



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 06:45 PM JST

PDB ID : 7EU3
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:

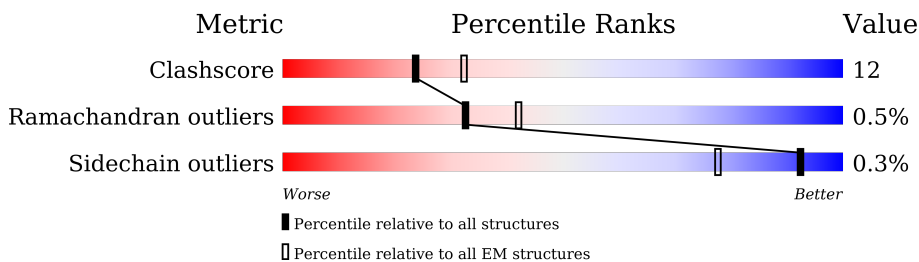
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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)
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	346	
2	B	483	
3	C	117	
4	D	499	
5	E	100	
6	F	777	
7	G	176	
8	H	383	

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Mol	Chain	Length	Quality of chain
9	I	165	30% 78% 22%
10	J	159	45% 63% 37%
11	K	245	25% 52% 27% 21%
12	L	192	23% 17% 18% 64%
13	M	213	19% 38% 15% 47%
14	N	233	17% 42% 20% 38%
15	T	61	93% 7%
16	1	154	69% 28% 2%
17	2	216	52% 8% 40%
18	3	227	46% 13% 41%
19	4	130	78% 22%
20	5	243	56% 14% 29%
21	6	469	51% 22% 27%
22	7	361	56% 30% 12%
23	8	119	71% 26% 3%
24	9	83	71% 28% 1%
25	0	155	85% 11% 4%

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
			Total	C	N	O	S		
1	A	346	2608	1744	393	463	8	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 15 is a protein called Unidentified stromal protein.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

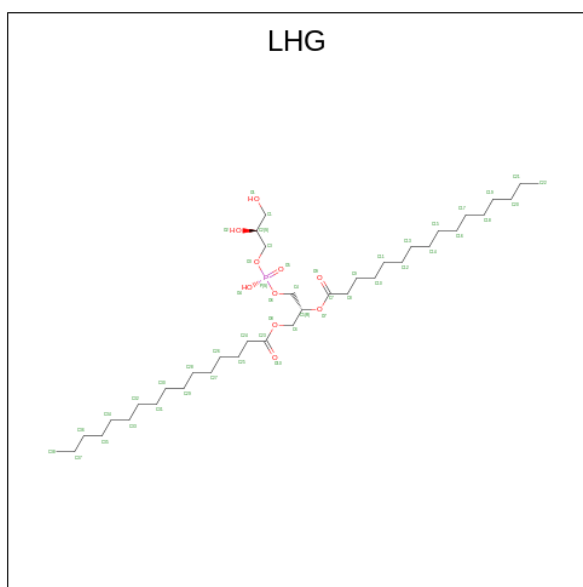
- Molecule 24 is a protein called Photosynthetic NDH subunit of subcomplex B4.

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

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

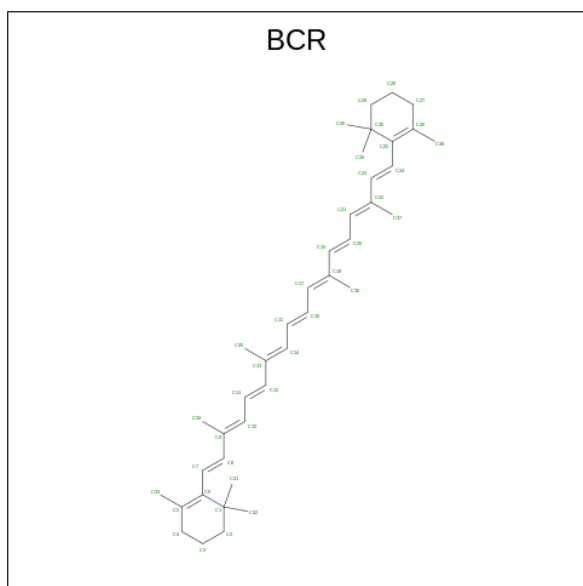
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	149	1089	704	175	204	6	0	0

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



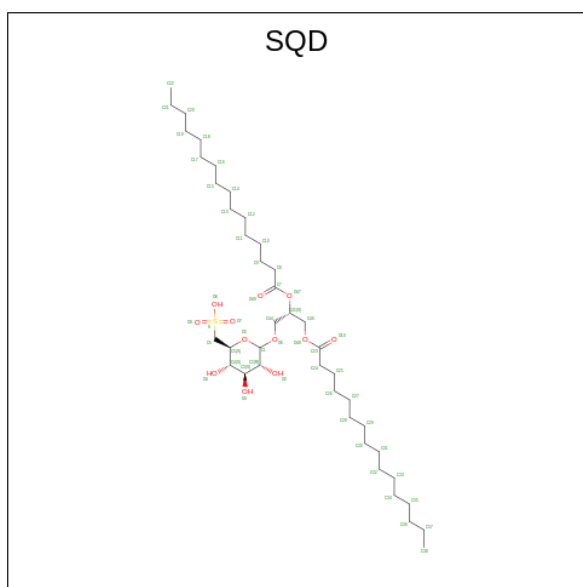
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
26	D	1	24	15	8	1	0

- Molecule 27 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



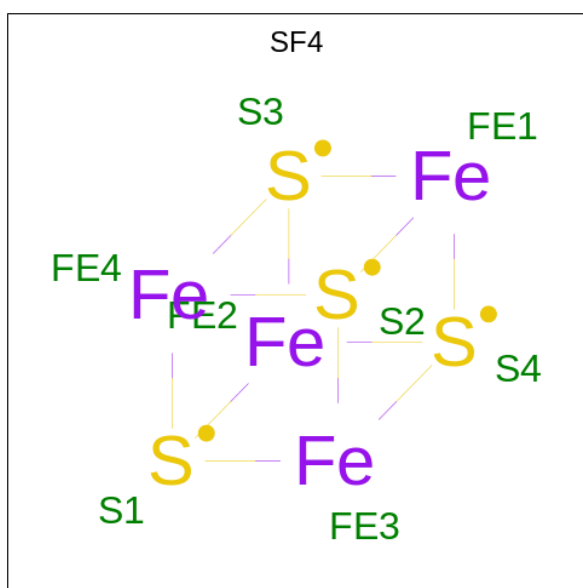
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
27	F	1	39	39	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		S
28	F	1	100	74	24	2	0
28	F	1	100	74	24	2	0

- Molecule 29 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

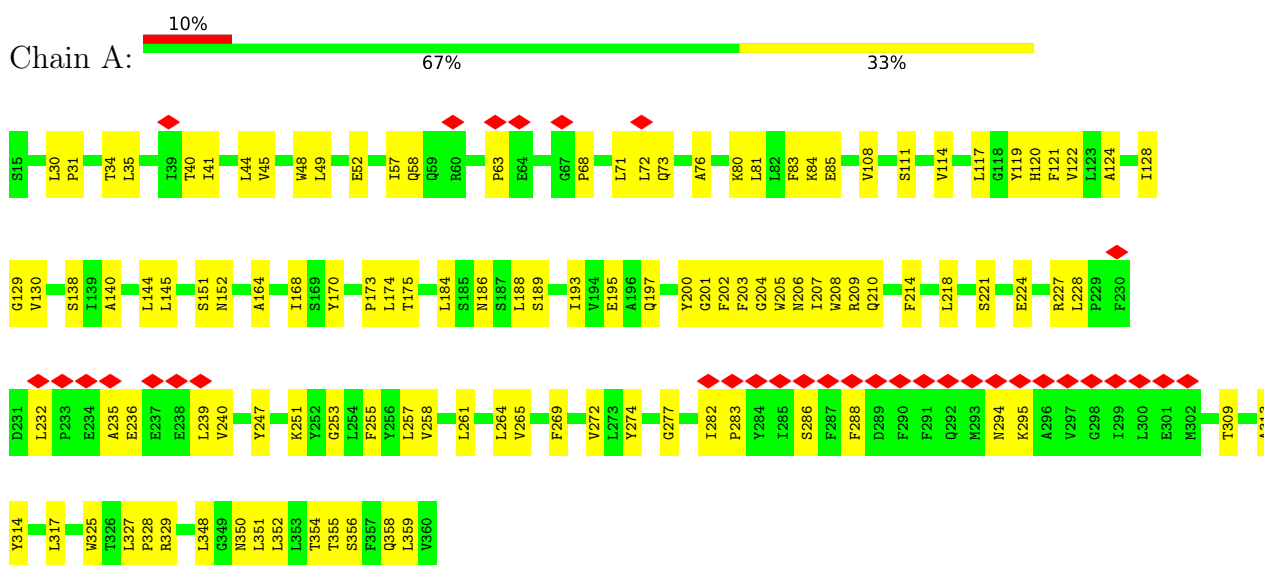


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
29	8	1	8	4	4	0

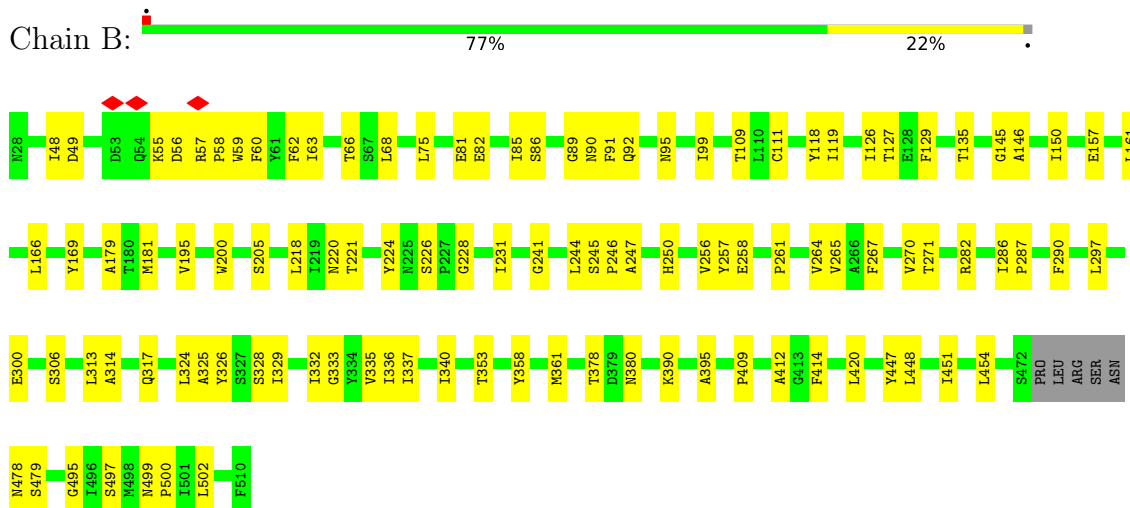
3 Residue-property plots

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

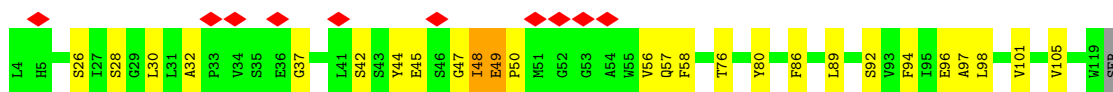
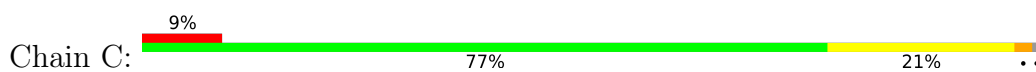
- Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic



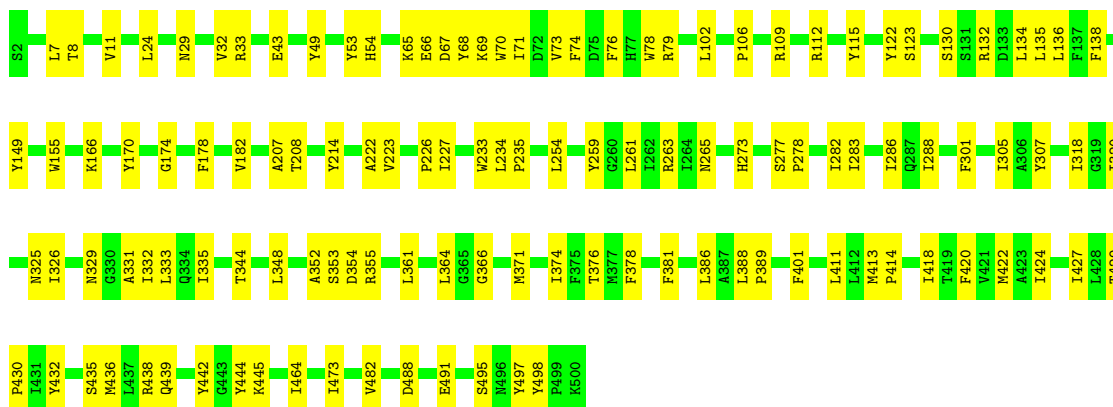
- Molecule 2: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic



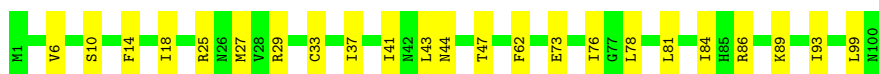
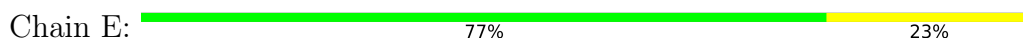
- Molecule 3: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



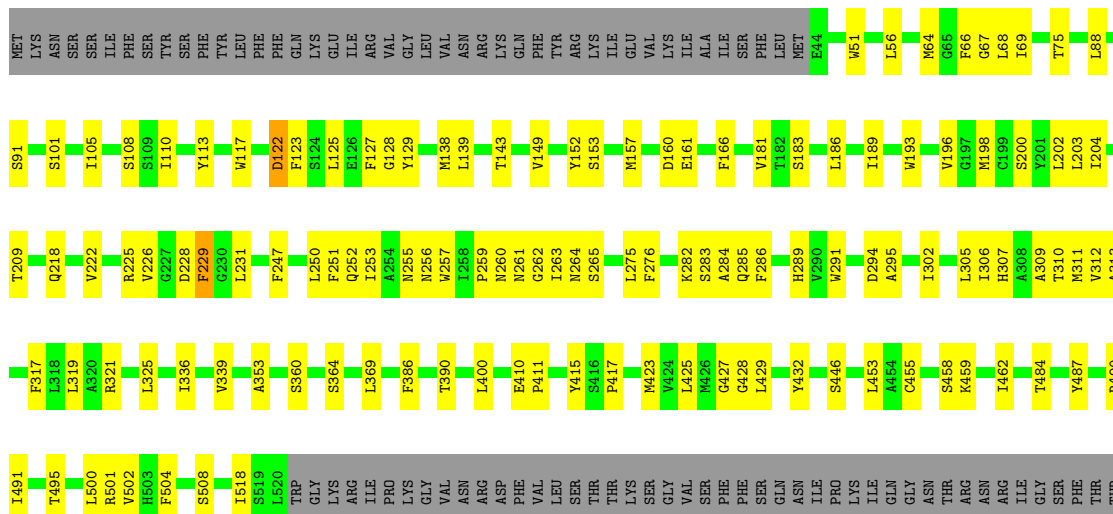
- Molecule 4: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

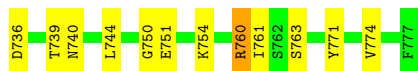


- Molecule 5: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

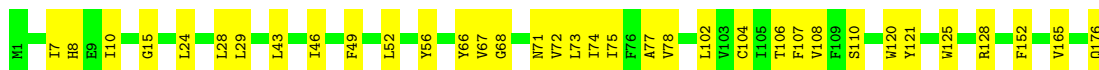
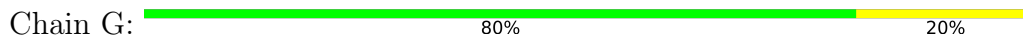


- Molecule 6: NAD(P)H-quinone oxidoreductase subunit F

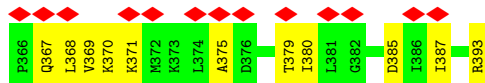
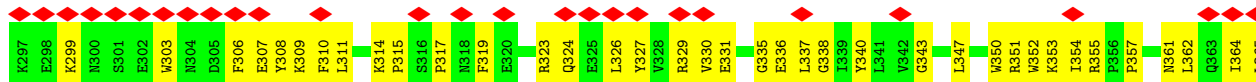
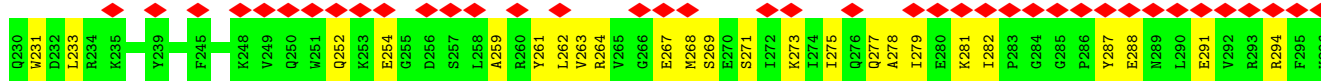
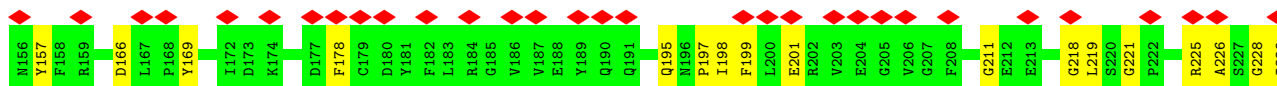
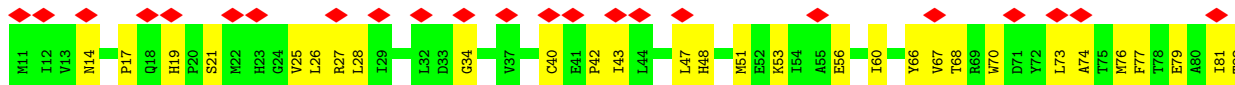
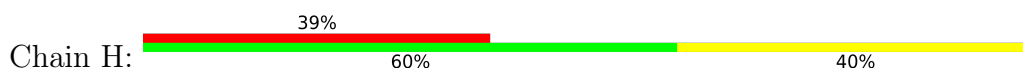




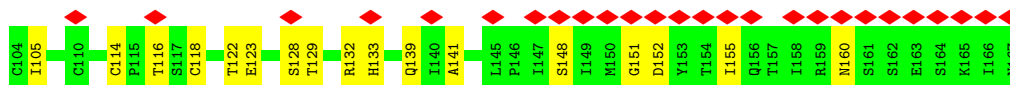
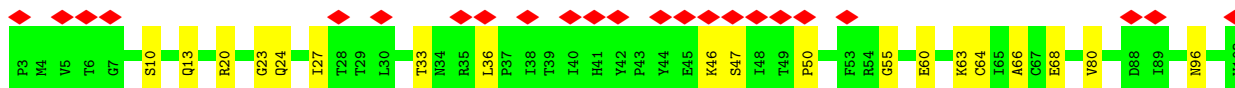
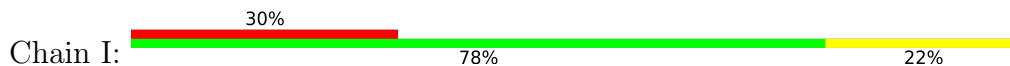
- Molecule 7: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic



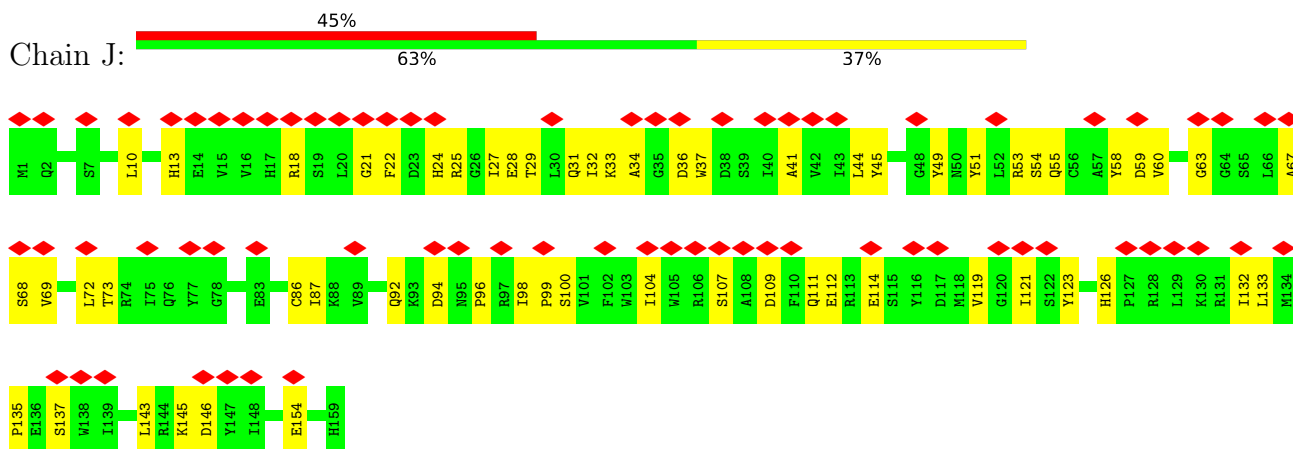
- Molecule 8: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic



