



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 06:13 am BST

PDB ID : 7BKD / pdb_00007bkd
EMDB ID : EMD-12210
Title : Formate dehydrogenase - heterodisulfide reductase - formylmethanofuran dehydrogenase complex from Methanospirillum hungatei (heterodisulfide reductase core and mobile arm in conformational state 1, composite structure)
Authors : Pfeil-Gardiner, O.; Watanabe, T.; Shima, S.; Murphy, B.J.
Deposited on : 2021-01-15
Resolution : 3.00 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

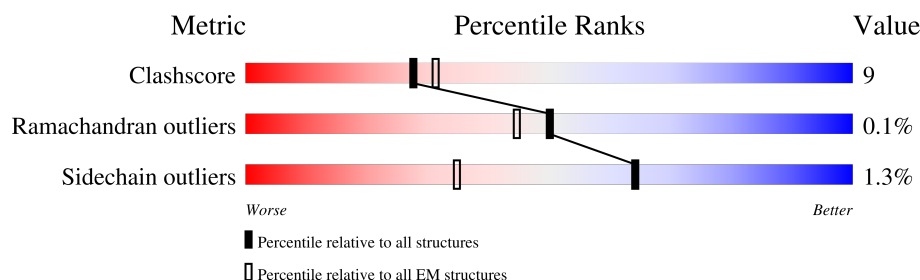
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	671	
1	a	671	
2	C	191	
2	c	191	
3	B	296	
3	b	296	
4	F	140	
5	E	414	

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Mol	Chain	Length	Quality of chain
6	D	686	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SF4	a	703	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 24799 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 CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	664	Total	C	N	O	S	0	0
			5013	3168	852	937	56		
1	a	446	Total	C	N	O	S	0	0
			3368	2133	570	632	33		

- Molecule 2 is a protein called CoB–CoM heterodisulfide reductase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		
2	c	189	Total	C	N	O	S	0	0
			1498	936	271	278	13		

- Molecule 3 is a protein called CoB–CoM heterodisulfide reductase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		
3	b	296	Total	C	N	O	S	0	0
			2304	1470	387	426	21		

- Molecule 4 is a protein called F420-non-reducing hydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	137	Total	C	N	O	S	0	0
			1073	687	188	186	12		

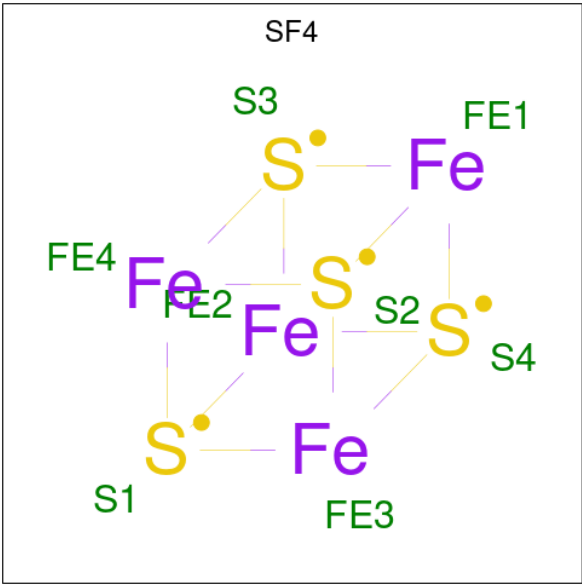
- Molecule 5 is a protein called Formate dehydrogenase, beta subunit (F420).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	411	Total	C	N	O	S	0	0
			3151	1985	542	589	35		

- Molecule 6 is a protein called Formate dehydrogenase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	D	549	4251	2691	737	795	28	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



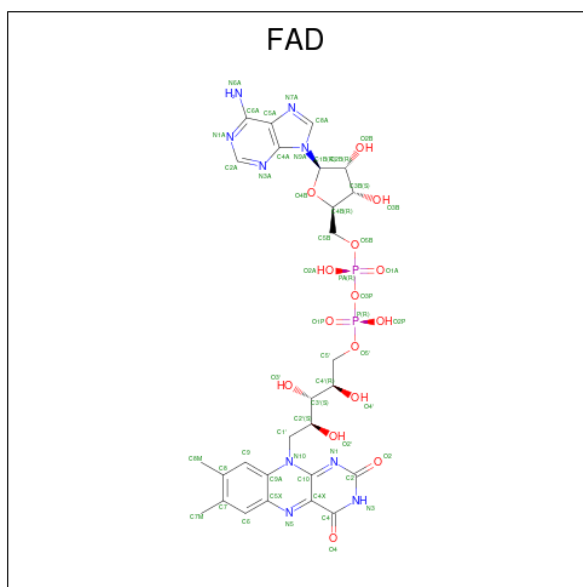
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
7	A	1	Total 8	Fe 4	S 4	0
7	A	1	Total 8	Fe 4	S 4	0
7	A	1	Total 8	Fe 4	S 4	0
7	A	1	Total 8	Fe 4	S 4	0
7	A	1	Total 8	Fe 4	S 4	0
7	A	1	Total 8	Fe 4	S 4	0
7	C	1	Total 8	Fe 4	S 4	0
7	C	1	Total 8	Fe 4	S 4	0
7	a	1	Total 8	Fe 4	S 4	0
7	a	1	Total 8	Fe 4	S 4	0

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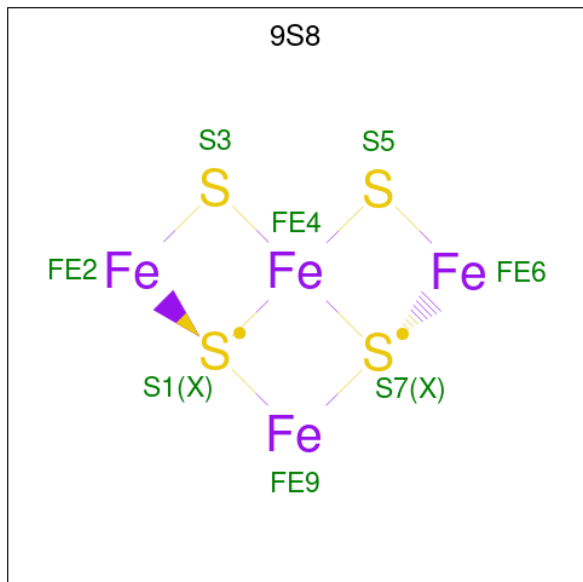
Mol	Chain	Residues	Atoms			AltConf
7	a	1	Total 8	Fe 4	S 4	0
7	c	1	Total 8	Fe 4	S 4	0
7	c	1	Total 8	Fe 4	S 4	0
7	E	1	Total 8	Fe 4	S 4	0
7	E	1	Total 8	Fe 4	S 4	0
7	E	1	Total 8	Fe 4	S 4	0
7	E	1	Total 8	Fe 4	S 4	0
7	D	1	Total 8	Fe 4	S 4	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total 53	C 27	N 9	O 15	P 2	0
8	a	1	Total 53	C 27	N 9	O 15	P 2	0
8	E	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 9 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).

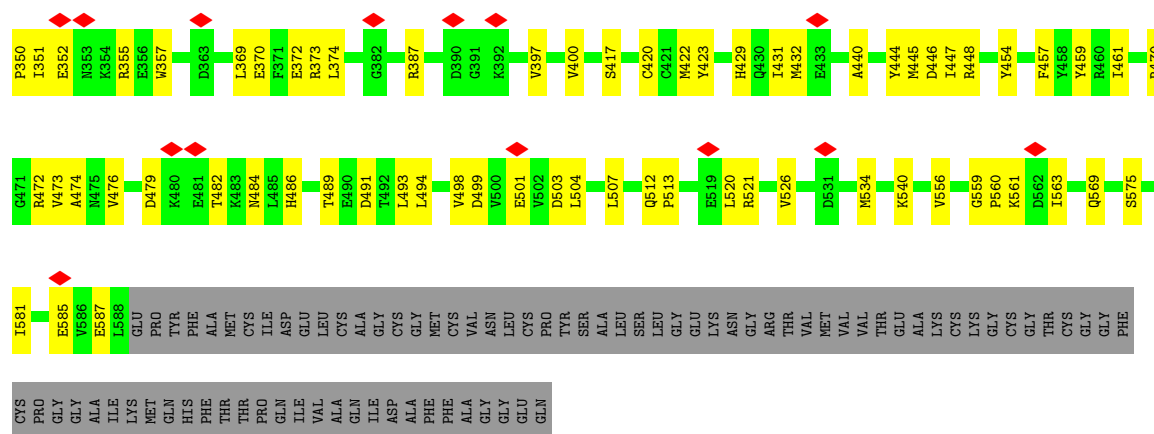


Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	Fe	S	0
			8	4	4	
9	B	1	Total	Fe	S	0
			8	4	4	
9	b	1	Total	Fe	S	0
			8	4	4	
9	b	1	Total	Fe	S	0
			8	4	4	

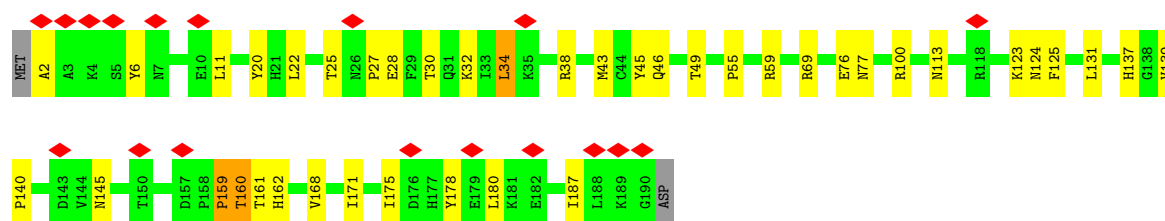
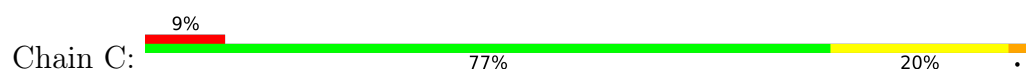
- Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



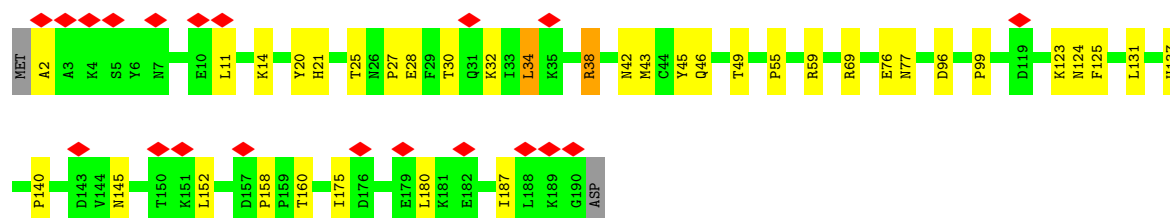
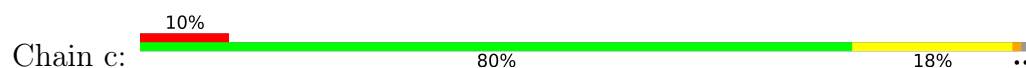
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
10	F	1	4	2	2	0



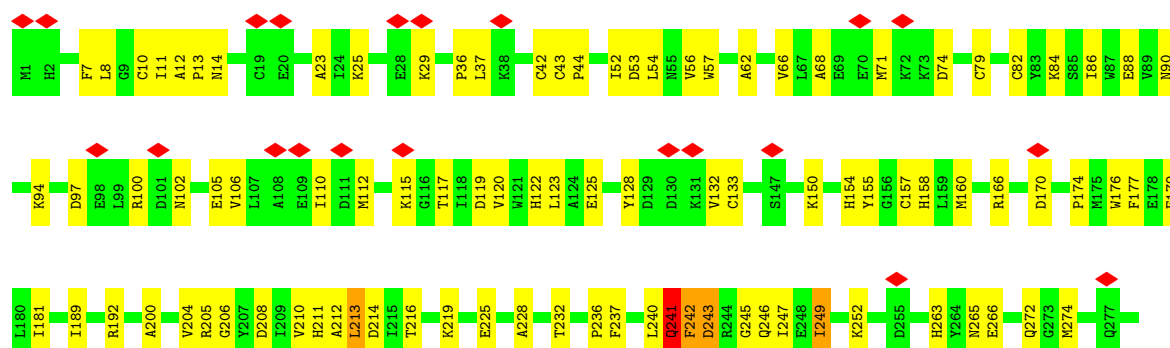
• Molecule 2: CoB-CoM heterodisulfide reductase subunit C

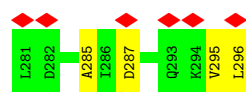


• Molecule 2: CoB-CoM heterodisulfide reductase subunit C

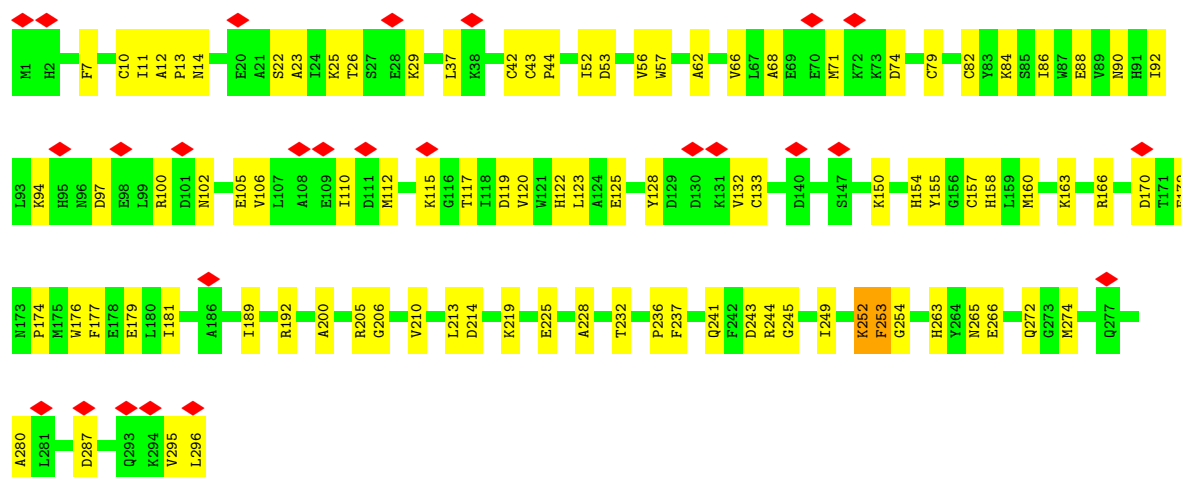


• Molecule 3: CoB-CoM heterodisulfide reductase subunit B

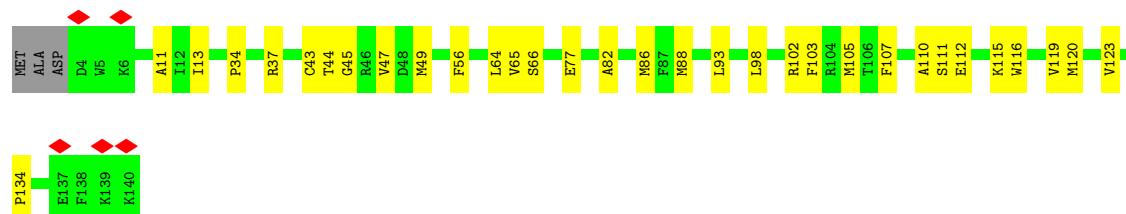
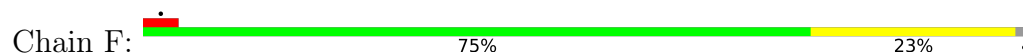




