2	23:8:165:ARG:HG2	2.02	0.41
25:0:137:VAL:HG12	25:0:137:VAL:O	2.20	0.41
2:B:75:LEU:HD23	2:B:75:LEU:HA	1.85	0.41
2:B:361:MET:HE2	2:B:405:LEU:HA	2.02	0.41
7:G:107:PHE:O	7:G:110:SER:OG	2.35	0.41
14:N:196:PRO:HG3	14:N:204:VAL:HG22	2.01	0.41
20:5:240:LEU:HD12	20:5:241:PRO:HD2	2.00	0.41
21:6:416:SER:C	21:6:418:GLU:H	2.27	0.41
2:B:218:LEU:O	2:B:224:TYR:HB3	2.20	0.41
6:F:353:ALA:HB2	23:8:123:LEU:HB3	2.01	0.41
12:L:157:PHE:O	12:L:159:ARG:HD2	2.20	0.41
20:5:235:SER:OG	20:5:236:GLU:N	2.53	0.41
21:6:336:GLU:HG2	21:6:448:ILE:HD12	2.01	0.41
22:7:288:ALA:HA	22:7:289:PRO:HD3	1.91	0.41
24:9:148:TRP:O	24:9:150:TYR:N	2.53	0.41
1:A:63:PRO:HB3	1:A:73:GLN:HG2	2.02	0.41
2:B:447:TYR:O	2:B:451:ILE:HG12	2.20	0.41
4:D:226:PRO:HG2	4:D:234:LEU:HD22	2.03	0.41
6:F:286:PHE:O	6:F:289:HIS:ND1	2.53	0.41
8:H:47:LEU:HD21	11:K:61:THR:HB	2.02	0.41
10:J:32:ILE:HG12	10:J:87:ILE:HD12	2.02	0.41
11:K:63:CYS:SG	11:K:100:THR:OG1	2.76	0.41
14:N:74:PRO:HB3	14:N:214:PHE:HD1	1.86	0.41
14:N:210:ASN:CG	14:N:211:TRP:H	2.27	0.41
20:5:79:TYR:HB2	20:5:94:ARG:HD2	2.02	0.41
21:6:325:ASP:CG	21:6:443:LEU:H	2.29	0.41
21:6:366:ILE:N	21:6:370:GLU:OE2	2.53	0.41
2:B:390:LYS:HD2	2:B:390:LYS:HA	1.90	0.41
4:D:388:LEU:HD11	6:F:198:MET:HB2	2.02	0.41
8:H:25:VAL:O	8:H:26:LEU:HD23	2.21	0.41
11:K:138:ASP:N	11:K:138:ASP:OD1	2.53	0.41
12:L:112:PRO:CB	12:L:148:TRP:HB2	2.51	0.41
4:D:29:ASN:ND2	4:D:33:ARG:HD3	2.35	0.41
19:4:128:ALA:N	19:4:239:CYS:SG	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:6:250:ALA:C	21:6:252:GLY:H	2.29	0.41
21:6:309:HIS:ND1	21:6:399:ALA:HB2	2.34	0.41
25:0:101:GLU:HG2	25:0:102:GLY:N	2.34	0.41
2:B:478:ASN:HB3	2:B:479:SER:H	1.61	0.41
4:D:288:ILE:HD12	4:D:422:MET:HG3	2.03	0.41
4:D:401:PHE:HE1	4:D:422:MET:SD	2.43	0.41
7:G:121:TYR:HD2	17:2:147:LEU:HD13	1.86	0.41
8:H:116:LEU:HD21	8:H:138:ARG:CZ	2.51	0.41
8:H:197:PRO:O	8:H:201:GLU:N	2.34	0.41
10:J:44:LEU:HD13	10:J:49:TYR:HD2	1.84	0.41
12:L:110:VAL:O	12:L:113:PRO:HD2	2.21	0.41
22:7:73:ARG:HG3	22:7:75:ASN:H	1.85	0.41
23:8:107:ILE:HD12	23:8:107:ILE:HA	1.88	0.41
1:A:68:PRO:HA	12:L:120:ARG:HH12	1.85	0.41
8:H:219:LEU:HD23	8:H:219:LEU:HA	1.96	0.41
8:H:221:GLY:O	8:H:225:ARG:HG3	2.21	0.41
9:I:141:ALA:HA	14:N:183:VAL:HG22	2.03	0.41
15:T:58:UNK:HA	15:T:95:UNK:CB	2.51	0.41
21:6:290:VAL:HG23	21:6:291:VAL:N	2.36	0.41
21:6:311:ILE:HG22	21:6:312:GLU:HG2	2.02	0.41
1:A:71:LEU:HD12	1:A:71:LEU:H	1.86	0.41
1:A:197:GLN:HE21	1:A:206:ASN:H	1.69	0.41
3:C:56:VAL:HG13	8:H:34:GLY:H	1.86	0.41
3:C:89:LEU:HD23	3:C:89:LEU:HA	1.96	0.41
4:D:65:LYS:HB3	4:D:65:LYS:HE2	1.85	0.41
4:D:174:GLY:HA3	4:D:223:VAL:HG11	2.03	0.41
4:D:282:ILE:HD13	4:D:418:ILE:HD11	2.03	0.41
6:F:160:ASP:OD1	6:F:161:GLU:N	2.46	0.41
6:F:417:PRO:HD2	25:0:93:TYR:CD2	2.55	0.41
8:H:84:ASN:HA	8:H:88:PHE:HB3	2.02	0.41
8:H:101:ILE:O	8:H:105:MET:HG3	2.20	0.41
10:J:137:SER:OG	13:M:161:GLU:HB2	2.20	0.41
11:K:105:MET:O	11:K:109:LEU:HB2	2.21	0.41
11:K:117:PRO:O	11:K:120:LYS:HG2	2.21	0.41
12:L:149:ALA:C	12:L:151:PHE:N	2.78	0.41
16:1:185:ALA:HA	16:1:201:VAL:O	2.21	0.41
20:5:114:LEU:HD22	20:5:121:PHE:O	2.21	0.41
22:7:55:THR:C	22:7:57:ALA:H	2.28	0.41
22:7:109:VAL:HG12	22:7:231:ALA:O	2.20	0.41
22:7:186:PRO:HG3	22:7:346:PRO:HD3	2.03	0.41
22:7:229:THR:O	22:7:231:ALA:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:GLU:HA	16:1:96:ARG:HH11	1.85	0.41
6:F:428:GLY:C	6:F:429:LEU:HD12	2.46	0.41
8:H:225:ARG:NH2	8:H:267:GLU:OE2	2.53	0.41
18:3:155:TYR:CZ	18:3:159:LYS:HG3	2.56	0.41
21:6:192:LYS:HB2	21:6:192:LYS:HE2	1.88	0.41
21:6:416:SER:O	21:6:418:GLU:N	2.54	0.41
22:7:103:GLY:H	22:7:107:GLY:HA2	1.86	0.41
6:F:306:ILE:HG13	6:F:307:HIS:ND1	2.37	0.40
7:G:8:HIS:CD2	7:G:52:LEU:HD11	2.56	0.40
8:H:129:THR:N	8:H:130:PRO:HD3	2.36	0.40
9:I:114:CYS:SG	9:I:118:CYS:HB3	2.61	0.40
11:K:25:GLU:HG3	13:M:185:LYS:CB	2.50	0.40
16:1:189:ILE:HG12	16:1:198:THR:HG22	2.03	0.40
21:6:228:ASN:HA	21:6:232:ALA:HB2	2.03	0.40
22:7:201:LYS:C	22:7:203:ARG:H	2.29	0.40
2:B:332:ILE:C	2:B:334:TYR:H	2.28	0.40
4:D:348:LEU:HD13	4:D:378:PHE:HA	2.03	0.40
6:F:152:TYR:CD1	6:F:400:LEU:HD22	2.56	0.40
6:F:305:LEU:HD12	6:F:305:LEU:HA	1.93	0.40
8:H:269:SER:O	8:H:273:LYS:HG2	2.20	0.40
10:J:10:LEU:HA	10:J:13:HIS:CD2	2.53	0.40
14:N:219:LEU:O	14:N:223:SER:N	2.53	0.40
17:2:149:SER:O	17:2:153:ASP:N	2.54	0.40
18:3:135:PHE:HE1	24:9:84:ASN:HB3	1.85	0.40
21:6:172:TYR:CD2	21:6:173:ASP:HB3	2.56	0.40
21:6:319:MET:HE2	21:6:319:MET:HB2	2.01	0.40
22:7:215:TYR:HA	22:7:273:TYR:HA	2.02	0.40
1:A:261:LEU:O	1:A:265:VAL:HG13	2.22	0.40
6:F:364:SER:HB2	6:F:487:TYR:HE1	1.85	0.40
14:N:99:SER:HA	14:N:154:TYR:HB3	2.02	0.40
21:6:319:MET:C	21:6:321:SER:H	2.29	0.40
22:7:78:LEU:HD21	22:7:110:ARG:HG3	2.03	0.40
22:7:158:SER:OG	22:7:159:LYS:N	2.54	0.40
2:B:244:LEU:HD12	2:B:246:PRO:HD3	2.03	0.40
2:B:502:LEU:HD23	2:B:502:LEU:HA	1.88	0.40
4:D:76:PHE:HE1	4:D:136:LEU:HB2	1.87	0.40
8:H:74:ALA:HB1	8:H:77:PHE:CD2	2.56	0.40
8:H:128:GLN:HG2	8:H:129:THR:N	2.37	0.40
10:J:45:TYR:HA	10:J:49:TYR:H	1.87	0.40
22:7:70:LEU:HD23	22:7:168:LEU:HD22	2.03	0.40
22:7:109:VAL:HB	22:7:232:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:7:311:GLU:N	22:7:336:ALA:O	2.35	0.40
24:9:144:GLY:O	24:9:148:TRP:N	2.54	0.40
2:B:324:LEU:HD23	2:B:324:LEU:HA	1.88	0.40
4:D:261:LEU:O	4:D:265:ASN:HB2	2.20	0.40
6:F:149:VAL:HG11	6:F:305:LEU:HD22	2.03	0.40
8:H:337:LEU:HA	8:H:355:ARG:O	2.22	0.40
8:H:361:ASN:O	8:H:364:ILE:HG22	2.21	0.40
12:L:96:ILE:O	12:L:99:PRO:HD2	2.22	0.40
12:L:97:LEU:HB3	12:L:98:PRO:HD3	2.04	0.40
12:L:119:MET:HA	12:L:119:MET:HE2	2.03	0.40
14:N:73:TYR:HB3	14:N:210:ASN:HB3	2.04	0.40
15:T:95:UNK:O	15:T:96:UNK:C	2.68	0.40
16:1:117:VAL:HA	16:1:200:ILE:O	2.22	0.40
16:1:173:GLU:HB2	16:1:186:PHE:CE1	2.57	0.40
17:2:132:MET:HE1	17:2:140:TYR:CD2	2.57	0.40
22:7:207:VAL:HG13	22:7:293:THR:O	2.21	0.40
24:9:113:THR:HG22	25:0:141:MET:HE1	2.03	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	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	36	65
2	B	474/483 (98%)	424 (90%)	50 (10%)	0	100	100
3	C	114/117 (97%)	96 (84%)	15 (13%)	3 (3%)	4	28
4	D	497/499 (100%)	450 (90%)	46 (9%)	1 (0%)	43	72
5	E	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
6	F	665/777 (86%)	598 (90%)	65 (10%)	2 (0%)	36	65
7	G	174/176 (99%)	148 (85%)	26 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	381/383 (100%)	339 (89%)	42 (11%)	0	100	100
9	I	163/165 (99%)	123 (76%)	40 (24%)	0	100	100
10	J	157/159 (99%)	141 (90%)	16 (10%)	0	100	100
11	K	192/245 (78%)	174 (91%)	17 (9%)	1 (0%)	24	56
12	L	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	8	36
13	M	110/213 (52%)	92 (84%)	18 (16%)	0	100	100
14	N	139/233 (60%)	116 (84%)	20 (14%)	3 (2%)	5	31
16	1	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	18	50
17	2	127/216 (59%)	106 (84%)	21 (16%)	0	100	100
18	3	132/227 (58%)	116 (88%)	16 (12%)	0	100	100
19	4	128/130 (98%)	102 (80%)	26 (20%)	0	100	100
20	5	170/243 (70%)	156 (92%)	13 (8%)	1 (1%)	21	52
21	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	21	52
22	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	36	65
23	8	117/119 (98%)	79 (68%)	33 (28%)	5 (4%)	2	19
24	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	9	38
25	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	18	50
All	All	5280/6245 (84%)	4465 (85%)	791 (15%)	24 (0%)	26	56

