



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:46 PM UTC

PDB ID : 7OSE / pdb_00007ose
EMDB ID : EMD-13048
Title : cytochrome bd-II type oxidase with bound aurachin D
Authors : Grauel, A.; Kaegi, J.; Rasmussen, T.; Wohlwend, D.; Boettcher, B.; Friedrich, T.
Deposited on : 2021-06-08
Resolution : 3.00 Å(reported)
Based on initial model : 6RX4

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:

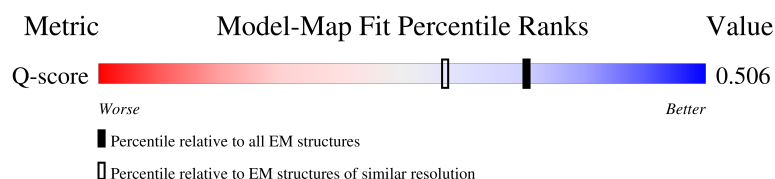
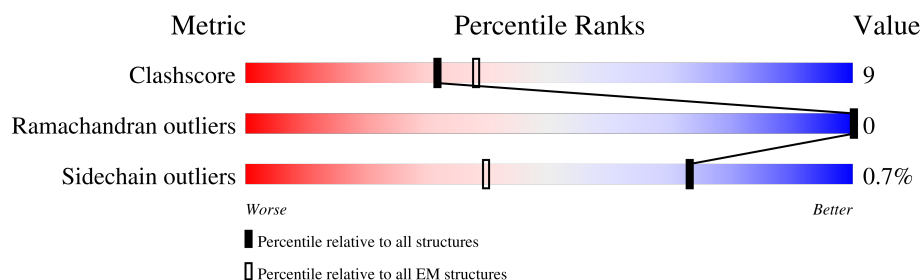
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	514	 79% 19% .
1	D	514	 78% 20% .
2	B	378	 75% 25%
2	E	378	 77% 22%

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Mol	Chain	Length	Quality of chain
3	C	30	
3	F	30	

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
4	HEB	A	601	X	-	-	-
4	HEB	A	602	X	-	-	-
4	HEB	D	601	X	-	-	-
4	HEB	D	602	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14882 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 Cytochrome bd-II ubiquinol oxidase subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	503	Total	C	N	O	S	0	0
			4003	2644	656	677	26		
1	D	503	Total	C	N	O	S	0	0
			4003	2644	656	677	26		

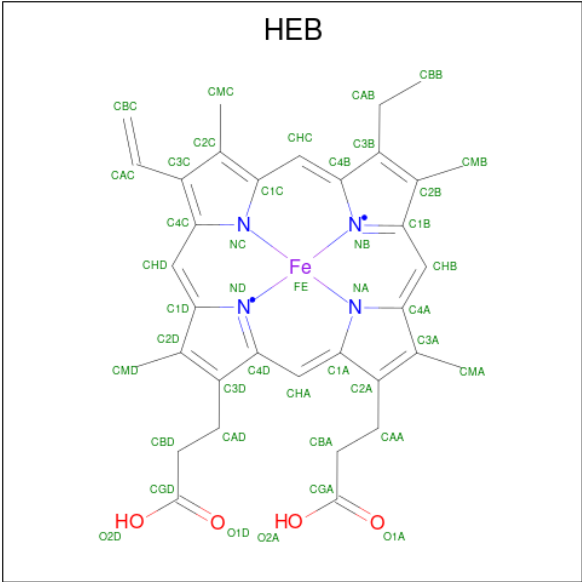
- Molecule 2 is a protein called Cytochrome bd-II ubiquinol oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	377	Total	C	N	O	S	0	0
			2990	2015	474	481	20		
2	E	377	Total	C	N	O	S	0	0
			2990	2015	474	481	20		

- Molecule 3 is a protein called Putative cytochrome bd-II ubiquinol oxidase subunit AppX.