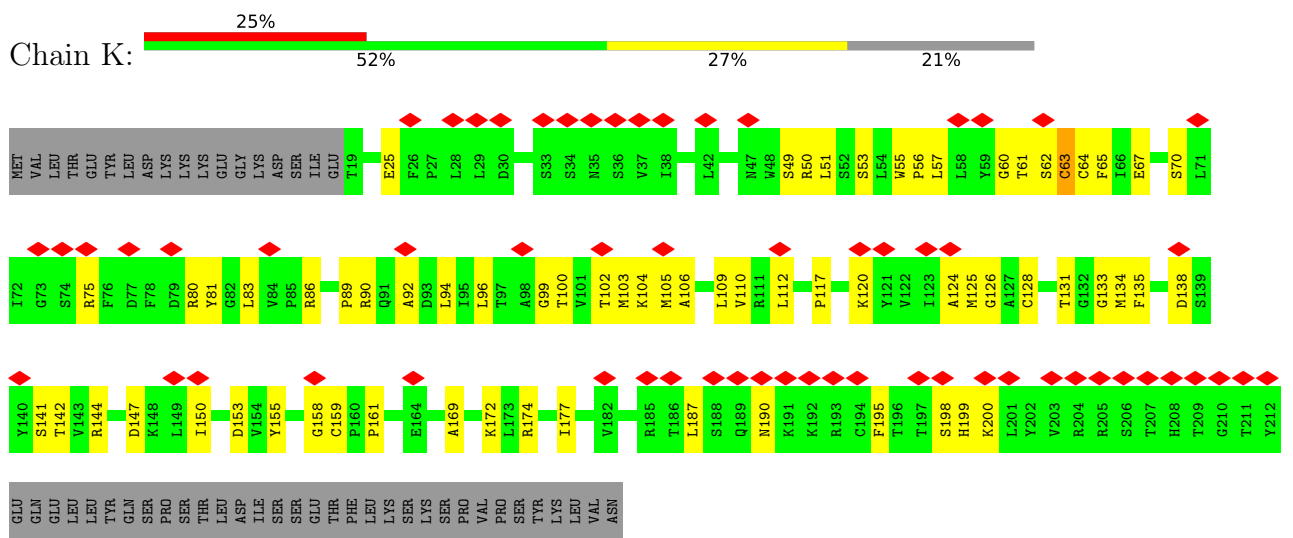
- Molecule 9: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic



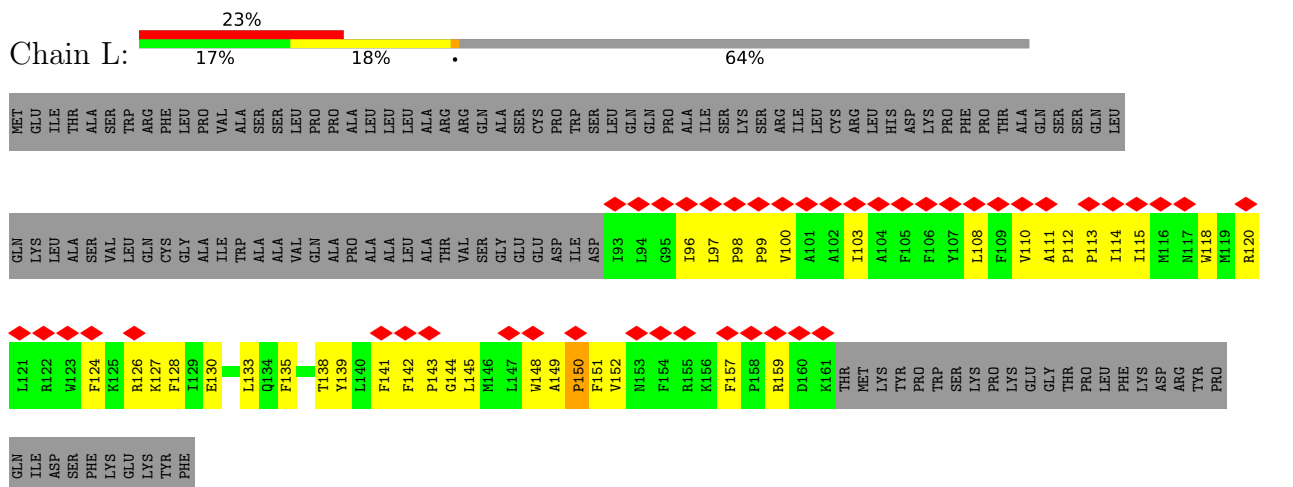
- Molecule 10: NAD(P)H-quinone oxidoreductase subunit J



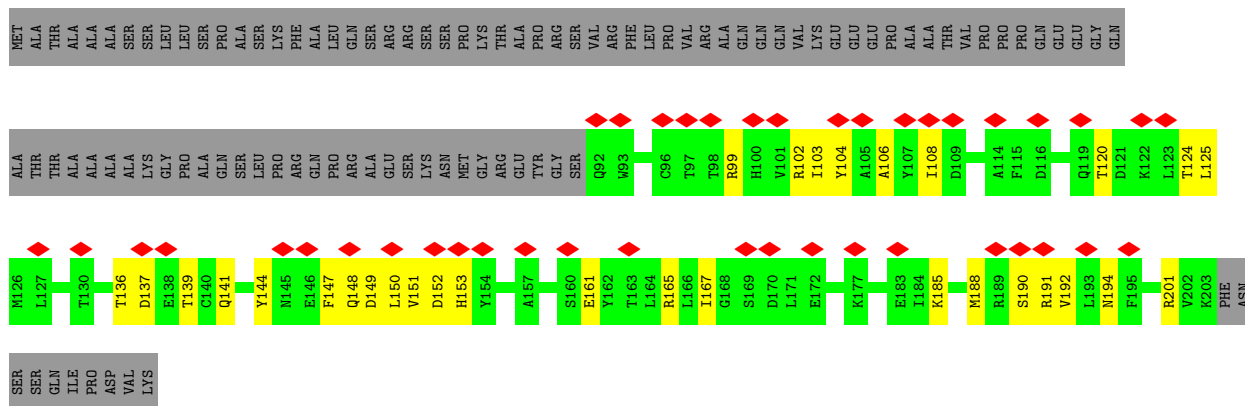
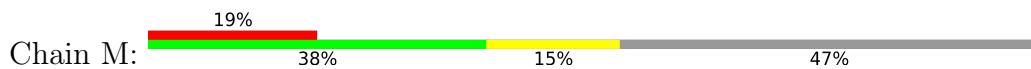
- Molecule 11: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic



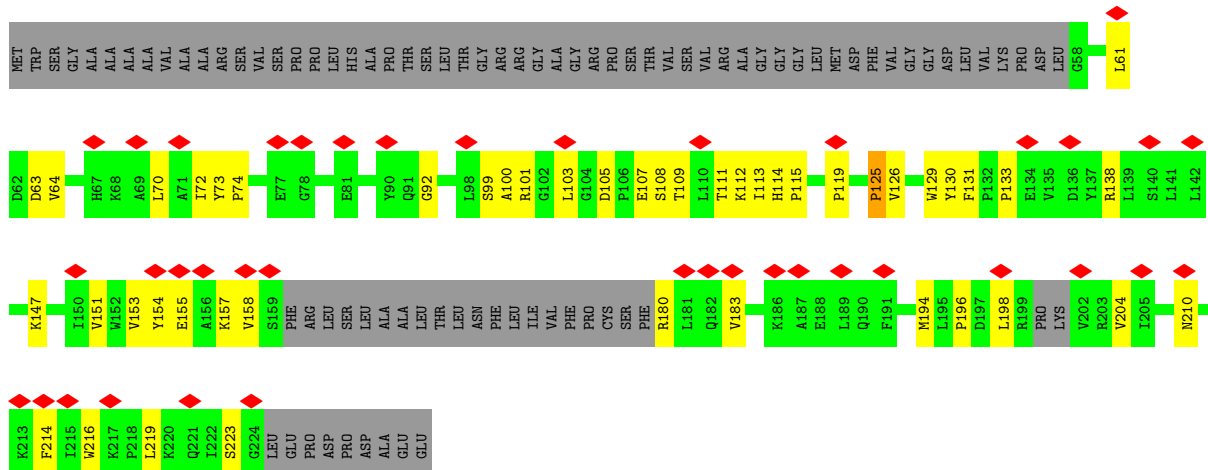
- Molecule 12: NAD(P)H-quinone oxidoreductase subunit L



- Molecule 13: NAD(P)H-quinone oxidoreductase subunit M



- Molecule 14: NAD(P)H-quinone oxidoreductase subunit N



- Molecule 15: Unidentified stromal protein



- Molecule 16: Photosynthetic NDH subunit of subcomplex L1



- Molecule 17: Photosynthetic NDH subunit of subcomplex L2

Chain 2:  52% 8% 40%

MET ALA THR LEU VAL HIS LEU ILE LEU CYS SER THR THR SER SER SER THR ALA THR PRO SER PRO ASN ARG ARG PRO PRO SER SER PRO ASP GLY ALA ASP LYS ARG ALA HIS LEU THR GLN SER SER THR VAL ALA MET VAL ALA

THR ALA LEU SER ALA ARG PRO ALA PRO PRO MET THR SER ALA GLU ALA THR VAL ARG LEU PRO VAL P88 R94 W95 G96 T97 R102 R118 A123 R130 Y140 L147 K148 S149 D153 K193 Y198 L199 L208 G216

- Molecule 18: Photosynthetic NDH subunit of subcomplex L3


Chain 3:  46% 13% 41%

MET ALA THR PRO THR LEU SER PHE GLN ASP GLY ALA ALA PRO ALA THR THR SER GLY GLY ALA THR TRP TRP LEU ARG PRO ARG ARG ARG PRO PRO VAL VAL THR CYS THR SER GLU PRO SER GLY ARG SER ALA CYS LEU SER LEU GLY LEU GLY LEU THR ALA VAL VAL LEU

HIS THR THR PRO ALA ARG ILE ASP GLY ASP GLU PRO PRO ASN ASN GLY TRP TRP THR GLU PHE LEU VAL ARG K93 A125 R129 V130 R131 F135 D136 L137 A148 Y155 L158 K159 Y164 Y165 D166 F167 D168 I171 D177

P180 L185 A186 M187 R188 F190 V200 D205 T206 I207 Y212 T215 L219 M223 V226 ALA

- Molecule 19: Photosynthetic NDH subunit of subcomplex L4

Chain 4:  78% 22%

A128 E133 L134 S137 L151 Q152 V153 D155 S160 V161 S162 M163 V164 V165 A172 R173 F174 P175 D176 G177 D181 R186 L200 V213 G220 A231 G238 C239 F240 S241 E242 A257

- Molecule 20: Photosynthetic NDH subunit of subcomplex L5

Chain 5:  56% 14% 29%

MET ALA ALA THR SER PHE ALA THR LEU VAL VAL ALA ARG PRO ALA ALA ALA ALA ALA ALA GLN ARG ALA ALA SER SER ALA LEU SER LEU ARG GLY VAL GLY ARG VAL ALA SER PRO ALA LEU SER VAL SER LEU GLN THR ARG ALA PHE VAL ALA SER