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	LYS
3	C	49	GLU
21	6	275	PRO
23	8	124	LEU
3	C	48	ILE
6	F	707	TYR
24	9	149	TYR
4	D	498	TYR
14	N	158	VAL
16	1	96	ARG
3	C	44	TYR
11	K	63	CYS
23	8	90	THR
23	8	125	ASN

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Mol	Chain	Res	Type
25	0	213	THR
20	5	87	PRO
22	7	289	PRO
21	6	267	PRO
23	8	122	LEU
12	L	150	PRO
6	F	263	ILE
14	N	125	PRO
23	8	91	PRO
14	N	126	VAL

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	271/301 (90%)	271 (100%)	0	100	100
2	B	397/419 (95%)	397 (100%)	0	100	100
3	C	71/100 (71%)	71 (100%)	0	100	100
4	D	399/427 (93%)	399 (100%)	0	100	100
5	E	78/88 (89%)	78 (100%)	0	100	100
6	F	513/674 (76%)	513 (100%)	0	100	100
7	G	119/154 (77%)	119 (100%)	0	100	100
8	H	298/336 (89%)	297 (100%)	1 (0%)	86	83
9	I	123/155 (79%)	123 (100%)	0	100	100
10	J	126/141 (89%)	126 (100%)	0	100	100
11	K	162/226 (72%)	162 (100%)	0	100	100
12	L	55/167 (33%)	55 (100%)	0	100	100
13	M	86/184 (47%)	86 (100%)	0	100	100
14	N	115/192 (60%)	115 (100%)	0	100	100
16	1	116/132 (88%)	116 (100%)	0	100	100
17	2	74/181 (41%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	3	92/183 (50%)	92 (100%)	0	100	100
19	4	80/102 (78%)	80 (100%)	0	100	100
20	5	135/191 (71%)	135 (100%)	0	100	100
21	6	250/389 (64%)	250 (100%)	0	100	100
22	7	233/279 (84%)	233 (100%)	0	100	100
23	8	69/102 (68%)	69 (100%)	0	100	100
24	9	55/70 (79%)	54 (98%)	1 (2%)	51	67
25	0	93/137 (68%)	93 (100%)	0	100	100
All	All	4010/5330 (75%)	4008 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	362	LEU
24	9	106	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	120	HIS
1	A	197	GLN
1	A	262	ASN
1	A	294	ASN
1	A	358	GLN
2	B	92	GLN
2	B	147	ASN
2	B	317	GLN
2	B	362	ASN
4	D	26	HIS
4	D	29	ASN
4	D	265	ASN
6	F	174	ASN
6	F	391	HIS
6	F	465	ASN
6	F	503	HIS
6	F	646	ASN
6	F	679	ASN

