



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:27 AM UTC

PDB ID : 7D3F / pdb_00007d3f
EMDB ID : EMD-30556
Title : Cryo-EM structure of human DUOX1-DUOXA1 in high-calcium state
Authors : Chen, L.; Wu, J.X.
Deposited on : 2020-09-19
Resolution : 2.60 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:

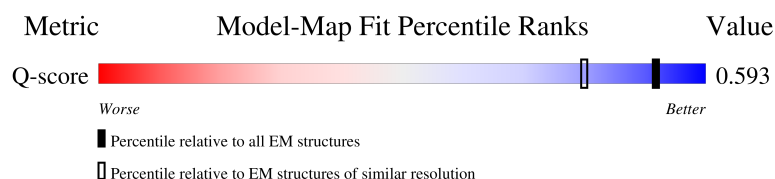
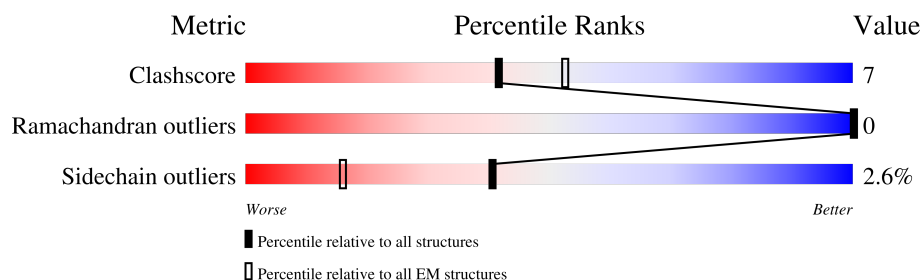
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	1551	
1	C	1551	
2	B	483	
2	D	483	

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Mol	Chain	Length	Quality of chain
3	E	10	20%70%10%
3	F	10	20%70%10%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 26466 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 Dual oxidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1369	Total	C	N	O	S	0	0
			10770	6947	1882	1903	38		
1	C	1369	Total	C	N	O	S	0	0
			10770	6947	1882	1903	38		

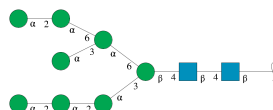
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1178	PHE	LEU	variant	UNP Q9NRD9
C	1178	PHE	LEU	variant	UNP Q9NRD9

- Molecule 2 is a protein called Isoform 2 of Dual oxidase maturation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	272	Total	C	N	O	S	0	0
			2085	1379	330	364	12		
2	D	272	Total	C	N	O	S	0	0
			2085	1379	330	364	12		

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



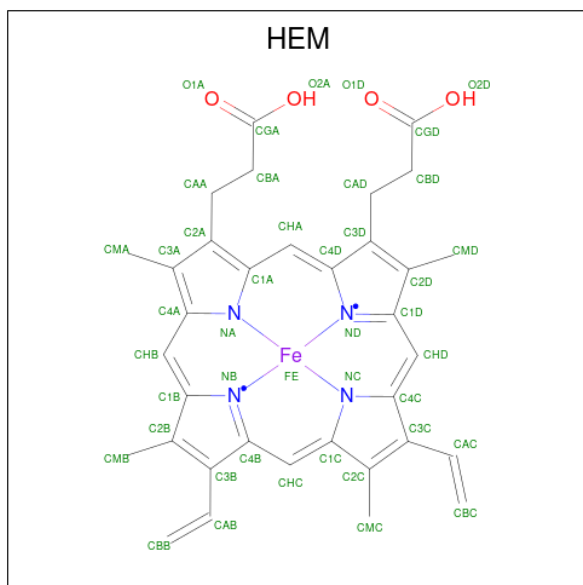
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	10	Total	C	N	O	0	0
			116	64	2	50		

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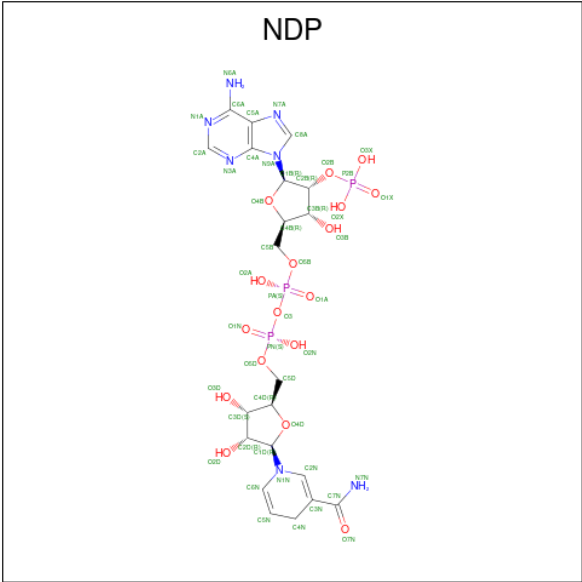
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



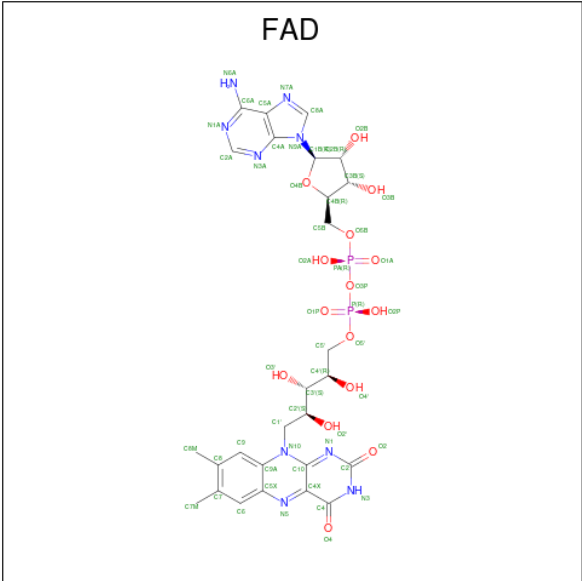
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	Fe	N	O
			43	34	1	4	4
4	A	1	Total	C	Fe	N	O
			43	34	1	4	4
4	C	1	Total	C	Fe	N	O
			43	34	1	4	4
4	C	1	Total	C	Fe	N	O
			43	34	1	4	4

- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
5	C	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 6 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
6	A	1	Total	C	N	O	P	0
			53	27	9	15	2	

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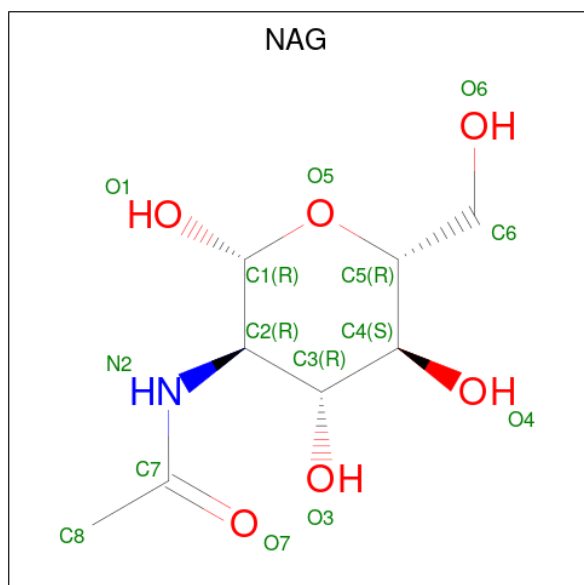
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Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	Ca	0
			2	2	
7	C	2	Total	Ca	0
			2	2	

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	A	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
9	A	2	Total	Na	0
			2	2	
9	C	2	Total	Na	0
			2	2	

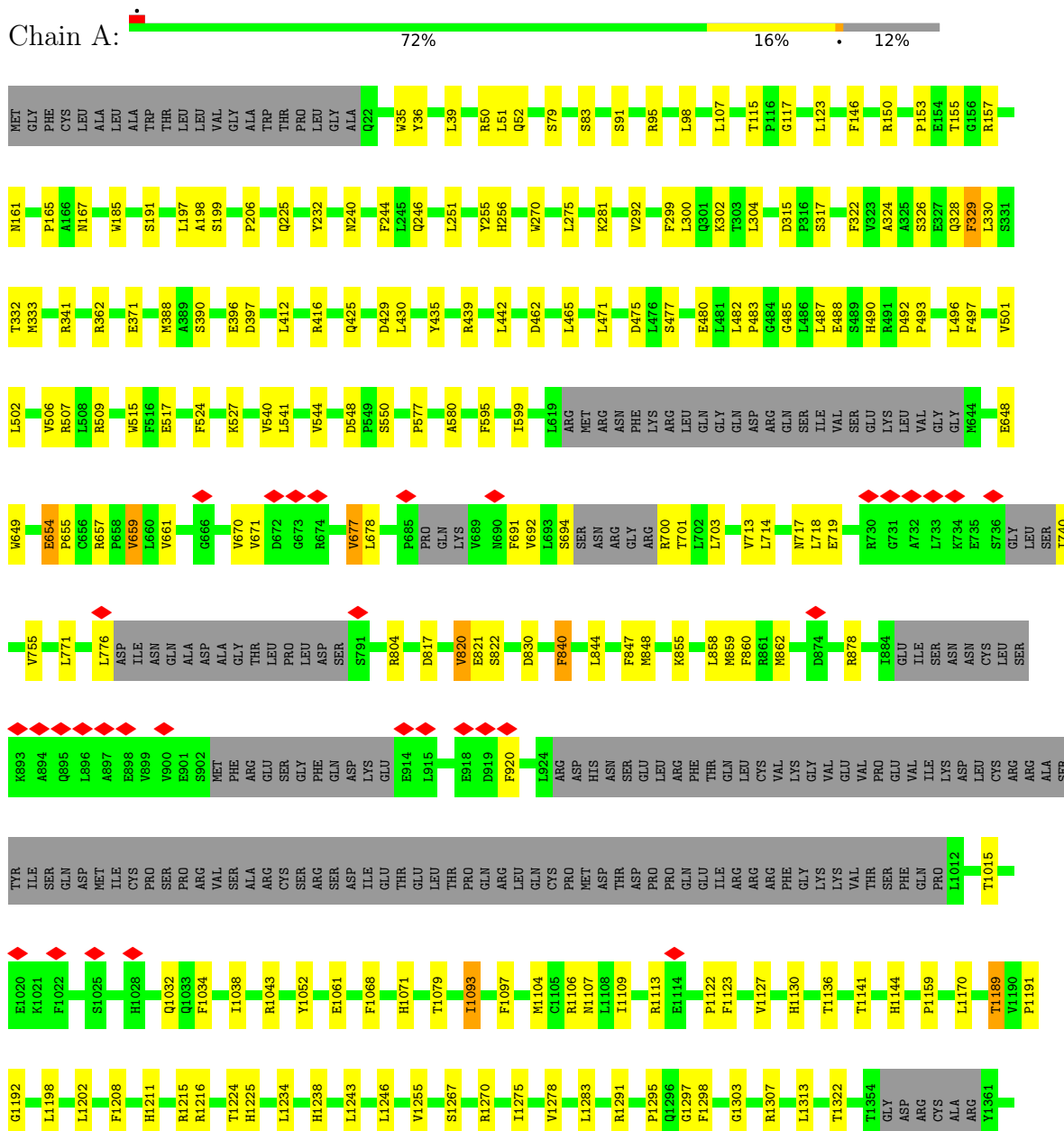
- Molecule 10 is water.

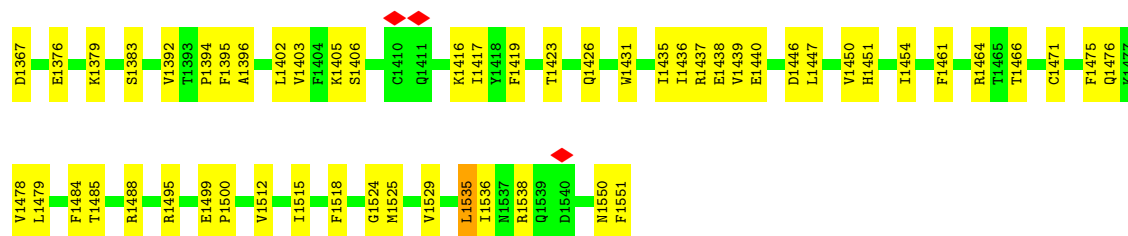
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	O	0
			1	1	
10	C	1	Total	O	0
			1	1	

3 Residue-property plots [i](#)

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

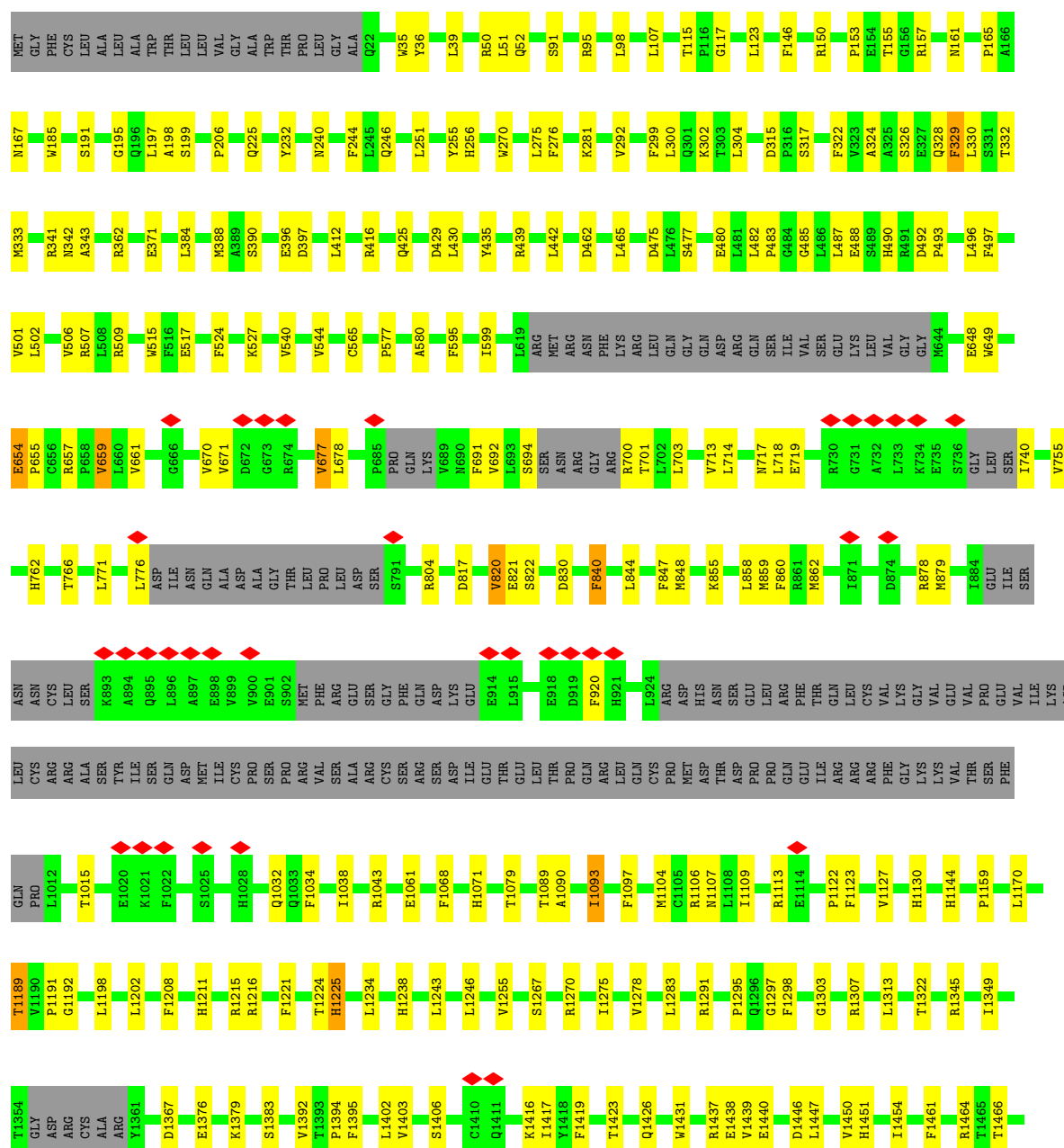
• Molecule 1: Dual oxidase 1





• Molecule 1: Dual oxidase 1

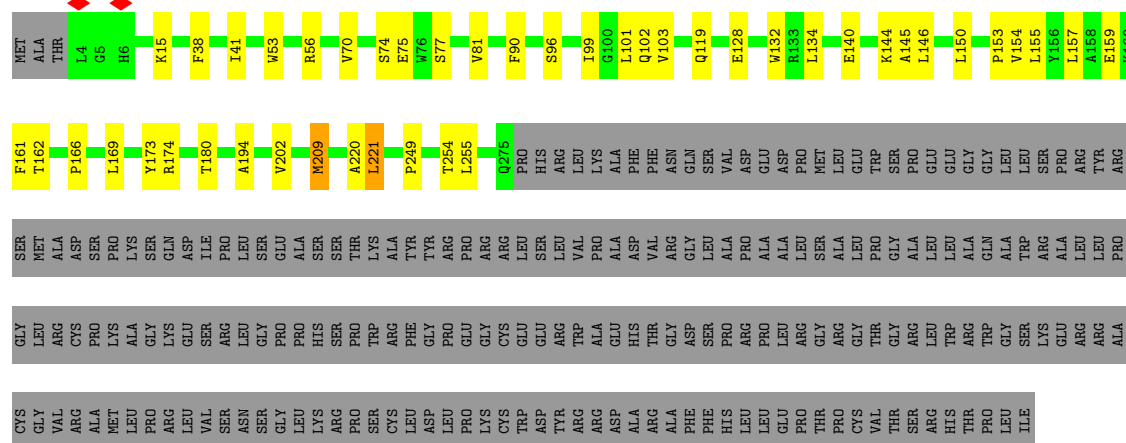
Chain C: 72% 16% 12%





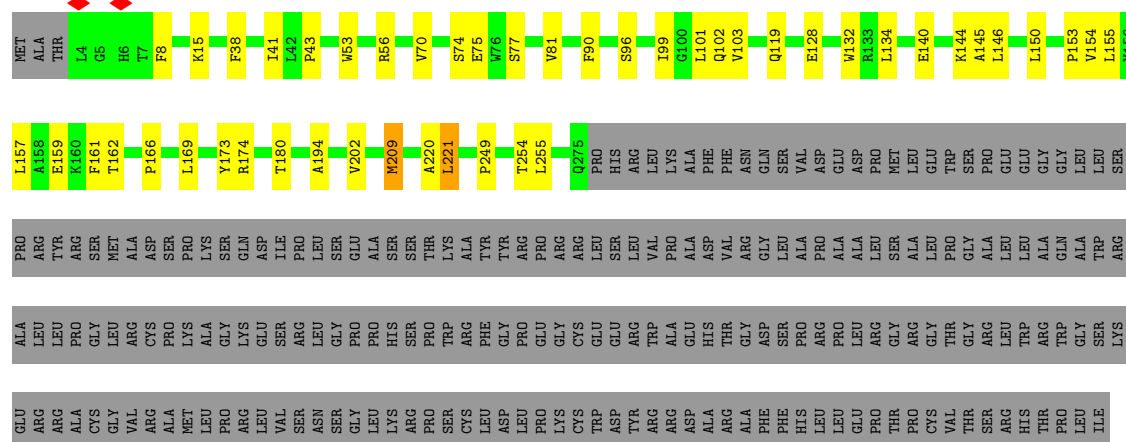
- Molecule 2: Isoform 2 of Dual oxidase maturation factor 1