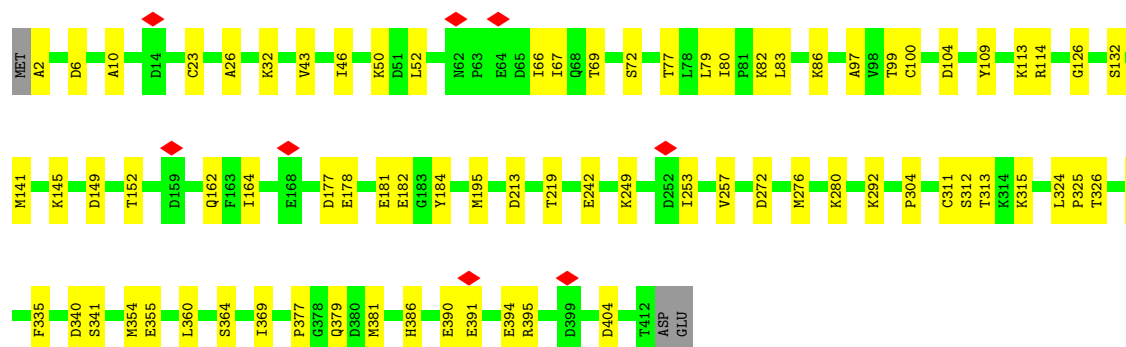
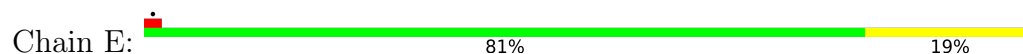
• Molecule 3: CoB–CoM heterodisulfide reductase subunit B



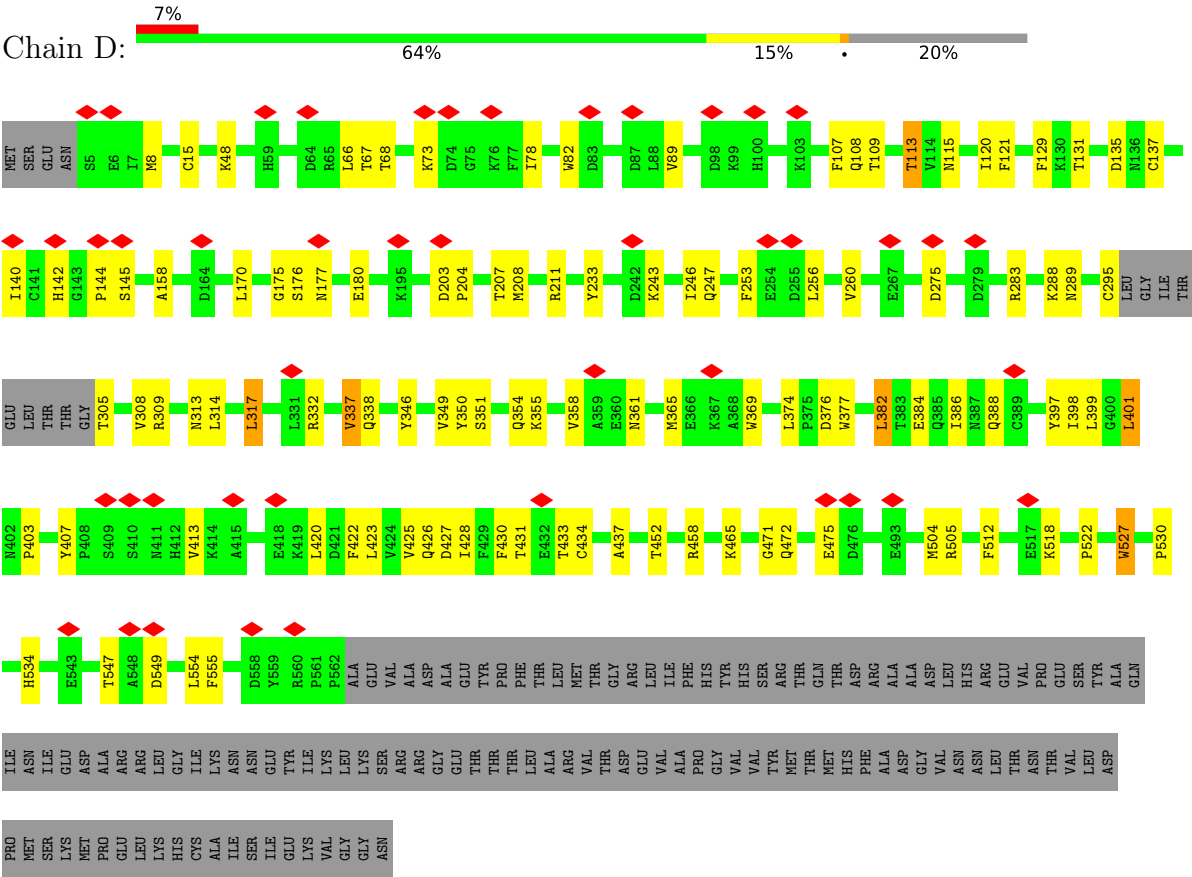
• Molecule 4: F420-non-reducing hydrogenase subunit D



• Molecule 5: Formate dehydrogenase, beta subunit (F420)



• Molecule 6: Formate dehydrogenase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	277450	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 K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	101.016	Depositor
Minimum map value	-70.139	Depositor
Average map value	0.005	Depositor
Map value standard deviation	1.185	Depositor
Recommended contour level	8	Depositor
Map size (Å)	361.584, 361.584, 361.584	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: 9S8, FES, SF4, FAD

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	0.28	0/5116	0.50	2/6925 (0.0%)
1	a	0.29	0/3435	0.50	0/4649
2	C	0.29	0/1529	0.53	1/2072 (0.0%)
2	c	0.19	0/1529	0.43	0/2072
3	B	0.43	3/2355 (0.1%)	0.66	5/3187 (0.2%)
3	b	0.40	3/2355 (0.1%)	0.62	2/3187 (0.1%)
4	F	0.27	0/1096	0.48	0/1474
5	E	0.24	0/3208	0.41	0/4314
6	D	0.33	0/4345	0.54	3/5889 (0.1%)
All	All	0.31	6/24968 (0.0%)	0.52	13/33769 (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
3	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	241	GLN	C-O	-7.47	1.15	1.24
3	B	243	ASP	C-O	6.94	1.32	1.24
3	B	241	GLN	C-O	-6.88	1.16	1.24
3	B	245	GLY	C-O	-5.88	1.16	1.23
3	b	245	GLY	C-O	-5.53	1.17	1.23
3	b	253	PHE	C-O	5.32	1.31	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	249	ILE	N-CA-C	-8.94	102.11	111.58
2	C	159	PRO	CB-CA-C	-7.35	103.09	113.09
1	A	591	TYR	CB-CA-C	-7.23	101.22	111.85
3	B	241	GLN	CA-C-O	-6.55	114.13	121.00
3	b	252	LYS	CA-C-N	-6.52	112.98	121.79
3	b	252	LYS	C-N-CA	-6.52	112.98	121.79
3	B	246	GLN	N-CA-C	-6.00	104.73	111.28
6	D	530	PRO	N-CA-C	5.85	121.24	113.40
6	D	337	VAL	N-CA-C	-5.71	103.79	111.44
6	D	527	TRP	N-CA-C	5.28	120.66	113.16
3	B	242	PHE	CA-C-O	-5.13	115.44	120.82
3	B	240	LEU	CA-C-O	-5.06	115.50	120.82
1	A	406	ARG	N-CA-C	-5.04	105.25	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	241	GLN	Mainchain