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Mol	Chain	Res	Type
7	G	71	ASN
8	H	14	ASN
8	H	19	HIS
8	H	48	HIS
8	H	367	GLN
9	I	14	GLN
10	J	13	HIS
10	J	50	ASN
10	J	95	ASN
11	K	91	GLN
13	M	145	ASN
13	M	148	GLN
13	M	194	ASN
14	N	143	HIS
14	N	182	GLN
16	1	113	GLN
16	1	141	ASN
20	5	138	GLN
20	5	206	GLN
21	6	381	GLN
22	7	252	GLN
22	7	297	GLN
23	8	184	GLN
24	9	147	HIS
25	0	97	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 ligands 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$
27	BCR	F	801	-	40,40,41	0.77	0	54,54,56	2.99	21 (38%)
26	LHG	D	601	-	23,23,48	1.32	2 (8%)	26,28,54	1.32	3 (11%)
29	SF4	8	201	23	0,12,12	-	-	-	-	-
28	SQD	F	802	-	53,54,54	1.18	4 (7%)	62,65,65	1.04	4 (6%)
28	SQD	F	803	-	45,46,54	1.28	4 (8%)	54,57,65	1.15	7 (12%)

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
27	BCR	F	801	-	-	10/27/61/63	0/2/2/2
26	LHG	D	601	-	-	3/27/27/53	-
29	SF4	8	201	23	-	-	0/6/5/5
28	SQD	F	802	-	-	9/49/69/69	0/1/1/1
28	SQD	F	803	-	-	9/41/61/69	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	802	SQD	O8-S	4.60	1.63	1.47
28	F	803	SQD	O8-S	4.59	1.63	1.47
28	F	803	SQD	O47-C7	4.28	1.46	1.34
28	F	802	SQD	O48-C23	4.24	1.45	1.33
28	F	803	SQD	O48-C23	4.24	1.45	1.33
26	D	601	LHG	O8-C23	4.14	1.45	1.33
26	D	601	LHG	O7-C7	4.12	1.45	1.34
28	F	802	SQD	O47-C7	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	803	SQD	C6-S	-2.96	1.66	1.77
28	F	802	SQD	C6-S	-2.92	1.66	1.77

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	801	BCR	C11-C10-C9	-10.58	112.21	127.31
27	F	801	BCR	C7-C8-C9	-8.72	113.06	126.23
27	F	801	BCR	C24-C23-C22	-5.98	117.20	126.23
27	F	801	BCR	C13-C12-C11	-5.67	112.19	124.81
27	F	801	BCR	C15-C16-C17	-5.01	113.22	123.47
27	F	801	BCR	C20-C21-C22	-4.94	120.25	127.31
27	F	801	BCR	C15-C14-C13	-4.78	114.18	124.81
26	D	601	LHG	O7-C7-C8	4.16	120.46	111.50
27	F	801	BCR	C8-C9-C10	3.93	124.97	118.94
27	F	801	BCR	C3-C4-C5	-3.78	107.33	114.08
28	F	803	SQD	O47-C7-C8	3.72	119.52	111.50
27	F	801	BCR	C34-C9-C10	-3.53	117.97	122.92
28	F	802	SQD	O47-C7-C8	3.40	118.82	111.50
27	F	801	BCR	C33-C5-C4	3.35	120.06	113.62
27	F	801	BCR	C38-C26-C27	3.26	119.88	113.62
27	F	801	BCR	C28-C27-C26	-3.17	108.42	114.08
27	F	801	BCR	C27-C26-C25	-3.07	118.27	122.73
27	F	801	BCR	C4-C5-C6	-3.04	118.31	122.73
28	F	803	SQD	O48-C23-C24	2.89	120.99	111.91
27	F	801	BCR	C12-C11-C10	2.85	129.30	123.47
27	F	801	BCR	C30-C25-C26	-2.73	118.77	122.61
26	D	601	LHG	C5-O7-C7	-2.64	111.30	117.79
28	F	802	SQD	O48-C23-C24	2.60	120.08	111.91
27	F	801	BCR	C33-C5-C6	-2.58	121.63	124.53
28	F	802	SQD	O8-S-C6	2.50	109.72	105.74
27	F	801	BCR	C38-C26-C25	-2.38	121.86	124.53
28	F	803	SQD	O7-S-C6	2.32	109.69	106.94
28	F	802	SQD	O9-S-C6	2.28	109.65	106.94
27	F	801	BCR	C36-C18-C19	2.25	121.63	118.08
28	F	803	SQD	O9-S-C6	2.17	109.52	106.94
26	D	601	LHG	O8-C23-C24	2.12	118.56	111.91
28	F	803	SQD	O8-S-C6	2.11	109.10	105.74
28	F	803	SQD	O48-C23-O10	-2.08	118.34	123.59
27	F	801	BCR	C37-C22-C21	-2.08	120.01	122.92
28	F	803	SQD	C9-C8-C7	-2.01	106.29	113.62

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	F	801	BCR	C37-C22-C23-C24
28	F	802	SQD	O5-C1-O6-C44
28	F	803	SQD	C2-C1-O6-C44
28	F	803	SQD	O5-C1-O6-C44
27	F	801	BCR	C21-C22-C23-C24
27	F	801	BCR	C1-C6-C7-C8
27	F	801	BCR	C5-C6-C7-C8
28	F	802	SQD	C28-C29-C30-C31
28	F	803	SQD	O49-C7-O47-C45
28	F	803	SQD	C8-C7-O47-C45
28	F	802	SQD	C7-C8-C9-C10
28	F	803	SQD	C44-C45-O47-C7
28	F	803	SQD	O47-C45-C46-O48
27	F	801	BCR	C36-C18-C19-C20
28	F	802	SQD	C8-C7-O47-C45
28	F	803	SQD	C44-C45-C46-O48
28	F	802	SQD	O47-C7-C8-C9
27	F	801	BCR	C23-C24-C25-C26
27	F	801	BCR	C23-C24-C25-C30
27	F	801	BCR	C17-C18-C19-C20
28	F	802	SQD	O49-C7-O47-C45
28	F	803	SQD	O6-C44-C45-O47
26	D	601	LHG	C4-O6-P-O3
27	F	801	BCR	C19-C20-C21-C22
28	F	802	SQD	O49-C7-C8-C9
27	F	801	BCR	C15-C16-C17-C18
28	F	802	SQD	C29-C30-C31-C32
26	D	601	LHG	C7-C8-C9-C10
28	F	803	SQD	C7-C8-C9-C10
26	D	601	LHG	C4-O6-P-O5
28	F	802	SQD	C11-C10-C9-C8

There are no ring outliers.

5 monomers are involved in 13 short contacts:

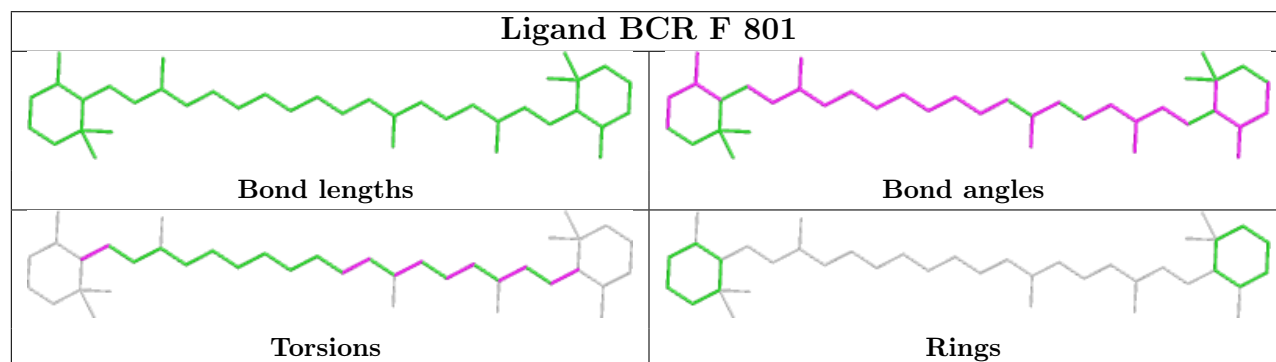
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	F	801	BCR	6	0
26	D	601	LHG	1	0
29	8	201	SF4	1	0
28	F	802	SQD	1	0