Chain B: 47% 9% 44%



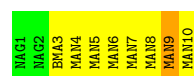
- Molecule 2: Isoform 2 of Dual oxidase maturation factor 1

Chain D: 47% 9% 44%

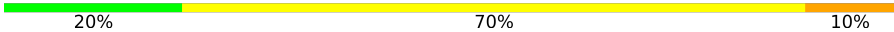


- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 20% 70% 10%



- Molecule 3: α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-2)- α -D-mannopyranose-(1-6)-[α -D-mannopyranose-(1-3)] α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain F:  20% 70% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125948	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	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	0.274	Depositor
Minimum map value	-0.157	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	188.09999, 188.09999, 188.09999	wwPDB
Map dimensions	180, 180, 180	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	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: NDP, CA, HEM, NAG, BMA, FAD, MAN, NA

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	0.10	0/11076	0.28	0/15074
1	C	0.10	0/11076	0.28	0/15074
2	B	0.12	0/2146	0.28	0/2938
2	D	0.12	0/2146	0.28	0/2938
All	All	0.11	0/26444	0.28	0/36024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10770	0	10321	153	0
1	C	10770	0	10321	149	0
2	B	2085	0	2082	28	0
2	D	2085	0	2082	30	0
3	E	116	0	97	2	0
3	F	116	0	97	2	0
4	A	86	0	60	10	0
4	C	86	0	60	8	0
5	A	48	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	48	0	26	2	0
6	A	53	0	31	1	0
6	C	53	0	31	1	0
7	A	2	0	0	0	0
7	C	2	0	0	0	0
8	A	42	0	39	0	0
8	B	28	0	26	0	0
8	C	42	0	39	0	0
8	D	28	0	26	0	0
9	A	2	0	0	0	0
9	C	2	0	0	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
All	All	26466	0	25364	350	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 7.