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	5013	0	4948	94	0
1	a	3368	0	3343	75	0
2	C	1498	0	1495	34	0
2	c	1498	0	1495	33	0
3	B	2304	0	2272	66	0
3	b	2304	0	2272	62	0
4	F	1073	0	1082	24	0
5	E	3151	0	3162	54	0
6	D	4251	0	4204	79	0
7	A	48	0	0	2	0
7	C	16	0	0	0	0
7	D	8	0	0	1	0
7	E	32	0	0	0	0
7	a	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	c	16	0	0	0	0
8	A	53	0	31	1	0
8	E	53	0	31	5	0
8	a	53	0	31	2	0
9	B	16	0	0	2	0
9	b	16	0	0	2	0
10	F	4	0	0	0	0
All	All	24799	0	24366	465	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 9.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:SER:HB2	1:a:575:SER:HB2	1.56	0.87
1:a:431:ILE:HD11	1:a:440:ALA:HB2	1.58	0.86
1:A:432:MET:HE3	1:A:440:ALA:H	1.46	0.78
6:D:427:ASP:OD2	6:D:428:ILE:N	2.20	0.74
5:E:355:GLU:OE2	6:D:48:LYS:NZ	2.20	0.74
2:c:175:ILE:HG23	2:c:180:LEU:HB3	1.69	0.73
2:C:175:ILE:HG23	2:C:180:LEU:HB3	1.70	0.73
3:B:66:VAL:HG23	3:B:112:MET:HE2	1.71	0.72
6:D:108:GLN:HG2	6:D:382:LEU:HD22	1.71	0.72
3:b:66:VAL:HG23	3:b:112:MET:HE2	1.71	0.72
6:D:158:ALA:O	6:D:458:ARG:NH1	2.23	0.72
6:D:113:THR:HG21	6:D:399:LEU:HD21	1.72	0.72
4:F:13:ILE:HG22	4:F:66:SER:HB3	1.73	0.70
1:a:556:VAL:HG13	1:a:560:PRO:HA	1.73	0.70
6:D:354:GLN:O	6:D:361:ASN:ND2	2.24	0.69
6:D:365:MET:O	6:D:369:TRP:HB2	1.92	0.69
6:D:144:PRO:HB2	6:D:305:THR:HG22	1.76	0.68
1:A:161:GLN:HG2	1:A:567:VAL:HG13	1.76	0.68
3:b:23:ALA:HA	3:b:265:ASN:HD22	1.59	0.68
6:D:465:LYS:NZ	6:D:475:GLU:OE2	2.24	0.68
1:A:226:LYS:HA	1:A:523:LYS:HD3	1.75	0.67
3:B:23:ALA:HA	3:B:265:ASN:HD22	1.59	0.67
3:B:192:ARG:NH1	3:B:225:GLU:OE1	2.28	0.67
1:a:153:VAL:HG11	1:a:520:LEU:HD11	1.75	0.67
3:b:295:VAL:HG23	3:b:296:LEU:HG	1.77	0.66
1:A:33:ALA:HA	1:A:36:LEU:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:LEU:HB3	6:D:8:MET:HE1	1.77	0.66
6:D:420:LEU:HD11	6:D:423:LEU:HB2	1.78	0.66
1:A:261:CYS:HA	7:A:706:SF4:S3	2.36	0.66
6:D:67:THR:HG23	6:D:68:THR:HG23	1.77	0.66
3:B:295:VAL:HG23	3:B:296:LEU:HG	1.77	0.65
3:b:192:ARG:NH1	3:b:225:GLU:OE1	2.28	0.65
3:B:157:CYS:HB2	9:B:302:9S8:S3	2.37	0.65
3:b:97:ASP:OD1	3:b:100:ARG:NH2	2.30	0.65
1:A:387:ARG:HD2	1:A:503:ASP:HB3	1.79	0.65
3:b:84:LYS:O	3:b:88:GLU:HB2	1.97	0.64
5:E:177:ASP:OD1	5:E:178:GLU:N	2.30	0.64
5:E:276:MET:HE1	5:E:364:SER:HB3	1.78	0.64
1:A:76:PRO:O	1:A:80:GLU:HB2	1.97	0.64
3:B:53:ASP:HB3	3:B:56:VAL:HG12	1.80	0.64
3:b:110:ILE:HG13	3:b:112:MET:HG2	1.79	0.64
3:B:84:LYS:O	3:B:88:GLU:HB2	1.97	0.64
6:D:142:HIS:CD2	6:D:332:ARG:HH11	2.16	0.64
3:b:157:CYS:HB2	9:b:302:9S8:S3	2.37	0.63
6:D:175:GLY:HA2	6:D:203:ASP:HA	1.80	0.63
3:B:97:ASP:OD1	3:B:100:ARG:NH2	2.30	0.63
3:B:110:ILE:HG13	3:B:112:MET:HG2	1.79	0.63
2:c:180:LEU:HD11	3:b:52:ILE:HD12	1.80	0.63
1:A:127:ARG:NH1	1:A:664:ALA:O	2.31	0.63
3:b:53:ASP:HB3	3:b:56:VAL:HG12	1.80	0.63
5:E:391:GLU:OE2	5:E:395:ARG:NH1	2.31	0.63
1:A:615:LEU:HD22	1:A:626:MET:SD	2.39	0.62
5:E:312:SER:HA	5:E:315:LYS:HD2	1.79	0.62
3:B:200:ALA:HA	3:B:205:ARG:HB2	1.82	0.62
3:b:213:LEU:HD13	3:b:249:ILE:HG13	1.82	0.62
3:b:84:LYS:HB2	3:b:158:HIS:HB3	1.82	0.62
5:E:79:LEU:HD21	5:E:304:PRO:HG3	1.80	0.62
1:A:474:ALA:HA	2:c:49:THR:HG23	1.82	0.62
3:B:84:LYS:HB2	3:B:158:HIS:HB3	1.82	0.62
5:E:2:ALA:N	5:E:6:ASP:OD2	2.32	0.62
6:D:177:ASN:HB3	6:D:180:GLU:HB2	1.81	0.62
1:a:277:ASN:O	1:a:281:MET:N	2.32	0.61
6:D:505:ARG:NH1	6:D:512:PHE:O	2.33	0.61
1:A:431:ILE:HD11	1:A:440:ALA:HB2	1.82	0.61
5:E:113:LYS:NZ	5:E:377:PRO:O	2.29	0.61
3:B:7:PHE:HA	3:B:37:LEU:HD12	1.83	0.61
3:b:7:PHE:HA	3:b:37:LEU:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:200:ALA:HA	3:b:205:ARG:HB2	1.82	0.61
1:A:243:ARG:NE	1:A:302:THR:OG1	2.35	0.60
1:A:473:VAL:HA	1:A:489:THR:HB	1.81	0.60
2:C:160:THR:HG23	2:C:162:HIS:HB2	1.82	0.60
6:D:89:VAL:HA	6:D:422:PHE:HZ	1.66	0.60
3:B:213:LEU:HD13	3:B:249:ILE:HG13	1.84	0.60
1:a:432:MET:HE3	1:a:440:ALA:H	1.67	0.60
4:F:82:ALA:O	4:F:86:MET:HG2	2.00	0.60
1:A:444:TYR:CD1	1:A:447:ILE:HG12	2.36	0.60
8:E:505:FAD:O4'	8:E:505:FAD:O2'	2.16	0.60
6:D:108:GLN:HG2	6:D:382:LEU:CD2	2.31	0.60
1:a:155:GLY:N	1:a:177:GLU:OE1	2.31	0.59
2:C:27:PRO:O	2:C:30:THR:HG22	2.03	0.59
3:b:88:GLU:OE2	3:b:166:ARG:NH1	2.35	0.59
1:A:387:ARG:NH1	1:A:484:ASN:OD1	2.35	0.59
1:A:420:CYS:HA	1:A:423:TYR:CE1	2.37	0.59
6:D:89:VAL:HA	6:D:422:PHE:CZ	2.38	0.59
3:B:88:GLU:OE2	3:B:166:ARG:NH1	2.35	0.58
6:D:66:LEU:HD11	6:D:430:PHE:HB2	1.85	0.58
1:a:486:HIS:NE2	1:a:501:GLU:OE2	2.37	0.58
2:c:27:PRO:O	2:c:30:THR:HG22	2.03	0.58
2:c:124:ASN:OD1	2:c:125:PHE:N	2.37	0.58
1:A:96:ARG:NH2	1:A:138:ASP:OD1	2.36	0.58
2:C:124:ASN:OD1	2:C:125:PHE:N	2.37	0.57
3:B:177:PHE:O	3:B:181:ILE:HD12	2.05	0.57
1:a:276:PRO:HB3	1:a:282:GLY:HA2	1.86	0.57
4:F:43:CYS:O	4:F:44:THR:HG22	2.05	0.57
6:D:135:ASP:HB3	6:D:382:LEU:CD2	2.34	0.57
6:D:246:ILE:HD11	6:D:317:LEU:HD23	1.86	0.57
1:a:444:TYR:CD2	1:a:447:ILE:HG12	2.40	0.57
3:b:160:MET:HE1	3:b:174:PRO:HB3	1.87	0.57
6:D:309:ARG:HD3	6:D:555:PHE:HD2	1.69	0.57
2:C:11:LEU:HD22	3:b:210:VAL:HG11	1.86	0.57
3:B:160:MET:HE1	3:B:174:PRO:HB3	1.87	0.57
2:C:137:HIS:HA	3:B:42:CYS:HB2	1.86	0.56
1:a:143:SER:N	1:a:585:GLU:OE2	2.38	0.56
1:a:445:MET:HE1	1:a:472:ARG:HD2	1.86	0.56
1:A:186:MET:HG2	1:A:203:LEU:HD22	1.87	0.56
2:C:45:TYR:HE2	1:a:445:MET:SD	2.28	0.56
1:A:110:HIS:HA	1:A:114:MET:HE3	1.87	0.56
3:b:177:PHE:O	3:b:181:ILE:HD12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:180:LEU:HD11	3:B:52:ILE:HD12	1.87	0.56
2:c:137:HIS:HA	3:b:42:CYS:HB2	1.88	0.56
3:b:154:HIS:ND1	3:b:219:LYS:HE2	2.21	0.56
3:B:154:HIS:ND1	3:B:219:LYS:HE2	2.21	0.56
6:D:346:TYR:HB3	6:D:349:VAL:HG22	1.86	0.56
6:D:386:ILE:HG13	6:D:407:TYR:HE2	1.71	0.56
1:a:261:CYS:HA	7:a:703:SF4:S3	2.46	0.55
5:E:311:CYS:SG	5:E:313:THR:OG1	2.59	0.55
3:B:10:CYS:HB2	9:B:301:9S8:S3	2.47	0.55
1:A:49:CYS:HB3	7:A:703:SF4:S3	2.47	0.55
3:b:66:VAL:CG2	3:b:112:MET:HE2	2.37	0.55
5:E:213:ASP:OD1	5:E:213:ASP:N	2.40	0.55
5:E:340:ASP:OD1	5:E:341:SER:N	2.40	0.55
3:b:123:LEU:HD23	3:b:265:ASN:HD21	1.71	0.55
4:F:134:PRO:HB3	5:E:280:LYS:HE3	1.88	0.55
1:a:184:GLY:O	1:a:187:SER:OG	2.24	0.55
5:E:177:ASP:O	5:E:181:GLU:HG2	2.07	0.55
3:B:123:LEU:HD23	3:B:265:ASN:HD21	1.71	0.54
3:B:189:ILE:HD11	3:B:228:ALA:HB2	1.90	0.54
6:D:350:TYR:HB3	6:D:365:MET:HE3	1.90	0.54
1:A:457:PHE:O	1:A:461:ILE:HG12	2.06	0.54
3:B:66:VAL:CG2	3:B:112:MET:HE2	2.37	0.54
4:F:43:CYS:C	4:F:45:GLY:H	2.15	0.54
3:B:128:TYR:HD1	3:B:128:TYR:O	1.91	0.54
1:A:193:PHE:O	1:a:540:LYS:NZ	2.23	0.54
2:C:145:ASN:HD22	3:B:14:ASN:C	2.16	0.54
1:a:400:VAL:HG22	1:a:473:VAL:HG21	1.90	0.54
2:c:145:ASN:HD22	3:b:14:ASN:C	2.15	0.54
3:b:128:TYR:HD1	3:b:128:TYR:O	1.91	0.54
3:b:189:ILE:HD11	3:b:228:ALA:HB2	1.90	0.54
3:b:10:CYS:HB2	9:b:301:9S8:S3	2.47	0.53
5:E:100:CYS:HB2	5:E:104:ASP:HB2	1.89	0.53
6:D:233:TYR:HB2	6:D:260:VAL:HG22	1.91	0.53
1:a:267:CYS:HB3	7:a:703:SF4:S4	2.49	0.53
1:A:611:PRO:HG3	4:F:77:GLU:HB2	1.90	0.53
3:B:128:TYR:CE2	3:B:176:TRP:HB2	2.44	0.53
1:A:233:ASN:HB2	1:A:336:LYS:NZ	2.23	0.53
5:E:145:LYS:HE3	5:E:182:GLU:HG2	1.91	0.53
1:A:20:ILE:HG22	1:A:26:ILE:HD11	1.90	0.53
3:b:128:TYR:CE2	3:b:176:TRP:HB2	2.44	0.53
6:D:425:VAL:HG12	6:D:425:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:90:ASN:OD1	3:B:94:LYS:HE3	2.09	0.52
6:D:384:GLU:O	6:D:388:GLN:HG2	2.10	0.52
2:C:49:THR:HG23	1:a:474:ALA:HA	1.91	0.52
3:b:44:PRO:HB2	3:b:57:TRP:HD1	1.74	0.52
6:D:137:CYS:HB3	6:D:401:LEU:HD11	1.90	0.52
1:A:124:ASP:OD1	1:A:127:ARG:NH2	2.43	0.52
6:D:431:THR:N	6:D:434:CYS:SG	2.81	0.52
5:E:249:LYS:O	5:E:253:ILE:HD12	2.10	0.52
1:A:226:LYS:HG2	1:A:237:THR:HB	1.92	0.52
3:B:44:PRO:HB2	3:B:57:TRP:HD1	1.74	0.52
6:D:309:ARG:HD3	6:D:555:PHE:CD2	2.44	0.52
1:a:154:GLY:O	1:a:159:GLY:HA3	2.10	0.51
5:E:50:LYS:HD2	6:D:522:PRO:HG3	1.91	0.51
6:D:135:ASP:HB3	6:D:382:LEU:HD23	1.92	0.51
3:b:90:ASN:OD1	3:b:94:LYS:HE3	2.09	0.51
4:F:65:VAL:O	4:F:105:MET:HA	2.10	0.51
1:A:179:THR:OG1	1:A:181:THR:O	2.29	0.51
1:A:536:GLU:CD	1:A:558:GLN:HE21	2.19	0.51
6:D:518:LYS:NZ	6:D:534:HIS:O	2.40	0.51
3:B:79:CYS:HB3	3:B:82:CYS:HB2	1.92	0.51
1:a:493:LEU:O	1:a:494:LEU:HB3	2.11	0.51
4:F:86:MET:SD	4:F:103:PHE:HZ	2.33	0.51
6:D:288:LYS:HE2	6:D:289:ASN:ND2	2.26	0.51
1:a:201:CYS:SG	4:F:110:ALA:HB3	2.50	0.51
2:c:152:LEU:HD21	3:b:280:ALA:HB2	1.93	0.51
6:D:203:ASP:OD1	6:D:204:PRO:HD2	2.11	0.51
6:D:203:ASP:OD2	6:D:207:THR:OG1	2.28	0.51
2:C:161:THR:HB	2:C:168:VAL:HG22	1.93	0.50
3:b:79:CYS:HB3	3:b:82:CYS:HB2	1.92	0.50
1:A:224:VAL:HA	1:A:238:LEU:HD23	1.93	0.50
3:b:74:ASP:HB2	3:b:119:ASP:O	2.12	0.50
1:A:358:GLY:HA3	1:A:362:PHE:CD2	2.47	0.50
5:E:10:ALA:HA	5:E:242:GLU:O	2.11	0.50
2:c:38:ARG:HH12	3:b:92:ILE:HG12	1.76	0.50
1:A:142:LYS:HG3	1:A:588:LEU:HD12	1.93	0.49
1:a:387:ARG:HD3	1:a:503:ASP:HB3	1.93	0.49
6:D:170:LEU:O	6:D:170:LEU:HD23	2.12	0.49
1:A:575:SER:OG	1:a:165:ASP:OD1	2.30	0.49
3:B:74:ASP:HB2	3:B:119:ASP:O	2.12	0.49
3:B:263:HIS:HB3	3:B:266:GLU:OE1	2.12	0.49
1:a:349:PHE:CD1	1:a:350:PRO:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:THR:HB	1:A:656:PRO:HD2	1.94	0.49
2:C:161:THR:HG21	2:C:171:ILE:HD11	1.94	0.49
1:a:351:ILE:HD12	1:a:507:LEU:HD12	1.95	0.49
1:a:429:HIS:HB2	1:a:461:ILE:HD12	1.95	0.49
1:a:473:VAL:HA	1:a:489:THR:HB	1.93	0.49
1:A:320:ASP:HA	1:A:322:LYS:HZ3	1.78	0.49
3:B:29:LYS:HD3	3:B:272:GLN:CD	2.38	0.49
3:b:263:HIS:HB3	3:b:266:GLU:OE1	2.12	0.49
2:C:55:PRO:O	2:C:59:ARG:NH1	2.46	0.49
2:c:55:PRO:O	2:c:59:ARG:NH1	2.46	0.49
3:b:29:LYS:HD3	3:b:272:GLN:CD	2.38	0.49
4:F:112:GLU:HB3	4:F:115:LYS:HB3	1.94	0.49
5:E:46:ILE:HD11	5:E:80:ILE:HD11	1.95	0.49
5:E:272:ASP:HB3	5:E:360:LEU:HD11	1.95	0.49
1:A:605:MET:HE3	5:E:114:ARG:HG2	1.93	0.49
4:F:88:MET:SD	5:E:386:HIS:NE2	2.74	0.49
6:D:107:PHE:CZ	6:D:129:PHE:HZ	2.30	0.49
2:c:20:TYR:HH	2:c:25:THR:HG1	1.55	0.48
6:D:420:LEU:HD21	6:D:423:LEU:HD13	1.95	0.48
1:A:242:ALA:N	1:A:330:ASP:OD1	2.46	0.48
4:F:107:PHE:O	4:F:115:LYS:NZ	2.46	0.48
1:A:555:GLY:H	1:A:569:GLN:HG2	1.78	0.48
3:B:25:LYS:HE2	3:B:274:MET:HG2	1.96	0.48
3:B:208:ASP:OD1	3:B:211:HIS:HB2	2.14	0.48
3:B:247:ILE:HG13	3:B:285:ALA:HB1	1.94	0.48
2:C:159:PRO:HG3	3:B:36:PRO:HB3	1.95	0.48
1:A:51:THR:OG1	1:A:52:PRO:HD3	2.14	0.48
1:A:605:MET:CE	5:E:114:ARG:HG2	2.43	0.48
2:C:30:THR:O	2:C:34:LEU:HD12	2.14	0.48
1:a:179:THR:OG1	1:a:181:THR:O	2.32	0.48
1:a:420:CYS:HA	1:a:423:TYR:CE1	2.49	0.48
3:b:22:SER:O	3:b:26:THR:OG1	2.25	0.48
3:b:25:LYS:HE2	3:b:274:MET:HG2	1.96	0.48
1:a:186:MET:HE3	1:a:563:ILE:HD13	1.96	0.48
1:a:499:ASP:HB3	2:c:21:HIS:CE1	2.49	0.48
3:B:68:ALA:HA	3:B:71:MET:HB3	1.96	0.48
6:D:107:PHE:CE2	6:D:129:PHE:HZ	2.31	0.48
5:E:100:CYS:HB2	5:E:104:ASP:CB	2.44	0.48
5:E:276:MET:HE1	5:E:364:SER:CB	2.41	0.48
1:A:425:LEU:HB3	1:A:461:ILE:HG13	1.95	0.47
5:E:23:CYS:O	5:E:219:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:142:HIS:CE1	6:D:332:ARG:HA	2.49	0.47
3:B:241:GLN:O	3:B:242:PHE:C	2.56	0.47
1:A:243:ARG:NH2	1:A:300:ILE:HB	2.28	0.47
4:F:56:PHE:CE2	4:F:93:LEU:HD21	2.49	0.47
3:B:287:ASP:OD1	3:B:287:ASP:N	2.47	0.47
3:b:287:ASP:OD1	3:b:287:ASP:N	2.47	0.47
3:b:68:ALA:HA	3:b:71:MET:HB3	1.96	0.47
3:B:204:VAL:HG12	3:B:212:ALA:HB2	1.96	0.47
1:a:422:MET:HE2	1:a:454:TYR:CD1	2.49	0.47
1:a:457:PHE:O	1:a:461:ILE:HG12	2.15	0.47
2:c:28:GLU:O	2:c:32:LYS:HG3	2.15	0.47
2:c:30:THR:O	2:c:34:LEU:HD12	2.14	0.47
1:A:417:SER:HB2	1:A:420:CYS:SG	2.55	0.47
5:E:66:ILE:O	5:E:69:THR:OG1	2.32	0.47
1:A:556:VAL:HG13	1:A:560:PRO:HA	1.95	0.47
6:D:313:ASN:ND2	6:D:555:PHE:O	2.48	0.47
2:C:139:VAL:HB	3:B:10:CYS:HB3	1.97	0.47
6:D:121:PHE:HE2	6:D:397:TYR:CD2	2.33	0.47
2:c:124:ASN:HD22	3:b:206:GLY:C	2.22	0.46
3:b:11:ILE:HD12	3:b:237:PHE:HD1	1.80	0.46
1:a:521:ARG:HB2	1:a:534:MET:HE2	1.97	0.46
2:c:131:LEU:HD22	2:c:140:PRO:HG2	1.97	0.46
6:D:115:ASN:ND2	6:D:452:THR:OG1	2.49	0.46
5:E:77:THR:HG22	5:E:132:SER:HB3	1.97	0.46
1:A:541:LEU:HD12	1:a:202:ILE:HG22	1.97	0.46
1:A:665:PHE:CE1	4:F:37:ARG:HD3	2.50	0.46
2:C:28:GLU:O	2:C:32:LYS:HG3	2.15	0.46
3:B:86:ILE:HG22	3:B:120:VAL:HG21	1.98	0.46
3:b:102:ASN:O	3:b:106:VAL:HG23	2.16	0.46
3:B:11:ILE:HD12	3:B:237:PHE:HD1	1.80	0.46
5:E:292:LYS:O	5:E:354:MET:HG3	2.14	0.46
6:D:423:LEU:HB3	6:D:437:ALA:HA	1.97	0.46
1:a:431:ILE:HG13	1:a:432:MET:N	2.30	0.46
6:D:275:ASP:OD1	6:D:275:ASP:N	2.48	0.46
3:B:155:TYR:CZ	3:B:177:PHE:HB3	2.51	0.46
1:A:244:GLY:HA3	1:A:303:VAL:CG1	2.45	0.46
5:E:332:LEU:HD23	5:E:335:PHE:HD2	1.81	0.46
6:D:253:PHE:HE1	6:D:317:LEU:HD21	1.81	0.46
6:D:332:ARG:HB3	6:D:337:VAL:HG11	1.98	0.46
1:a:417:SER:HB2	1:a:420:CYS:SG	2.56	0.46
6:D:120:ILE:HD12	6:D:120:ILE:HA	1.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:NH2	1:A:104:GLU:OE2	2.32	0.46
1:A:357:TRP:HE1	1:A:473:VAL:CG1	2.29	0.46
1:a:188:GLN:O	1:a:373:ARG:NH1	2.42	0.46
6:D:170:LEU:HD11	6:D:283:ARG:HB3	1.97	0.46
1:A:223:GLU:OE1	1:A:223:GLU:N	2.49	0.45
1:a:372:GLU:OE1	8:a:702:FAD:H6	2.16	0.45
5:E:26:ALA:N	8:E:505:FAD:O2P	2.49	0.45
5:E:195:MET:HE1	5:E:379:GLN:HE21	1.81	0.45
2:c:145:ASN:ND2	3:b:14:ASN:C	2.74	0.45
6:D:504:MET:HE3	6:D:504:MET:HB3	1.89	0.45
3:B:210:VAL:HG11	2:c:11:LEU:HD22	1.99	0.45
1:a:143:SER:HB3	1:a:587:GLU:HA	1.98	0.45
1:a:561:LYS:HE2	1:a:569:GLN:HG3	1.98	0.45
6:D:351:SER:O	6:D:354:GLN:HG3	2.16	0.45
1:A:390:ASP:OD1	1:A:390:ASP:N	2.48	0.45
1:A:498:VAL:HG23	2:C:20:TYR:HD2	1.82	0.45
1:a:244:GLY:HA3	1:a:303:VAL:HG12	1.98	0.45
1:a:512:GLN:HG2	1:a:513:PRO:HD2	1.98	0.45
5:E:340:ASP:HA	5:E:369:ILE:HG21	1.98	0.45
1:A:521:ARG:HB3	1:A:534:MET:HE2	1.99	0.45
2:C:131:LEU:HD22	2:C:140:PRO:HG2	1.98	0.45
4:F:49:MET:HE1	5:E:386:HIS:NE2	2.32	0.45
3:B:102:ASN:O	3:B:106:VAL:HG23	2.16	0.45
1:a:222:THR:HG22	1:a:240:LYS:HA	1.99	0.45
1:a:281:MET:HE1	1:a:369:LEU:HB3	1.99	0.45
3:b:12:ALA:HB3	3:b:13:PRO:HD3	1.98	0.45
5:E:162:GLN:HG2	5:E:164:ILE:HD11	1.98	0.45
1:A:88:LYS:HD3	1:A:94:PRO:HG3	1.99	0.45
1:A:639:CYS:HB2	1:A:648:ILE:HD13	1.98	0.45
2:C:160:THR:OG1	2:C:161:THR:N	2.50	0.45
3:B:12:ALA:HB3	3:B:13:PRO:HD3	1.98	0.45
3:b:86:ILE:HG22	3:b:120:VAL:HG21	1.98	0.45
2:C:123:LYS:NZ	2:C:187:ILE:O	2.50	0.45
1:a:397:VAL:HA	1:a:504:LEU:O	2.17	0.45
3:b:155:TYR:CZ	3:b:177:PHE:HB3	2.51	0.45
4:F:11:ALA:HA	4:F:64:LEU:O	2.17	0.45
6:D:403:PRO:HD2	6:D:433:THR:HG21	1.99	0.45
5:E:253:ILE:O	5:E:257:VAL:HG23	2.17	0.44
6:D:15:CYS:HB3	7:D:701:SF4:S3	2.56	0.44
1:A:429:HIS:HB2	1:A:461:ILE:CD1	2.47	0.44
2:c:123:LYS:NZ	2:c:187:ILE:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:b:123:LEU:CD2	3:b:265:ASN:HD21	2.30	0.44
5:E:43:VAL:HG22	5:E:97:ALA:HB3	2.00	0.44
5:E:82:LYS:O	5:E:86:LYS:HG3	2.17	0.44
5:E:390:GLU:O	5:E:394:GLU:HG2	2.17	0.44
2:C:20:TYR:OH	2:C:25:THR:OG1	2.34	0.44
4:F:64:LEU:HD22	4:F:123:VAL:HG21	2.00	0.44
1:A:472:ARG:NH1	2:c:99:PRO:HG3	2.33	0.44
1:A:494:LEU:O	1:A:496:ARG:HG3	2.18	0.44
1:A:151:MET:HB2	1:A:337:VAL:HG11	2.00	0.44
1:A:244:GLY:HA3	1:A:303:VAL:HG12	1.99	0.44
2:C:2:ALA:N	3:b:214:ASP:OD2	2.51	0.44
1:a:357:TRP:HD1	1:a:476:VAL:HG23	1.82	0.44
6:D:73:LYS:HD2	6:D:78:ILE:HG13	2.00	0.44
1:A:109:VAL:HG23	1:A:110:HIS:CE1	2.53	0.44
2:C:76:GLU:O	2:C:77:ASN:HB2	2.18	0.44
3:B:43:CYS:SG	3:B:82:CYS:HA	2.58	0.44
1:a:281:MET:HE3	1:a:370:GLU:HG3	1.99	0.44
4:F:93:LEU:HD23	4:F:98:LEU:HD23	2.00	0.44
1:A:114:MET:SD	4:F:34:PRO:HD3	2.57	0.43
1:a:482:THR:O	1:a:484:ASN:N	2.46	0.43
5:E:32:LYS:HA	5:E:66:ILE:HD12	2.00	0.43
1:a:155:GLY:O	1:a:160:MET:HG3	2.17	0.43
5:E:324:LEU:HD12	5:E:324:LEU:HA	1.71	0.43
1:a:521:ARG:HG3	1:a:526:VAL:HB	2.00	0.43
6:D:131:THR:HG1	6:D:377:TRP:HH2	1.64	0.43
1:A:445:MET:SD	2:c:45:TYR:HE2	2.41	0.43
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.73	0.43
2:C:6:TYR:CD1	3:b:253:PHE:HB3	2.54	0.43
2:C:46:GLN:O	1:a:470:ARG:NH1	2.49	0.43
3:B:214:ASP:OD2	2:c:2:ALA:N	2.52	0.43
4:F:119:VAL:HG12	4:F:120:MET:HE2	1.99	0.43
6:D:145:SER:HA	6:D:308:VAL:HG11	2.01	0.43
6:D:547:THR:OG1	6:D:549:ASP:O	2.33	0.43
3:b:102:ASN:O	3:b:105:GLU:HG3	2.18	0.43
1:A:500:VAL:HG13	2:C:22:LEU:HD11	2.01	0.43
3:b:43:CYS:SG	3:b:82:CYS:HA	2.58	0.43
6:D:82:TRP:NE1	6:D:472:GLN:O	2.44	0.43
6:D:355:LYS:O	6:D:358:VAL:HG22	2.19	0.43
1:A:375:ILE:HD11	1:A:430:GLN:HB3	2.01	0.43
1:A:476:VAL:CG1	1:A:485:LEU:HD12	2.49	0.43
3:B:102:ASN:O	3:B:105:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:446:ASP:O	1:a:448:ARG:HG3	2.18	0.43
5:E:67:ILE:HD12	5:E:67:ILE:H	1.82	0.43
5:E:276:MET:HE2	5:E:360:LEU:HG	2.00	0.43
1:A:489:THR:OG1	1:A:490:GLU:N	2.52	0.43
1:a:491:ASP:HB2	1:a:498:VAL:HG21	2.01	0.43
3:B:115:LYS:HG3	3:B:117:THR:HG23	2.01	0.43
3:b:170:ASP:OD1	3:b:170:ASP:N	2.52	0.43
4:F:102:ARG:HG2	4:F:102:ARG:HH11	1.84	0.43
6:D:142:HIS:ND1	6:D:332:ARG:HA	2.34	0.43
1:A:153:VAL:HG11	1:A:520:LEU:HD21	2.01	0.43
1:A:494:LEU:HB2	2:C:69:ARG:HG2	2.00	0.43
3:B:123:LEU:CD2	3:B:265:ASN:HD21	2.30	0.43
1:a:281:MET:HE1	1:a:369:LEU:CB	2.48	0.43
2:c:96:ASP:OD1	3:b:163:LYS:HG3	2.19	0.43
6:D:256:LEU:HB2	6:D:554:LEU:CD1	2.49	0.43
2:C:124:ASN:HD22	3:B:206:GLY:C	2.27	0.42
4:F:116:TRP:O	4:F:120:MET:HG2	2.19	0.42
1:A:556:VAL:HA	1:A:559:GLY:O	2.19	0.42
3:B:79:CYS:SG	3:B:236:PRO:HD2	2.59	0.42
1:a:271:CYS:HB3	1:a:287:LYS:HB3	2.00	0.42
1:a:479:ASP:OD2	1:a:486:HIS:HE1	2.02	0.42
1:a:352:GLU:OE2	1:a:355:ARG:NH1	2.52	0.42
5:E:100:CYS:O	5:E:126:GLY:HA2	2.19	0.42
3:B:62:ALA:O	3:B:66:VAL:HG13	2.19	0.42
5:E:99:THR:HG21	8:E:505:FAD:H1B	2.01	0.42
6:D:208:MET:HA	6:D:211:ARG:HD2	2.00	0.42
1:A:95:PHE:CD2	1:A:139:LEU:HB2	2.54	0.42
1:A:538:HIS:CE1	1:a:202:ILE:HG21	2.55	0.42
3:B:170:ASP:OD1	3:B:170:ASP:N	2.52	0.42
2:c:76:GLU:O	2:c:77:ASN:HB2	2.18	0.42
1:A:192:THR:HA	8:A:702:FAD:O4	2.20	0.42
1:A:432:MET:HE1	1:A:465:GLY:O	2.20	0.42
1:a:226:LYS:HB3	1:a:237:THR:CG2	2.48	0.42
1:a:397:VAL:HG23	1:a:504:LEU:HB3	2.02	0.42
1:a:459:TYR:CE1	2:c:43:MET:HE2	2.55	0.42
6:D:332:ARG:HB3	6:D:337:VAL:CG1	2.50	0.42
3:B:132:VAL:HG12	3:B:133:CYS:H	1.85	0.42
3:b:79:CYS:SG	3:b:236:PRO:HD2	2.59	0.42
5:E:52:LEU:H	5:E:52:LEU:HD23	1.85	0.42
6:D:121:PHE:HE2	6:D:397:TYR:HD2	1.66	0.42
6:D:243:LYS:O	6:D:247:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:167:ALA:HB2	1:a:216:ILE:HG13	2.02	0.42
3:b:132:VAL:HG12	3:b:133:CYS:H	1.85	0.42
1:A:12:PHE:HB3	1:A:48:MET:HE1	2.02	0.42
3:B:219:LYS:HE3	3:B:219:LYS:HB3	1.93	0.42
1:a:192:THR:HA	8:a:702:FAD:O4	2.20	0.42
4:F:44:THR:HA	4:F:47:VAL:HG23	2.01	0.42
1:A:597:ASP:OD1	1:A:597:ASP:N	2.53	0.42
2:C:28:GLU:C	2:C:32:LYS:HZ3	2.28	0.42
2:C:178:TYR:OH	3:B:106:VAL:HG21	2.19	0.42
3:B:122:HIS:O	3:B:125:GLU:HB3	2.19	0.42
3:b:128:TYR:CD2	3:b:176:TRP:HB2	2.55	0.42
5:E:325:PRO:HA	6:D:208:MET:HE1	2.01	0.42
1:A:12:PHE:CB	1:A:48:MET:HE1	2.50	0.41
1:A:356:GLU:N	3:b:172:GLU:OE1	2.53	0.41
1:A:523:LYS:HE3	1:A:523:LYS:HB2	1.61	0.41
3:B:128:TYR:CD2	3:B:176:TRP:HB2	2.55	0.41
3:b:122:HIS:O	3:b:125:GLU:HB3	2.19	0.41
5:E:141:MET:HG2	5:E:184:TYR:HB3	2.02	0.41
1:A:154:GLY:O	1:A:159:GLY:HA3	2.20	0.41
1:A:281:MET:HB2	1:A:283:MET:HE2	2.02	0.41
2:c:158:PRO:C	2:c:160:THR:H	2.28	0.41
3:b:62:ALA:O	3:b:66:VAL:HG13	2.19	0.41
6:D:398:ILE:HD12	6:D:423:LEU:HD11	2.02	0.41
1:A:375:ILE:CD1	1:A:430:GLN:HB3	2.51	0.41
1:a:499:ASP:HB3	2:c:21:HIS:HE1	1.85	0.41
3:b:115:LYS:HG3	3:b:117:THR:HG23	2.01	0.41
3:b:243:ASP:O	3:b:244:ARG:C	2.63	0.41
1:A:139:LEU:HD11	1:A:652:HIS:HB2	2.02	0.41
1:A:470:ARG:NH1	2:c:46:GLN:O	2.44	0.41
3:B:208:ASP:OD1	2:c:14:LYS:NZ	2.40	0.41
1:a:283:MET:HE1	1:a:374:LEU:HG	2.01	0.41
2:c:28:GLU:C	2:c:32:LYS:HZ3	2.28	0.41
5:E:72:SER:HA	8:E:505:FAD:H8A	2.02	0.41
5:E:324:LEU:O	5:E:326:THR:N	2.53	0.41
1:A:354:LYS:HG2	1:A:357:TRP:CZ3	2.55	0.41
1:A:518:ASN:HA	1:A:521:ARG:HG3	2.03	0.41
2:C:43:MET:O	2:C:100:ARG:NH1	2.51	0.41
6:D:407:TYR:HB2	6:D:413:VAL:HG21	2.02	0.41
3:B:8:LEU:HA	3:B:8:LEU:HD23	1.77	0.41
5:E:109:TYR:HD1	5:E:381:MET:HG3	1.86	0.41
8:E:505:FAD:H9	8:E:505:FAD:H1'1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:ALA:HB2	1:A:650:MET:HE1	2.03	0.41
1:a:148:LYS:HA	1:a:581:ILE:HG23	2.02	0.41
1:a:164:LEU:HD23	1:a:164:LEU:HA	1.92	0.41
1:a:494:LEU:HB2	2:c:69:ARG:HG2	2.02	0.41
1:a:556:VAL:HA	1:a:559:GLY:O	2.21	0.41
6:D:67:THR:OG1	6:D:471:GLY:HA3	2.21	0.41
1:A:110:HIS:CD2	4:F:34:PRO:HB3	2.55	0.41
2:C:145:ASN:ND2	3:B:14:ASN:C	2.79	0.41
1:a:225:GLU:OE2	1:a:239:ARG:HD2	2.21	0.41
1:A:472:ARG:CZ	2:c:99:PRO:HG3	2.51	0.41
1:a:230:TYR:HD1	1:a:232:GLY:H	1.69	0.41
6:D:332:ARG:O	6:D:337:VAL:HG11	2.21	0.41
6:D:399:LEU:HG	6:D:426:GLN:NE2	2.36	0.41
6:D:422:PHE:HD1	6:D:422:PHE:O	2.04	0.41
3:B:177:PHE:HZ	3:B:232:THR:HG22	1.86	0.40
6:D:332:ARG:NE	6:D:338:GLN:OE1	2.54	0.40
2:C:113:ASN:HD21	3:B:54:LEU:HG	1.86	0.40
1:a:202:ILE:H	1:a:202:ILE:HG13	1.63	0.40
5:E:404:ASP:OD1	5:E:404:ASP:N	2.54	0.40
1:A:335:VAL:HG12	1:A:337:VAL:HG13	2.03	0.40
3:b:177:PHE:HZ	3:b:232:THR:HG22	1.86	0.40
6:D:109:THR:HA	6:D:399:LEU:HB3	2.03	0.40
1:a:203:LEU:HD12	1:a:203:LEU:HA	1.93	0.40
2:c:34:LEU:HD21	2:c:42:ASN:OD1	2.22	0.40
6:D:176:SER:HA	6:D:295:CYS:HB3	2.03	0.40
6:D:288:LYS:HE2	6:D:289:ASN:HD21	1.87	0.40
1:A:36:LEU:HD21	1:A:127:ARG:HA	2.02	0.40
1:A:636:CYS:SG	1:A:637:GLY:N	2.94	0.40
5:E:149:ASP:HB3	5:E:152:THR:HG23	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	662/671 (99%)	627 (95%)	34 (5%)	1 (0%)	44	77
1	a	444/671 (66%)	417 (94%)	27 (6%)	0	100	100
2	C	187/191 (98%)	180 (96%)	7 (4%)	0	100	100
2	c	187/191 (98%)	179 (96%)	8 (4%)	0	100	100
3	B	294/296 (99%)	280 (95%)	14 (5%)	0	100	100
3	b	294/296 (99%)	280 (95%)	13 (4%)	1 (0%)	37	70
4	F	135/140 (96%)	125 (93%)	10 (7%)	0	100	100
5	E	409/414 (99%)	393 (96%)	16 (4%)	0	100	100
6	D	545/686 (79%)	501 (92%)	44 (8%)	0	100	100
All	All	3157/3556 (89%)	2982 (94%)	173 (6%)	2 (0%)	50	81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	446	ASP
3	b	254	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/543 (98%)	530 (99%)	3 (1%)	84	93
1	a	358/543 (66%)	352 (98%)	6 (2%)	56	81
2	C	168/170 (99%)	165 (98%)	3 (2%)	54	80
2	c	168/170 (99%)	166 (99%)	2 (1%)	67	86
3	B	245/245 (100%)	239 (98%)	6 (2%)	44	74
3	b	245/245 (100%)	242 (99%)	3 (1%)	67	86
4	F	112/114 (98%)	111 (99%)	1 (1%)	75	89
5	E	338/341 (99%)	338 (100%)	0	100	100
6	D	454/571 (80%)	445 (98%)	9 (2%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2621/2942 (89%)	2588 (99%)	33 (1%)	64 85