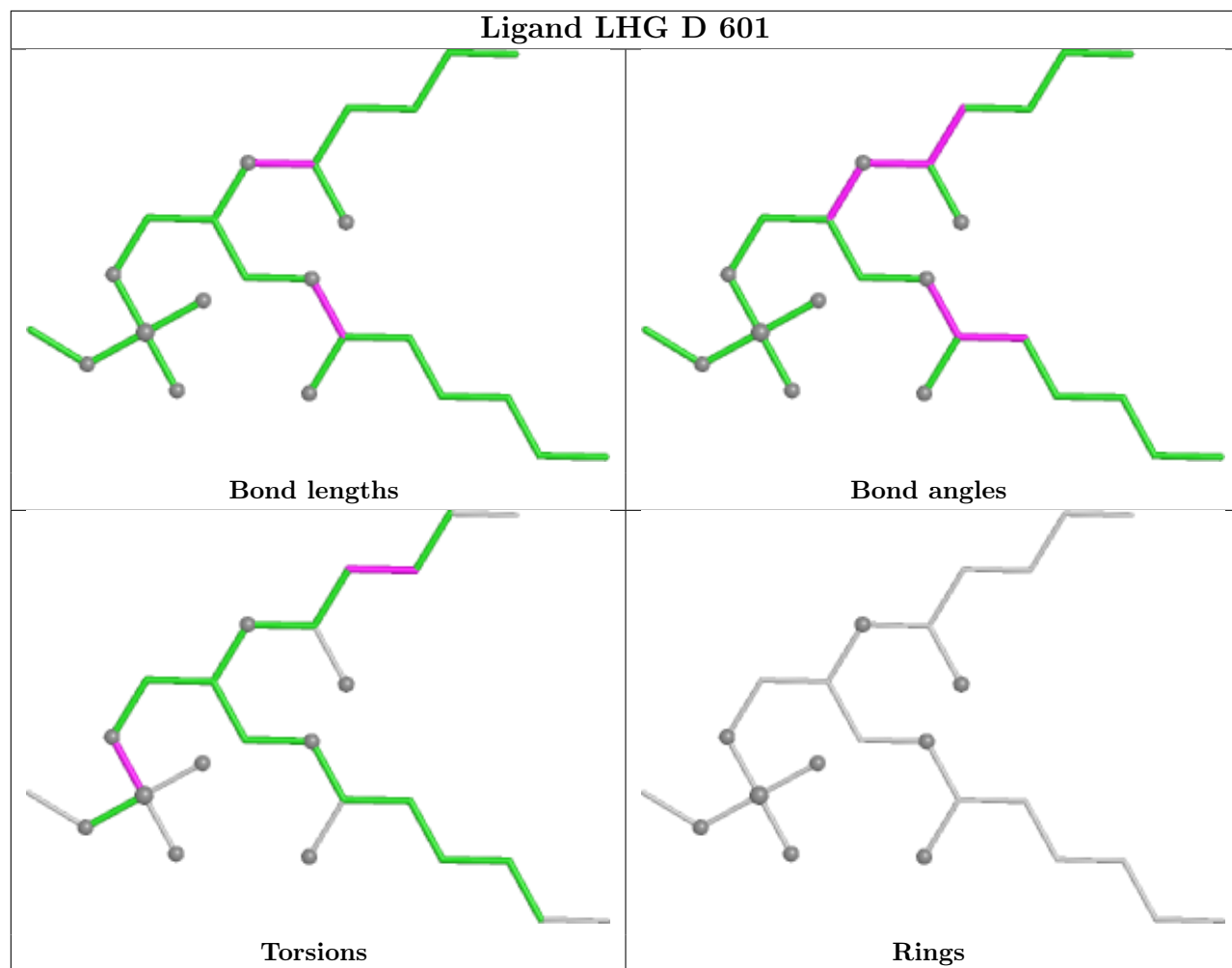
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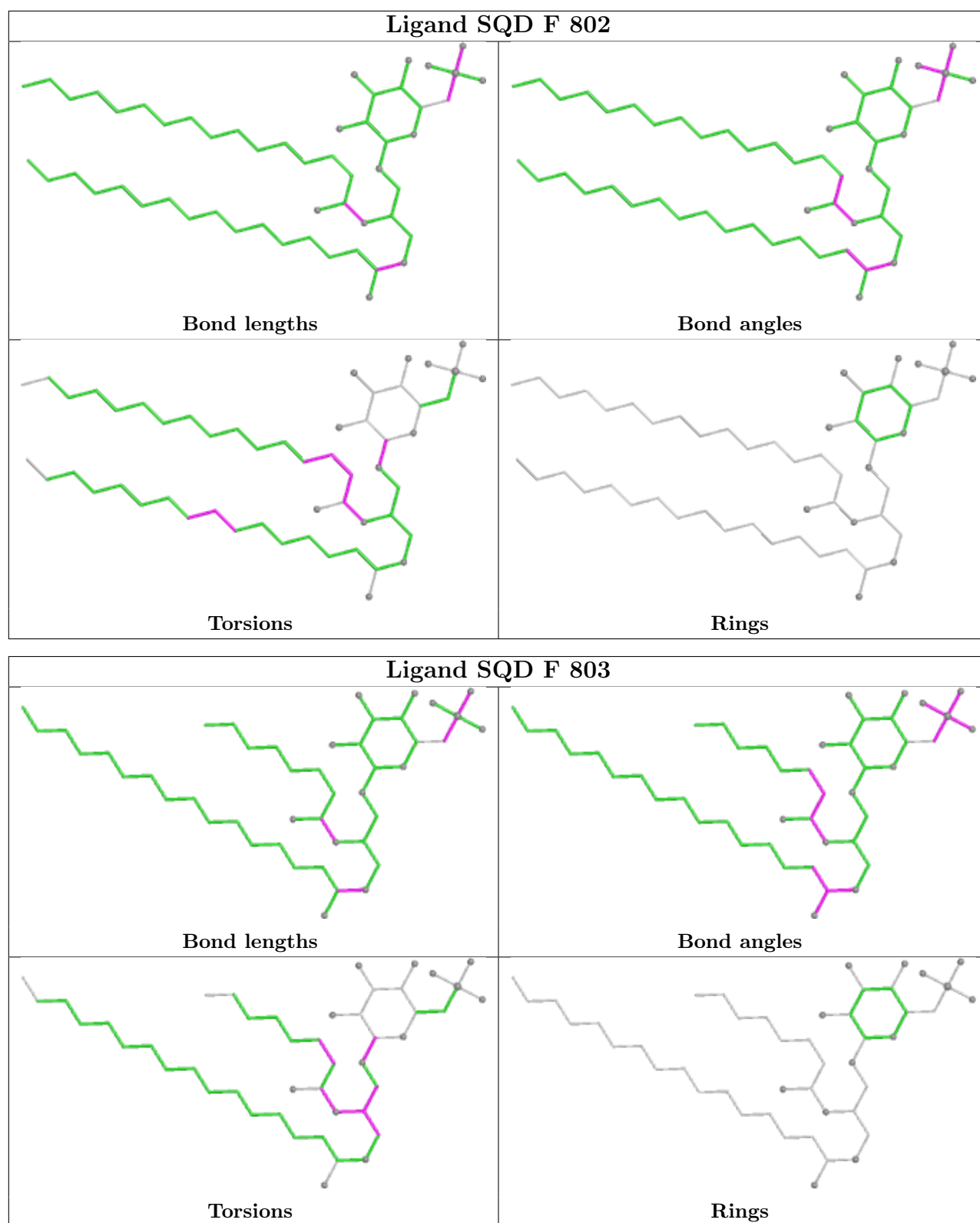
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	803	SQD	5	0

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

There are no chain breaks in this entry.