All (350) 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:694:SER:HB3	1:A:701:THR:HB	1.74	0.69
1:C:694:SER:HB3	1:C:701:THR:HB	1.74	0.69
1:A:771:LEU:HD11	1:A:840:PHE:HB3	1.77	0.67
1:C:1437:ARG:NH2	1:C:1485:THR:O	2.28	0.67
1:C:324:ALA:HB1	1:C:482:LEU:HD13	1.77	0.66
1:C:771:LEU:HD11	1:C:840:PHE:HB3	1.77	0.66
1:A:1437:ARG:NH2	1:A:1485:THR:O	2.28	0.66
1:C:804:ARG:NH1	1:C:821:GLU:OE1	2.28	0.66
1:A:324:ALA:HB1	1:A:482:LEU:HD13	1.77	0.66
1:A:804:ARG:NH1	1:A:821:GLU:OE1	2.29	0.65
1:A:1113:ARG:NH1	1:A:1550:ASN:O	2.31	0.63
1:A:1127:VAL:O	1:A:1130:HIS:HB3	1.98	0.63
1:C:412:LEU:HD11	1:C:1159:PRO:HB3	1.79	0.63
1:A:412:LEU:HD11	1:A:1159:PRO:HB3	1.79	0.63
1:A:847:PHE:O	1:A:855:LYS:NZ	2.32	0.62
1:C:1113:ARG:NH1	1:C:1550:ASN:O	2.32	0.62
1:A:52:GLN:NE2	1:A:315:ASP:OD2	2.33	0.62
1:C:847:PHE:O	1:C:855:LYS:NZ	2.33	0.61
1:A:692:VAL:HB	1:A:703:LEU:HB3	1.82	0.61
2:D:15:LYS:HE3	3:F:9:MAN:H62	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LYS:HE3	3:E:9:MAN:H62	1.82	0.60
1:C:692:VAL:HB	1:C:703:LEU:HB3	1.82	0.60
1:C:1303:GLY:HA2	1:C:1394:PRO:HB3	1.83	0.60
1:A:1303:GLY:HA2	1:A:1394:PRO:HB3	1.83	0.60
1:A:416:ARG:HH21	1:A:580:ALA:HB3	1.66	0.60
1:C:52:GLN:NE2	1:C:315:ASP:OD2	2.34	0.60
1:A:317:SER:O	1:A:507:ARG:NH1	2.35	0.59
2:B:77:SER:HB2	2:B:103:VAL:HB	1.85	0.59
1:C:416:ARG:HH21	1:C:580:ALA:HB3	1.66	0.59
2:D:77:SER:HB2	2:D:103:VAL:HB	1.85	0.58
1:C:317:SER:O	1:C:507:ARG:NH1	2.36	0.58
1:A:1535:LEU:HD13	1:A:1538:ARG:HE	1.68	0.58
2:D:194:ALA:HB2	2:D:209:MET:HB3	1.86	0.57
1:C:1535:LEU:HD13	1:C:1538:ARG:HE	1.68	0.57
1:C:1403:VAL:HG11	1:C:1439:VAL:HG13	1.87	0.57
1:C:1238:HIS:NE2	4:C:1602:HEM:NA	2.53	0.57
1:C:326:SER:HA	1:C:329:PHE:HD2	1.70	0.56
1:A:1394:PRO:HG2	1:A:1551:PHE:HB2	1.87	0.56
4:C:1602:HEM:HMB2	4:C:1602:HEM:HBB2	1.86	0.56
1:A:1093:ILE:HG23	1:A:1097:PHE:CD2	2.40	0.56
1:C:1090:ALA:HB2	1:C:1144:HIS:CE1	2.40	0.56
1:C:1093:ILE:HG23	1:C:1097:PHE:CD2	2.40	0.56
1:A:326:SER:HA	1:A:329:PHE:HD2	1.69	0.56
1:A:341:ARG:NH2	1:A:390:SER:OG	2.38	0.56
1:A:1295:PRO:HB2	1:A:1298:PHE:HB2	1.88	0.56
1:C:251:LEU:HD12	1:C:544:VAL:HG21	1.88	0.56
1:A:694:SER:O	1:A:700:ARG:N	2.39	0.56
4:A:1601:HEM:HMC1	4:A:1601:HEM:HBC2	1.88	0.56
1:C:659:VAL:HG11	1:C:670:VAL:HG12	1.88	0.56
1:C:1394:PRO:HG2	1:C:1551:PHE:HB2	1.87	0.56
1:A:1403:VAL:HG11	1:A:1439:VAL:HG13	1.87	0.56
1:A:153:PRO:O	1:A:157:ARG:NH1	2.35	0.56
2:B:194:ALA:HB2	2:B:209:MET:HB3	1.86	0.56
1:C:341:ARG:NH2	1:C:390:SER:OG	2.38	0.55
1:C:1189:THR:HG22	1:C:1192:GLY:H	1.71	0.55
1:A:1189:THR:HG22	1:A:1192:GLY:H	1.72	0.55
4:A:1602:HEM:HMB2	4:A:1602:HEM:HBB2	1.87	0.55
1:C:1170:LEU:HD22	1:C:1243:LEU:HD11	1.88	0.55
1:A:659:VAL:HG11	1:A:670:VAL:HG12	1.88	0.55
1:A:661:VAL:HG21	1:A:714:LEU:HD21	1.89	0.55
1:C:661:VAL:HG21	1:C:714:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1107:ASN:OD1	1:A:1270:ARG:NH1	2.40	0.55
1:A:251:LEU:HD12	1:A:544:VAL:HG21	1.89	0.55
1:A:1043:ARG:HB3	1:A:1122:PRO:HD3	1.89	0.55
1:C:694:SER:O	1:C:700:ARG:N	2.39	0.55
1:C:1107:ASN:OD1	1:C:1270:ARG:NH1	2.39	0.55
1:C:1295:PRO:HB2	1:C:1298:PHE:HB2	1.88	0.54
1:A:191:SER:HB3	1:A:198:ALA:HA	1.89	0.54
4:C:1601:HEM:HMC1	4:C:1601:HEM:HBC2	1.88	0.54
1:A:36:TYR:OH	2:B:146:LEU:O	2.21	0.54
1:A:1189:THR:HG23	1:A:1191:PRO:HD2	1.89	0.54
1:C:1043:ARG:HB3	1:C:1122:PRO:HD3	1.89	0.54
1:C:1376:GLU:HB3	1:C:1518:PHE:CE1	2.43	0.54
1:A:1109:ILE:HG23	1:A:1123:PHE:HB3	1.90	0.54
1:C:191:SER:HB3	1:C:198:ALA:HA	1.89	0.54
1:C:509:ARG:HG3	1:C:515:TRP:CE2	2.43	0.54
1:A:1170:LEU:HD22	1:A:1243:LEU:HD11	1.89	0.54
1:A:509:ARG:HG3	1:A:515:TRP:CE2	2.43	0.53
1:A:700:ARG:N	1:A:719:GLU:OE1	2.41	0.53
1:C:95:ARG:HD3	1:C:299:PHE:HA	1.91	0.53
1:C:1109:ILE:HG23	1:C:1123:PHE:HB3	1.89	0.53
1:C:1322:THR:HG21	1:C:1394:PRO:HG3	1.91	0.53
1:A:95:ARG:HD3	1:A:299:PHE:HA	1.91	0.53
1:A:197:LEU:HG	1:A:256:HIS:CD2	2.44	0.53
2:B:140:GLU:HG2	2:B:144:LYS:HE2	1.90	0.53
1:C:700:ARG:N	1:C:719:GLU:OE1	2.41	0.53
1:C:117:GLY:HA2	1:C:150:ARG:HG2	1.91	0.53
1:C:1189:THR:HG23	1:C:1191:PRO:HD2	1.90	0.53
1:A:1376:GLU:HB3	1:A:1518:PHE:CE1	2.43	0.53
2:D:140:GLU:HG2	2:D:144:LYS:HE2	1.90	0.53
2:D:53:TRP:CD1	2:D:56:ARG:HH11	2.27	0.53
1:A:1535:LEU:HD22	1:A:1538:ARG:HH21	1.74	0.52
1:C:197:LEU:HG	1:C:256:HIS:CD2	2.44	0.52
1:C:206:PRO:HG2	1:C:232:TYR:HB3	1.91	0.52
1:C:1535:LEU:HD22	1:C:1538:ARG:HH21	1.74	0.52
1:A:1208:PHE:CG	1:A:1224:THR:HG21	2.44	0.52
1:C:1093:ILE:HG23	1:C:1097:PHE:HD2	1.75	0.52
1:A:1322:THR:HG21	1:A:1394:PRO:HG3	1.91	0.52
2:B:75:GLU:HB3	2:B:249:PRO:HG2	1.92	0.52
1:C:691:PHE:HE2	1:C:740:ILE:HG23	1.75	0.52
1:A:117:GLY:HA2	1:A:150:ARG:HG2	1.91	0.52
2:D:75:GLU:HB3	2:D:249:PRO:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:TRP:CD1	2:B:56:ARG:HH11	2.27	0.51
1:A:1093:ILE:HG23	1:A:1097:PHE:HD2	1.75	0.51
2:B:180:THR:HG23	2:B:220:ALA:HB1	1.92	0.51
1:A:691:PHE:HE2	1:A:740:ILE:HG23	1.75	0.51
1:C:153:PRO:O	1:C:157:ARG:NH1	2.35	0.51
1:C:475:ASP:OD2	1:C:477:SER:OG	2.26	0.51
1:A:199:SER:HA	1:A:206:PRO:HA	1.93	0.51
1:A:281:LYS:HG2	1:A:524:PHE:CZ	2.46	0.51
1:A:206:PRO:HG2	1:A:232:TYR:HB3	1.92	0.51
1:C:199:SER:HA	1:C:206:PRO:HA	1.93	0.51
1:C:822:SER:HB3	1:C:862:MET:HG2	1.93	0.51
2:D:74:SER:O	2:D:102:GLN:HB3	2.10	0.51
2:D:180:THR:HG23	2:D:220:ALA:HB1	1.92	0.51
1:C:1090:ALA:HB2	1:C:1144:HIS:HE1	1.75	0.51
1:A:822:SER:HB3	1:A:862:MET:HG2	1.93	0.51
1:A:1015:THR:HG21	1:A:1451:HIS:CE1	2.46	0.51
1:C:332:THR:OG1	1:C:397:ASP:O	2.25	0.51
2:B:74:SER:O	2:B:102:GLN:HB3	2.10	0.50
1:C:1015:THR:HG21	1:C:1451:HIS:CE1	2.46	0.50
2:D:99:ILE:HD13	2:D:153:PRO:HB3	1.93	0.50
1:C:1106:ARG:NH2	4:C:1601:HEM:O1A	2.42	0.50
1:A:322:PHE:HE2	1:A:501:VAL:HG13	1.76	0.50
1:C:281:LYS:HG2	1:C:524:PHE:CZ	2.46	0.50
1:A:1106:ARG:NH2	4:A:1601:HEM:O1A	2.42	0.50
1:C:107:LEU:HD22	1:C:330:LEU:HD12	1.92	0.50
1:A:107:LEU:HD22	1:A:330:LEU:HD12	1.92	0.50
2:B:99:ILE:HD13	2:B:153:PRO:HB3	1.93	0.50
1:C:123:LEU:HD23	1:C:425:GLN:HG3	1.94	0.49
1:C:1211:HIS:NE2	1:C:1215:ARG:HD2	2.27	0.49
1:A:1211:HIS:NE2	1:A:1215:ARG:HD2	2.27	0.49
1:A:123:LEU:HD23	1:A:425:GLN:HG3	1.94	0.49
1:A:776:LEU:HD12	1:A:848:MET:HE1	1.93	0.49
1:A:860:PHE:HD2	1:A:920:PHE:HD1	1.60	0.49
1:C:322:PHE:HE2	1:C:501:VAL:HG13	1.76	0.49
1:C:776:LEU:HD12	1:C:848:MET:HE1	1.93	0.49
1:C:1495:ARG:HH12	5:C:1603:NDP:P2B	2.35	0.49
1:A:475:ASP:OD2	1:A:477:SER:OG	2.26	0.49
1:A:332:THR:OG1	1:A:397:ASP:O	2.25	0.49
1:A:1495:ARG:HH12	5:A:1603:NDP:P2B	2.35	0.49
1:A:1499:GLU:HB3	1:A:1500:PRO:HD3	1.95	0.48
1:C:860:PHE:HD2	1:C:920:PHE:HD1	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:HA	1:C:388:MET:HE2	1.95	0.48
1:A:1034:PHE:CZ	1:A:1038:ILE:HD11	2.48	0.48
1:C:1499:GLU:HB3	1:C:1500:PRO:HD3	1.95	0.48
1:C:36:TYR:OH	2:D:146:LEU:O	2.21	0.48
1:A:657:ARG:HH21	1:A:678:LEU:HD13	1.79	0.47
1:A:1402:LEU:HD13	1:A:1417:ILE:HG13	1.95	0.47
1:C:1402:LEU:HD13	1:C:1417:ILE:HG13	1.96	0.47
2:D:128:GLU:HG3	2:D:154:VAL:HG11	1.96	0.47
1:C:1034:PHE:CZ	1:C:1038:ILE:HD11	2.49	0.47
1:C:1221:PHE:O	1:C:1225:HIS:HB2	2.14	0.47
1:C:91:SER:OG	1:C:396:GLU:OE2	2.32	0.47
1:A:98:LEU:HA	1:A:388:MET:HE2	1.95	0.47
1:A:302:LYS:HD3	1:A:502:LEU:HD22	1.97	0.47
2:B:15:LYS:HB3	1:C:1071:HIS:CE1	2.49	0.47
1:A:91:SER:OG	1:A:396:GLU:OE2	2.32	0.47
1:A:648:GLU:HB2	1:A:659:VAL:HG21	1.97	0.47
2:B:128:GLU:HG3	2:B:154:VAL:HG11	1.96	0.47
1:C:225:GLN:NE2	1:C:371:GLU:OE1	2.48	0.47
1:A:35:TRP:CE2	2:B:146:LEU:HD13	2.50	0.47
1:A:1379:LYS:HG2	1:C:1297:GLY:HA3	1.96	0.47
1:C:302:LYS:HD3	1:C:502:LEU:HD22	1.97	0.47
1:A:1524:GLY:HA3	5:A:1603:NDP:N6A	2.30	0.46
1:C:717:ASN:HB3	1:C:718:LEU:HD22	1.97	0.46
1:C:1208:PHE:CG	1:C:1224:THR:HG21	2.49	0.46
1:A:225:GLN:NE2	1:A:371:GLU:OE1	2.48	0.46
1:C:657:ARG:HH21	1:C:678:LEU:HD13	1.79	0.46
1:C:1524:GLY:HA3	5:C:1603:NDP:N6A	2.30	0.46
1:A:717:ASN:HB3	1:A:718:LEU:HD22	1.97	0.46
1:C:35:TRP:CE2	2:D:146:LEU:HD13	2.50	0.46
2:D:159:GLU:HA	2:D:162:THR:HG23	1.98	0.46
1:C:1093:ILE:HG21	4:C:1602:HEM:HHD	1.98	0.46
2:B:221:LEU:HD11	2:B:255:LEU:HB2	1.98	0.46
1:C:1127:VAL:O	1:C:1130:HIS:HB3	2.16	0.46
1:A:1071:HIS:CE1	2:D:15:LYS:HB3	2.51	0.46
1:A:1512:VAL:HG21	1:A:1515:ILE:HD11	1.98	0.45
1:C:648:GLU:HB2	1:C:659:VAL:HG21	1.97	0.45
1:C:1093:ILE:HD13	1:C:1093:ILE:HA	1.74	0.45
1:C:1478:VAL:HG12	1:C:1479:LEU:HD22	1.98	0.45
1:C:435:TYR:CZ	1:C:439:ARG:HD2	2.52	0.45
1:A:1225:HIS:HE1	4:A:1601:HEM:NC	2.12	0.45
1:A:1297:GLY:HA3	1:C:1379:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:GLU:HA	2:B:162:THR:HG23	1.98	0.45
1:A:1419:PHE:HD2	1:A:1450:VAL:HG13	1.82	0.45
1:C:95:ARG:HD2	1:C:333:MET:HE1	1.99	0.45
1:C:527:LYS:HB3	1:C:527:LYS:HE3	1.76	0.45
1:A:435:TYR:CZ	1:A:439:ARG:HD2	2.52	0.45
1:A:1104:MET:HG3	4:A:1601:HEM:C2A	2.52	0.45
1:A:1478:VAL:HG12	1:A:1479:LEU:HD22	1.98	0.45
1:C:1406:SER:HB2	1:C:1447:LEU:HD22	1.99	0.45
6:C:1604:FAD:O1A	6:C:1604:FAD:H8A	2.17	0.45
1:C:1278:VAL:N	1:C:1291:ARG:O	2.51	0.44
1:C:1307:ARG:HB2	1:C:1367:ASP:HB3	1.99	0.44
1:A:79:SER:O	1:A:83:SER:OG	2.33	0.44
1:C:1419:PHE:HD2	1:C:1450:VAL:HG13	1.82	0.44
1:C:1512:VAL:HG21	1:C:1515:ILE:HD11	1.98	0.44
2:D:221:LEU:HD11	2:D:255:LEU:HB2	1.98	0.44
1:A:1283:LEU:HD13	1:A:1431:TRP:HB3	2.00	0.44
1:A:1307:ARG:HB2	1:A:1367:ASP:HB3	1.99	0.44
1:C:240:ASN:OD1	1:C:246:GLN:NE2	2.49	0.44
1:C:1104:MET:HG3	4:C:1601:HEM:C2A	2.51	0.44
1:C:1283:LEU:HD13	1:C:1431:TRP:HB3	2.00	0.44
1:A:240:ASN:OD1	1:A:246:GLN:NE2	2.50	0.44
1:A:649:TRP:HE3	1:A:713:VAL:HG11	1.83	0.44
1:A:1093:ILE:HG21	4:A:1602:HEM:HHH	1.98	0.44
1:A:1406:SER:HB2	1:A:1447:LEU:HD22	1.99	0.44
1:C:649:TRP:HE3	1:C:713:VAL:HG11	1.83	0.44
1:A:859:MET:HE1	1:A:1476:GLN:HE21	1.83	0.44
1:A:1471:CYS:SG	1:A:1484:PHE:HB2	2.58	0.44
1:A:1141:THR:O	1:A:1144:HIS:HB3	2.18	0.44
6:A:1604:FAD:O1A	6:A:1604:FAD:H8A	2.17	0.44
1:C:1471:CYS:SG	1:C:1484:PHE:HB2	2.58	0.44
1:A:817:ASP:HB3	1:A:820:VAL:HG13	2.00	0.44
1:C:485:GLY:HA3	1:C:497:PHE:CZ	2.53	0.44
1:C:1198:LEU:HB3	4:C:1602:HEM:HMC3	2.00	0.44
1:C:817:ASP:HB3	1:C:820:VAL:HG13	2.00	0.44
1:A:1034:PHE:O	1:A:1038:ILE:HG13	2.17	0.43
1:A:95:ARG:HD2	1:A:333:MET:HE1	1.99	0.43
1:C:859:MET:HE1	1:C:1476:GLN:HE21	1.83	0.43
2:B:103:VAL:HG13	2:B:132:TRP:HH2	1.83	0.43
1:C:1034:PHE:O	1:C:1038:ILE:HG13	2.19	0.43
1:C:1234:LEU:O	1:C:1238:HIS:HB2	2.18	0.43
1:A:485:GLY:HA3	1:A:497:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:PHE:O	1:A:599:ILE:HG12	2.19	0.43
1:C:165:PRO:HB3	1:C:430:LEU:HD22	2.01	0.43
1:C:1416:LYS:NZ	1:C:1446:ASP:OD2	2.52	0.43
1:A:255:TYR:CD1	1:A:540:VAL:HG13	2.54	0.43
1:C:1246:LEU:HD11	2:D:134:LEU:HB3	2.00	0.43
1:A:859:MET:HE2	1:A:1475:PHE:CE2	2.54	0.43
1:C:859:MET:HE2	1:C:1475:PHE:CE2	2.54	0.43
2:D:103:VAL:HG13	2:D:132:TRP:HH2	1.84	0.43
1:A:1234:LEU:O	1:A:1238:HIS:HB2	2.19	0.43
2:B:145:ALA:HB1	2:B:150:LEU:HD12	2.01	0.43
1:C:435:TYR:OH	1:C:488:GLU:OE2	2.24	0.43
2:B:169:LEU:O	2:B:173:TYR:HB2	2.19	0.42
1:A:300:LEU:HD23	1:A:493:PRO:HG2	2.01	0.42
1:A:490:HIS:C	1:A:492:ASP:H	2.28	0.42
1:A:251:LEU:HD11	1:A:540:VAL:HG12	2.01	0.42
1:A:1416:LYS:NZ	1:A:1446:ASP:OD2	2.52	0.42
1:C:655:PRO:HB3	1:C:1216:ARG:CZ	2.49	0.42
1:A:1426:GLN:OE1	1:A:1464:ARG:NH1	2.52	0.42
2:B:38:PHE:HA	2:B:41:ILE:HG12	2.01	0.42
2:B:96:SER:O	2:B:119:GLN:NE2	2.37	0.42
2:B:101:LEU:HD21	2:B:161:PHE:CE2	2.54	0.42
1:C:255:TYR:CD1	1:C:540:VAL:HG13	2.54	0.42
1:C:1426:GLN:OE1	1:C:1464:ARG:NH1	2.52	0.42
1:A:304:LEU:HD22	1:A:506:VAL:HG23	2.01	0.42
1:A:1278:VAL:N	1:A:1291:ARG:O	2.51	0.42
1:A:39:LEU:HA	2:B:90:PHE:CZ	2.55	0.42
1:A:185:TRP:HA	2:B:166:PRO:HG2	2.02	0.42
1:A:1246:LEU:HD11	2:B:134:LEU:HB3	2.00	0.42
2:B:101:LEU:HD13	2:B:157:LEU:HD13	2.02	0.42
2:D:169:LEU:O	2:D:173:TYR:HB2	2.19	0.42
1:A:412:LEU:HD12	1:A:412:LEU:HA	1.74	0.42
1:A:465:LEU:HD23	1:A:487:LEU:HD13	2.01	0.42
1:A:1383:SER:HB2	1:A:1417:ILE:HD13	2.01	0.42
1:A:1426:GLN:HG3	1:A:1454:ILE:HD11	2.02	0.42
1:C:362:ARG:NH1	1:C:577:PRO:O	2.53	0.42
2:D:132:TRP:HB2	2:D:174:ARG:HD2	2.02	0.42
1:A:52:GLN:HG2	1:A:317:SER:HB2	2.02	0.42
1:A:165:PRO:HB3	1:A:430:LEU:HD22	2.01	0.42
1:A:671:VAL:HG22	1:A:677:VAL:HA	2.02	0.42
1:C:300:LEU:HD23	1:C:493:PRO:HG2	2.01	0.42
1:C:515:TRP:CD1	1:C:517:GLU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:MET:HE3	1:C:879:MET:HB3	1.95	0.42
1:C:1525:MET:O	1:C:1529:VAL:HG23	2.20	0.42
1:A:270:TRP:HE3	1:A:275:LEU:HD23	1.85	0.42
1:A:655:PRO:HB3	1:A:1216:ARG:CZ	2.49	0.42
1:A:1107:ASN:ND2	1:A:1267:SER:OG	2.52	0.42
2:B:132:TRP:HB2	2:B:174:ARG:HD2	2.02	0.42
2:D:38:PHE:HA	2:D:41:ILE:HG12	2.01	0.42
2:D:101:LEU:HD21	2:D:161:PHE:CE2	2.54	0.42
1:A:362:ARG:NH1	1:A:577:PRO:O	2.53	0.42
1:A:1461:PHE:HB3	1:A:1466:THR:HG23	2.02	0.42
1:C:123:LEU:O	1:C:146:PHE:HB3	2.20	0.42
1:C:270:TRP:HE3	1:C:275:LEU:HD23	1.85	0.42
1:C:465:LEU:HD23	1:C:487:LEU:HD13	2.01	0.42
1:C:671:VAL:HG22	1:C:677:VAL:HA	2.02	0.42
1:A:1159:PRO:HD3	2:D:8:PHE:CE1	2.55	0.41
1:C:595:PHE:O	1:C:599:ILE:HG12	2.19	0.41
1:C:1383:SER:HB2	1:C:1417:ILE:HD13	2.02	0.41
1:A:480:GLU:HB2	1:A:483:PRO:HD2	2.02	0.41
1:A:1392:VAL:HA	1:A:1395:PHE:HD2	1.84	0.41
2:B:146:LEU:HD23	2:B:155:LEU:HD13	2.02	0.41
1:C:107:LEU:HD11	1:C:326:SER:HB2	2.02	0.41
1:C:439:ARG:NH1	1:C:488:GLU:OE2	2.53	0.41
1:A:439:ARG:NH1	1:A:488:GLU:OE2	2.54	0.41
1:C:51:LEU:HD21	1:C:167:ASN:HB2	2.02	0.41
1:C:1107:ASN:ND2	1:C:1267:SER:OG	2.52	0.41
1:C:1440:GLU:O	1:C:1488:ARG:NH2	2.53	0.41
1:A:107:LEU:HD11	1:A:326:SER:HB2	2.02	0.41
1:A:442:LEU:HD12	1:A:496:LEU:HD12	2.02	0.41
1:C:251:LEU:HD11	1:C:540:VAL:HG12	2.01	0.41
1:C:304:LEU:HD22	1:C:506:VAL:HG23	2.01	0.41
1:A:1198:LEU:HB3	4:A:1602:HEM:HMC3	2.01	0.41
1:C:39:LEU:HA	2:D:90:PHE:CZ	2.55	0.41
1:A:123:LEU:O	1:A:146:PHE:HB3	2.20	0.41
1:A:515:TRP:CD1	1:A:517:GLU:HB2	2.55	0.41
1:A:654:GLU:HG3	1:A:655:PRO:HD2	2.03	0.41
1:A:1052:TYR:OH	1:A:1136:THR:OG1	2.37	0.41
1:A:1225:HIS:HE1	4:A:1601:HEM:C1C	2.39	0.41
1:C:52:GLN:HG2	1:C:317:SER:HB2	2.02	0.41
1:C:480:GLU:HB2	1:C:483:PRO:HD2	2.02	0.41
2:D:145:ALA:HB1	2:D:150:LEU:HD12	2.01	0.41
1:A:51:LEU:HD21	1:A:167:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ASP:OD1	1:A:830:ASP:N	2.54	0.41
1:A:1243:LEU:H	4:A:1602:HEM:CGA	2.33	0.41
1:A:1436:ILE:HD13	1:A:1450:VAL:HG11	2.03	0.41
1:C:1089:THR:O	1:C:1093:ILE:HB	2.21	0.41
1:C:1426:GLN:HG3	1:C:1454:ILE:HD11	2.02	0.41
2:D:221:LEU:HD21	2:D:254:THR:HB	2.02	0.41
1:A:1038:ILE:HD12	2:D:43:PRO:HB2	2.01	0.41
1:A:1246:LEU:HD13	1:A:1246:LEU:HA	1.92	0.41
1:C:1345:ARG:O	1:C:1349:ILE:HG22	2.21	0.41
1:C:1392:VAL:HA	1:C:1395:PHE:HD2	1.84	0.41
1:A:1440:GLU:O	1:A:1488:ARG:NH2	2.53	0.41
1:C:185:TRP:HA	2:D:166:PRO:HG2	2.02	0.41
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.92	0.41
1:C:1461:PHE:HB3	1:C:1466:THR:HG23	2.02	0.41
2:D:96:SER:O	2:D:119:GLN:NE2	2.37	0.41
2:D:101:LEU:HD13	2:D:157:LEU:HD13	2.02	0.41
1:A:435:TYR:OH	1:A:488:GLU:OE2	2.24	0.41
1:A:527:LYS:HE3	1:A:527:LYS:HB3	1.76	0.41
1:A:1202:LEU:HD11	4:A:1602:HEM:CB	2.51	0.41
1:A:1525:MET:O	1:A:1529:VAL:HG23	2.20	0.41
1:C:341:ARG:HD2	1:C:565:CYS:CB	2.52	0.41
1:C:490:HIS:C	1:C:492:ASP:H	2.28	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.95	0.40
1:C:195:GLY:HA2	1:C:276:PHE:HB2	2.03	0.40
1:C:482:LEU:HA	1:C:482:LEU:HD12	1.89	0.40
1:A:155:THR:HG22	1:A:161:ASN:HD21	1.85	0.40
1:C:342:ASN:OD1	1:C:343:ALA:N	2.53	0.40
1:C:654:GLU:HG3	1:C:655:PRO:HD2	2.03	0.40
1:C:1068:PHE:O	3:E:3:BMA:H62	2.22	0.40
1:A:548:ASP:OD2	1:A:550:SER:OG	2.28	0.40
1:A:1396:ALA:HB1	1:A:1435:ILE:HG21	2.04	0.40
1:C:155:THR:HG22	1:C:161:ASN:HD21	1.86	0.40
1:C:442:LEU:HD12	1:C:496:LEU:HD12	2.02	0.40
1:C:830:ASP:OD1	1:C:830:ASP:N	2.54	0.40
1:C:1202:LEU:HD11	4:C:1602:HEM:CB	2.51	0.40
1:A:251:LEU:HD13	1:A:541:LEU:HD23	2.02	0.40
1:A:1376:GLU:HB3	1:A:1518:PHE:HE1	1.86	0.40
2:B:221:LEU:HD21	2:B:254:THR:HB	2.02	0.40
1:C:762:HIS:O	1:C:766:THR:HG22	2.22	0.40
1:A:1068:PHE:O	3:F:3:BMA:H62	2.22	0.40
1:A:1405:LYS:HE2	1:A:1405:LYS:HB2	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1535:LEU:HD13	1:A:1535:LEU:HA	1.97	0.40
2:D:146:LEU:HD23	2:D:155:LEU:HD13	2.02	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	1349/1551 (87%)	1324 (98%)	25 (2%)	0	100	100
1	C	1349/1551 (87%)	1324 (98%)	25 (2%)	0	100	100
2	B	270/483 (56%)	266 (98%)	4 (2%)	0	100	100
2	D	270/483 (56%)	267 (99%)	3 (1%)	0	100	100
All	All	3238/4068 (80%)	3181 (98%)	57 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1117/1360 (82%)	1088 (97%)	29 (3%)	40	68
1	C	1117/1360 (82%)	1087 (97%)	30 (3%)	39	67
2	B	219/400 (55%)	214 (98%)	5 (2%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	219/400 (55%)	214 (98%)	5 (2%)	44 71
All	All	2672/3520 (76%)	2603 (97%)	69 (3%)	41 68

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	115	THR
1	A	244	PHE
1	A	292	VAL
1	A	328	GLN
1	A	329	PHE
1	A	429	ASP
1	A	462	ASP
1	A	654	GLU
1	A	659	VAL
1	A	677	VAL
1	A	755	VAL
1	A	820	VAL
1	A	840	PHE
1	A	844	LEU
1	A	858	LEU
1	A	878	ARG
1	A	1032	GLN
1	A	1061	GLU
1	A	1079	THR
1	A	1093	ILE
1	A	1189	THR
1	A	1255	VAL
1	A	1275	ILE
1	A	1313	LEU
1	A	1423	THR
1	A	1438	GLU
1	A	1535	LEU
1	A	1536	ILE
2	B	70	VAL
2	B	81	VAL
2	B	202	VAL
2	B	209	MET
2	B	221	LEU
1	C	50	ARG
1	C	115	THR