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	CYS
1	A	405	SER
1	A	420	CYS
2	C	34	LEU
2	C	38	ARG
2	C	160	THR
3	B	150	LYS
3	B	179	GLU
3	B	213	LEU
3	B	216	THR
3	B	243	ASP
3	B	252	LYS
1	a	199	SER
1	a	202	ILE
1	a	204	THR
1	a	206	LYS
1	a	208	VAL
1	a	310	LYS
2	c	34	LEU
2	c	38	ARG
3	b	150	LYS
3	b	179	GLU
3	b	252	LYS
4	F	111	SER
6	D	113	THR
6	D	140	ILE
6	D	314	LEU
6	D	317	LEU
6	D	374	LEU
6	D	376	ASP
6	D	382	LEU
6	D	401	LEU
6	D	527	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	ASN
1	A	512	GLN
1	A	569	GLN
1	A	657	GLN
1	A	661	GLN
2	C	77	ASN
3	B	246	GLN
3	B	265	ASN
1	a	384	HIS
1	a	408	ASN
1	a	512	GLN
1	a	514	ASN
3	b	239	GLN
3	b	246	GLN
3	b	265	ASN
5	E	89	ASN
5	E	128	ASN
5	E	375	HIS
6	D	142	HIS
6	D	289	ASN
6	D	534	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 [i](#)