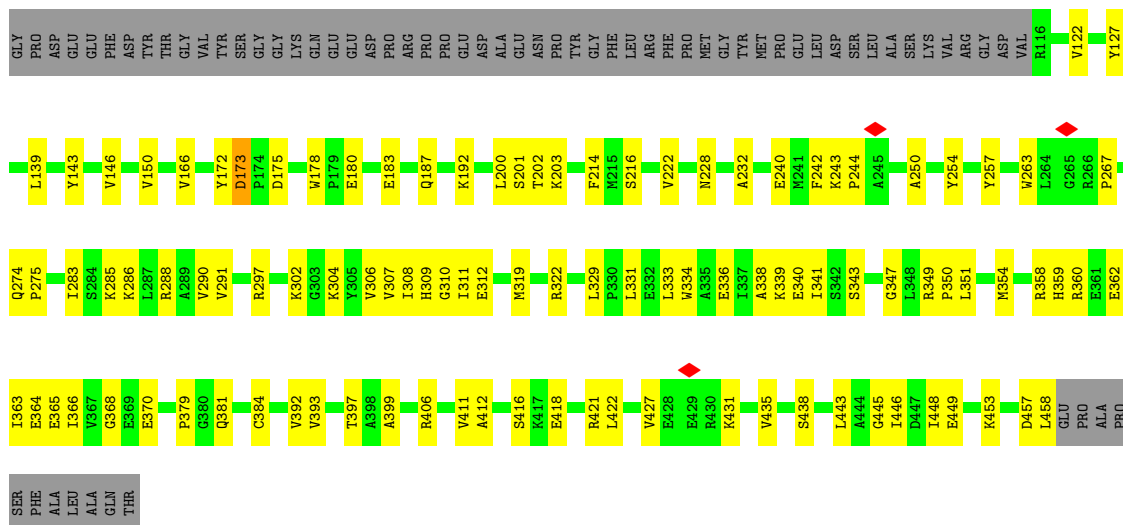
ALA SER ALA GLU PRO TYR ALA PRO GLU LEU Q71 K77 Y78 Y79 N83 N86 P87 V88 G89 R94 I95 V96 L99 V108 L114 F121 V131 M136 I137 Q138 M146 N162 F165 L173 S174 M175 A176 M177 A178 G179 P180 Q186 F187 F188 I189 C190

G205 E209 R227 S235 E236 L240 P241 V242 VAL

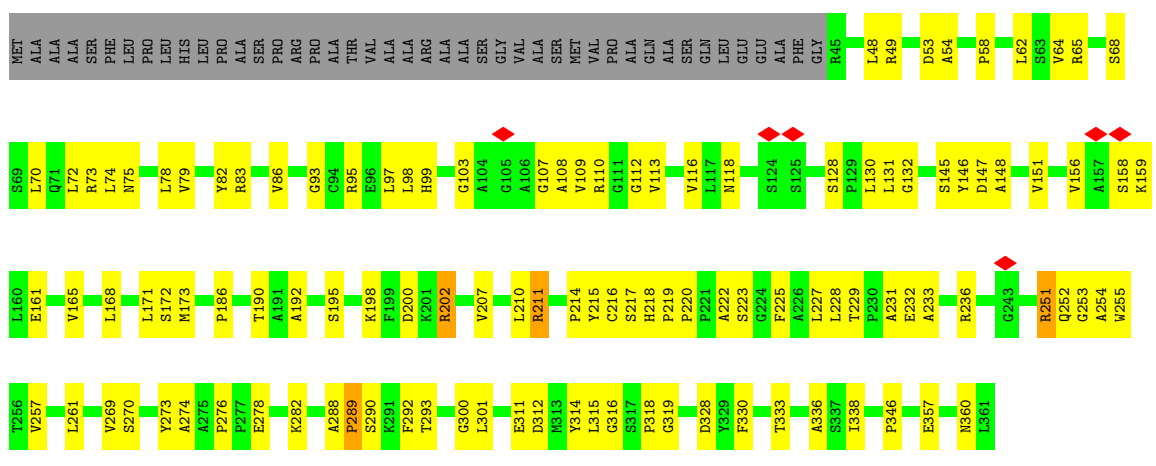
- Molecule 21: Photosynthetic NDH subunit of subcomplex B1

Chain 6:  51% 22% 27%

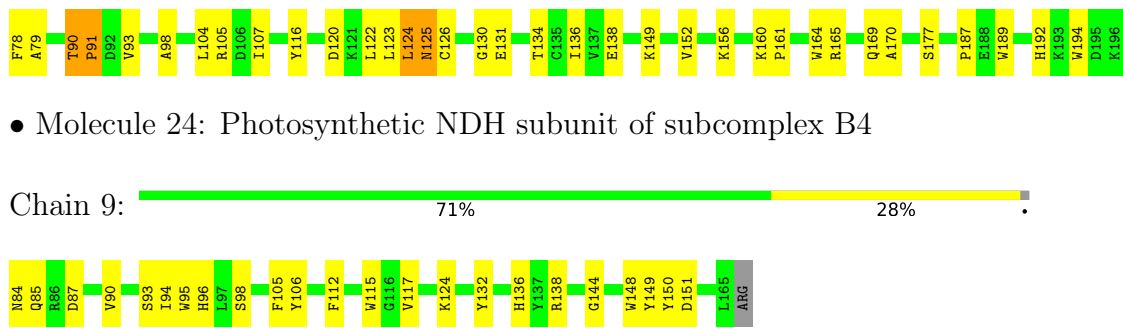
MET GLN THR PRO MET THR THR PRO MET ALA ARG PRO THR SER THR MET MET ALA THR LYS LEU PRO PRO ALA SER SER GLN CYS HIS LEU LEU PRO GLY ARG ARG VAL GLY ALA LEU LEU ALA ARG ALA SER SER LYS LYS ARG ASN PRO TRP LEU ASP PRO PHE ASP ASP



• Molecule 22: Photosynthetic NDH subunit of subcomplex B2



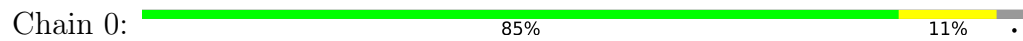
• Molecule 23: Photosynthetic NDH subunit of subcomplex B3



• 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 (Å)	575.08, 575.08, 575.08	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.307, 1.307, 1.307	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: SF4, BCR, SQD, LHG

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	0.25	0/2670	0.45	0/3644
2	B	0.27	0/3730	0.44	0/5082
3	C	0.30	0/865	0.50	0/1188
4	D	0.28	0/3987	0.47	1/5427 (0.0%)
5	E	0.26	0/759	0.41	0/1028
6	F	0.27	0/5270	0.45	0/7186
7	G	0.27	0/1288	0.45	0/1765
8	H	0.25	0/3070	0.46	0/4173
9	I	0.26	0/1254	0.52	0/1702
10	J	0.23	0/1297	0.45	0/1771
11	K	0.25	0/1505	0.47	0/2048
12	L	0.27	0/597	0.46	0/816
13	M	0.23	0/896	0.47	0/1218
14	N	0.29	0/1189	0.54	1/1617 (0.1%)
16	1	0.28	0/1213	0.55	0/1651
17	2	0.25	0/935	0.43	0/1276
18	3	0.26	0/1006	0.43	0/1365
19	4	0.26	0/894	0.54	0/1216
20	5	0.26	0/1314	0.47	0/1771
21	6	0.28	0/2589	0.50	0/3513
22	7	0.28	0/2358	0.57	0/3200
23	8	0.30	0/844	0.60	0/1145
24	9	0.27	0/636	0.48	0/868
25	0	0.27	0/1122	0.54	0/1536
All	All	0.27	0/41288	0.48	2/56206 (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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	N	157	LYS	N-CA-C	7.50	131.24	111.00
4	D	497	TYR	C-N-CA	-5.08	108.99	121.70

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	82	0
2	B	3646	0	3652	78	0
3	C	841	0	761	26	0
4	D	3874	0	3923	84	0
5	E	750	0	760	20	0
6	F	5124	0	4962	121	0
7	G	1260	0	1197	28	0
8	H	2991	0	2849	133	0
9	I	1229	0	1109	26	0
10	J	1258	0	1151	49	0
11	K	1474	0	1442	54	0
12	L	572	0	559	26	0
13	M	876	0	801	27	0
14	N	1154	0	1117	29	0
15	T	305	0	69	3	0
16	1	1185	0	1086	29	0
17	2	915	0	764	13	0
18	3	989	0	927	19	0
19	4	878	0	823	19	0
20	5	1289	0	1247	21	0
21	6	2541	0	2461	65	0
22	7	2311	0	2232	85	0
23	8	828	0	742	26	0
24	9	617	0	520	15	0
25	0	1089	0	901	12	0
26	D	24	0	19	1	0
27	F	39	0	53	6	0
28	F	100	0	137	5	0
29	8	8	0	0	1	0
All	All	40775	0	38873	967	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 (967) 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	0.85
23:8:123:LEU:C	23:8:124:LEU:O	2.15	0.85
18:3:148:ALA:HB3	24:9:105:PHE:HB2	1.67	0.76
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
3:C:47:GLY:O	3:C:50:PRO:N	2.22	0.72
3:C:47:GLY:O	3:C:48:ILE:C	2.28	0.70
6:F:669:TYR:HB3	22:7:300:GLY:HA2	1.74	0.69
23:8:123:LEU:O	23:8:124:LEU:C	2.31	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
22:7:251:ARG:HG2	22:7:276:PRO:HB3	1.85	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
22:7:220:PRO:HD2	22:7:225:PHE:CZ	2.40	0.57
8:H:51:MET:HE1	8:H:66:TYR:HD1	1.68	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
11:K:50:ARG:HH21	11:K:177:ILE:HG23	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:324:LEU:O	2:B:328:SER:OG	2.23	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
16:1:100:PHE:HB2	16:1:108:LYS:HZ3	1.74	0.51
22:7:314:TYR:OH	22:7:336:ALA:HB3	2.10	0.51
23:8:131:GLU:O	23:8:156:LYS:NZ	2.37	0.51
1:A:232:LEU:HB2	1:A:235:ALA:HB3	1.92	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
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
23:8:192:HIS:C	23:8:194:TRP:H	2.14	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
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
4:D:331:ALA:O	4:D:335:ILE:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
18:3:168:ASP:HA	18:3:171:ILE:HG22	1.94	0.50
1:A:236:GLU:HG3	1:A:239:LEU:C	2.33	0.49
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
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
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
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:427:ILE:HD11	6:F:229:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:51:MET:HE1	8:H:66:TYR:CD1	2.48	0.48
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:299:LYS:HD3	8:H:299:LYS:N	2.29	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
22:7:79:VAL:H	22:7:113:VAL:HG12	1.78	0.48
2:B:497:SER:O	2:B:497:SER:OG	2.28	0.48
5:E:78:LEU:HD12	7:G:73:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:268:MET:O	8:H:271:SER:OG	2.24	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
4:D:318:ILE:HG21	4:D:422:MET:HE1	1.96	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
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
24:9:115:TRP:C	24:9:117:VAL:H	2.17	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
21:6:379:PRO:C	21:6:381:GLN:H	2.18	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
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
1:A:80:LYS:HG3	11:K:50:ARG:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:PHE:HB2	2:B:146:ALA:H	1.80	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
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:326:LEU:HG	10:J:25:ARG:HH11	1.80	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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:118:TYR:OH	15:T:65:UNK:O	2.32	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
14:N:108:SER:HA	14:N:112:LYS:HB2	1.97	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
10:J:100:SER:OG	10:J:112:GLU:OE1	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:188:PHE:HE2	20:5:190:CYS:HG	1.65	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
21:6:216:SER:O	21:6:216:SER:OG	2.36	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
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
1:A:184:LEU:HD13	1:A:358:GLN:NE2	2.34	0.43
1:A:197:GLN:HE22	1:A:274:TYR:C	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:I:64:CYS:C	9:I:66:ALA:H	2.22	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
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
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: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
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
22:7:148:ALA:HA	22:7:168:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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
20:5:136:MET:HE1	20:5:188:PHE:HB2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
8:H:95:PRO:HG2	8:H:309:LYS:O	2.18	0.42
11:K:104:LYS:C	11:K:106:ALA:H	2.22	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
22:7:223:SER:HG	22:7:225:PHE:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
22:7:255:TRP:C	22:7:257:VAL:H	2.23	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:5:79:TYR:HB2	20:5:94:ARG:HD2	2.02	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
8:H:97:ARG:HH12	8:H:166:ASP:CG	2.24	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
12:L:141:PHE:C	12:L:145:LEU:HG	2.41	0.41
21:6:347:GLY:C	21:6:349:ARG:H	2.23	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
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
22:7:289:PRO:O	22:7:290:SER:OG	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
16:1:185:ALA:HA	16:1:201:VAL:O	2.21	0.41
20:5:83:ASN:HB3	20:5:89:GLY:C	2.41	0.41
20:5:114:LEU:HD22	20:5:121:PHE:O	2.21	0.41
21:6:445:GLY:C	21:6:446:ILE:HG13	2.42	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
1:A:195:GLU:HA	16:1:96:ARG:HH11	1.85	0.41
8:H:225:ARG:NH2	8:H:267:GLU:OE2	2.53	0.41
13:M:124:THR:C	13:M:125:LEU:HD12	2.42	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:283:PRO:O	1:A:286:SER:OG	2.27	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
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
22:7:207:VAL:HG13	22:7:293:THR:O	2.21	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	344/346 (99%)	303 (88%)	40 (12%)	1 (0%)	41 74
2	B	474/483 (98%)	424 (90%)	50 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	114/117 (97%)	96 (84%)	15 (13%)	3 (3%)	5	34
4	D	497/499 (100%)	450 (90%)	46 (9%)	1 (0%)	47	78
5	E	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
6	F	665/777 (86%)	598 (90%)	65 (10%)	2 (0%)	41	74
7	G	174/176 (99%)	148 (85%)	26 (15%)	0	100	100
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%)	29	66
12	L	67/192 (35%)	59 (88%)	7 (10%)	1 (2%)	10	44
13	M	110/213 (52%)	92 (84%)	18 (16%)	0	100	100
14	N	139/233 (60%)	116 (84%)	20 (14%)	3 (2%)	6	37
16	1	148/154 (96%)	112 (76%)	35 (24%)	1 (1%)	22	59
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%)	25	62
21	6	341/469 (73%)	249 (73%)	90 (26%)	2 (1%)	25	62
22	7	315/361 (87%)	226 (72%)	88 (28%)	1 (0%)	41	74
23	8	117/119 (98%)	79 (68%)	33 (28%)	5 (4%)	2	24
24	9	80/83 (96%)	65 (81%)	14 (18%)	1 (1%)	12	47
25	0	147/155 (95%)	98 (67%)	48 (33%)	1 (1%)	22	59
All	All	5280/6245 (84%)	4465 (85%)	791 (15%)	24 (0%)	32	66