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Mol	Chain	Res	Type
1	C	244	PHE
1	C	292	VAL
1	C	328	GLN
1	C	329	PHE
1	C	429	ASP
1	C	462	ASP
1	C	654	GLU
1	C	659	VAL
1	C	677	VAL
1	C	755	VAL
1	C	820	VAL
1	C	840	PHE
1	C	844	LEU
1	C	858	LEU
1	C	878	ARG
1	C	1032	GLN
1	C	1061	GLU
1	C	1079	THR
1	C	1093	ILE
1	C	1189	THR
1	C	1225	HIS
1	C	1255	VAL
1	C	1275	ILE
1	C	1313	LEU
1	C	1423	THR
1	C	1438	GLU
1	C	1535	LEU
1	C	1536	ILE
2	D	70	VAL
2	D	81	VAL
2	D	202	VAL
2	D	209	MET
2	D	221	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	ASN
1	A	301	GLN
1	A	555	ASN
1	A	1071	HIS
1	A	1451	HIS

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Mol	Chain	Res	Type
2	B	237	HIS
1	C	211	ASN
1	C	301	GLN
1	C	555	ASN
1	C	1071	HIS
1	C	1451	HIS
2	D	71	ASN
2	D	237	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](#)

20 monosaccharides 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	$\# Z > 2$
3	NAG	E	1	2,3	14,14,15	0.27	0	17,19,21	0.48	0
3	MAN	E	10	3	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
3	NAG	E	2	3	14,14,15	0.26	0	17,19,21	0.40	0
3	BMA	E	3	3	11,11,12	0.62	0	15,15,17	1.01	0
3	MAN	E	4	3	11,11,12	0.58	0	15,15,17	0.99	2 (13%)
3	MAN	E	5	3	11,11,12	0.58	0	15,15,17	1.12	2 (13%)
3	MAN	E	6	3	11,11,12	0.65	0	15,15,17	0.87	1 (6%)
3	MAN	E	7	3	11,11,12	0.71	0	15,15,17	1.12	2 (13%)
3	MAN	E	8	3	11,11,12	0.63	0	15,15,17	0.95	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	E	9	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
3	NAG	F	1	2,3	14,14,15	0.29	0	17,19,21	0.49	0
3	MAN	F	10	3	11,11,12	0.66	0	15,15,17	0.92	2 (13%)
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.40	0
3	BMA	F	3	3	11,11,12	0.62	0	15,15,17	1.01	0
3	MAN	F	4	3	11,11,12	0.57	0	15,15,17	0.99	2 (13%)
3	MAN	F	5	3	11,11,12	0.58	0	15,15,17	1.12	2 (13%)
3	MAN	F	6	3	11,11,12	0.67	0	15,15,17	0.85	1 (6%)
3	MAN	F	7	3	11,11,12	0.71	0	15,15,17	1.13	2 (13%)
3	MAN	F	8	3	11,11,12	0.62	0	15,15,17	0.96	2 (13%)
3	MAN	F	9	3	11,11,12	0.61	0	15,15,17	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	2,3	-	0/6/23/26	0/1/1/1
3	MAN	E	10	3	-	2/2/19/22	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	MAN	E	4	3	-	0/2/19/22	0/1/1/1
3	MAN	E	5	3	-	0/2/19/22	0/1/1/1
3	MAN	E	6	3	-	0/2/19/22	0/1/1/1
3	MAN	E	7	3	-	2/2/19/22	0/1/1/1
3	MAN	E	8	3	-	0/2/19/22	0/1/1/1
3	MAN	E	9	3	-	1/2/19/22	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	MAN	F	10	3	-	2/2/19/22	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	0/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
3	MAN	F	7	3	-	2/2/19/22	0/1/1/1
3	MAN	F	8	3	-	0/2/19/22	0/1/1/1
3	MAN	F	9	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	MAN	C1-O5-C5	2.95	116.14	112.19
3	F	5	MAN	C1-O5-C5	2.93	116.11	112.19
3	F	7	MAN	C1-O5-C5	2.86	116.02	112.19
3	E	7	MAN	C1-O5-C5	2.78	115.91	112.19
3	E	5	MAN	O2-C2-C3	-2.66	104.65	110.15
3	F	5	MAN	O2-C2-C3	-2.65	104.66	110.15
3	E	9	MAN	C1-O5-C5	2.54	115.59	112.19
3	F	9	MAN	C1-O5-C5	2.54	115.59	112.19
3	F	4	MAN	O2-C2-C3	-2.48	105.02	110.15
3	E	4	MAN	O2-C2-C3	-2.46	105.05	110.15
3	F	4	MAN	C1-O5-C5	2.41	115.41	112.19
3	E	4	MAN	C1-O5-C5	2.40	115.40	112.19
3	F	8	MAN	O2-C2-C3	-2.38	105.23	110.15
3	E	8	MAN	O2-C2-C3	-2.35	105.29	110.15
3	F	8	MAN	C1-O5-C5	2.31	115.28	112.19
3	E	8	MAN	C1-O5-C5	2.30	115.27	112.19
3	E	7	MAN	O2-C2-C3	-2.22	105.56	110.15
3	F	7	MAN	O2-C2-C3	-2.20	105.59	110.15
3	F	9	MAN	O2-C2-C3	-2.15	105.70	110.15
3	E	10	MAN	O2-C2-C3	-2.14	105.71	110.15
3	F	10	MAN	C1-O5-C5	2.14	115.05	112.19
3	E	10	MAN	C1-O5-C5	2.14	115.05	112.19
3	E	9	MAN	O2-C2-C3	-2.14	105.73	110.15
3	F	10	MAN	O2-C2-C3	-2.13	105.74	110.15
3	E	6	MAN	O2-C2-C3	-2.12	105.75	110.15
3	F	6	MAN	O2-C2-C3	-2.08	105.84	110.15

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	7	MAN	C4-C5-C6-O6
3	E	7	MAN	C4-C5-C6-O6
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	9	MAN	O5-C5-C6-O6
3	E	9	MAN	O5-C5-C6-O6
3	E	7	MAN	O5-C5-C6-O6

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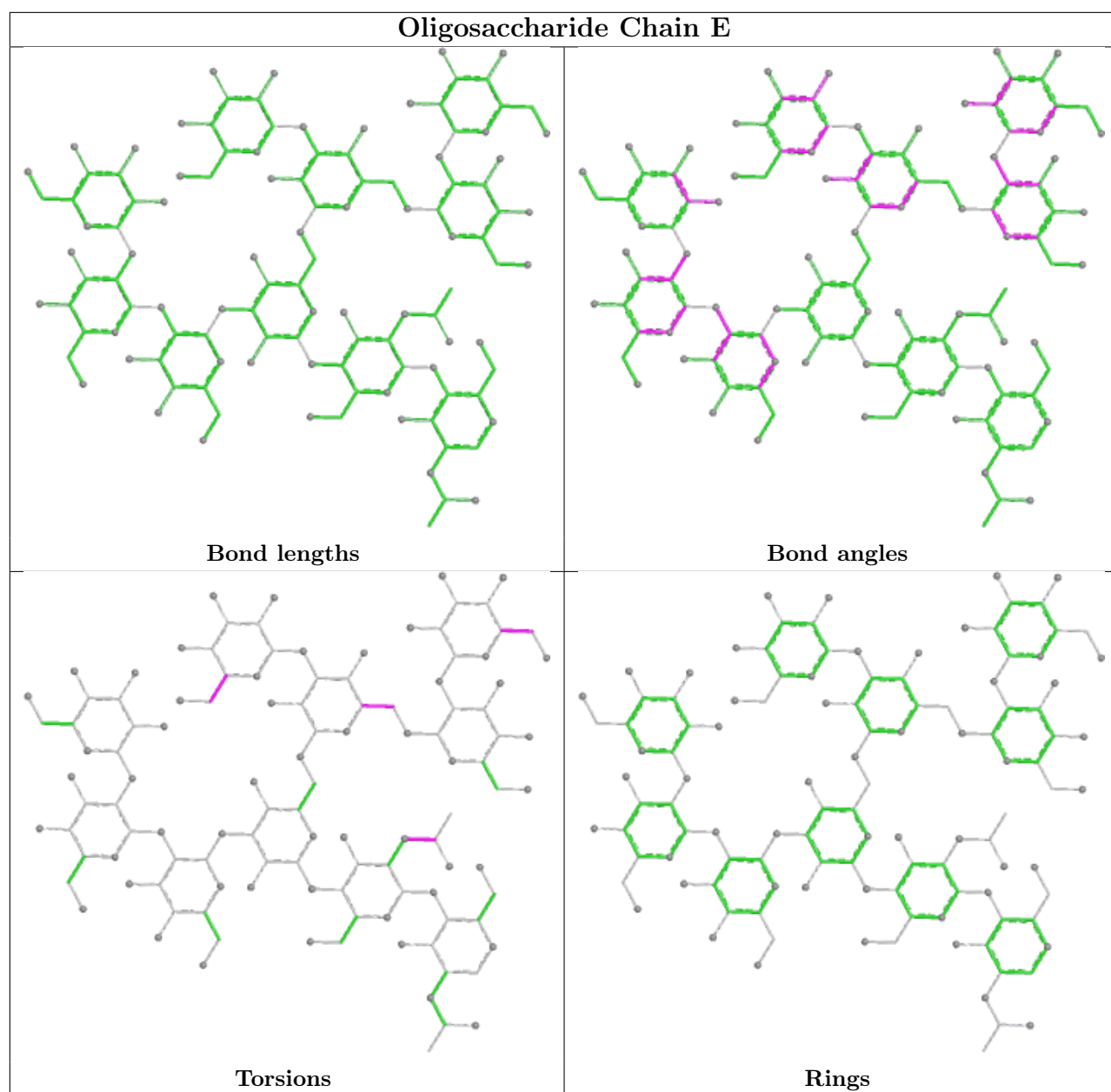
Mol	Chain	Res	Type	Atoms
3	F	7	MAN	O5-C5-C6-O6
3	F	10	MAN	O5-C5-C6-O6
3	F	10	MAN	C4-C5-C6-O6
3	E	10	MAN	O5-C5-C6-O6
3	E	10	MAN	C4-C5-C6-O6

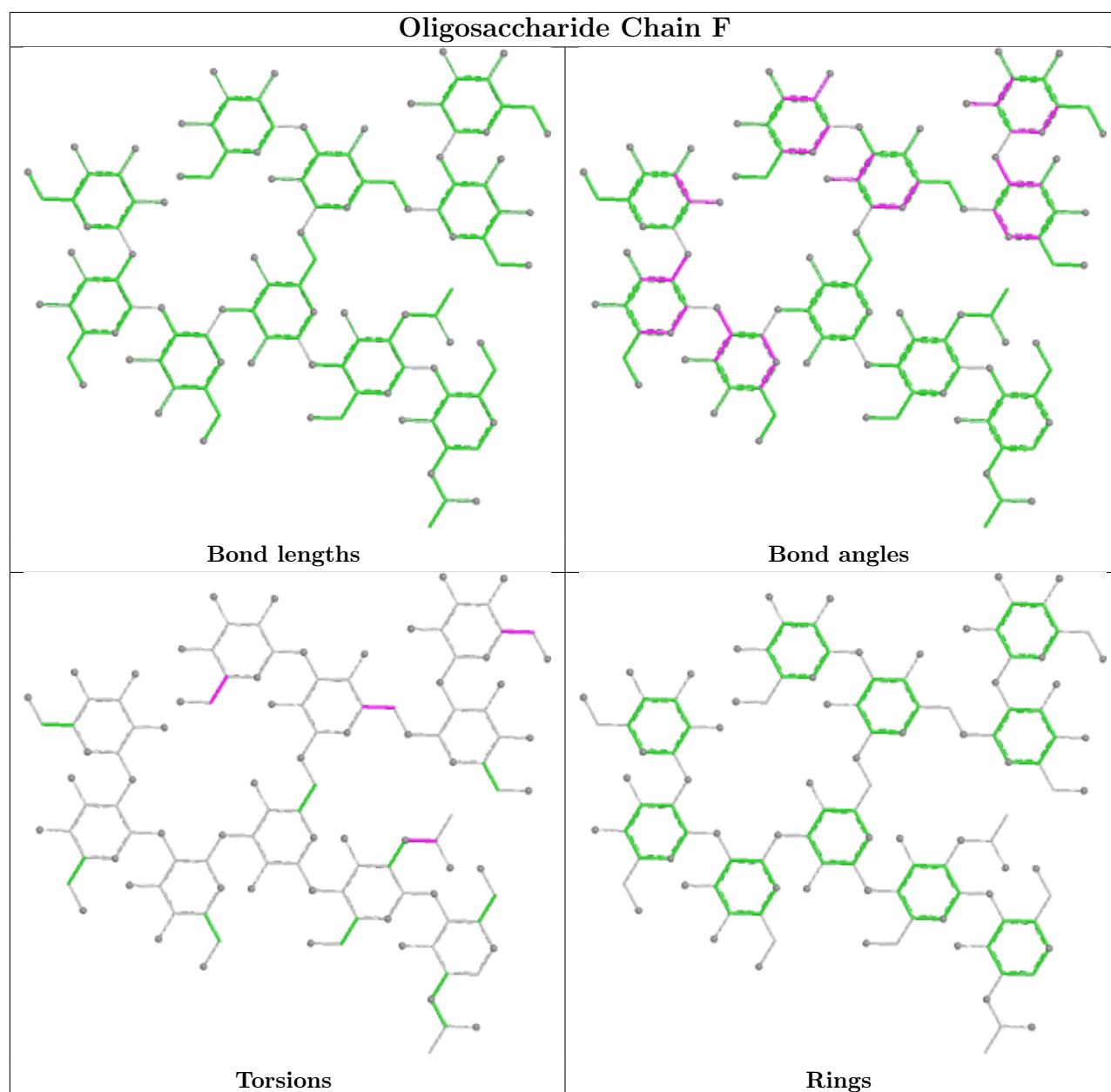
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	9	MAN	1	0
3	E	9	MAN	1	0
3	E	3	BMA	1	0
3	F	3	BMA	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 oligosaccharide.





5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	1602	1	50,50,50	1.43	9 (18%)	67,82,82	1.10	5 (7%)
6	FAD	A	1604	-	58,58,58	1.50	9 (15%)	85,89,89	1.57	16 (18%)
6	FAD	C	1604	-	58,58,58	1.50	10 (17%)	85,89,89	1.56	16 (18%)
5	NDP	C	1603	-	51,52,52	1.21	5 (9%)	71,80,80	1.60	10 (14%)
8	NAG	A	1608	1	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	B	502	2	14,14,15	0.24	0	17,19,21	0.55	0
8	NAG	C	1607	1	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	C	1609	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NDP	A	1603	-	51,52,52	1.20	5 (9%)	71,80,80	1.60	10 (14%)
4	HEM	A	1601	1	50,50,50	1.41	9 (18%)	67,82,82	1.14	5 (7%)
4	HEM	C	1601	1	50,50,50	1.41	8 (16%)	67,82,82	1.12	4 (5%)
8	NAG	C	1608	1	14,14,15	0.24	0	17,19,21	0.46	0
8	NAG	D	502	2	14,14,15	0.23	0	17,19,21	0.55	0
4	HEM	C	1602	1	50,50,50	1.45	9 (18%)	67,82,82	1.10	5 (7%)
8	NAG	A	1607	1	14,14,15	0.23	0	17,19,21	0.45	0
8	NAG	B	501	2	14,14,15	0.23	0	17,19,21	0.50	0
8	NAG	D	501	2	14,14,15	0.25	0	17,19,21	0.51	0
8	NAG	A	1609	1	14,14,15	0.27	0	17,19,21	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	1602	1	-	2/14/54/54	-
6	FAD	A	1604	-	-	14/34/50/50	0/6/6/6
6	FAD	C	1604	-	-	14/34/50/50	0/6/6/6
5	NDP	C	1603	-	-	6/34/77/77	0/5/5/5
8	NAG	A	1608	1	-	1/6/23/26	0/1/1/1
8	NAG	B	502	2	-	4/6/23/26	0/1/1/1
8	NAG	C	1607	1	-	0/6/23/26	0/1/1/1
8	NAG	C	1609	1	-	2/6/23/26	0/1/1/1
5	NDP	A	1603	-	-	6/34/77/77	0/5/5/5
4	HEM	A	1601	1	-	0/14/54/54	-
4	HEM	C	1601	1	-	0/14/54/54	-
8	NAG	C	1608	1	-	1/6/23/26	0/1/1/1
8	NAG	D	502	2	-	4/6/23/26	0/1/1/1
4	HEM	C	1602	1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1607	1	-	0/6/23/26	0/1/1/1
8	NAG	B	501	2	-	0/6/23/26	0/1/1/1
8	NAG	D	501	2	-	0/6/23/26	0/1/1/1
8	NAG	A	1609	1	-	2/6/23/26	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1604	FAD	C9A-C5X	5.39	1.49	1.41
6	A	1604	FAD	C9A-C5X	5.38	1.49	1.41
5	C	1603	NDP	C5A-C4A	4.76	1.47	1.39
5	A	1603	NDP	C5A-C4A	4.76	1.47	1.39
6	A	1604	FAD	C5A-C4A	4.75	1.47	1.39
6	C	1604	FAD	C5A-C4A	4.72	1.47	1.39
4	C	1602	HEM	FE-NA	3.61	2.07	1.95
4	A	1602	HEM	FE-ND	3.54	2.05	1.94
4	A	1602	HEM	FE-NB	3.50	2.05	1.94
4	C	1602	HEM	FE-NB	3.48	2.05	1.94
4	C	1601	HEM	FE-NB	3.47	2.05	1.94
4	C	1602	HEM	FE-ND	3.45	2.05	1.94
6	C	1604	FAD	C8-C7	3.32	1.48	1.40
6	A	1604	FAD	C8-C7	3.31	1.48	1.40
4	A	1601	HEM	FE-ND	3.15	2.04	1.94
4	C	1601	HEM	CAC-C3C	3.15	1.55	1.47
4	A	1601	HEM	FE-NC	3.13	2.05	1.95
4	A	1601	HEM	CAC-C3C	3.12	1.55	1.47
4	A	1602	HEM	CAB-C3B	3.12	1.55	1.47
4	C	1602	HEM	CAB-C3B	3.11	1.55	1.47
4	C	1601	HEM	FE-NA	3.09	2.05	1.95
4	C	1601	HEM	FE-NC	3.09	2.05	1.95
4	C	1602	HEM	CAC-C3C	3.07	1.55	1.47
4	A	1601	HEM	FE-NB	3.07	2.04	1.94
4	A	1602	HEM	CAC-C3C	3.06	1.55	1.47
4	A	1602	HEM	FE-NC	3.04	2.05	1.95
4	A	1601	HEM	FE-NA	3.04	2.05	1.95
4	A	1601	HEM	CAB-C3B	3.01	1.55	1.47
4	C	1601	HEM	CAB-C3B	2.98	1.55	1.47
4	A	1602	HEM	FE-NA	2.91	2.04	1.95
4	C	1601	HEM	FE-ND	2.86	2.03	1.94
6	C	1604	FAD	C5A-C6A	2.77	1.48	1.41
5	C	1603	NDP	C5A-C6A	2.76	1.48	1.41
6	A	1604	FAD	C5A-C6A	2.72	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1603	NDP	C5A-C6A	2.70	1.48	1.41
4	C	1602	HEM	FE-NC	2.53	2.03	1.95
6	C	1604	FAD	C4-N3	-2.46	1.34	1.38
6	A	1604	FAD	C4-N3	-2.45	1.34	1.38
5	C	1603	NDP	C8A-N7A	2.36	1.36	1.31
5	A	1603	NDP	C8A-N7A	2.35	1.36	1.31
6	C	1604	FAD	C8A-N7A	2.32	1.36	1.31
6	A	1604	FAD	C8A-N7A	2.31	1.36	1.31
5	C	1603	NDP	C5A-N7A	-2.28	1.34	1.39
6	C	1604	FAD	C5A-N7A	-2.27	1.34	1.39
6	A	1604	FAD	C5A-N7A	-2.25	1.35	1.39
5	A	1603	NDP	C5A-N7A	-2.24	1.35	1.39
4	C	1601	HEM	CMC-C2C	2.12	1.55	1.50
4	A	1602	HEM	CMB-C2B	2.12	1.55	1.50
5	C	1603	NDP	C6N-C5N	2.12	1.39	1.33
5	A	1603	NDP	C6N-C5N	2.12	1.39	1.33
6	C	1604	FAD	C5X-N5	-2.11	1.35	1.39
4	C	1602	HEM	CMB-C2B	2.11	1.55	1.50
4	A	1601	HEM	CMB-C2B	2.11	1.55	1.50
6	A	1604	FAD	C5X-N5	-2.11	1.35	1.39
6	A	1604	FAD	C4X-N5	2.11	1.35	1.30
4	C	1601	HEM	CMB-C2B	2.10	1.55	1.50
4	A	1601	HEM	CMC-C2C	2.09	1.55	1.50
6	C	1604	FAD	C4X-N5	2.09	1.35	1.30
4	C	1602	HEM	CMC-C2C	2.07	1.55	1.50
4	A	1602	HEM	CMC-C2C	2.05	1.55	1.50
4	C	1602	HEM	CMD-C2D	2.03	1.54	1.50
6	C	1604	FAD	PA-O3P	2.02	1.61	1.59
4	A	1602	HEM	CMA-C3A	2.01	1.54	1.50
4	A	1601	HEM	CMD-C2D	2.01	1.54	1.50