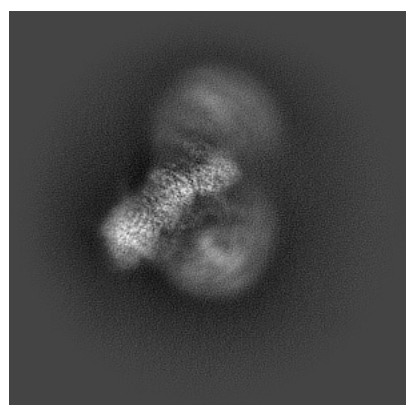
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31307. These allow visual inspection of the internal detail of the map and identification of artifacts.

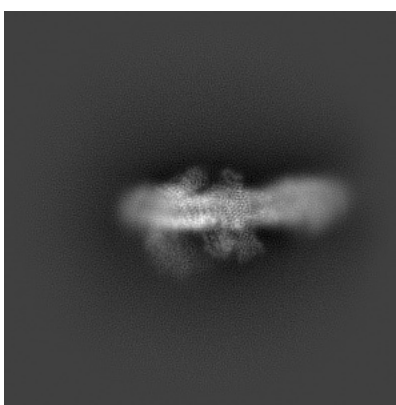
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

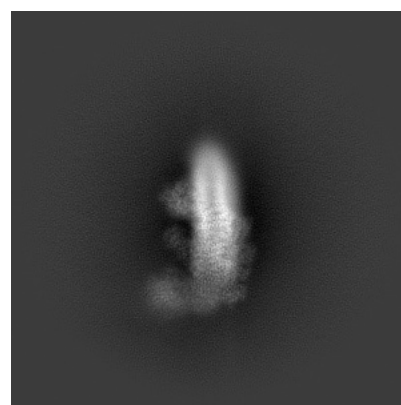
6.1.1 Primary map



X



Y

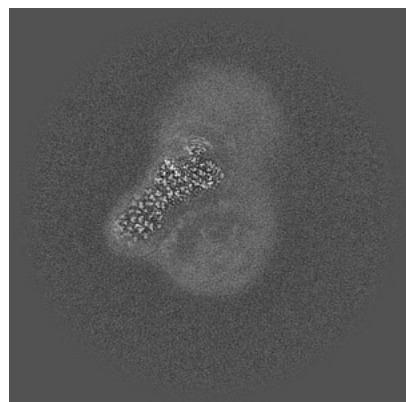


Z

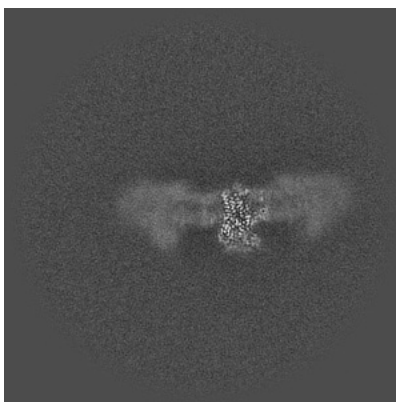
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

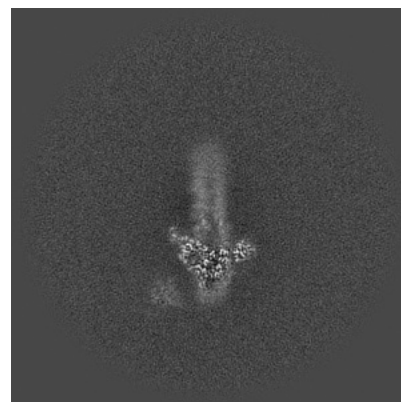
6.2.1 Primary map



X Index: 220



Y Index: 220

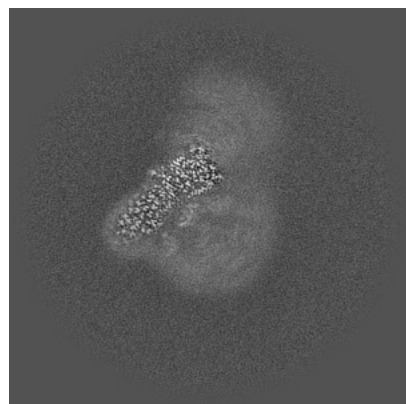


Z Index: 220

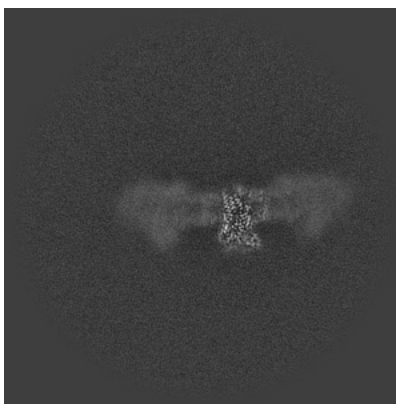
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

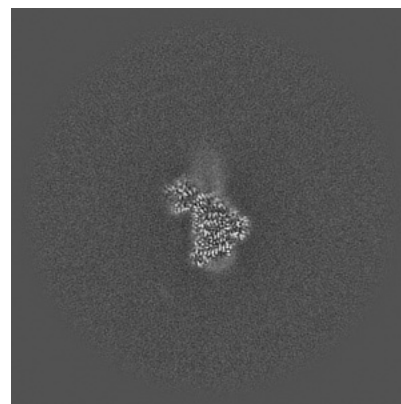
6.3.1 Primary map



X Index: 213



Y Index: 221

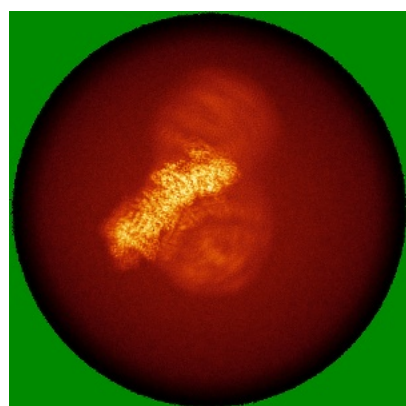


Z Index: 255

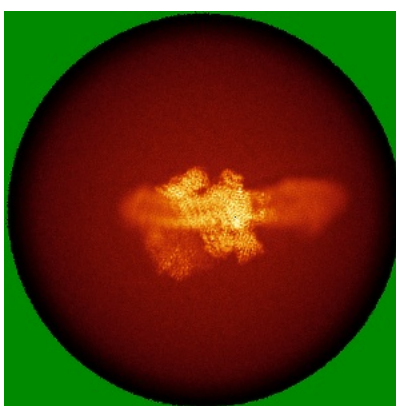
The images above show the largest variance slices of the map in three orthogonal directions.