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

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Mol	Chain	Res	Type
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
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 [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	271/301 (90%)	270 (100%)	1 (0%)	91	95
2	B	397/419 (95%)	396 (100%)	1 (0%)	92	96
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%)	77 (99%)	1 (1%)	69	83
6	F	513/674 (76%)	511 (100%)	2 (0%)	91	95
7	G	119/154 (77%)	119 (100%)	0	100	100
8	H	298/336 (89%)	298 (100%)	0	100	100
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%)	161 (99%)	1 (1%)	86	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	55/167 (33%)	54 (98%)	1 (2%)	59	77
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
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%)	230 (99%)	3 (1%)	69	83
23	8	69/102 (68%)	69 (100%)	0	100	100
24	9	55/70 (79%)	53 (96%)	2 (4%)	35	63
25	0	93/137 (68%)	93 (100%)	0	100	100
All	All	4010/5330 (75%)	3998 (100%)	12 (0%)	92	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	LYS
2	B	55	LYS
5	E	25	ARG
6	F	229	PHE
6	F	760	ARG
11	K	200	LYS
12	L	126	ARG
22	7	202	ARG
22	7	211	ARG
22	7	251	ARG
24	9	106	TYR
24	9	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	120	HIS

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Mol	Chain	Res	Type
1	A	197	GLN
1	A	262	ASN
1	A	294	ASN
1	A	358	GLN
2	B	222	GLN
2	B	317	GLN
6	F	218	GLN
6	F	646	ASN
7	G	71	ASN
8	H	14	ASN
8	H	48	HIS
8	H	367	GLN
10	J	13	HIS
11	K	91	GLN
13	M	145	ASN
13	M	194	ASN
14	N	143	HIS
14	N	182	GLN
16	1	113	GLN
20	5	206	GLN
21	6	129	ASN
21	6	381	GLN
22	7	252	GLN
22	7	297	GLN
22	7	360	ASN
23	8	184	GLN
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 monosaccharides 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
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%)
26	LHG	D	601	-	23,23,48	1.32	2 (8%)	26,28,54	1.32	3 (11%)
27	BCR	F	801	-	40,40,41	0.77	0	54,54,56	2.99	21 (38%)
29	SF4	8	201	23	0,12,12	-	-	-	-	-

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

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 12 short contacts:

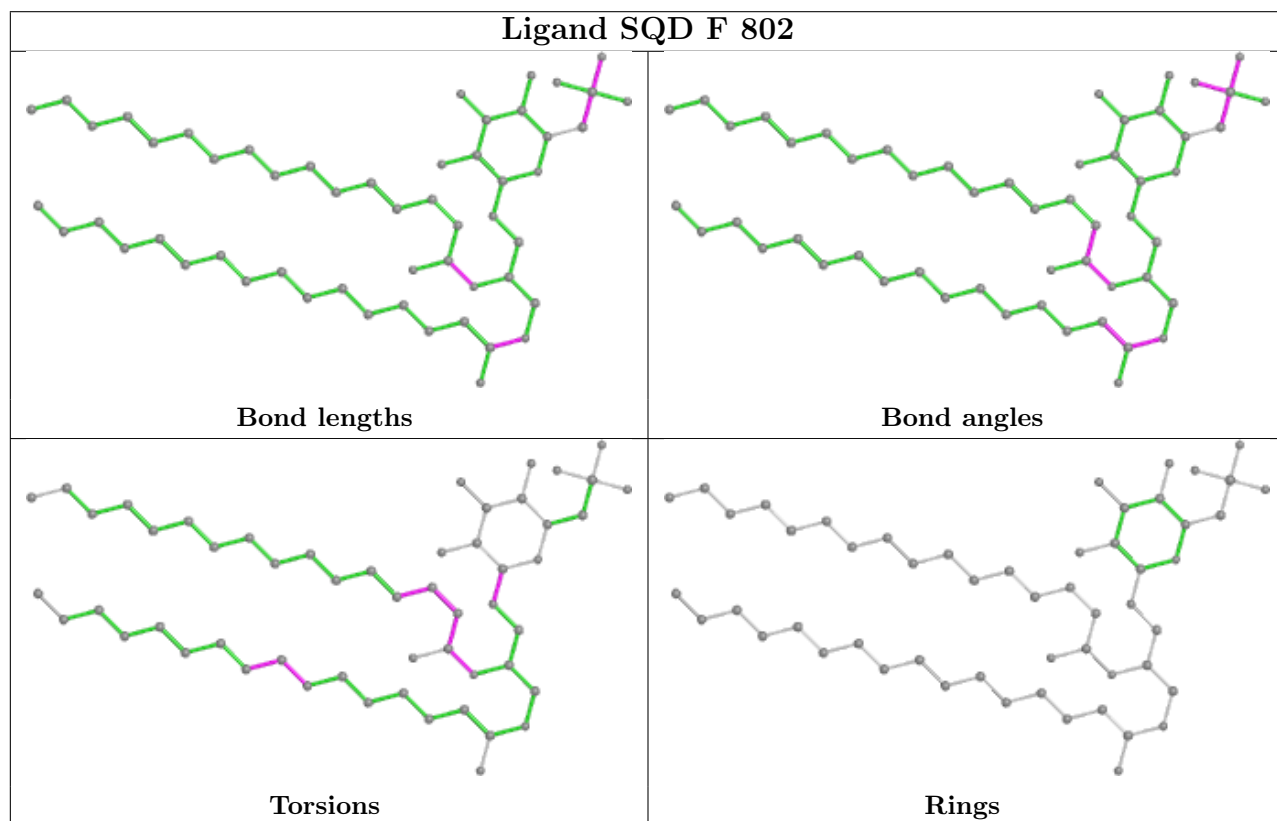
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	F	802	SQD	1	0
28	F	803	SQD	4	0
26	D	601	LHG	1	0
27	F	801	BCR	6	0