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1603	NDP	C5A-C4A-N3A	-5.86	118.64	126.72
6	A	1604	FAD	C5A-C4A-N3A	-5.86	118.65	126.72
5	C	1603	NDP	C5A-C4A-N3A	-5.84	118.67	126.72
6	C	1604	FAD	C5A-C4A-N3A	-5.83	118.70	126.72
5	C	1603	NDP	N3A-C4A-N9A	4.67	135.11	127.17
5	A	1603	NDP	N3A-C4A-N9A	4.65	135.07	127.17
6	C	1604	FAD	N3A-C4A-N9A	4.63	135.05	127.17
6	A	1604	FAD	N3A-C4A-N9A	4.63	135.05	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1603	NDP	C2A-N3A-C4A	3.71	120.88	111.83
5	A	1603	NDP	C2A-N3A-C4A	3.69	120.85	111.83
6	C	1604	FAD	C2A-N3A-C4A	3.69	120.85	111.83
6	A	1604	FAD	C2A-N3A-C4A	3.69	120.84	111.83
5	A	1603	NDP	C4A-C5A-N7A	-3.48	106.60	110.58
6	A	1604	FAD	C4A-C5A-N7A	-3.48	106.60	110.58
5	C	1603	NDP	C4A-C5A-N7A	-3.41	106.68	110.58
6	C	1604	FAD	C4A-C5A-N7A	-3.41	106.69	110.58
5	C	1603	NDP	N3A-C2A-N1A	-3.21	123.72	128.58
5	A	1603	NDP	N3A-C2A-N1A	-3.21	123.72	128.58
6	C	1604	FAD	N3A-C2A-N1A	-3.20	123.74	128.58
6	A	1604	FAD	N3A-C2A-N1A	-3.18	123.77	128.58
5	A	1603	NDP	C2B-C1B-N9A	-3.11	108.63	113.75
5	C	1603	NDP	C2B-C1B-N9A	-3.09	108.67	113.75
4	A	1601	HEM	C4D-ND-C1D	2.73	108.44	105.21
4	C	1601	HEM	C4D-ND-C1D	2.72	108.42	105.21
5	C	1603	NDP	C4A-N9A-C8A	2.70	108.57	105.74
6	A	1604	FAD	C4-C4X-N5	2.67	121.90	118.21
6	C	1604	FAD	C4-C4X-N5	2.67	121.89	118.21
5	A	1603	NDP	C4A-N9A-C8A	2.64	108.51	105.74
6	A	1604	FAD	C4A-N9A-C8A	2.59	108.45	105.74
6	A	1604	FAD	C4X-C10-N1	-2.58	118.27	124.59
6	C	1604	FAD	C4X-C10-N1	-2.56	118.32	124.59
6	C	1604	FAD	C4A-N9A-C8A	2.56	108.42	105.74
6	A	1604	FAD	C5A-N7A-C8A	2.55	107.46	103.45
5	C	1603	NDP	C5A-N7A-C8A	2.53	107.42	103.45
5	A	1603	NDP	C5A-N7A-C8A	2.53	107.42	103.45
6	C	1604	FAD	C5A-N7A-C8A	2.50	107.38	103.45
4	C	1601	HEM	C3D-C4D-ND	-2.48	107.45	110.17
4	A	1601	HEM	C3D-C4D-ND	-2.44	107.50	110.17
6	A	1604	FAD	C4X-C10-N10	2.42	119.94	116.48
6	C	1604	FAD	C4X-C10-N10	2.39	119.90	116.48
4	C	1602	HEM	C4D-ND-C1D	2.36	108.00	105.21
6	A	1604	FAD	C4'-C3'-C2'	-2.34	109.67	113.57
4	A	1602	HEM	C4D-ND-C1D	2.33	107.96	105.21
4	A	1601	HEM	C2A-C1A-NA	-2.32	107.58	110.15
4	A	1602	HEM	C2A-C1A-NA	-2.32	107.58	110.15
6	C	1604	FAD	C4'-C3'-C2'	-2.30	109.75	113.57
4	C	1601	HEM	C2A-C1A-NA	-2.30	107.61	110.15
4	C	1602	HEM	C1B-NB-C4B	2.29	107.92	105.21
4	A	1601	HEM	C1B-NB-C4B	2.29	107.92	105.21
4	A	1602	HEM	C1B-NB-C4B	2.26	107.88	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1602	HEM	C2A-C1A-NA	-2.23	107.67	110.15
6	C	1604	FAD	O4-C4-C4X	-2.17	120.80	126.53
4	C	1601	HEM	C1B-NB-C4B	2.17	107.77	105.21
6	A	1604	FAD	O4-C4-C4X	-2.16	120.82	126.53
6	C	1604	FAD	C10-N1-C2	2.14	121.48	116.85
6	A	1604	FAD	C10-N1-C2	2.14	121.47	116.85
5	A	1603	NDP	C3D-C2D-C1D	2.11	105.46	101.46
4	C	1602	HEM	C3D-C4D-ND	-2.11	107.86	110.17
5	C	1603	NDP	C3D-C2D-C1D	2.10	105.43	101.46
4	A	1602	HEM	C3D-C4D-ND	-2.08	107.89	110.17
6	C	1604	FAD	C3B-C2B-C1B	2.07	105.37	101.46
6	A	1604	FAD	C6A-C5A-N7A	2.06	136.07	132.09
5	A	1603	NDP	C6A-C5A-N7A	2.06	136.06	132.09
4	A	1602	HEM	C3B-C2B-C1B	2.05	107.95	106.41
6	A	1604	FAD	C3B-C2B-C1B	2.05	105.34	101.46
4	C	1602	HEM	C3B-C2B-C1B	2.05	107.95	106.41
5	C	1603	NDP	C6A-C5A-N7A	2.05	136.03	132.09
6	C	1604	FAD	C4X-C4-N3	2.03	118.43	113.25
6	C	1604	FAD	C6A-C5A-N7A	2.03	136.00	132.09
6	A	1604	FAD	C4X-C4-N3	2.02	118.39	113.25
4	A	1601	HEM	C2D-C1D-ND	-2.02	107.57	109.90

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1603	NDP	C5D-O5D-PN-O3
5	A	1603	NDP	C5D-O5D-PN-O1N
5	A	1603	NDP	C5D-O5D-PN-O2N
5	C	1603	NDP	C5D-O5D-PN-O3
5	C	1603	NDP	C5D-O5D-PN-O1N
5	C	1603	NDP	C5D-O5D-PN-O2N
6	A	1604	FAD	N10-C1'-C2'-O2'
6	A	1604	FAD	N10-C1'-C2'-C3'
6	A	1604	FAD	C1'-C2'-C3'-O3'
6	A	1604	FAD	C1'-C2'-C3'-C4'
6	A	1604	FAD	O2'-C2'-C3'-C4'
6	A	1604	FAD	C5'-O5'-P-O1P
6	C	1604	FAD	N10-C1'-C2'-O2'
6	C	1604	FAD	N10-C1'-C2'-C3'
6	C	1604	FAD	C1'-C2'-C3'-O3'
6	C	1604	FAD	C1'-C2'-C3'-C4'

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Mol	Chain	Res	Type	Atoms
6	C	1604	FAD	O2'-C2'-C3'-C4'
6	C	1604	FAD	C5'-O5'-P-O1P
6	A	1604	FAD	O2'-C2'-C3'-O3'
6	C	1604	FAD	O2'-C2'-C3'-O3'
6	A	1604	FAD	O4B-C4B-C5B-O5B
6	A	1604	FAD	C3B-C4B-C5B-O5B
6	C	1604	FAD	O4B-C4B-C5B-O5B
8	A	1609	NAG	O5-C5-C6-O6
8	C	1609	NAG	O5-C5-C6-O6
6	C	1604	FAD	C3B-C4B-C5B-O5B
8	B	502	NAG	O5-C5-C6-O6
8	D	502	NAG	O5-C5-C6-O6
8	A	1609	NAG	C4-C5-C6-O6
8	C	1609	NAG	C4-C5-C6-O6
8	B	502	NAG	C4-C5-C6-O6
8	D	502	NAG	C4-C5-C6-O6
5	A	1603	NDP	O4D-C1D-N1N-C2N
5	A	1603	NDP	O4B-C4B-C5B-O5B
5	C	1603	NDP	O4B-C4B-C5B-O5B
5	C	1603	NDP	O4D-C1D-N1N-C2N
6	A	1604	FAD	O3'-C3'-C4'-C5'
6	C	1604	FAD	O3'-C3'-C4'-C5'
6	C	1604	FAD	C2'-C3'-C4'-C5'
8	B	502	NAG	C1-C2-N2-C7
8	D	502	NAG	C1-C2-N2-C7
6	A	1604	FAD	C2'-C3'-C4'-C5'
6	A	1604	FAD	C2'-C3'-C4'-O4'
6	C	1604	FAD	C2'-C3'-C4'-O4'
6	A	1604	FAD	C5B-O5B-PA-O1A
6	C	1604	FAD	C5B-O5B-PA-O1A
8	B	502	NAG	C3-C2-N2-C7
8	D	502	NAG	C3-C2-N2-C7
5	A	1603	NDP	PA-O3-PN-O2N
5	C	1603	NDP	PA-O3-PN-O2N
6	C	1604	FAD	O3'-C3'-C4'-O4'
6	A	1604	FAD	O3'-C3'-C4'-O4'
4	A	1602	HEM	C2A-CAA-CBA-CGA
8	A	1608	NAG	O5-C5-C6-O6
8	C	1608	NAG	O5-C5-C6-O6
4	A	1602	HEM	CAD-CBD-CGD-O2D
4	C	1602	HEM	CAD-CBD-CGD-O2D

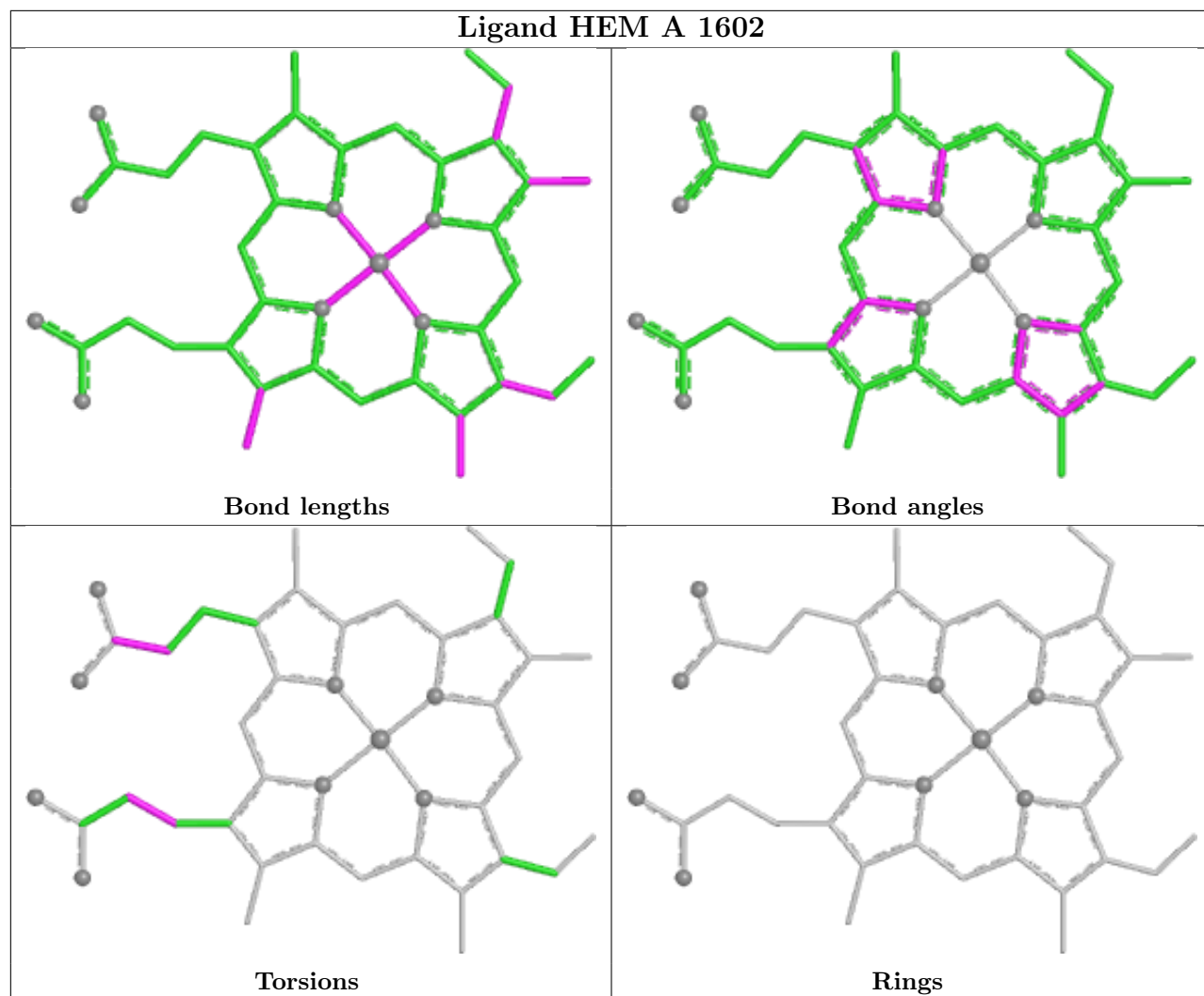
There are no ring outliers.