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

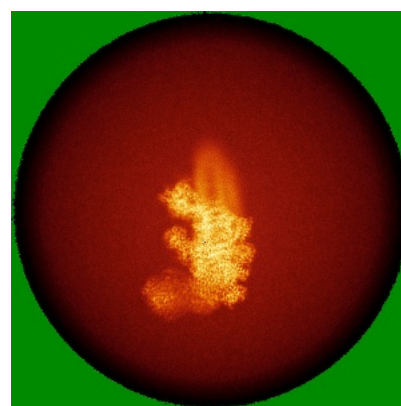
6.4.1 Primary map



X



Y

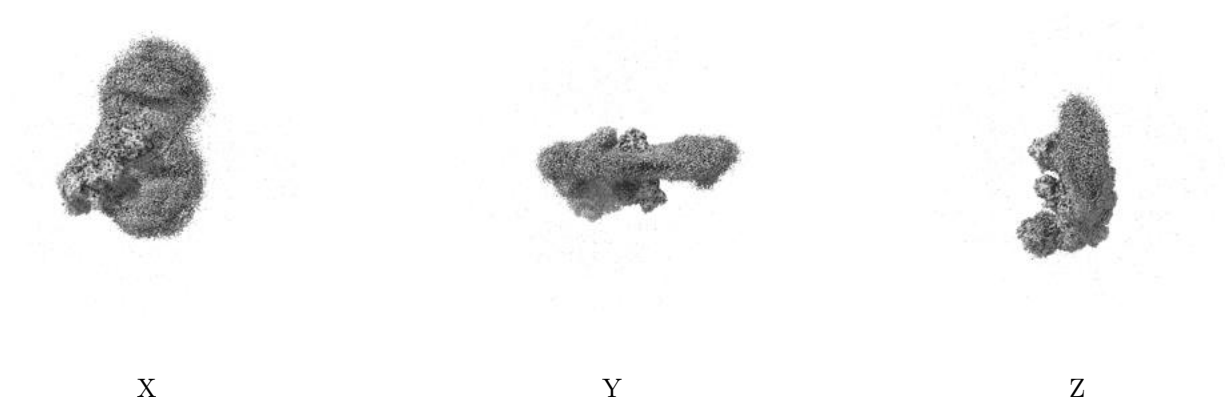


Z

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 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

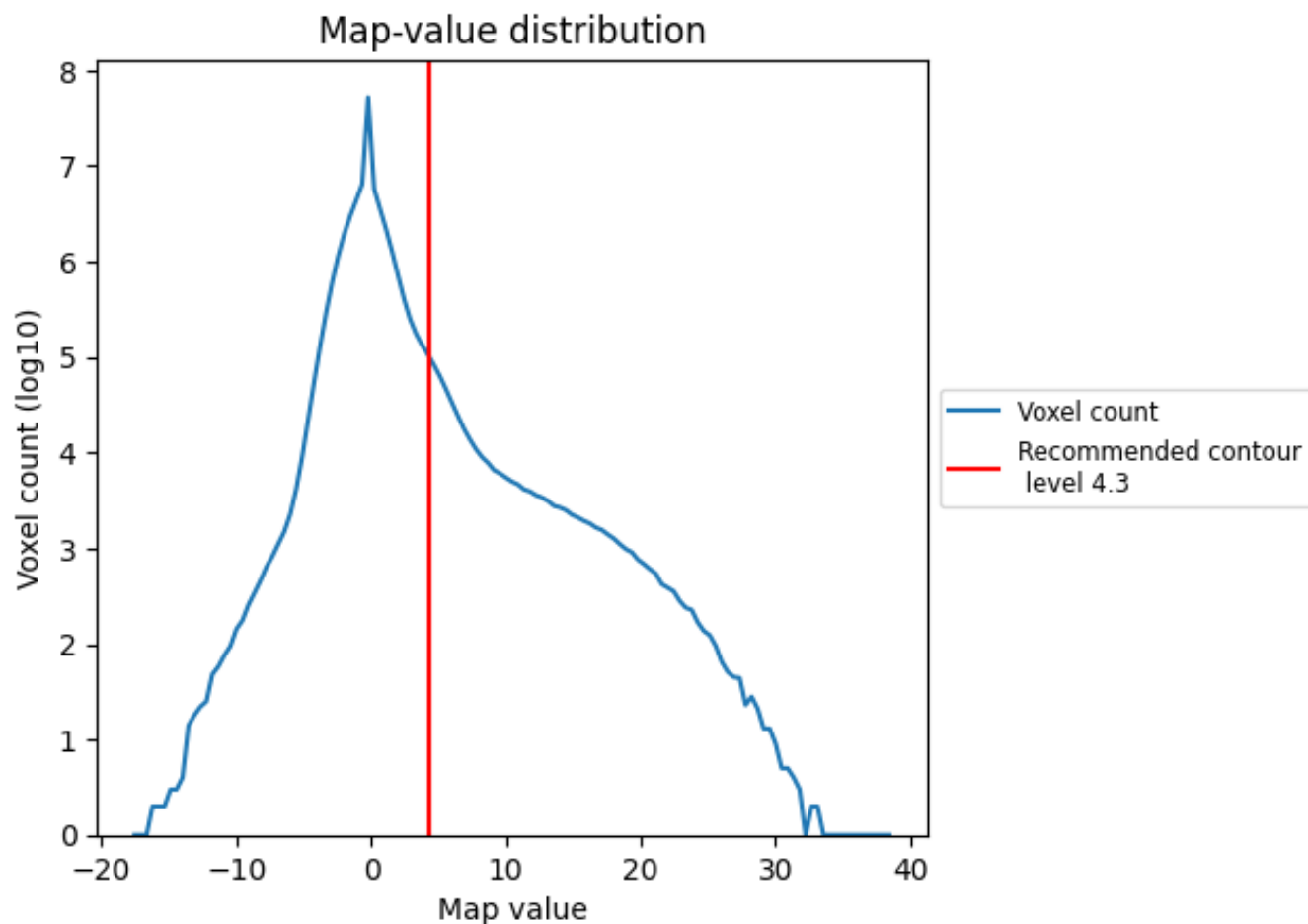
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

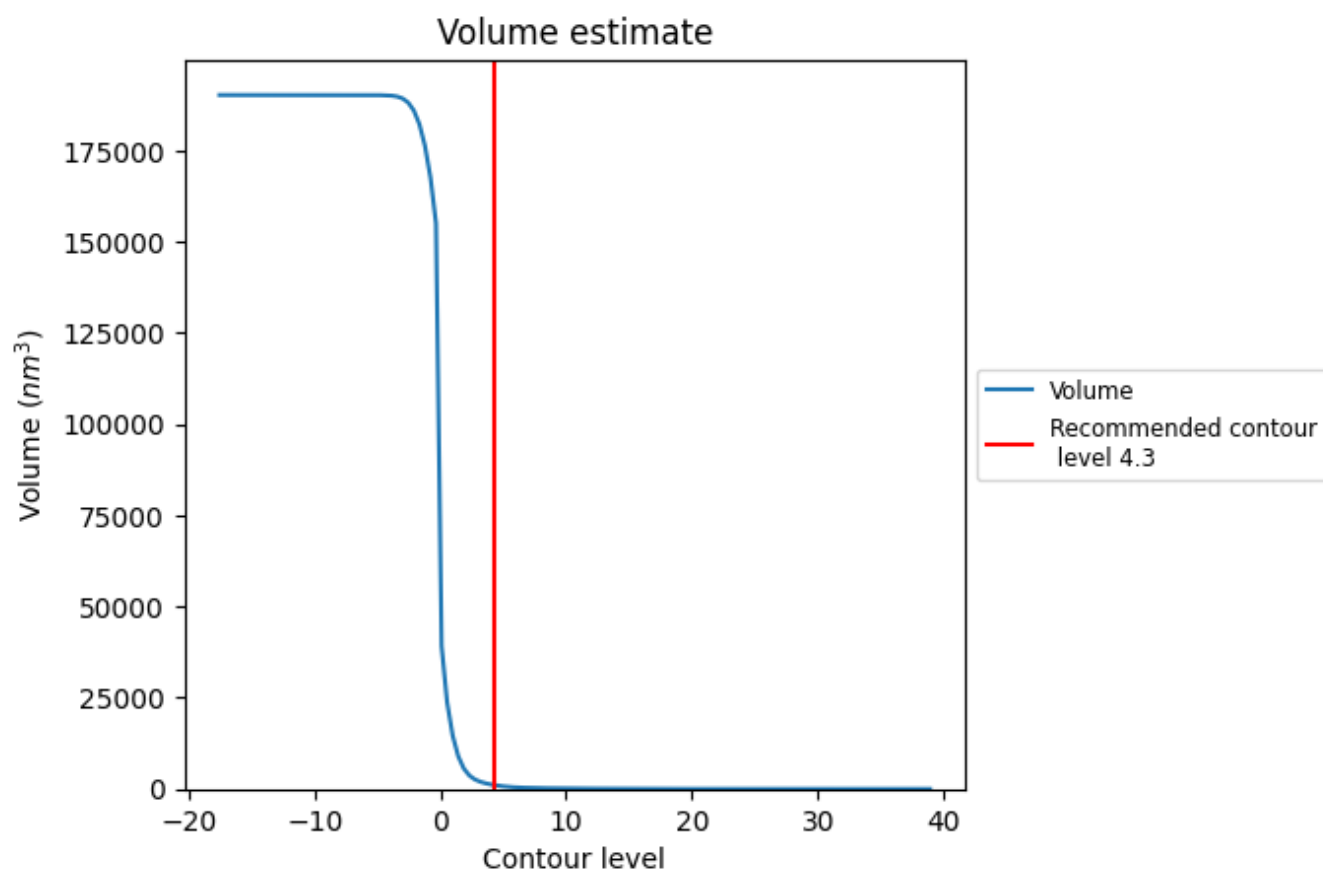
This section contains the results of statistical analysis of the map.