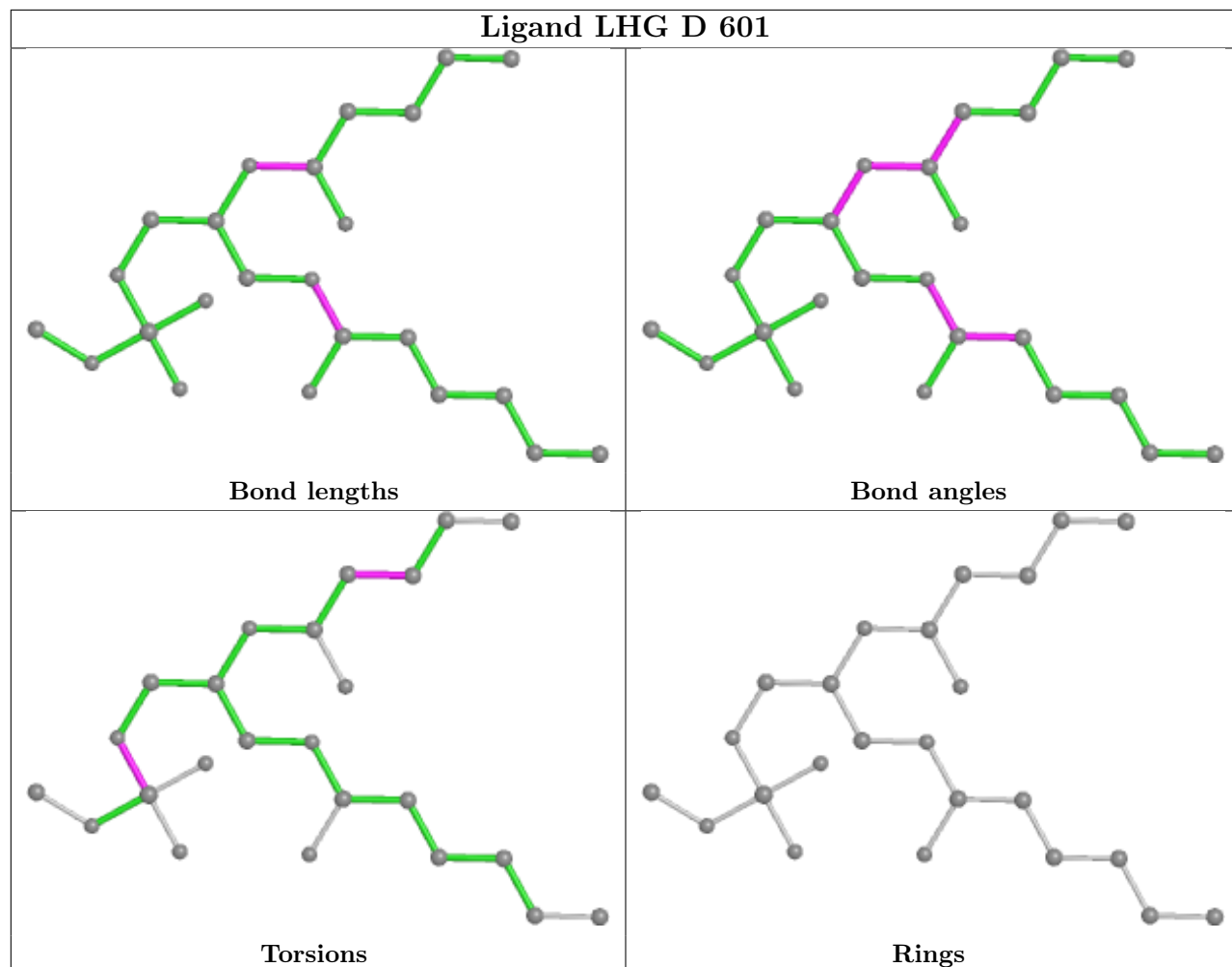
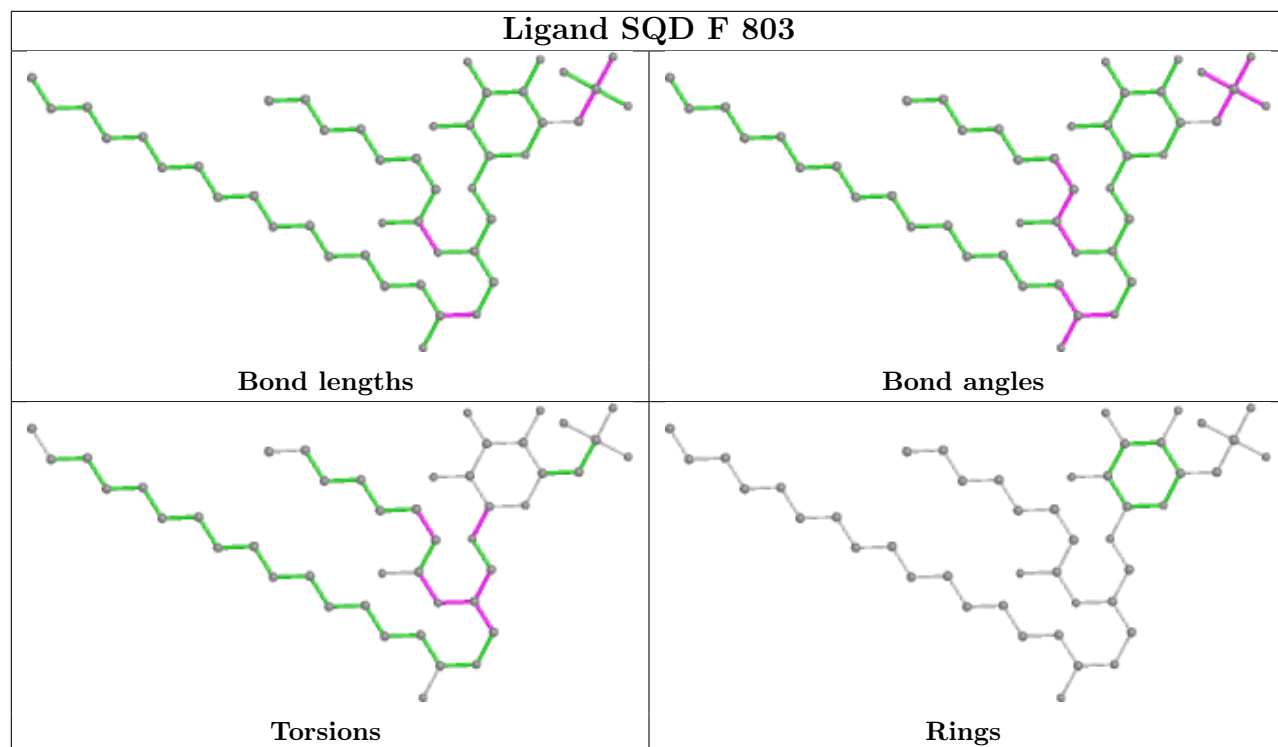
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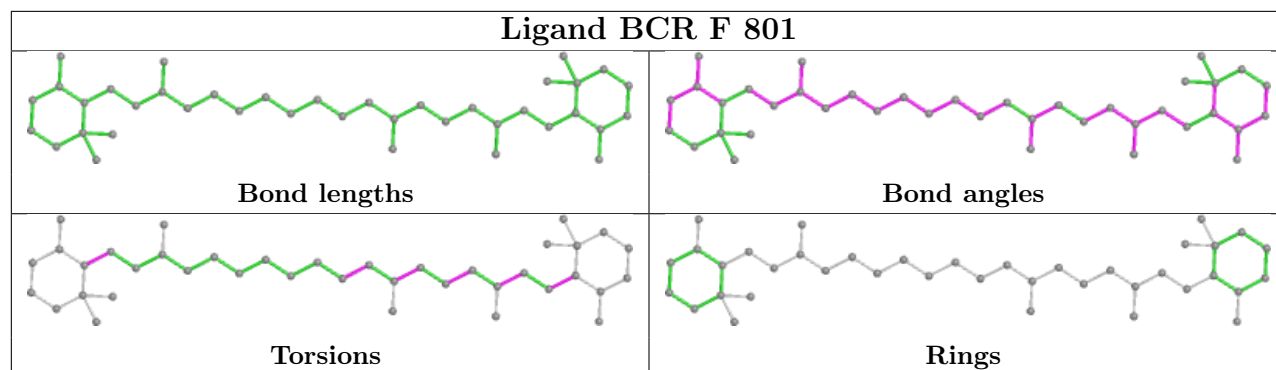
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	8	201	SF4	1	0

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](#)

There are no chain breaks in this entry.

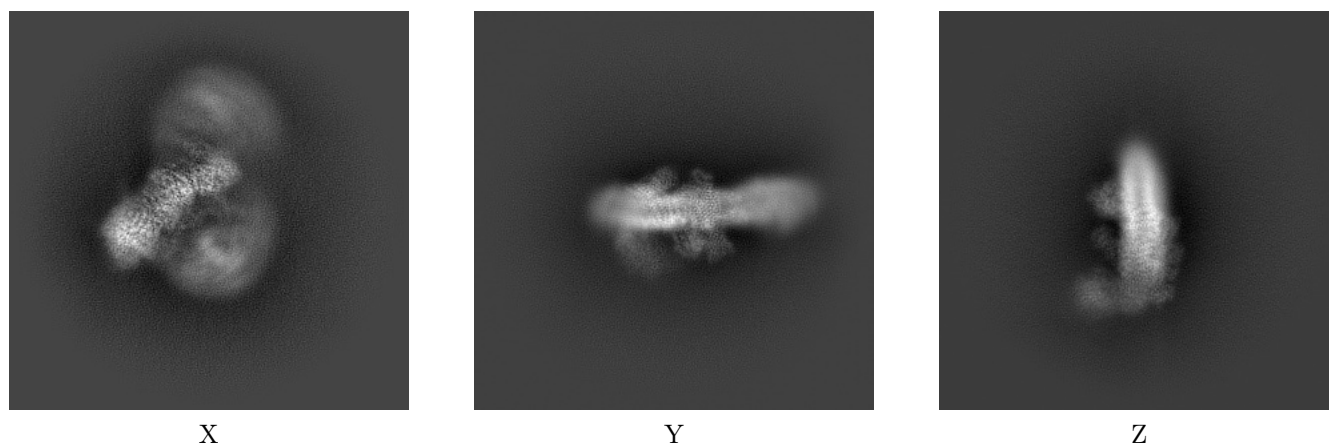
6 Map visualisation [i](#)

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](#)

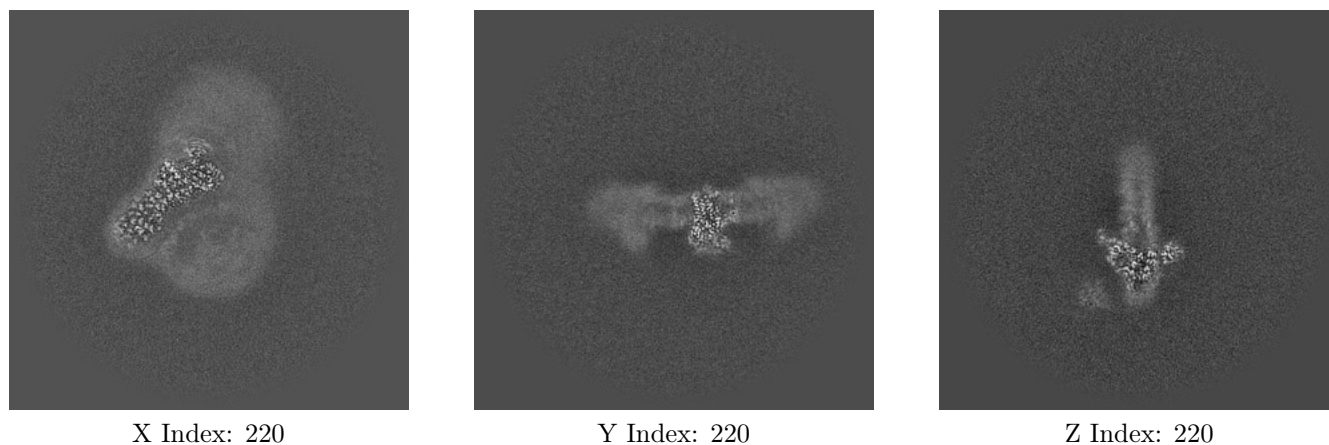
6.1.1 Primary map



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

6.2 Central slices [i](#)

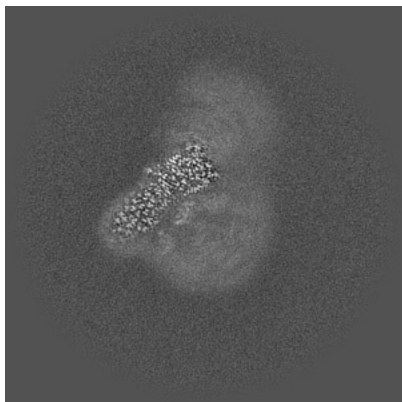
6.2.1 Primary map



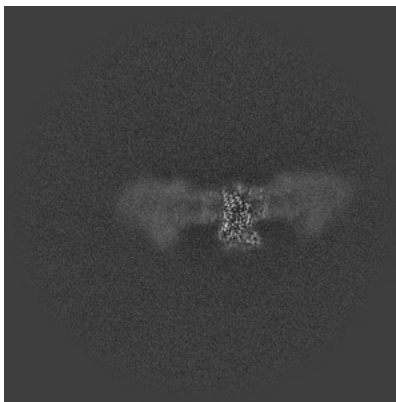
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