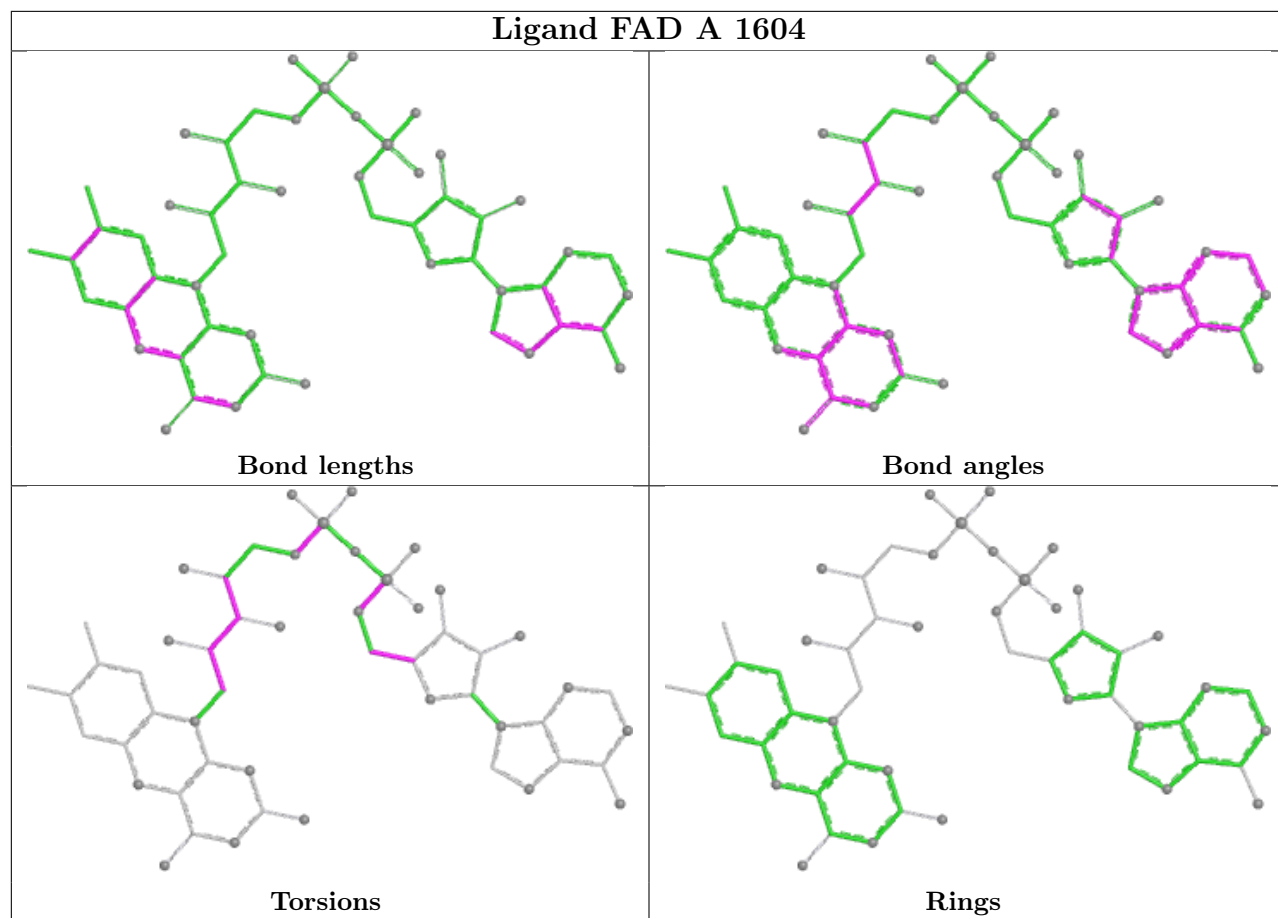
8 monomers are involved in 24 short contacts:

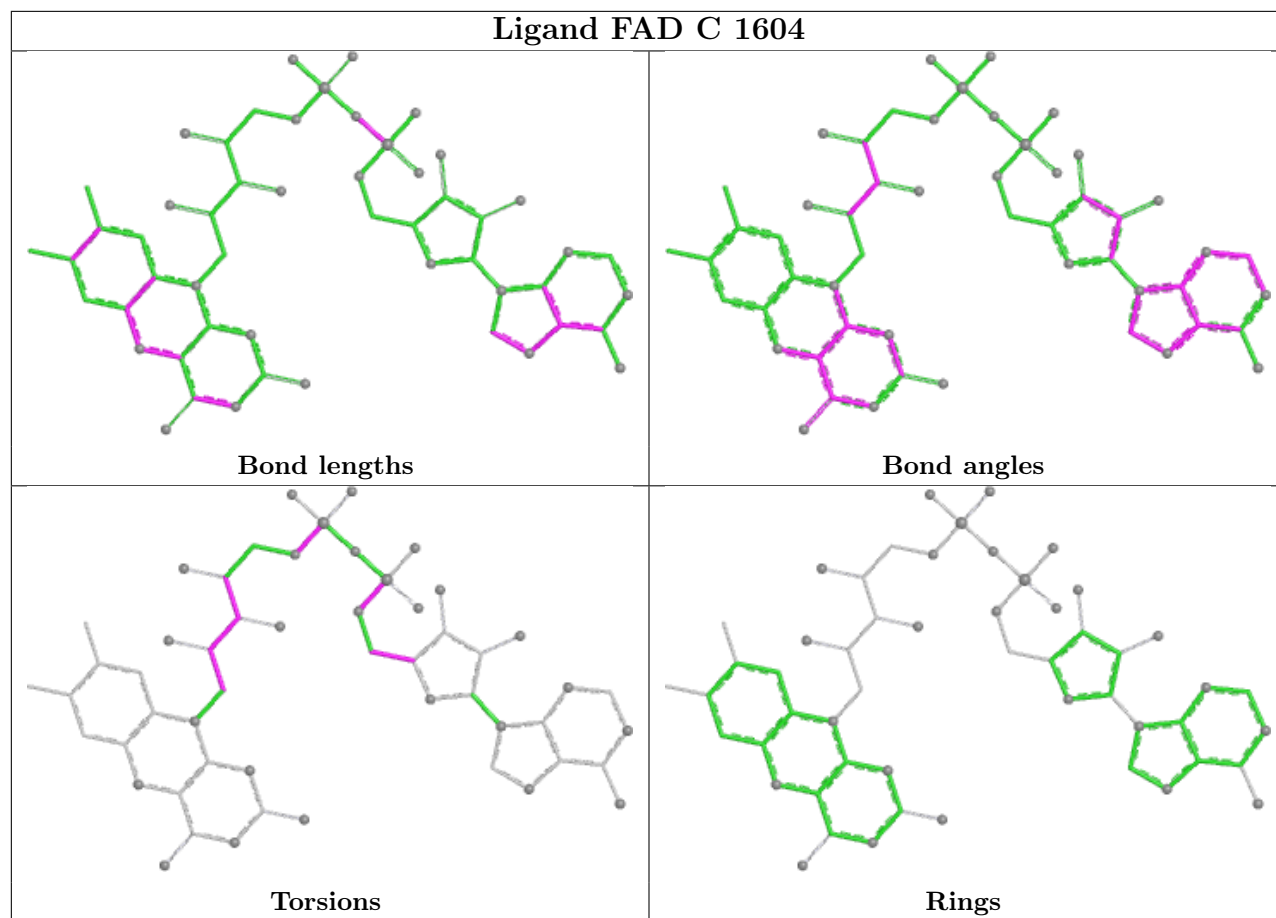
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1602	HEM	5	0
6	A	1604	FAD	1	0
6	C	1604	FAD	1	0
5	C	1603	NDP	2	0
5	A	1603	NDP	2	0
4	A	1601	HEM	5	0
4	C	1601	HEM	3	0
4	C	1602	HEM	5	0

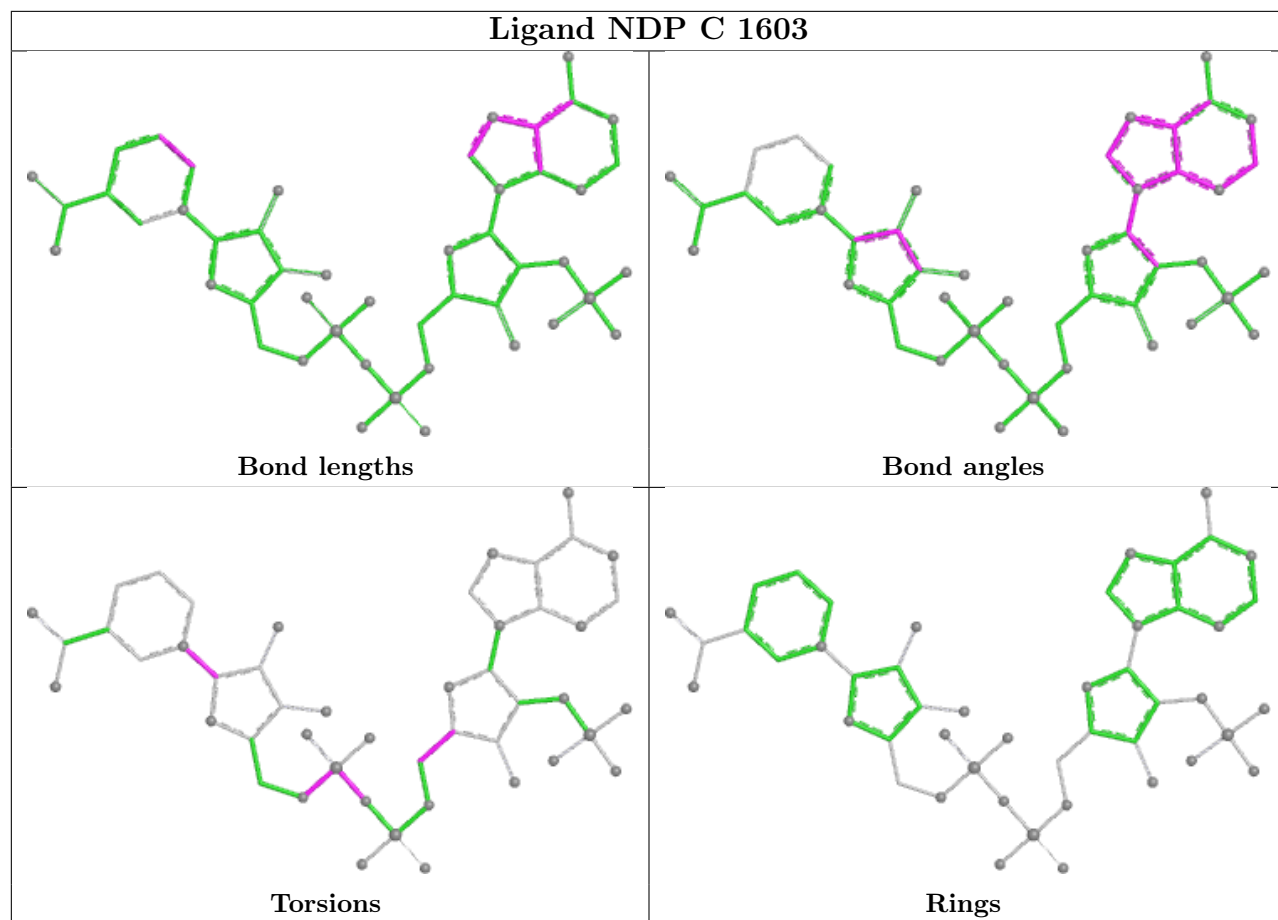
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