26 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
7	SF4	A	701	1	0,12,12	-	-	-		
7	SF4	C	201	2	0,12,12	-	-	-		
8	FAD	E	505	-	53,58,58	0.58	1 (1%)	68,89,89	0.53	2 (2%)
8	FAD	a	702	-	53,58,58	0.53	0	68,89,89	0.49	2 (2%)
7	SF4	A	703	1	0,12,12	-	-	-		
7	SF4	D	701	6	0,12,12	-	-	-		
7	SF4	a	703	1	0,12,12	-	-	-		
7	SF4	c	201	2	0,12,12	-	-	-		
7	SF4	A	706	1	0,12,12	-	-	-		
7	SF4	A	704	1	0,12,12	-	-	-		
9	9S8	b	301	3	2,10,10	1.06	0	-		
7	SF4	E	503	5	0,12,12	-	-	-		
7	SF4	a	704	1	0,12,12	-	-	-		
7	SF4	E	501	5	0,12,12	-	-	-		
9	9S8	B	301	3	2,10,10	1.07	0	-		
7	SF4	E	504	5	0,12,12	-	-	-		
9	9S8	B	302	3	2,10,10	1.11	0	-		
7	SF4	a	701	1	0,12,12	-	-	-		
8	FAD	A	702	-	53,58,58	0.53	0	68,89,89	0.48	2 (2%)
9	9S8	b	302	3	2,10,10	1.11	0	-		
7	SF4	c	202	2	0,12,12	-	-	-		
7	SF4	E	502	5	0,12,12	-	-	-		
7	SF4	A	707	1	0,12,12	-	-	-		
10	FES	F	201	4	0,4,4	-	-	-		
7	SF4	A	705	1	0,12,12	-	-	-		
7	SF4	C	202	2	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
7	SF4	A	701	1	-	-	0/6/5/5
7	SF4	C	201	2	-	-	0/6/5/5
8	FAD	E	505	-	-	15/30/50/50	0/6/6/6
8	FAD	a	702	-	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SF4	A	703	1	-	-	0/6/5/5
7	SF4	D	701	6	-	-	0/6/5/5
7	SF4	a	703	1	-	-	0/6/5/5
7	SF4	c	201	2	-	-	0/6/5/5
7	SF4	A	706	1	-	-	0/6/5/5
7	SF4	A	704	1	-	-	0/6/5/5
9	9S8	b	301	3	-	-	0/3/3/3
7	SF4	E	503	5	-	-	0/6/5/5
7	SF4	a	704	1	-	-	0/6/5/5
7	SF4	E	501	5	-	-	0/6/5/5
9	9S8	B	301	3	-	-	0/3/3/3
7	SF4	E	504	5	-	-	0/6/5/5
9	9S8	B	302	3	-	-	0/3/3/3
7	SF4	a	701	1	-	-	0/6/5/5
8	FAD	A	702	-	-	7/30/50/50	0/6/6/6
9	9S8	b	302	3	-	-	0/3/3/3
7	SF4	c	202	2	-	-	0/6/5/5
7	SF4	E	502	5	-	-	0/6/5/5
7	SF4	A	707	1	-	-	0/6/5/5
10	FES	F	201	4	-	-	0/1/1/1
7	SF4	A	705	1	-	-	0/6/5/5
7	SF4	C	202	2	-	-	0/6/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	505	FAD	P-O2P	-2.08	1.45	1.55

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	E	505	FAD	P-O3P-PA	-2.40	124.60	132.83
8	E	505	FAD	C5A-C6A-N6A	2.32	123.89	120.35
8	A	702	FAD	C5A-C6A-N6A	2.29	123.83	120.35
8	a	702	FAD	C5A-C6A-N6A	2.25	123.77	120.35
8	a	702	FAD	P-O3P-PA	-2.04	125.82	132.83
8	A	702	FAD	P-O3P-PA	-2.03	125.86	132.83

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	702	FAD	C5B-O5B-PA-O2A
8	A	702	FAD	P-O3P-PA-O5B
8	a	702	FAD	C5B-O5B-PA-O1A
8	a	702	FAD	C5B-O5B-PA-O2A
8	a	702	FAD	P-O3P-PA-O5B
8	E	505	FAD	C1'-C2'-C3'-O3'
8	E	505	FAD	C1'-C2'-C3'-C4'
8	E	505	FAD	O2'-C2'-C3'-O3'
8	E	505	FAD	O2'-C2'-C3'-C4'
8	E	505	FAD	C3'-C4'-C5'-O5'
8	E	505	FAD	O4'-C4'-C5'-O5'
8	E	505	FAD	C5'-O5'-P-O3P
8	A	702	FAD	O4B-C4B-C5B-O5B
8	A	702	FAD	C3B-C4B-C5B-O5B
8	a	702	FAD	O4B-C4B-C5B-O5B
8	a	702	FAD	C3B-C4B-C5B-O5B
8	E	505	FAD	C2'-C3'-C4'-O4'
8	A	702	FAD	C5B-O5B-PA-O3P
8	E	505	FAD	C4'-C5'-O5'-P
8	A	702	FAD	C5B-O5B-PA-O1A
8	E	505	FAD	C5'-O5'-P-O1P
8	E	505	FAD	C5'-O5'-P-O2P
8	E	505	FAD	O3'-C3'-C4'-O4'
8	a	702	FAD	C5B-O5B-PA-O3P
8	E	505	FAD	O3'-C3'-C4'-C5'
8	A	702	FAD	C4B-C5B-O5B-PA
8	a	702	FAD	PA-O3P-P-O1P
8	a	702	FAD	PA-O3P-P-O2P
8	E	505	FAD	C2'-C3'-C4'-C5'
8	a	702	FAD	C4B-C5B-O5B-PA
8	E	505	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

11 monomers are involved in 17 short contacts:

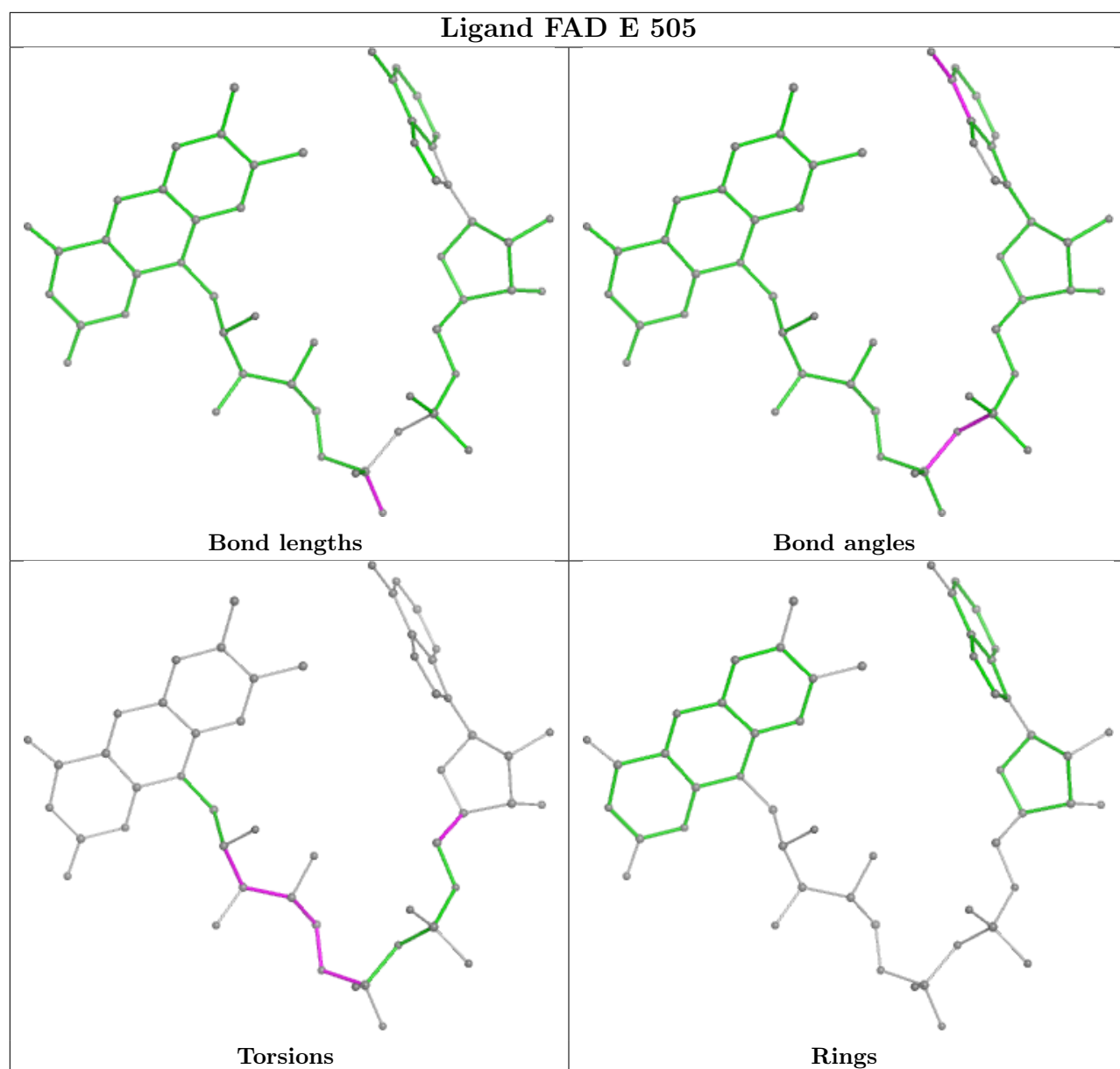
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	505	FAD	5	0
8	a	702	FAD	2	0
7	A	703	SF4	1	0
7	D	701	SF4	1	0
7	a	703	SF4	2	0
7	A	706	SF4	1	0
9	b	301	9S8	1	0