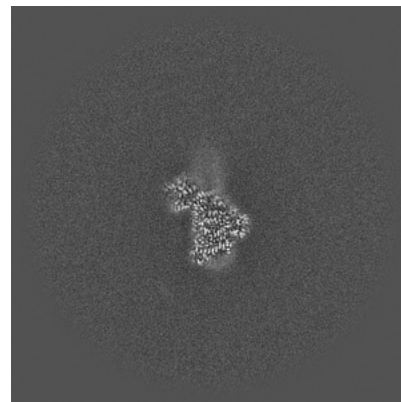
6.3.1 Primary map



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

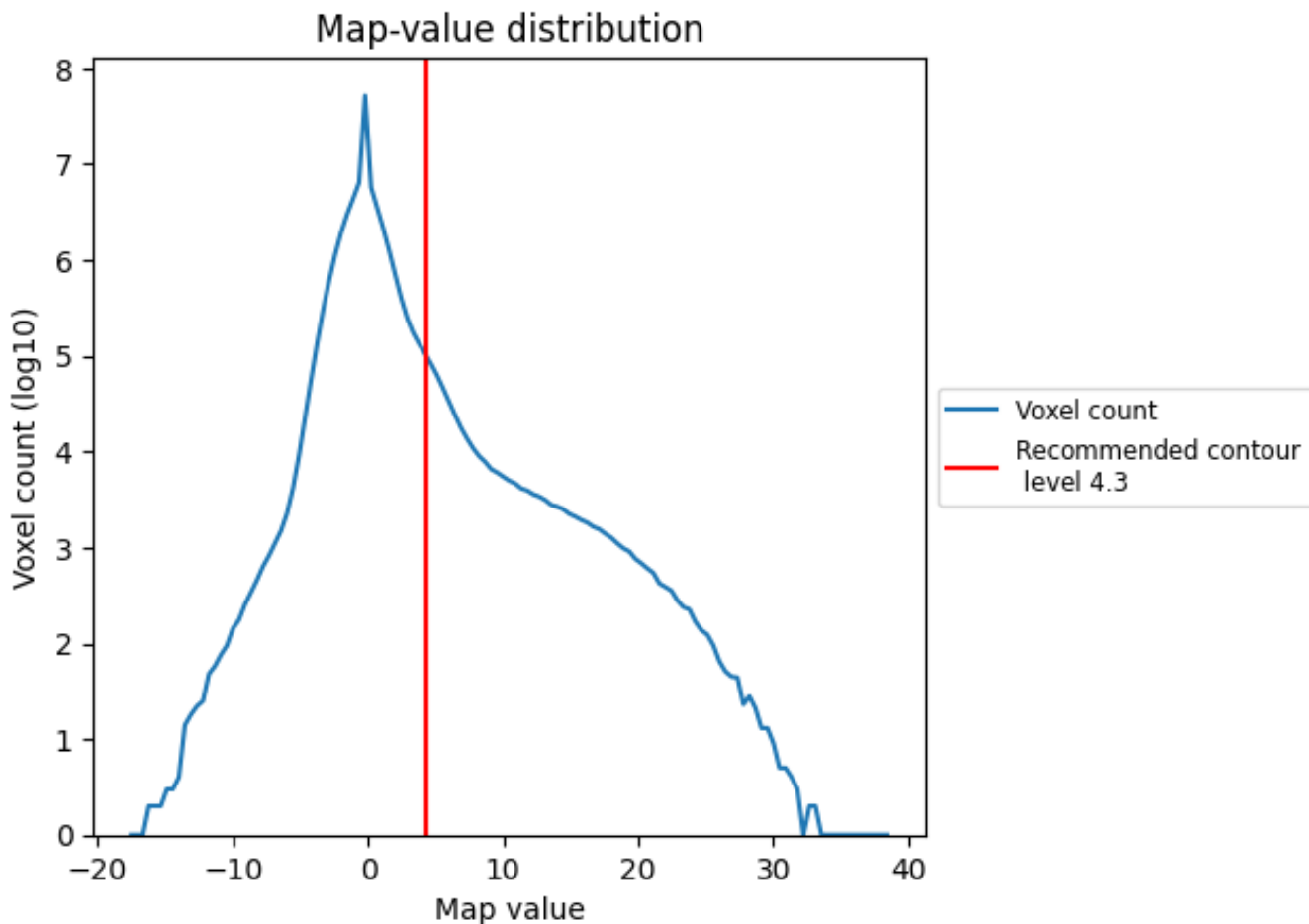
6.5 Mask visualisation

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

7 Map analysis [i](#)

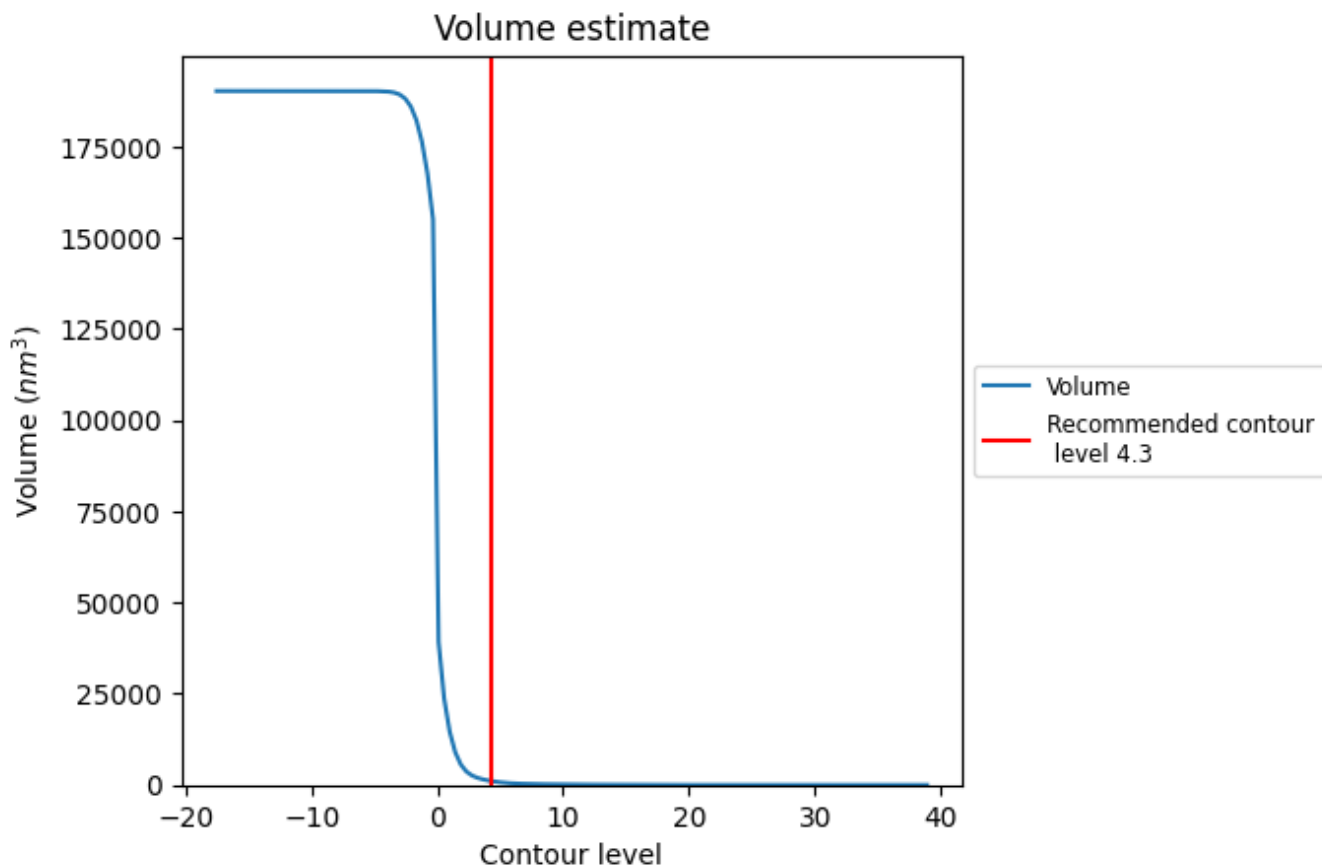
This section contains the results of statistical analysis of the map.

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.

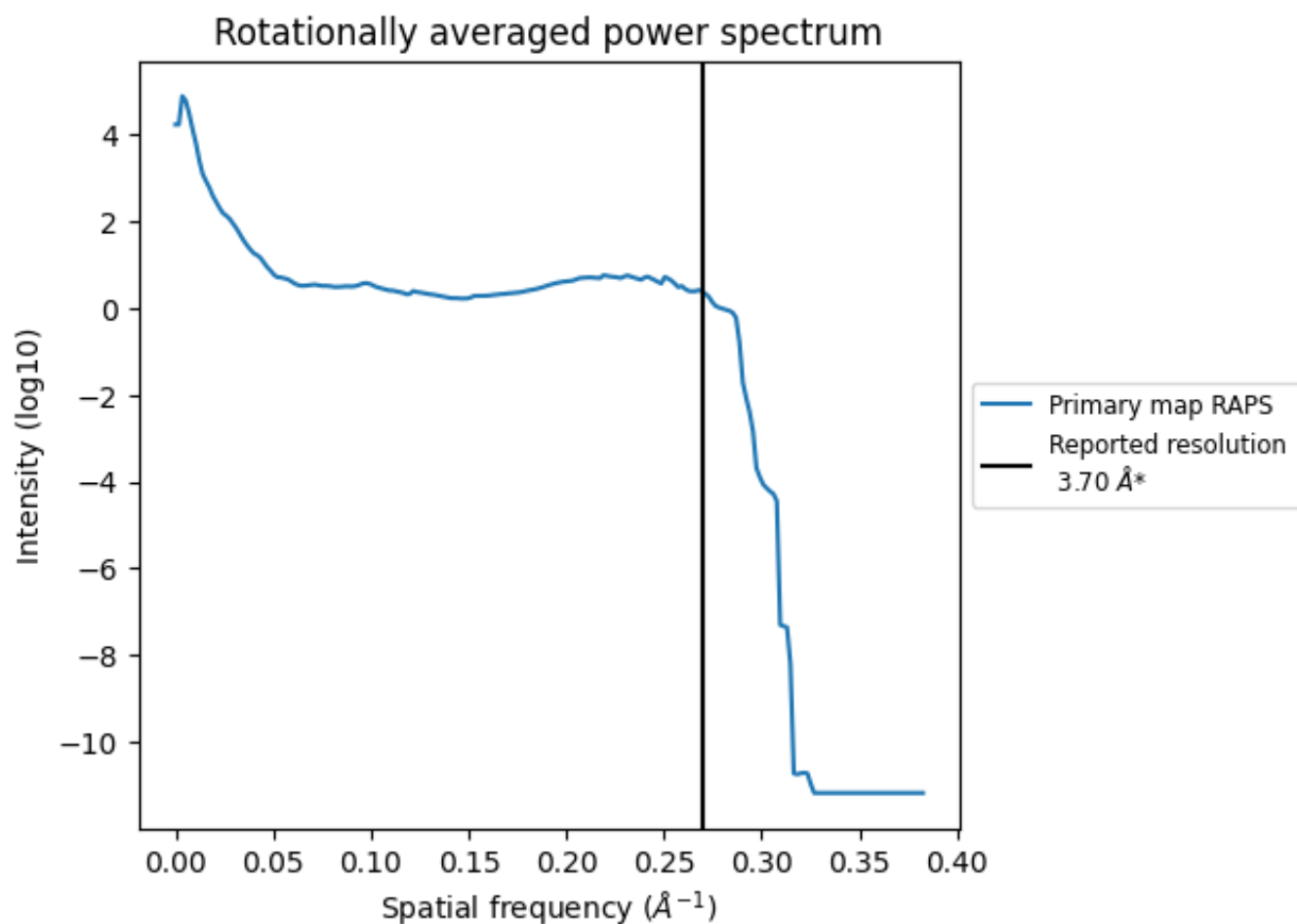
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 [\(i\)](#)