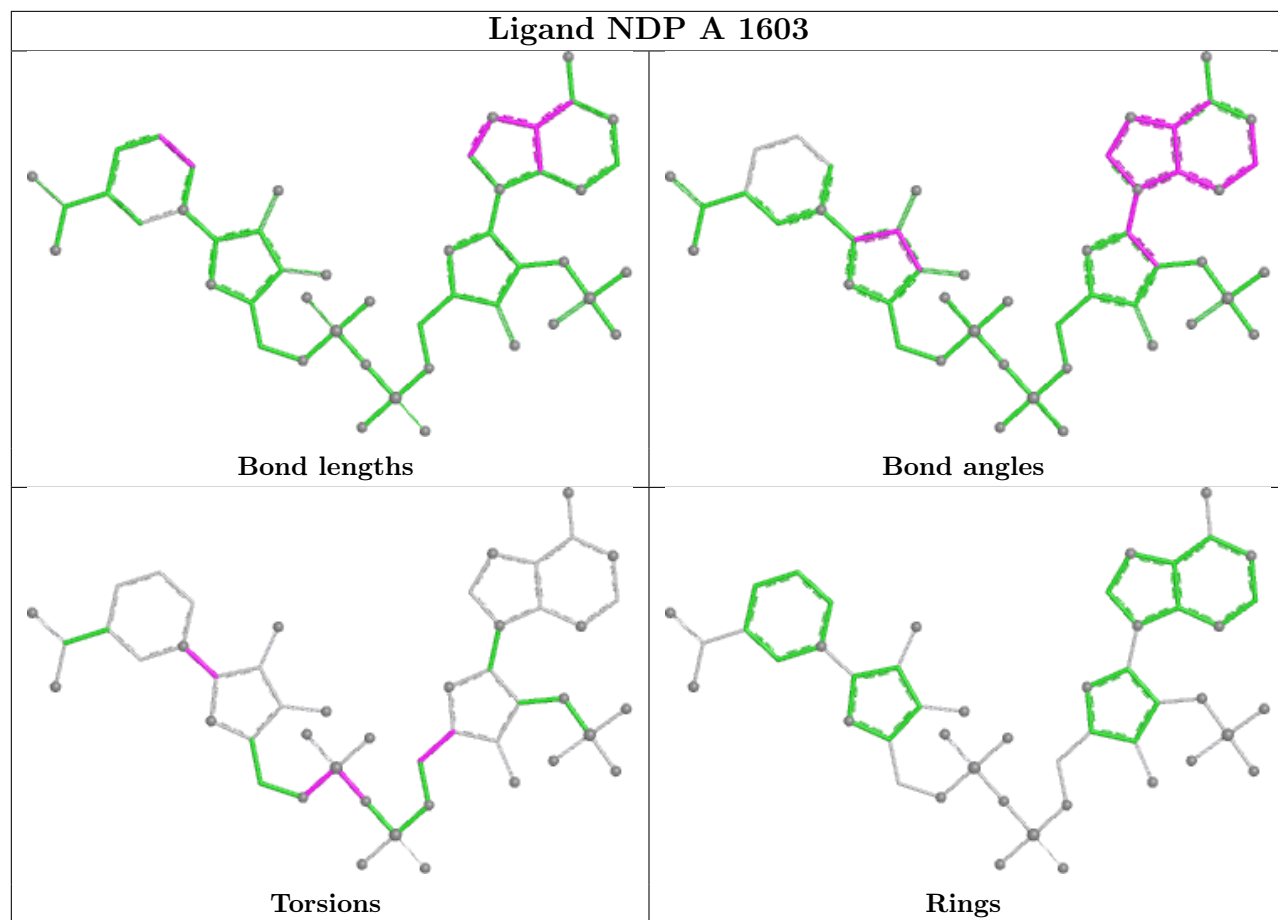
Ligand HEM A 1602

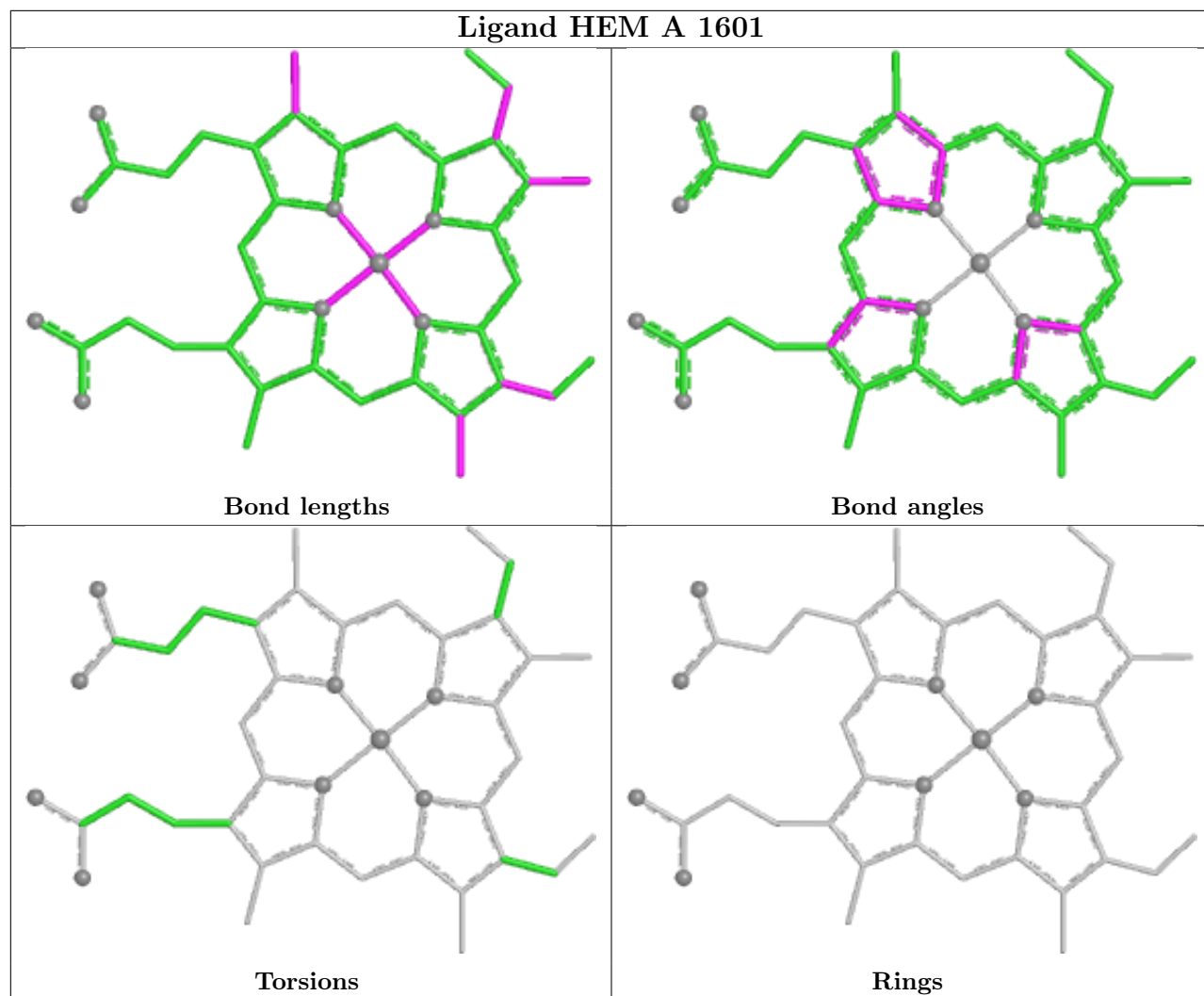


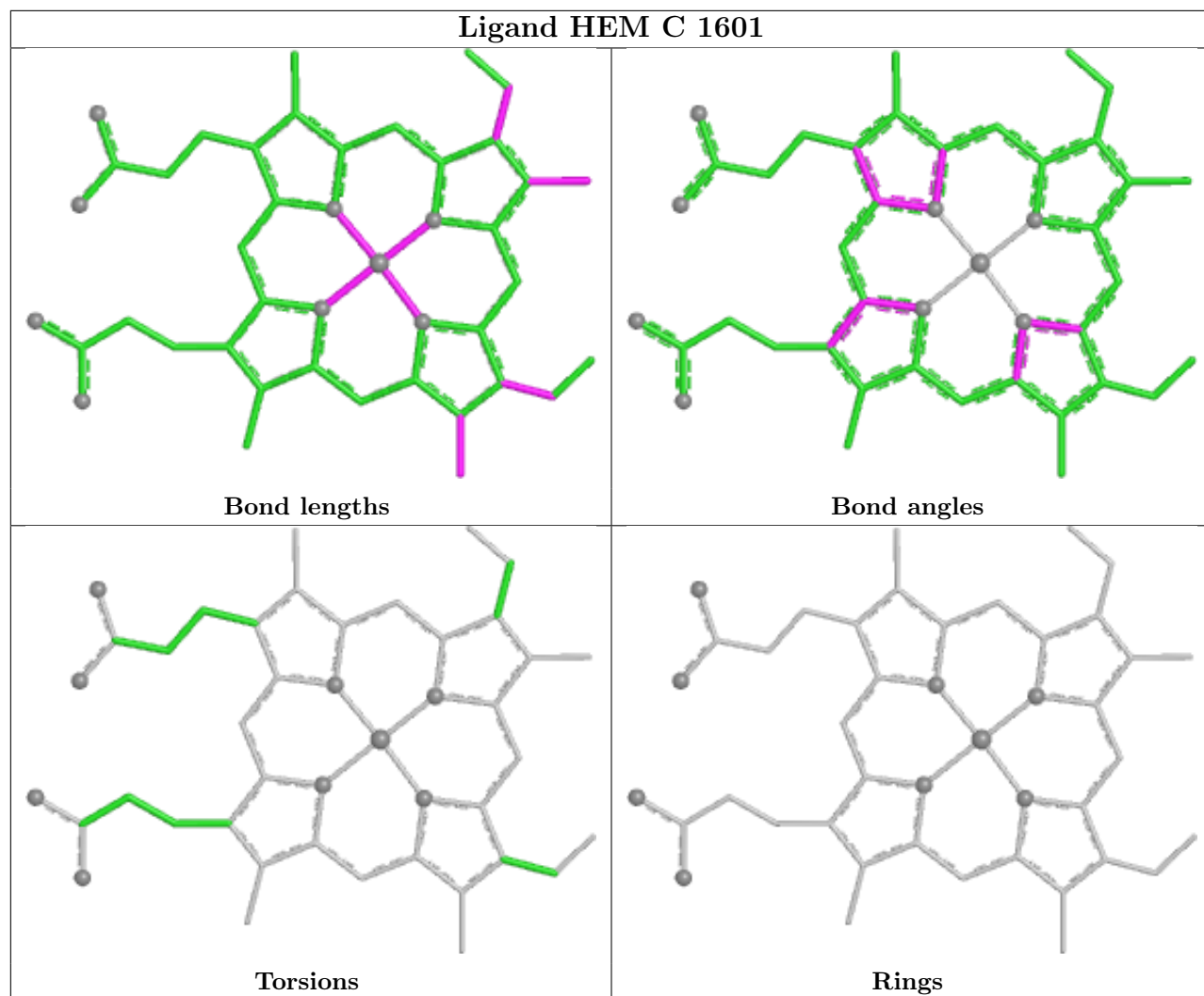


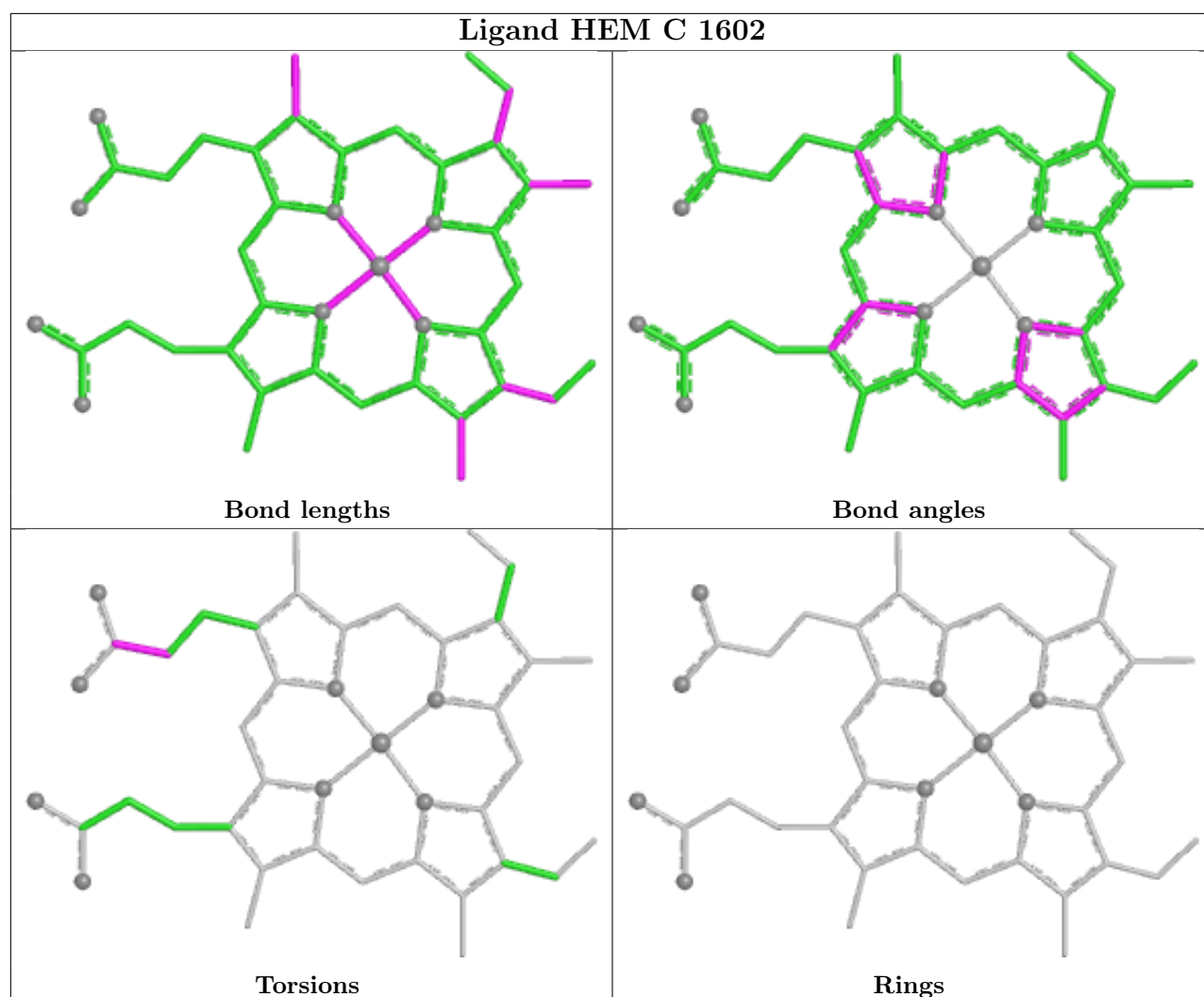












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

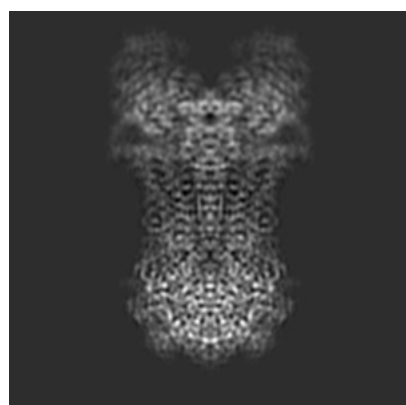
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30556. These allow visual inspection of the internal detail of the map and identification of artifacts.

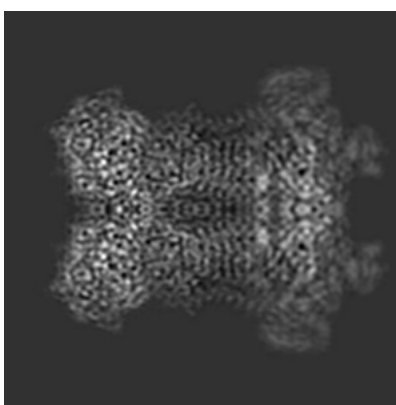
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

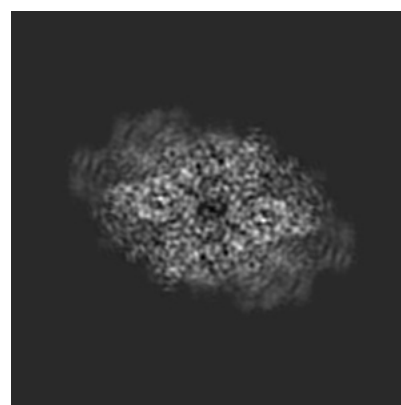
6.1.1 Primary map



X



Y



Z

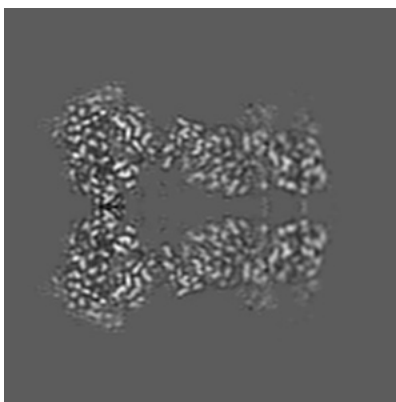
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

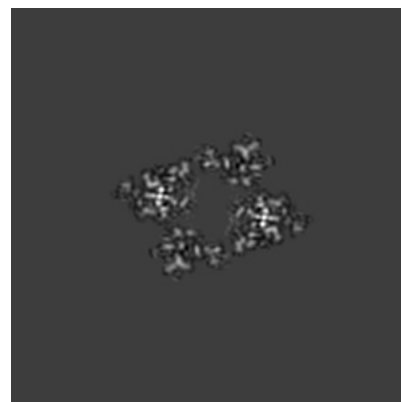
6.2.1 Primary map



X Index: 90



Y Index: 90

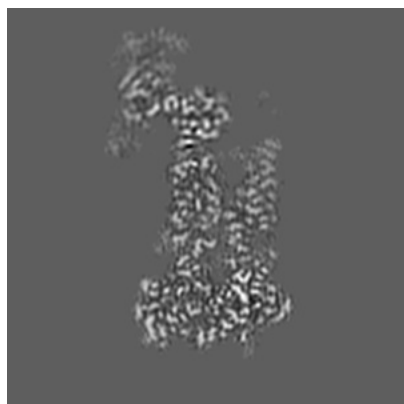


Z Index: 90

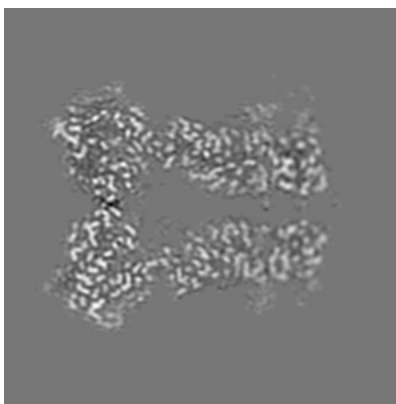
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

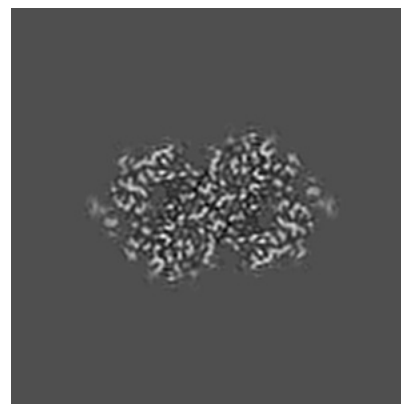
6.3.1 Primary map



X Index: 110



Y Index: 89

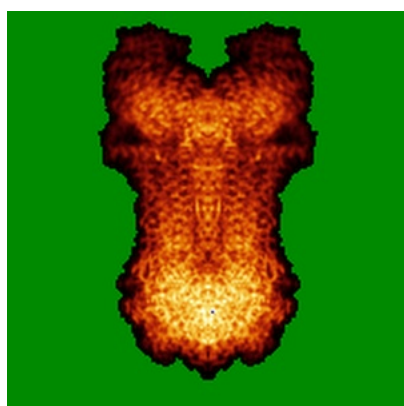


Z Index: 51

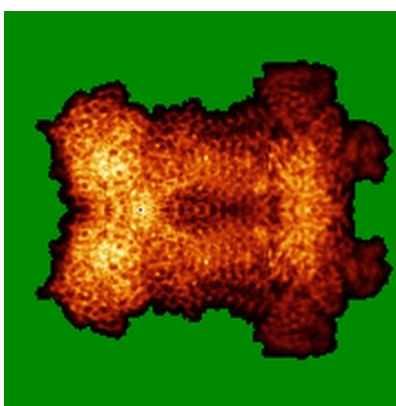
The images above show the largest variance slices of the map in three orthogonal directions.

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

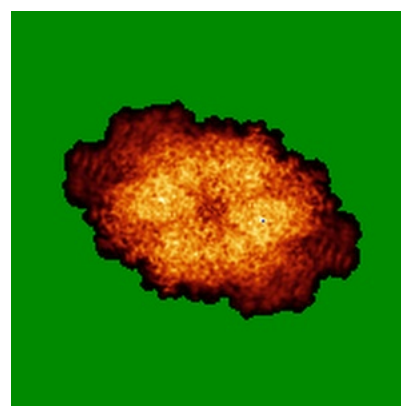
6.4.1 Primary map



X



Y

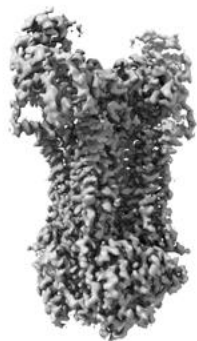


Z

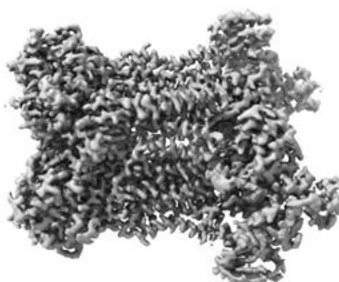
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

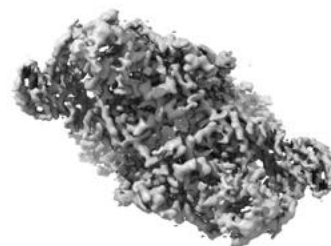
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

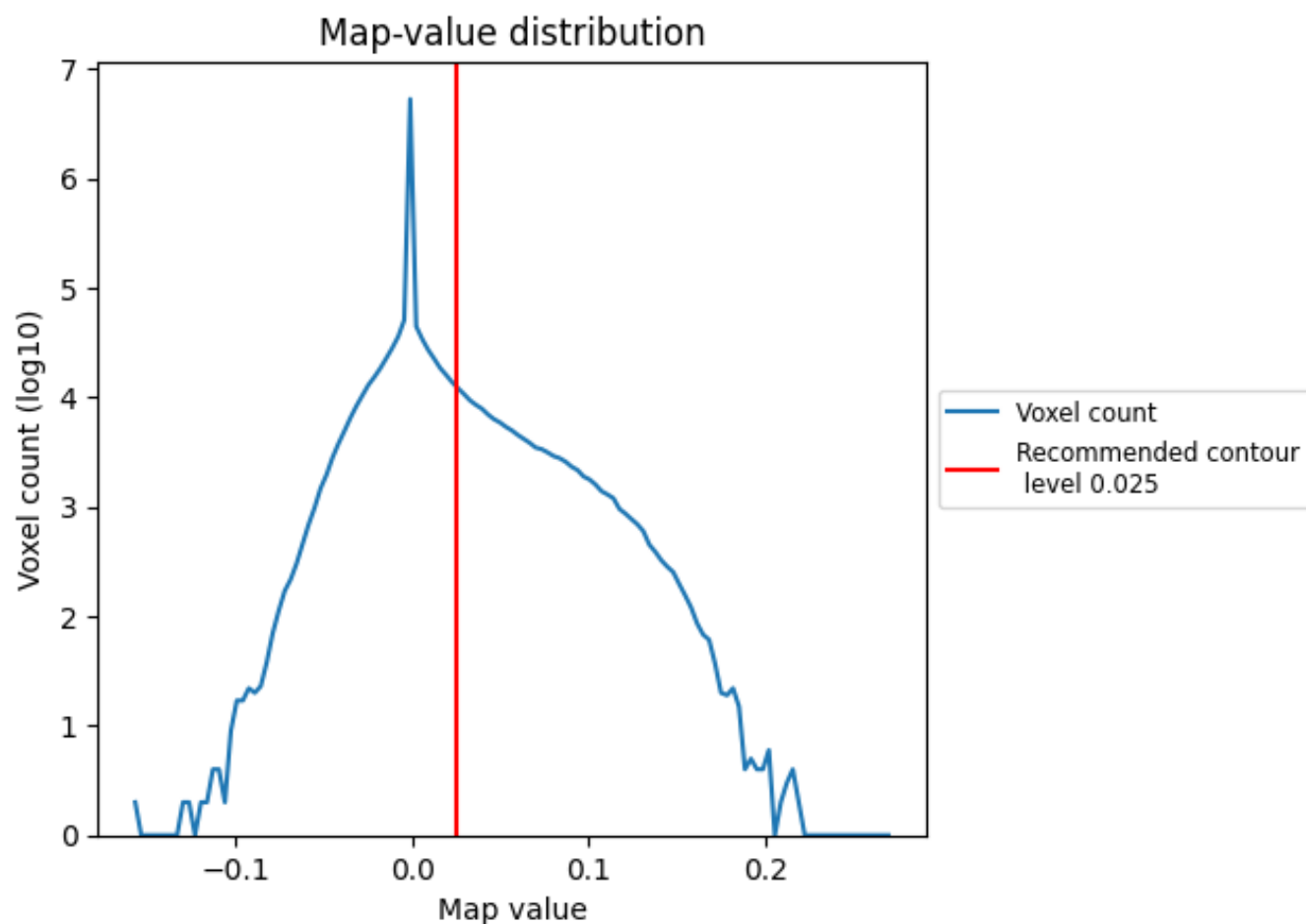
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