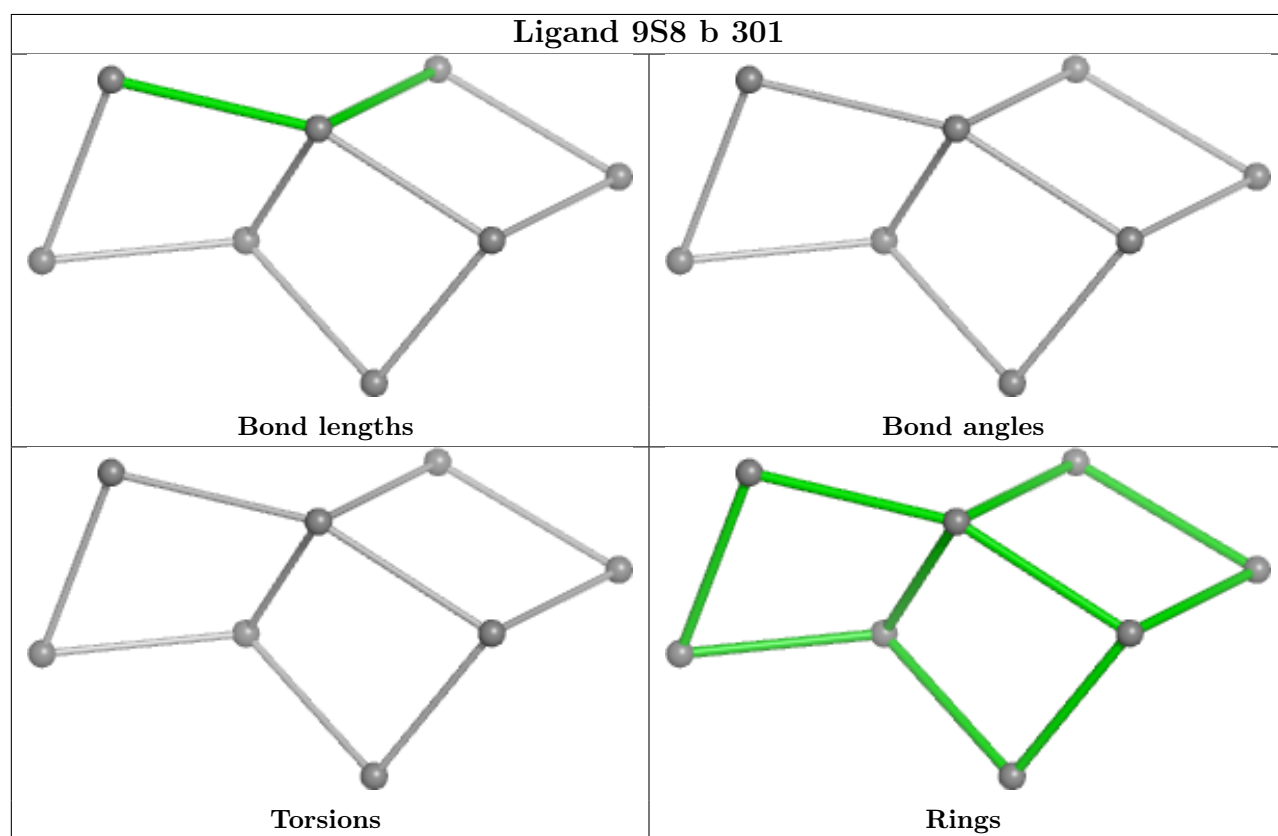
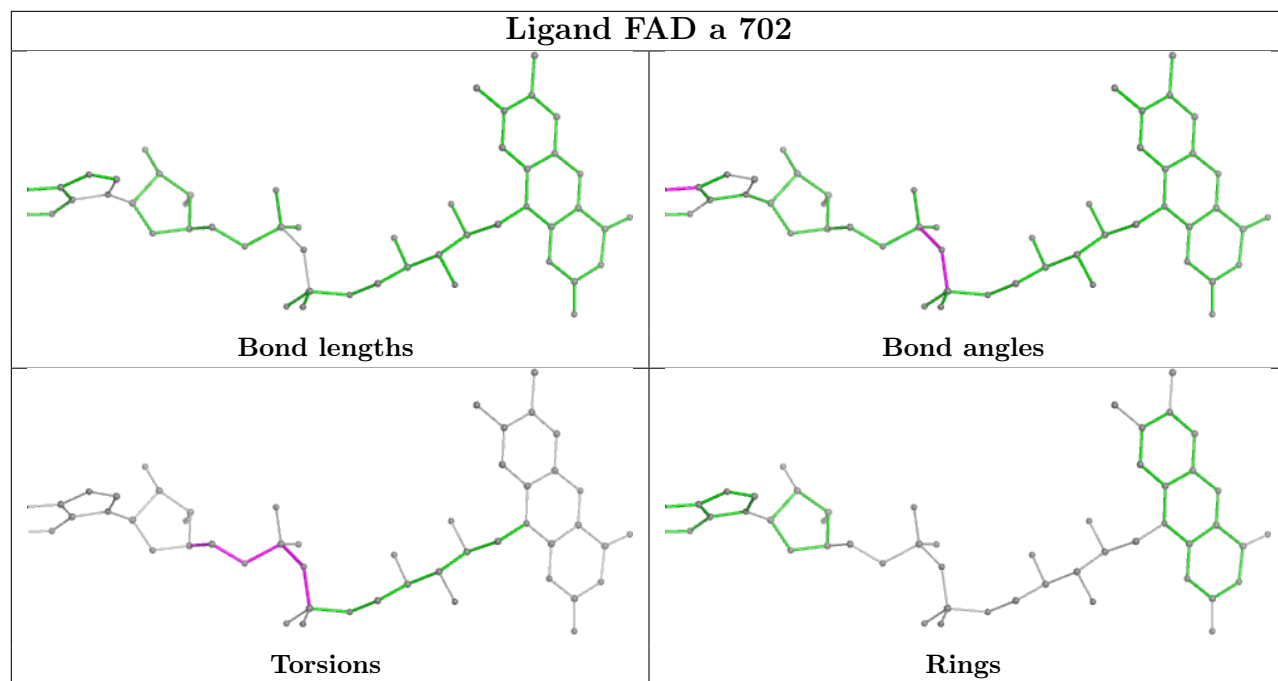
Continued on next page...

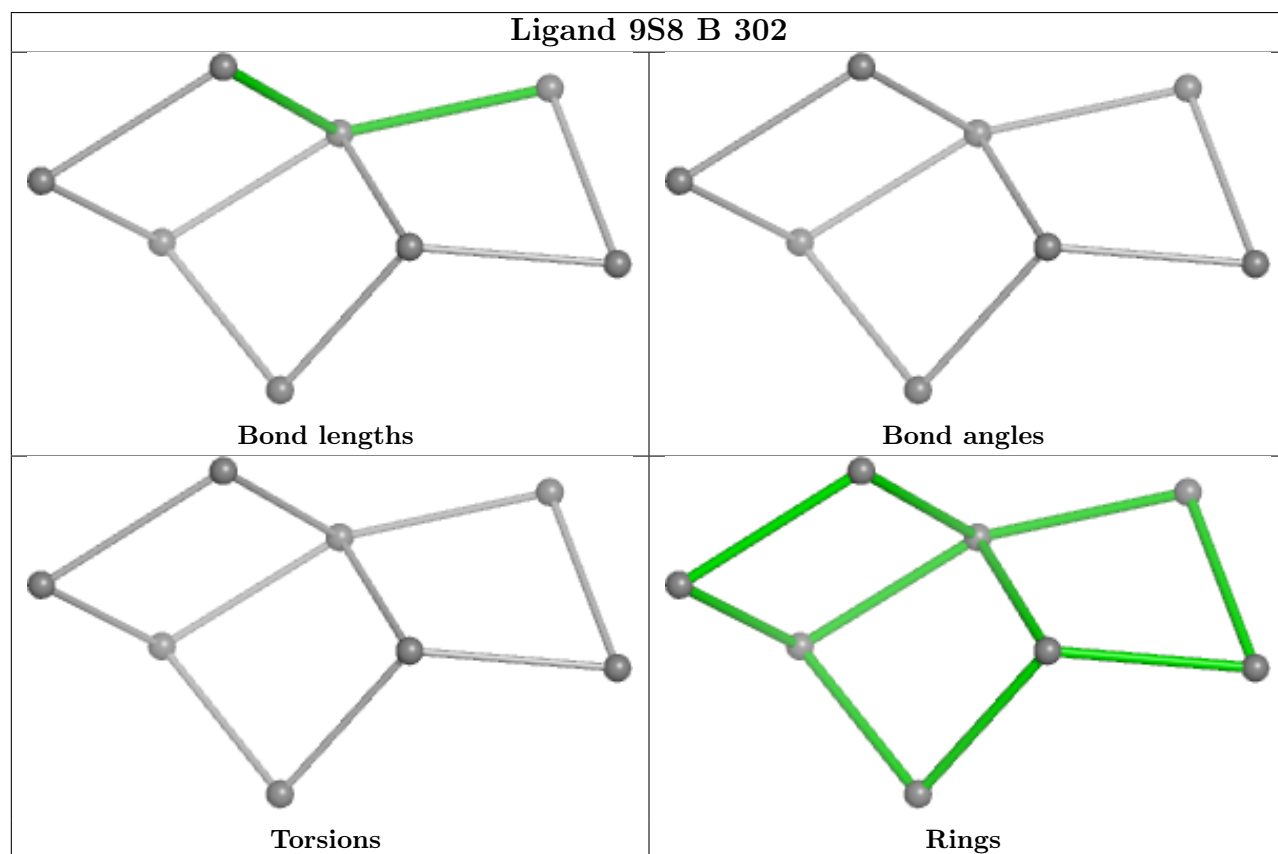
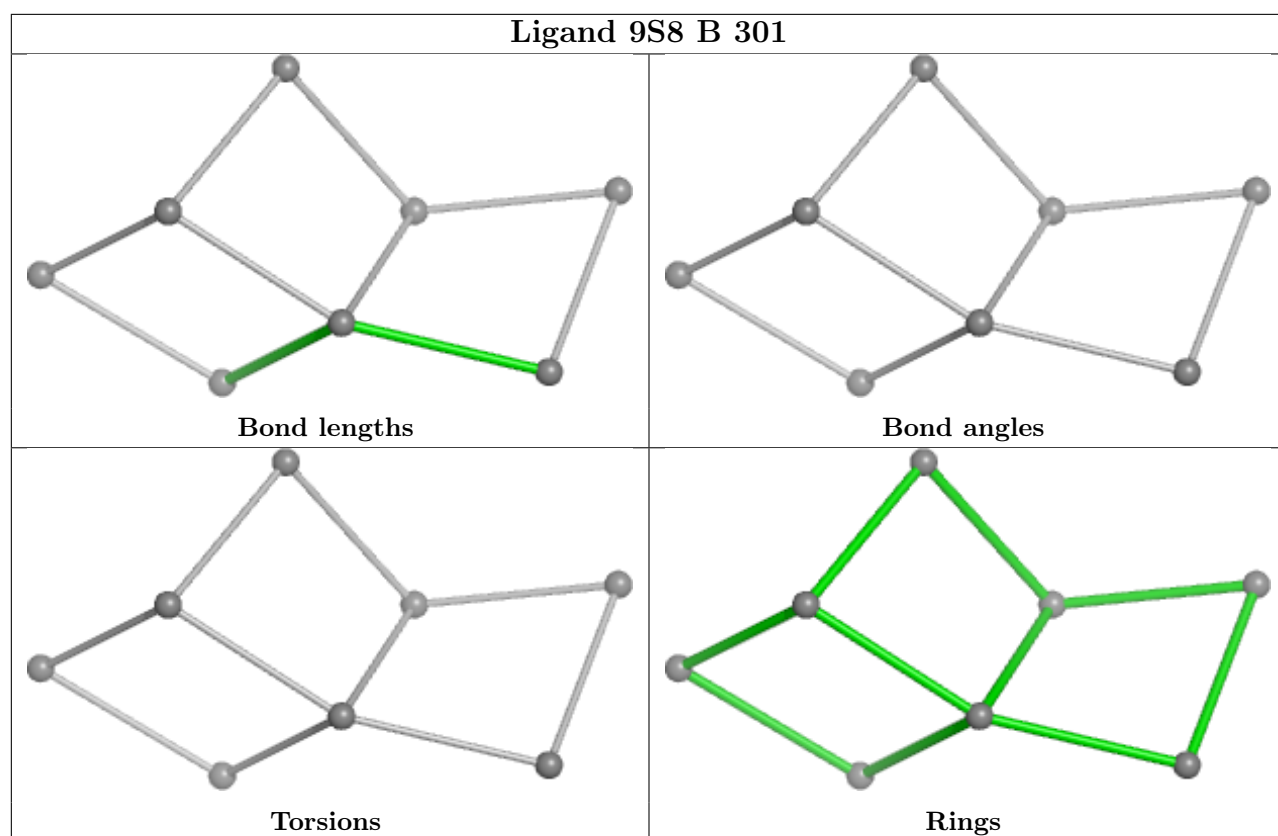
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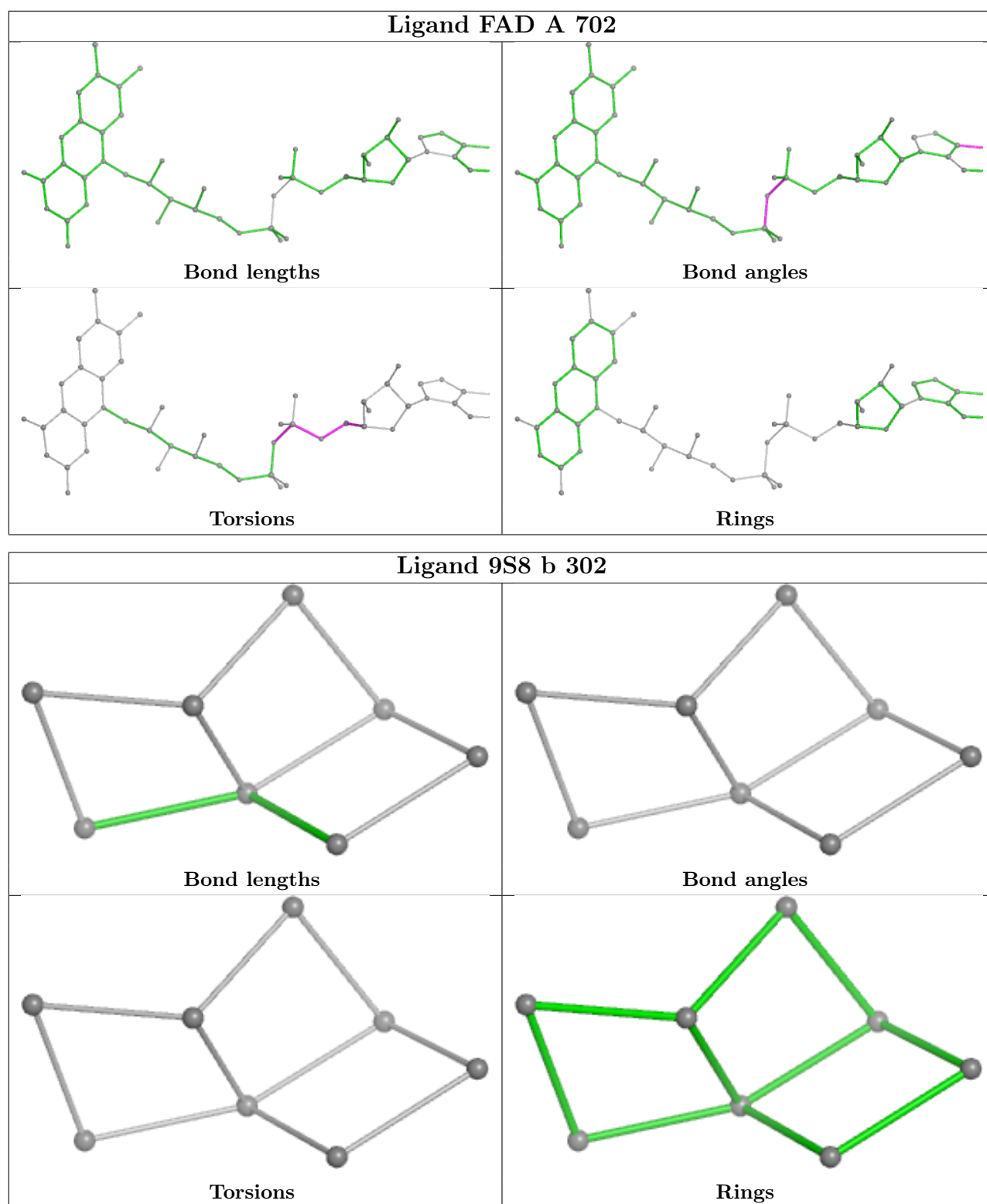
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	301	9S8	1	0
9	B	302	9S8	1	0
8	A	702	FAD	1	0
9	b	302	9S8	1	0