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

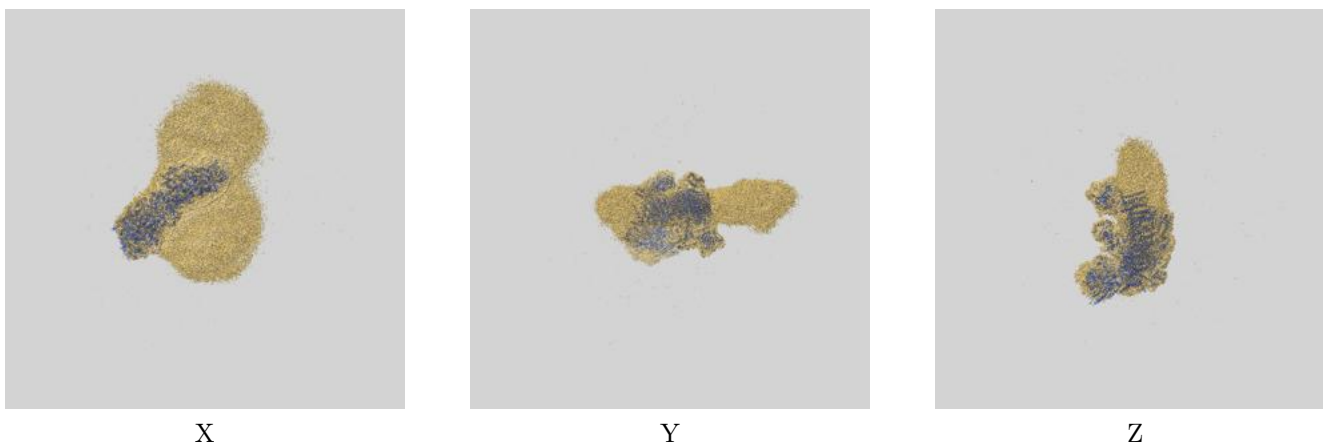
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

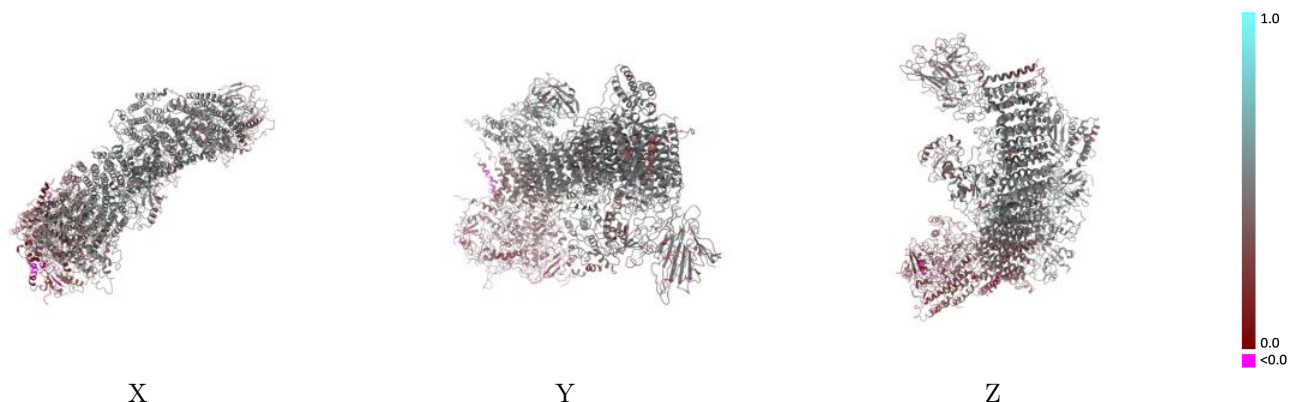
This section contains information regarding the fit between EMDB map EMD-31307 and PDB model 7EU3. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



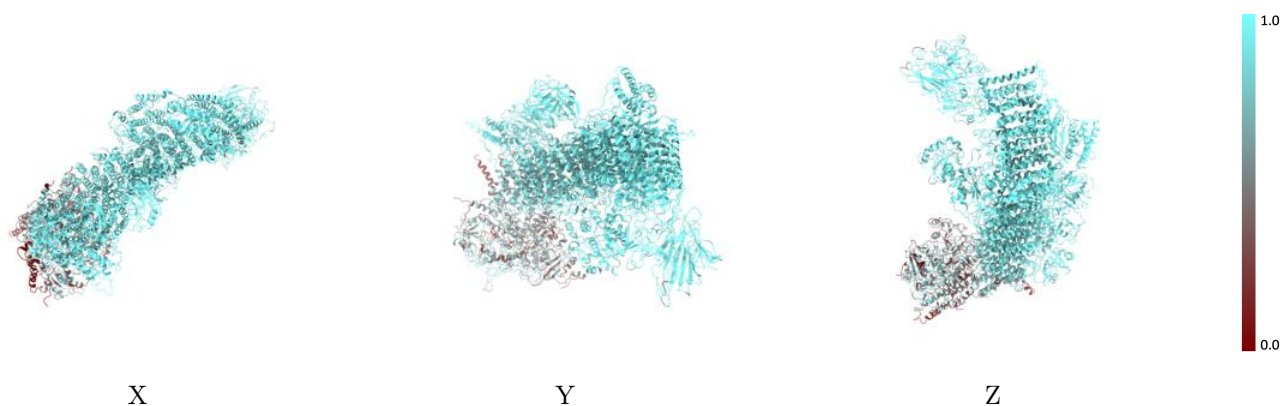
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



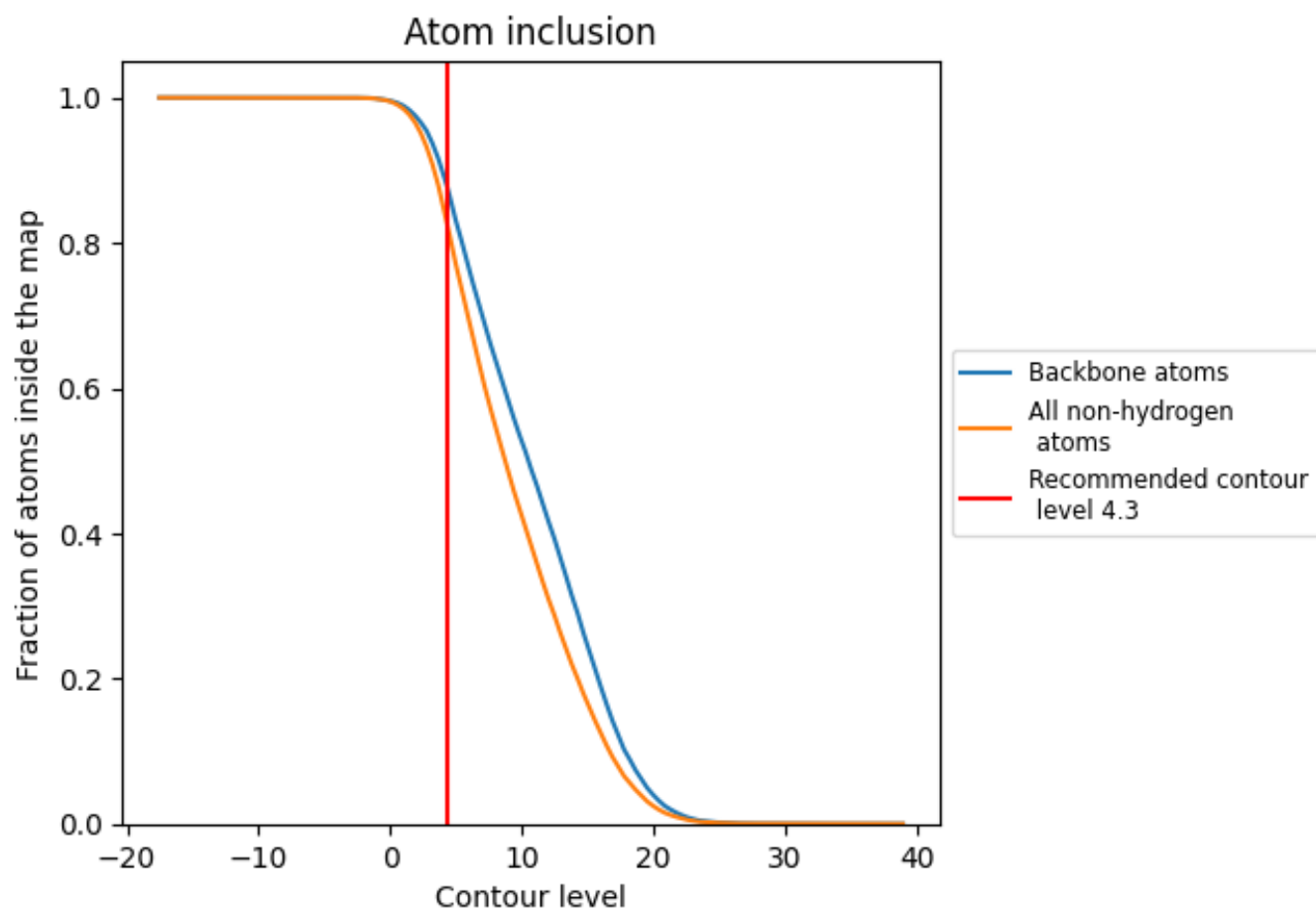
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8276	 0.4020
0	 0.9487	 0.4610
1	 0.9557	 0.4310
2	 0.9720	 0.4580
3	 0.9743	 0.4660
4	 0.9688	 0.4720
5	 0.9566	 0.4750
6	 0.9334	 0.4230
7	 0.9133	 0.4070
8	 0.9440	 0.4470
9	 0.9536	 0.4480
A	 0.7935	 0.3470
B	 0.9258	 0.4570
C	 0.8424	 0.3870
D	 0.9517	 0.4890
E	 0.9216	 0.4800
F	 0.9390	 0.4660
G	 0.9008	 0.4400
H	 0.4876	 0.2680
I	 0.5674	 0.2970
J	 0.4789	 0.2510
K	 0.5465	 0.2970
L	 0.3136	 0.0790
M	 0.4847	 0.2800
N	 0.5941	 0.2650
T	 0.9246	 0.4040