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.

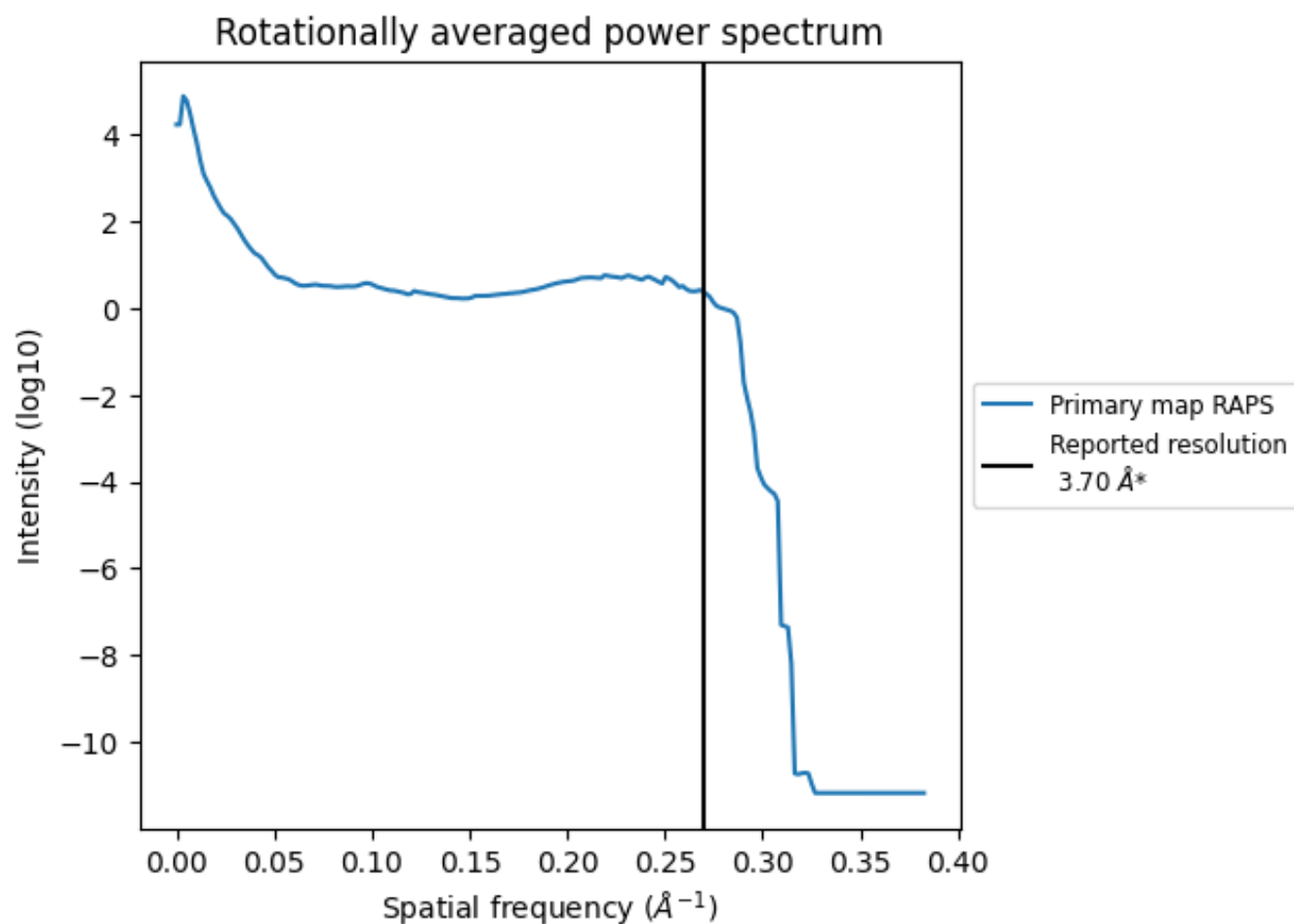
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1068 nm^3 ; this corresponds to an approximate mass of 965 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

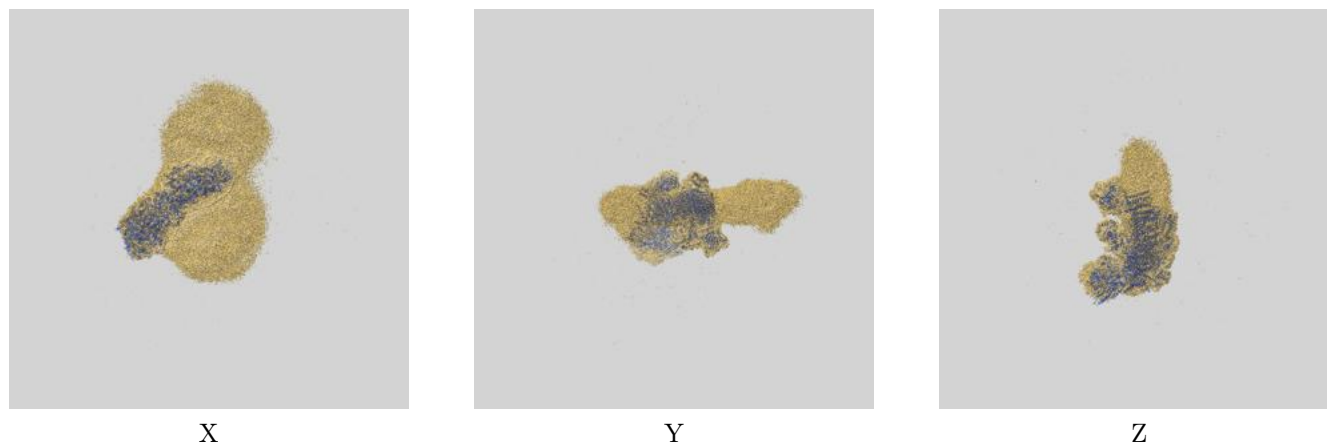
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