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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12210. These allow visual inspection of the internal detail of the map and identification of artifacts.

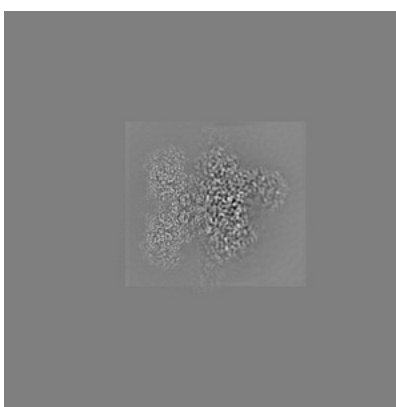
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

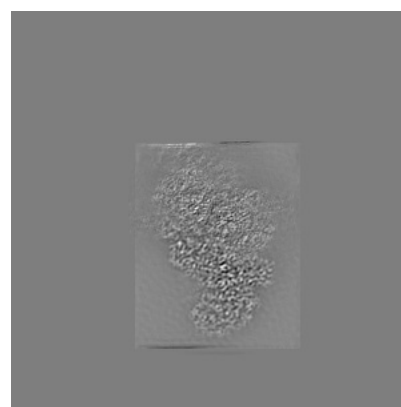
6.1.1 Primary map



X



Y

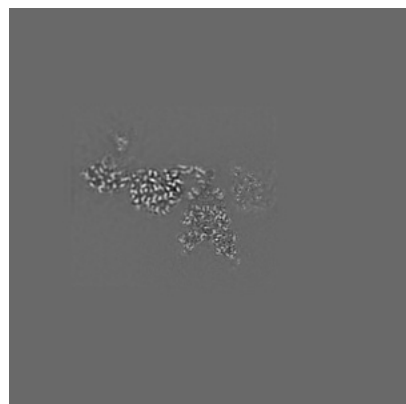


Z

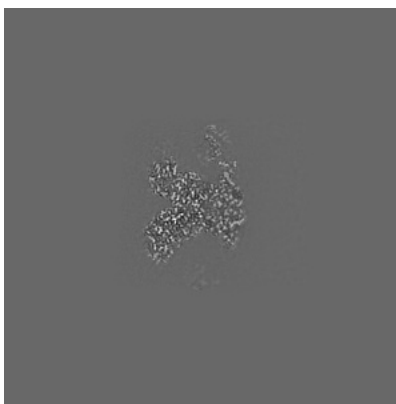
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

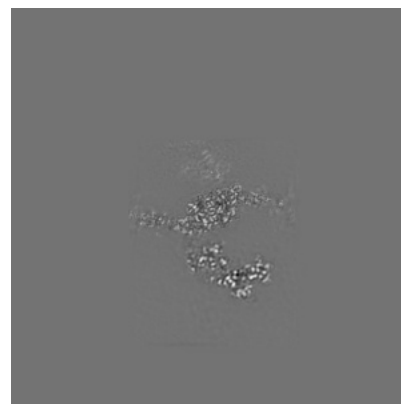
6.2.1 Primary map



X Index: 216



Y Index: 216

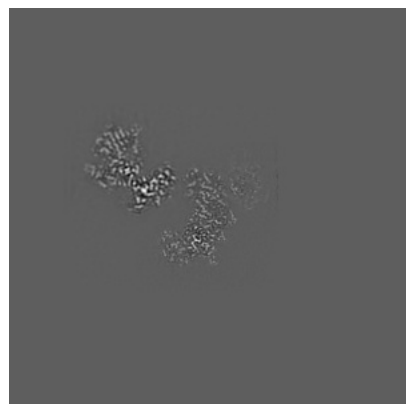


Z Index: 216

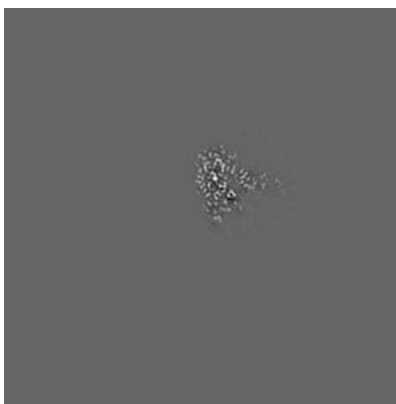
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 235



Y Index: 141

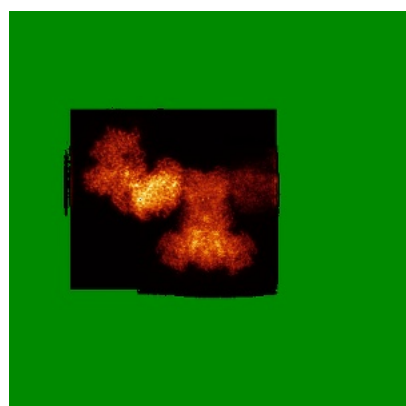


Z Index: 244

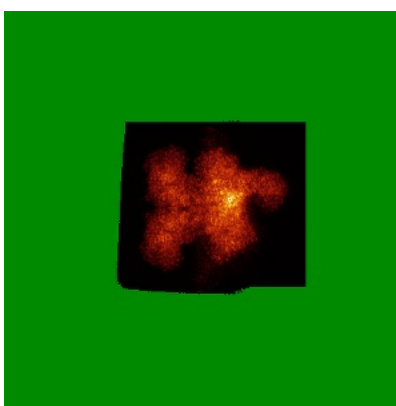
The images above show the largest variance slices of the map in three orthogonal directions.

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

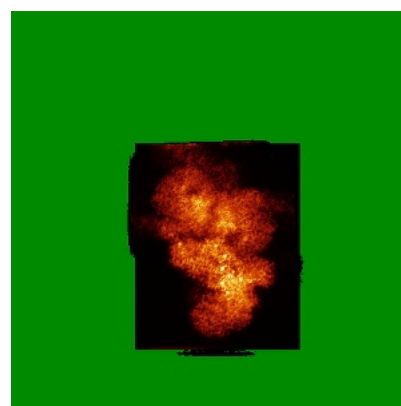
6.4.1 Primary map



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

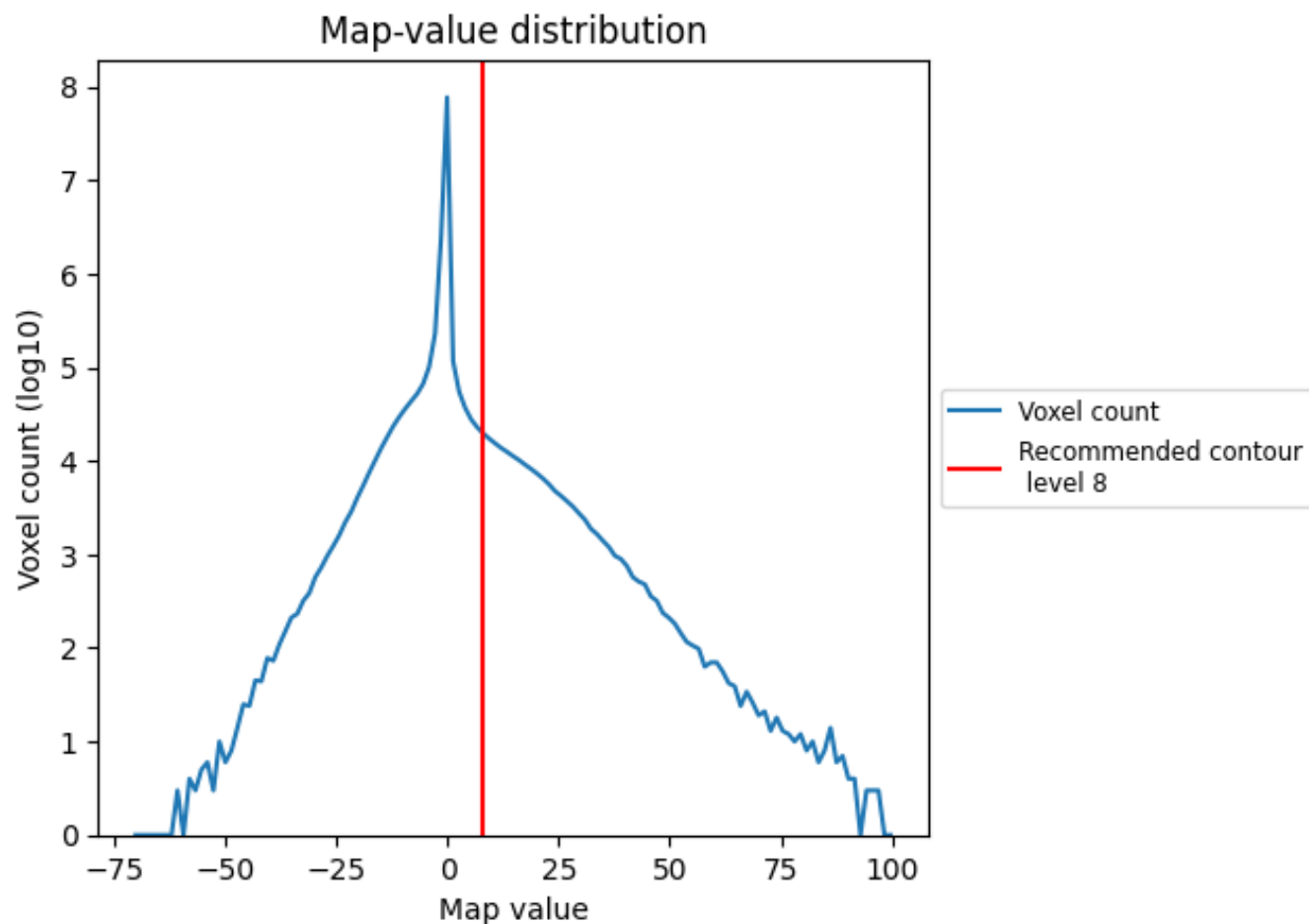
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

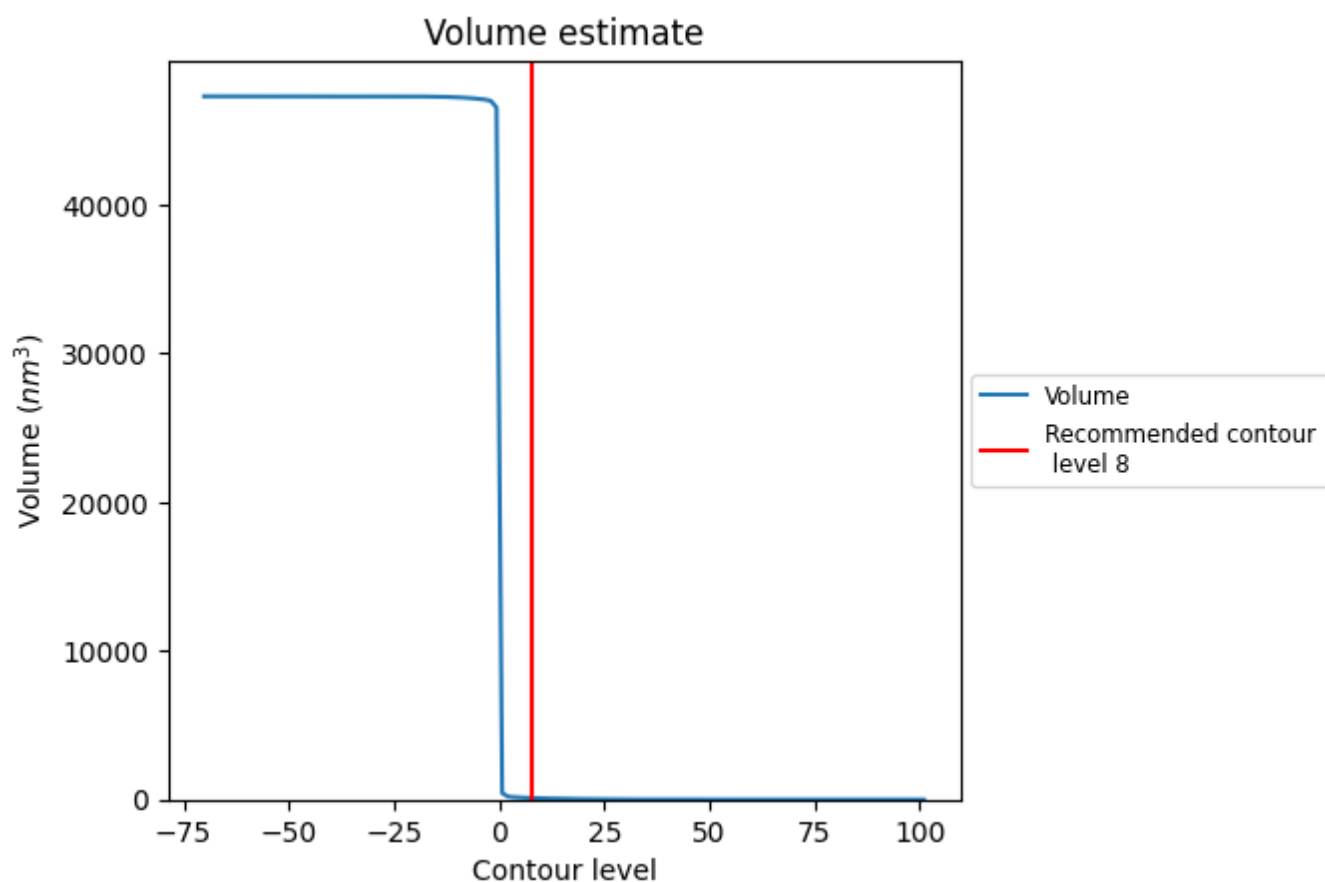
This section contains the results of statistical analysis of the map.