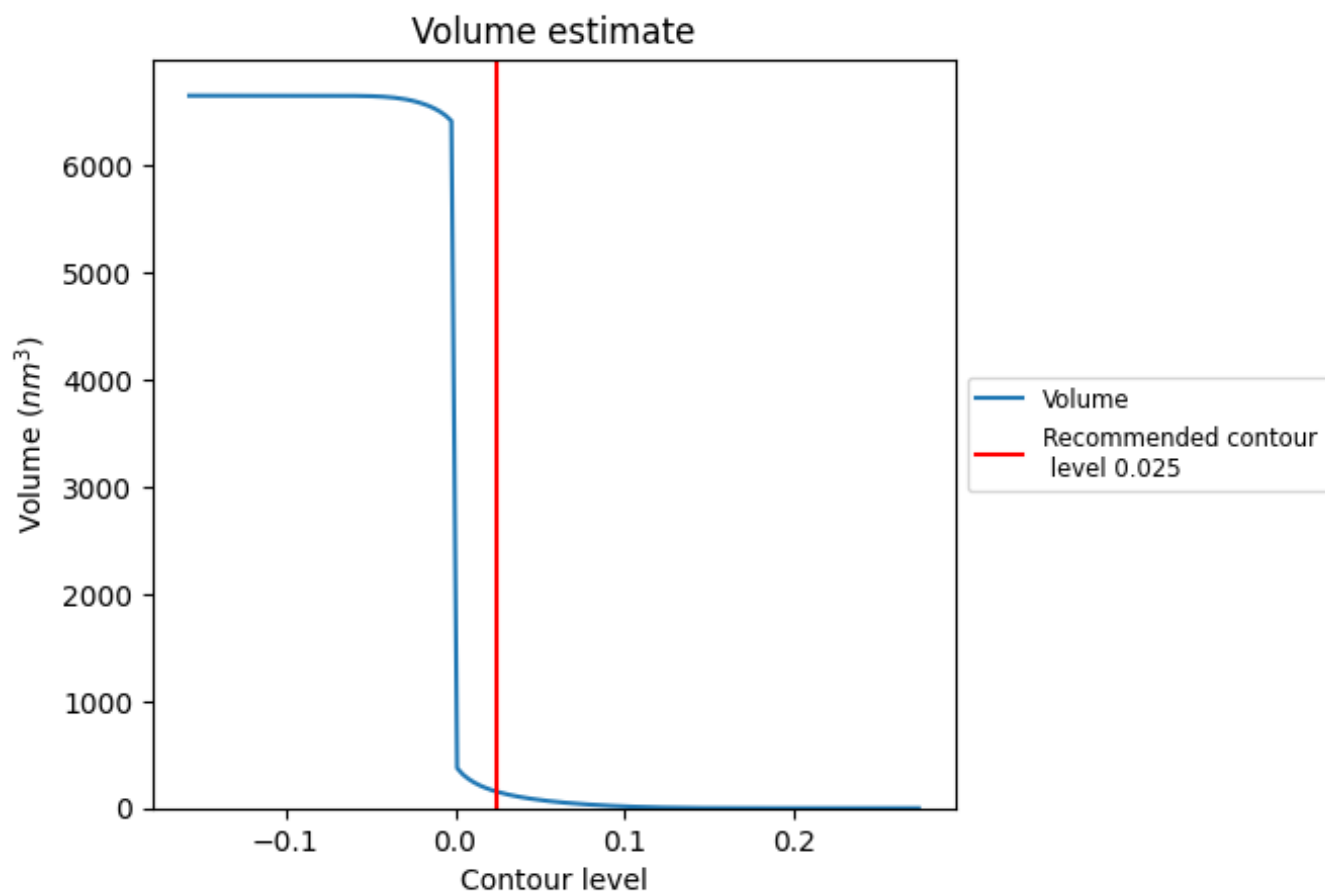
This section contains the results of statistical analysis of the map.

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.

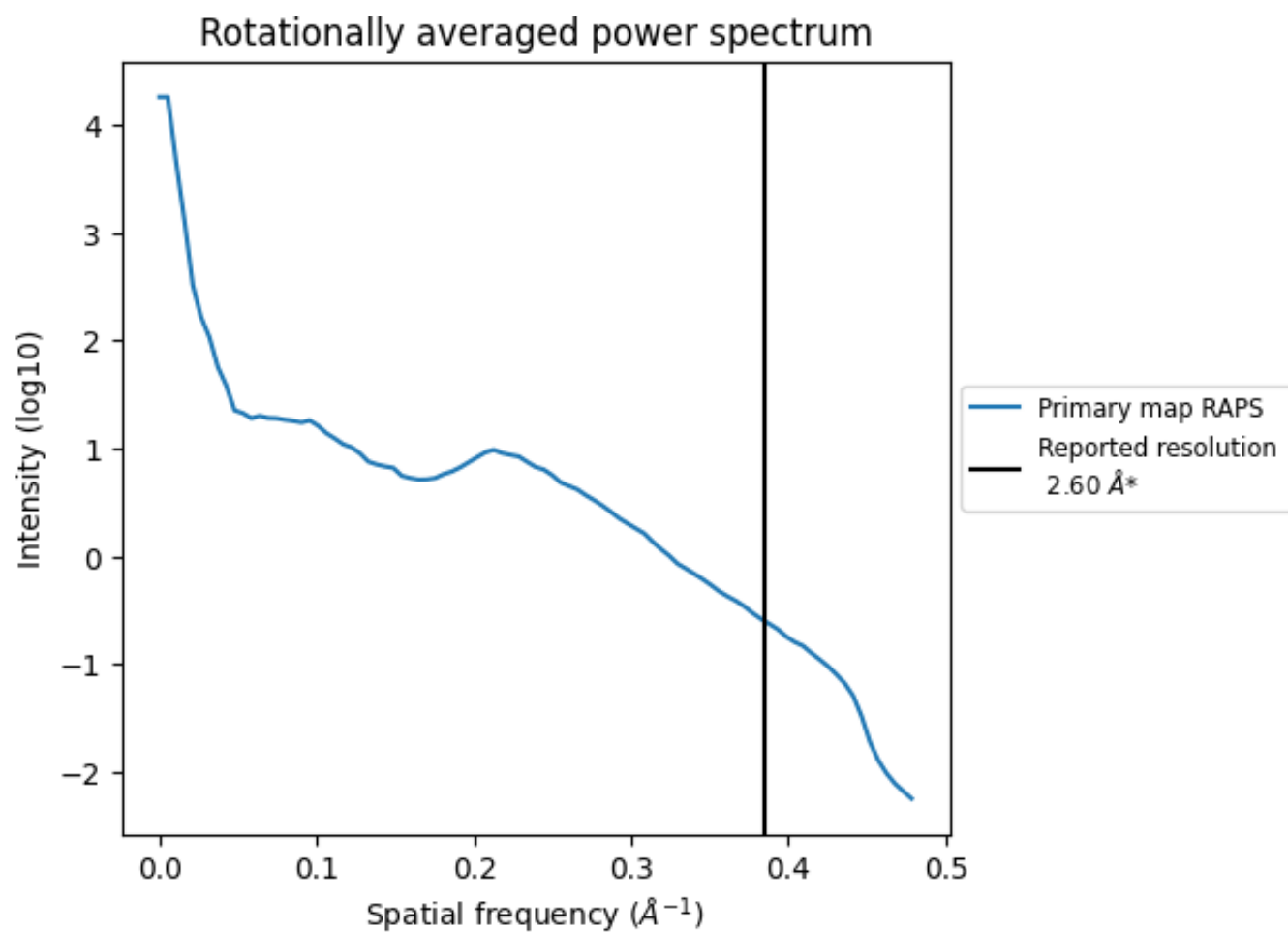
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 152 nm^3 ; this corresponds to an approximate mass of 137 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 0.385 Å⁻¹

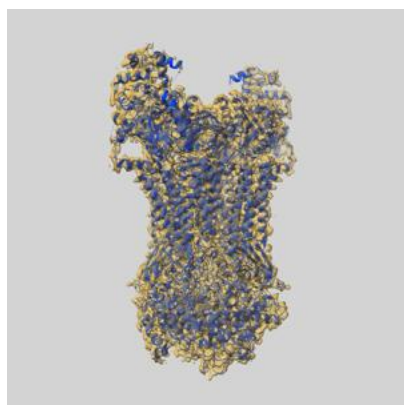
8 Fourier-Shell correlation ⓘ

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

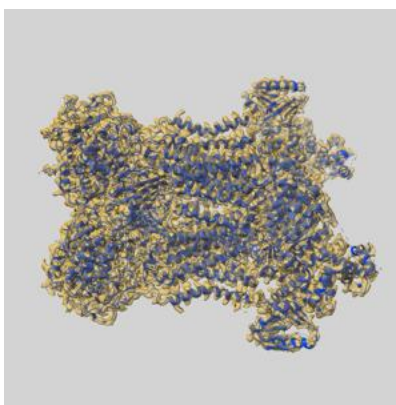
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30556 and PDB model 7D3F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

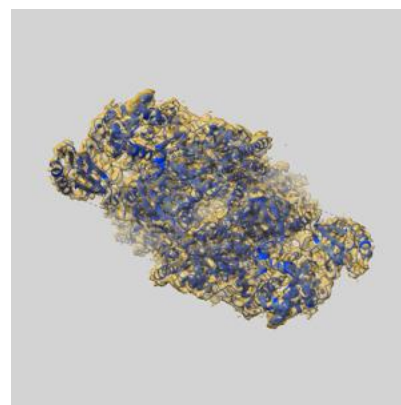
9.1 Map-model overlay [i](#)



X



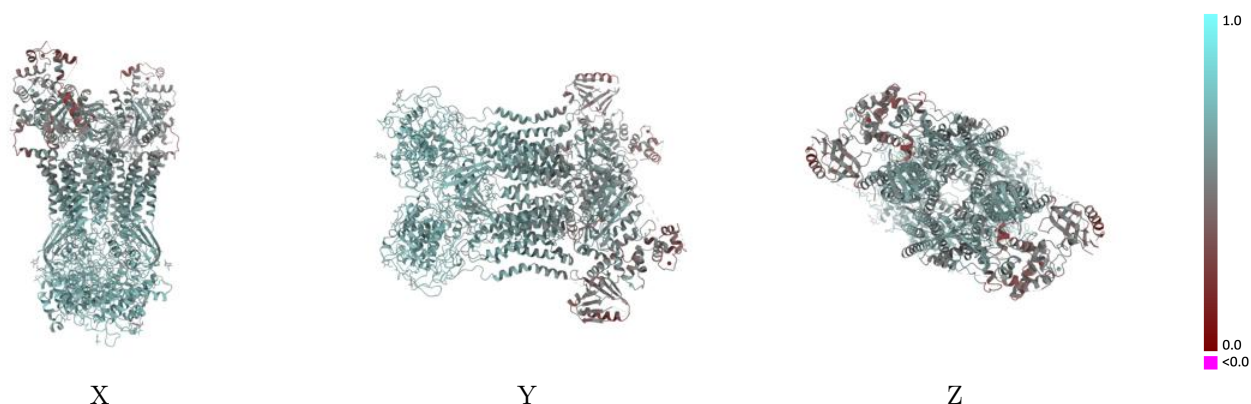
Y



Z

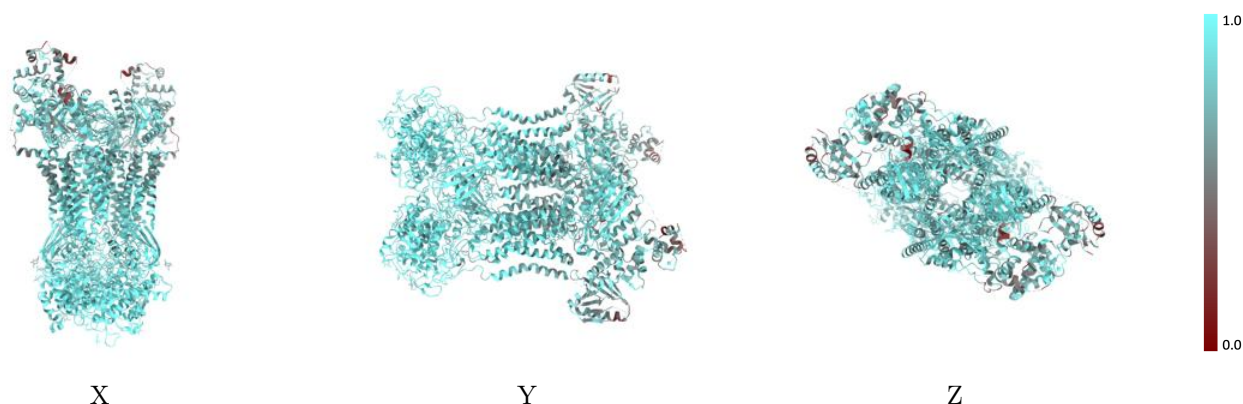
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



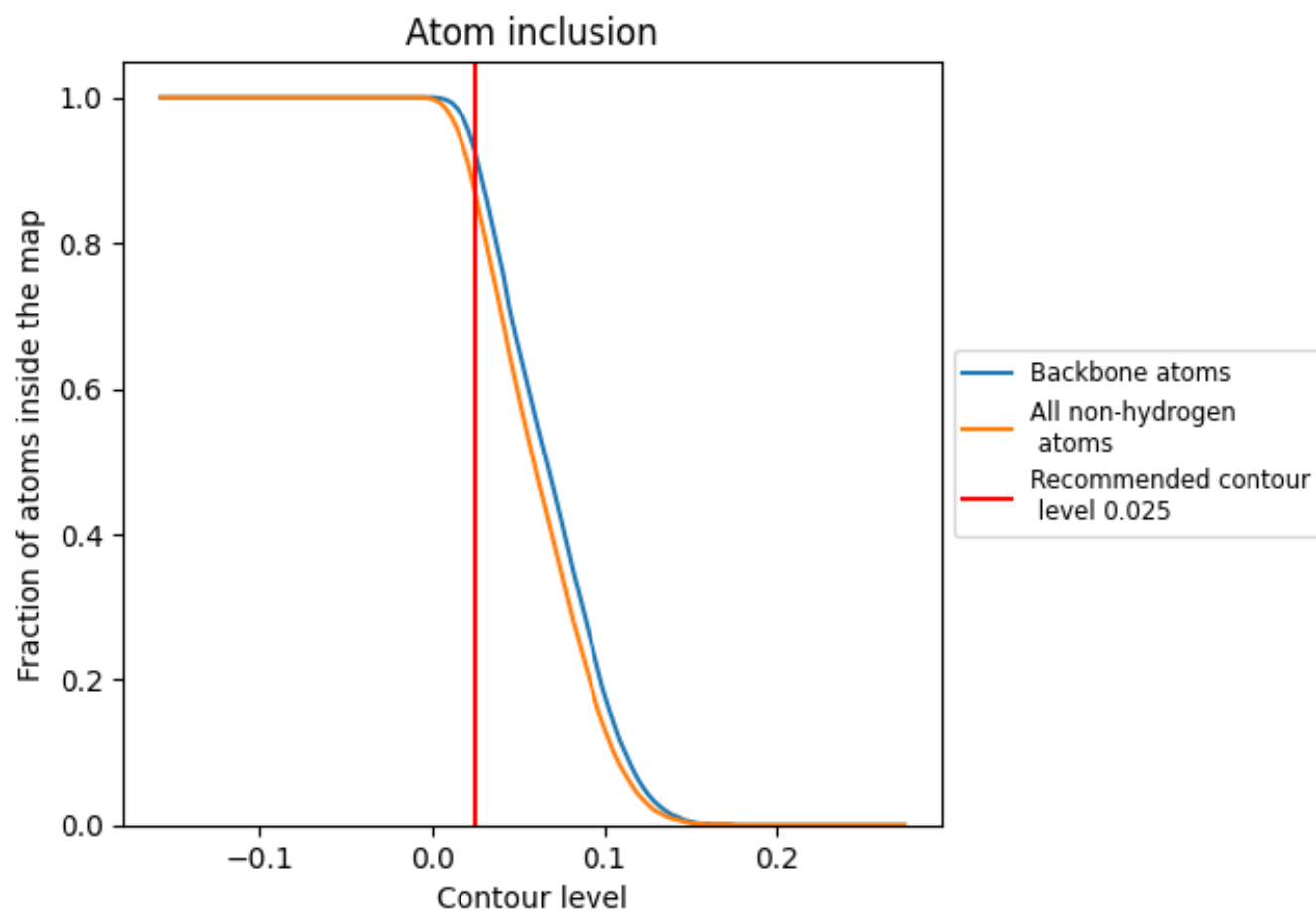
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8720	0.5930
A	0.8790	0.5900
B	0.8670	0.6140
C	0.8740	0.5880
D	0.8620	0.6080
E	0.9480	0.6390
F	0.9400	0.6380

1.0

0.0

<0.0