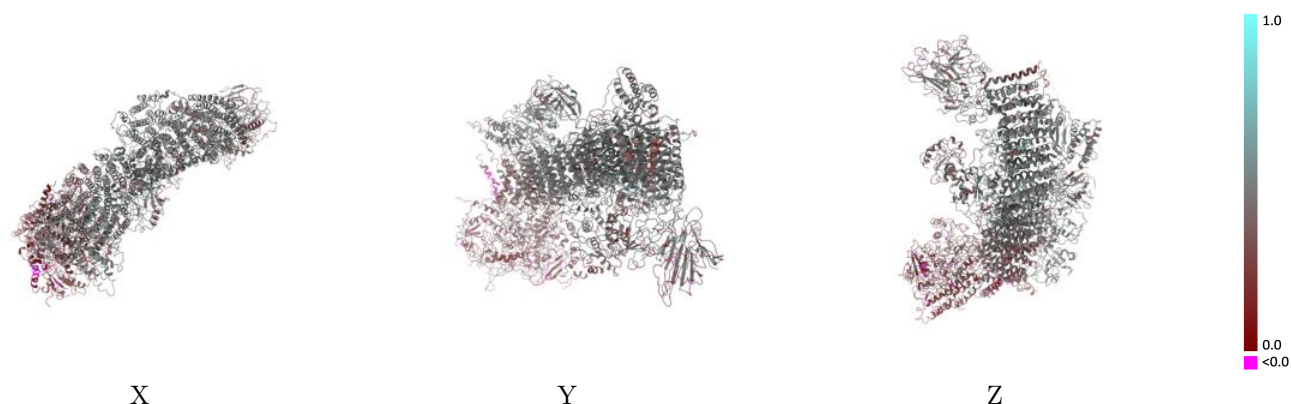
This section contains information regarding the fit between EMDB map EMD-31307 and PDB model 7EU3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



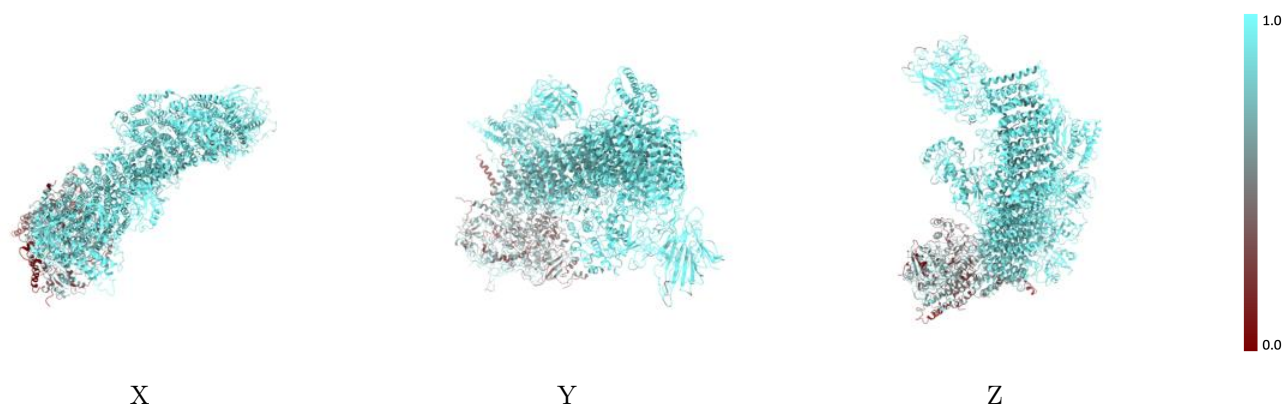
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



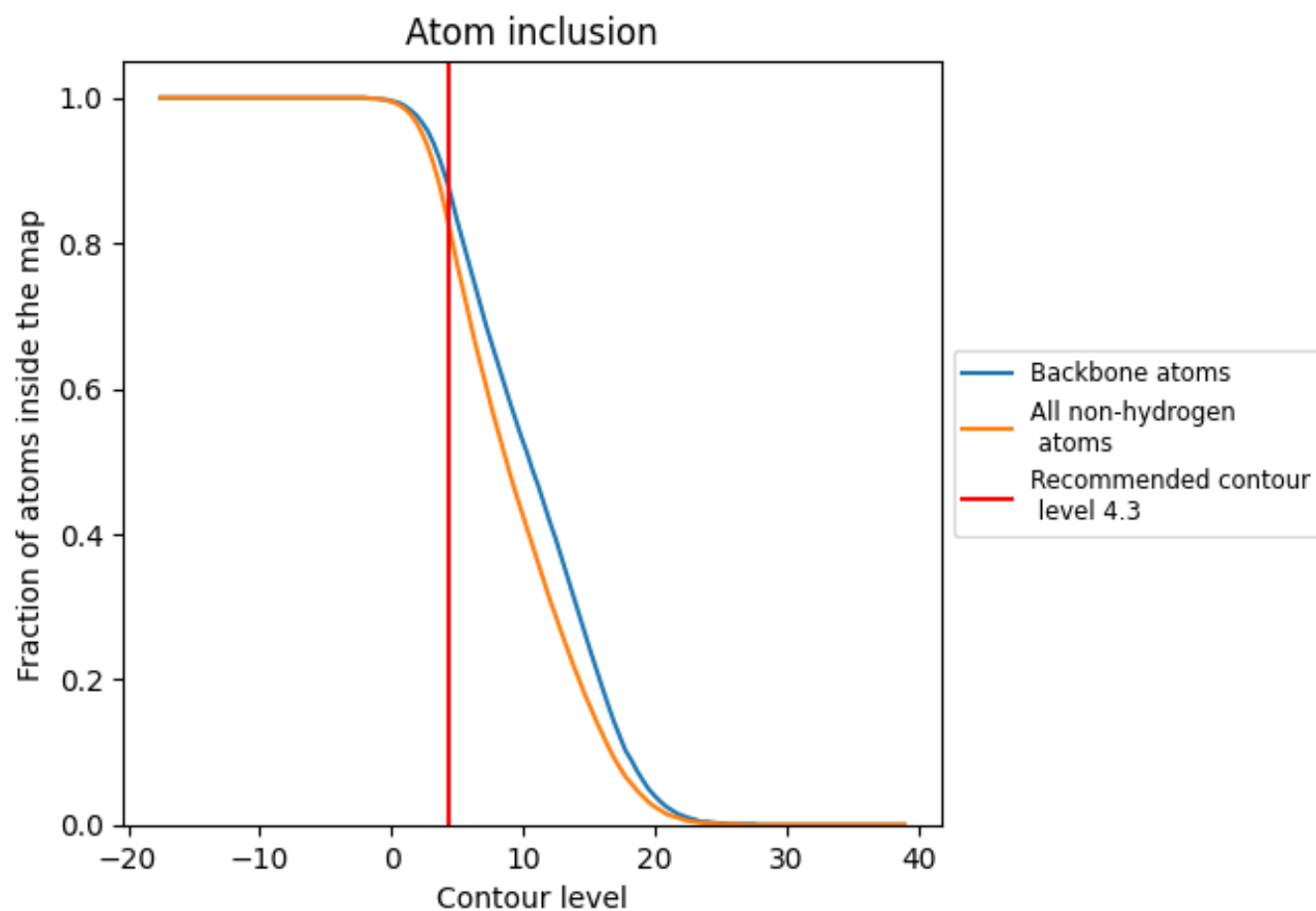
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 83% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8280	 0.4020
0	 0.9490	 0.4610
1	 0.9560	 0.4310
2	 0.9720	 0.4580
3	 0.9740	 0.4660
4	 0.9690	 0.4720
5	 0.9570	 0.4750
6	 0.9330	 0.4230
7	 0.9130	 0.4070
8	 0.9440	 0.4470
9	 0.9540	 0.4480
A	 0.7930	 0.3470
B	 0.9260	 0.4570
C	 0.8420	 0.3870
D	 0.9520	 0.4890
E	 0.9220	 0.4800
F	 0.9390	 0.4660
G	 0.9010	 0.4400
H	 0.4880	 0.2680
I	 0.5670	 0.2970
J	 0.4790	 0.2510
K	 0.5460	 0.2970
L	 0.3140	 0.0790
M	 0.4850	 0.2800
N	 0.5940	 0.2650
T	 0.9250	 0.4040