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.

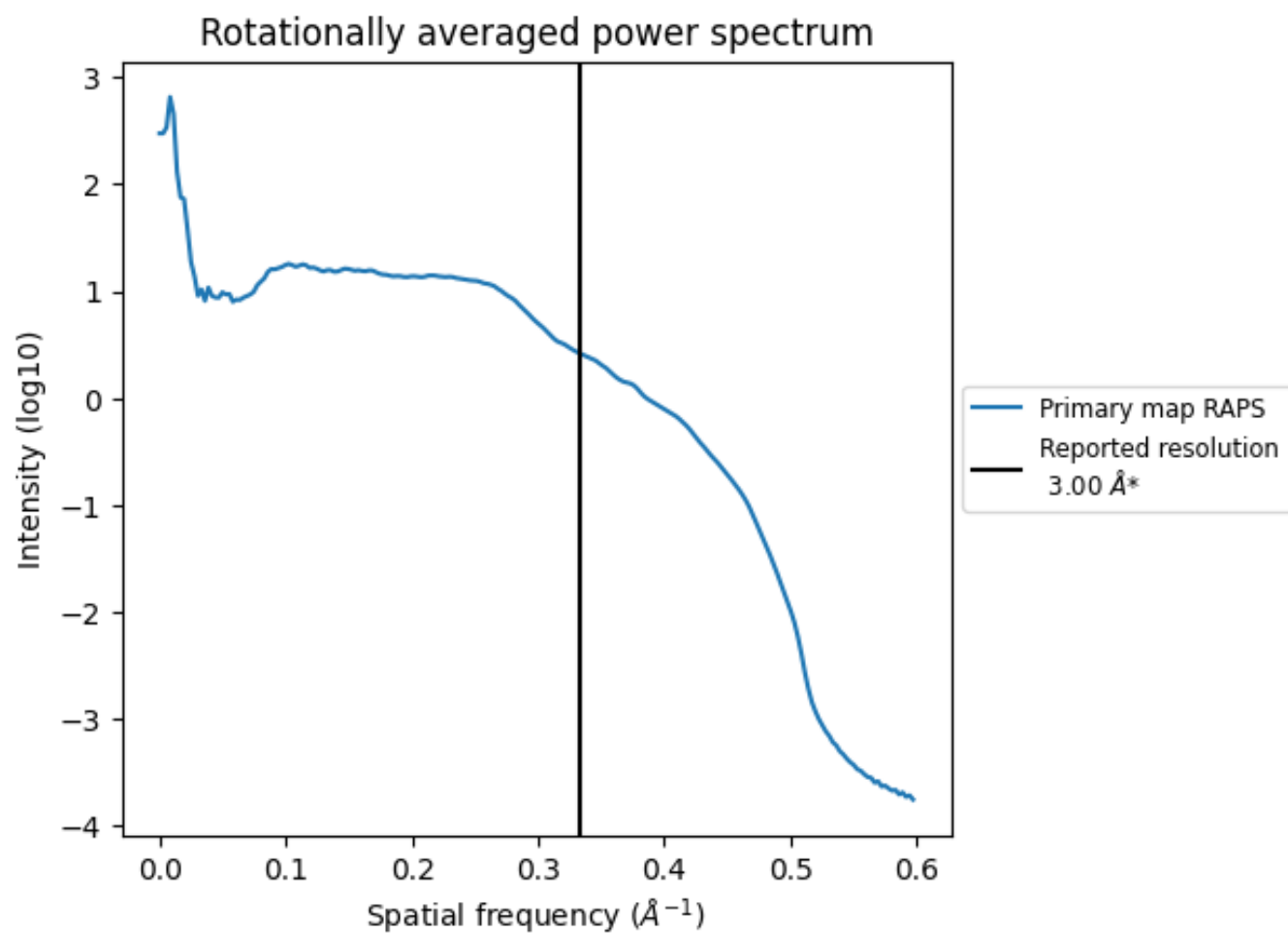
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 91 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 0.333 Å⁻¹

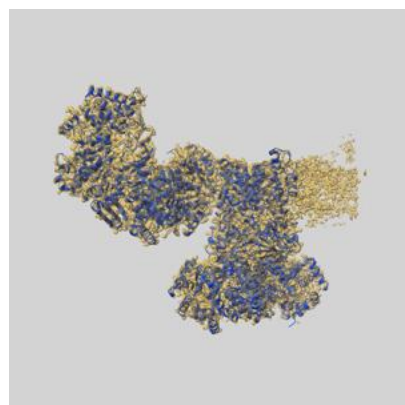
8 Fourier-Shell correlation

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

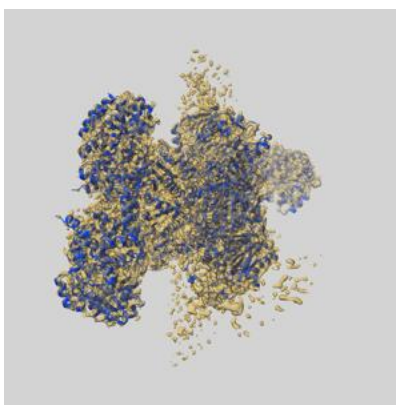
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12210 and PDB model 7BKD. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

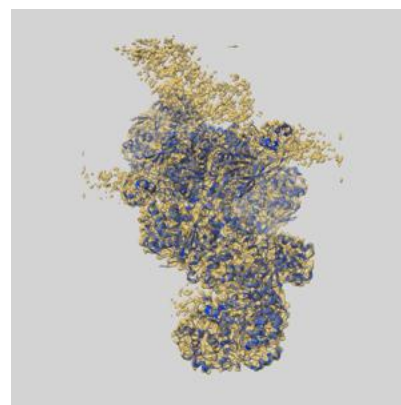
9.1 Map-model overlay [i](#)



X



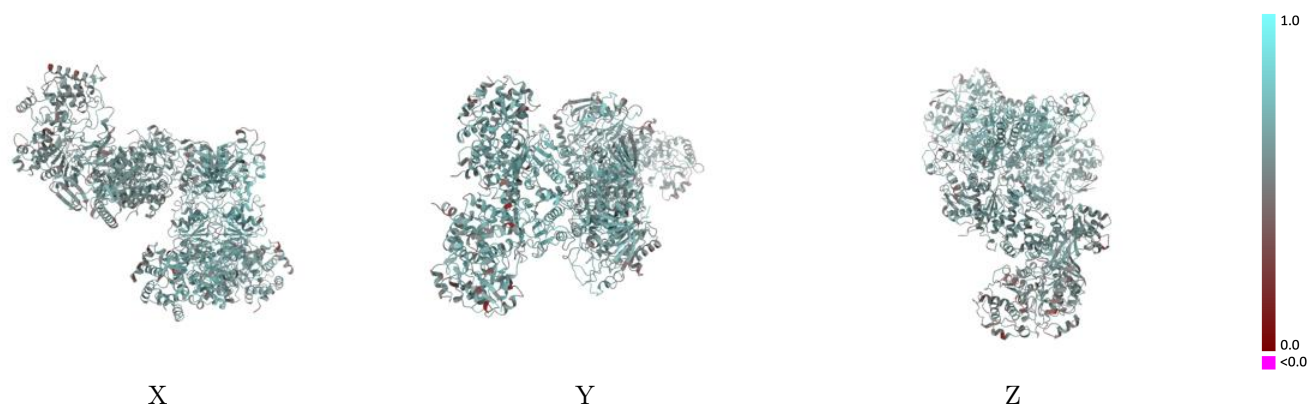
Y



Z

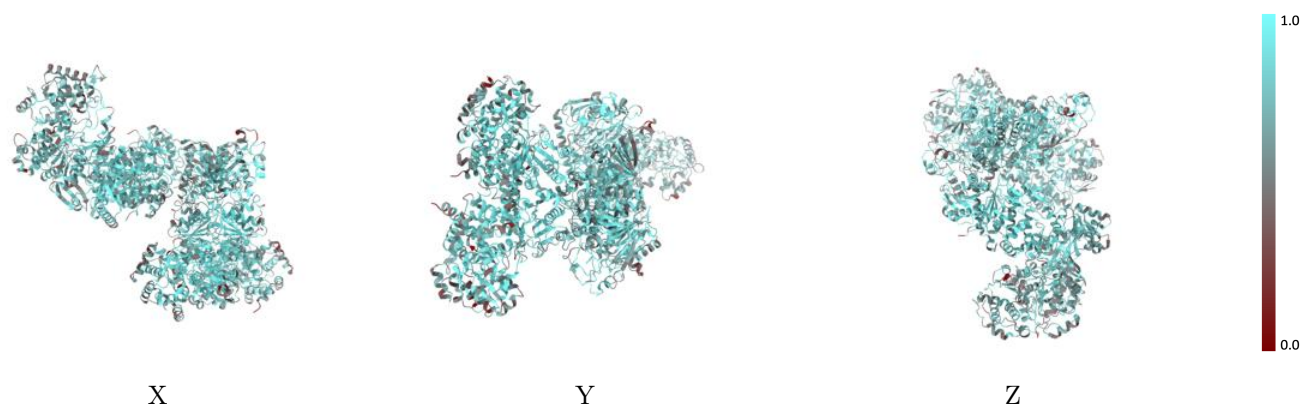
The images above show the 3D surface view of the map at the recommended contour level 8.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



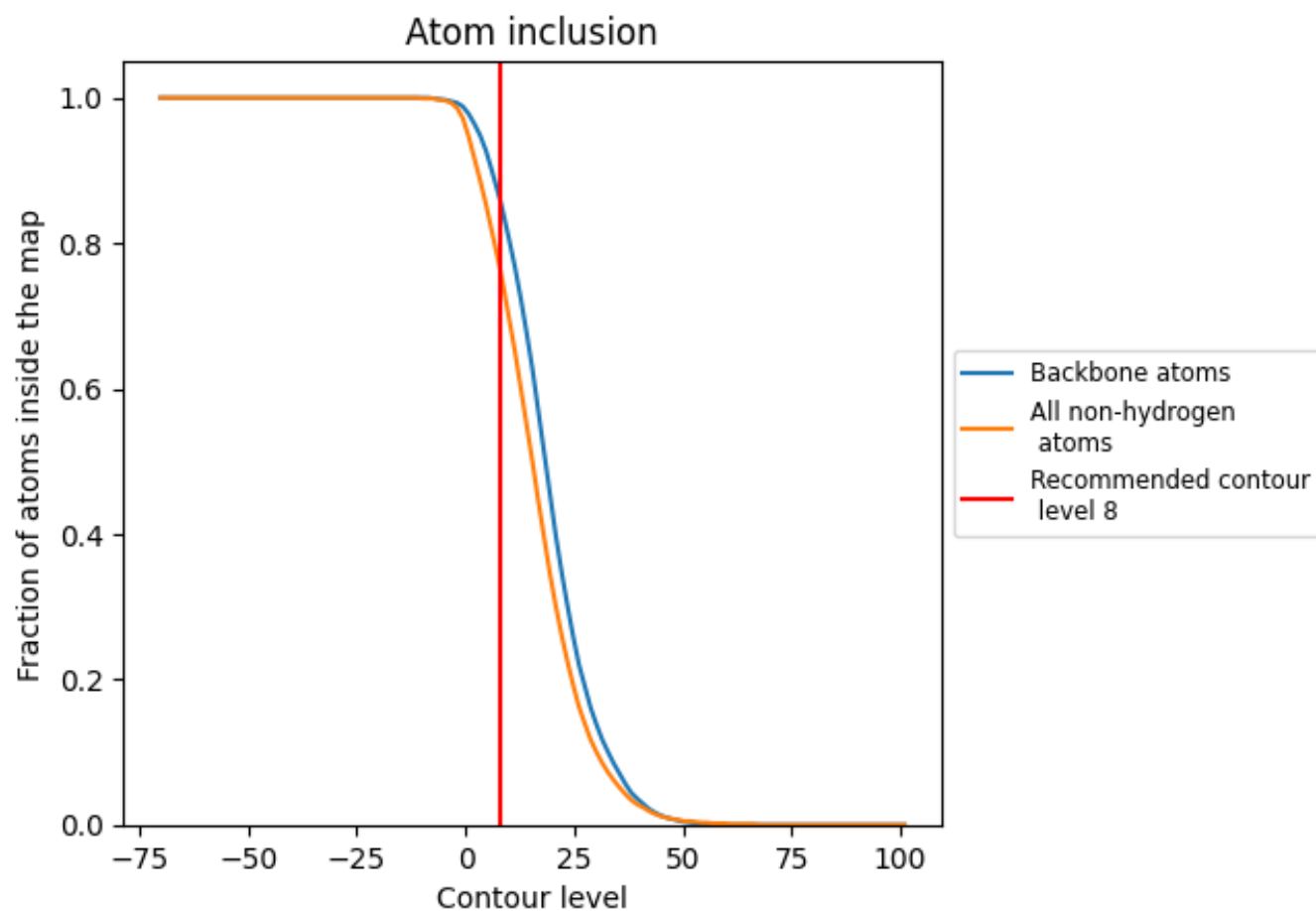
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 76% 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 (8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7640	<div><div></div></div> 0.5970
A	<div><div></div></div> 0.7970	<div><div></div></div> 0.6200
B	<div><div></div></div> 0.7660	<div><div></div></div> 0.6030
C	<div><div></div></div> 0.7650	<div><div></div></div> 0.6180
D	<div><div></div></div> 0.6870	<div><div></div></div> 0.5380
E	<div><div></div></div> 0.7930	<div><div></div></div> 0.5760
F	<div><div></div></div> 0.8020	<div><div></div></div> 0.5820
a	<div><div></div></div> 0.7690	<div><div></div></div> 0.6320
b	<div><div></div></div> 0.7660	<div><div></div></div> 0.6030
c	<div><div></div></div> 0.7620	<div><div></div></div> 0.6180

1.0

0.0

<0.0