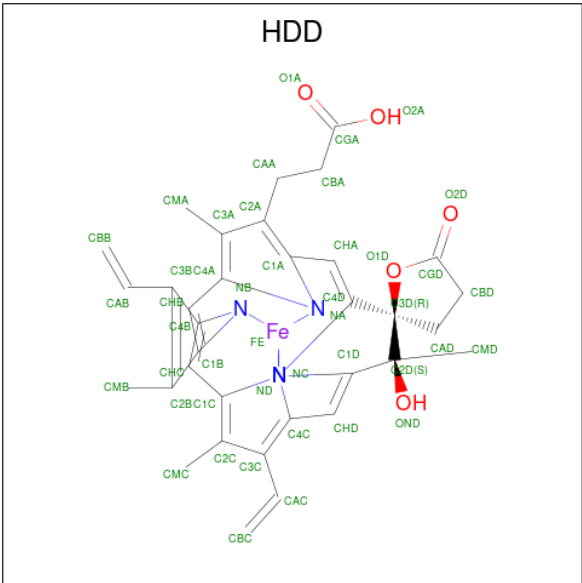
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	28	Total	C	N	O	S	0	0
			237	166	34	34	3		
3	F	28	Total	C	N	O	S	0	0
			237	166	34	34	3		

- Molecule 4 is HEME B/C (CCD ID: HEB) (formula: $C_{34}H_{34}FeN_4O_4$).



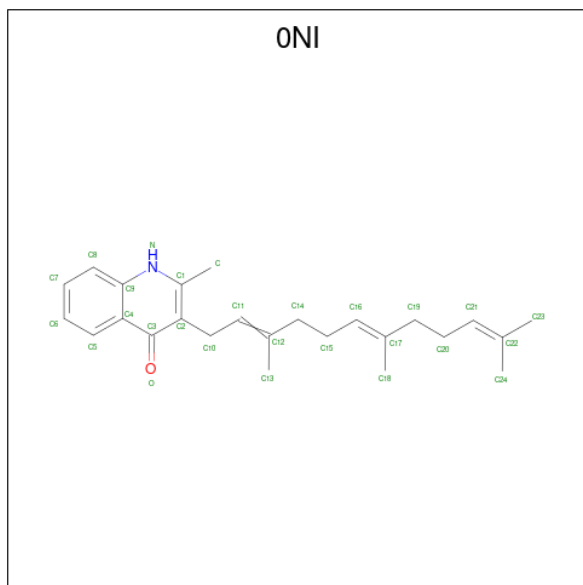
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0

- Molecule 5 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



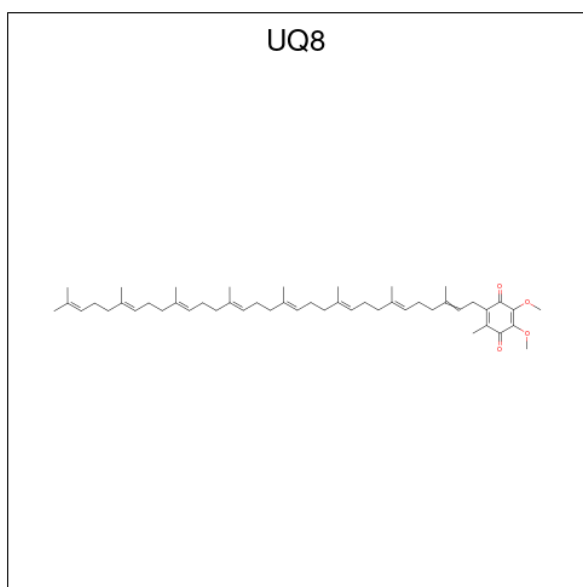
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	Fe	N	O	0
			44	34	1	4	5	
5	D	1	Total	C	Fe	N	O	0
			44	34	1	4	5	

- Molecule 6 is Aurachin D (CCD ID: 0NI) (formula: $C_{25}H_{33}NO$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			27	25	1	1	
6	D	1	Total	C	N	O	0
			27	25	1	1	

- Molecule 7 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	O	0
			53	49	4	
7	E	1	Total	C	O	0
			53	49	4	

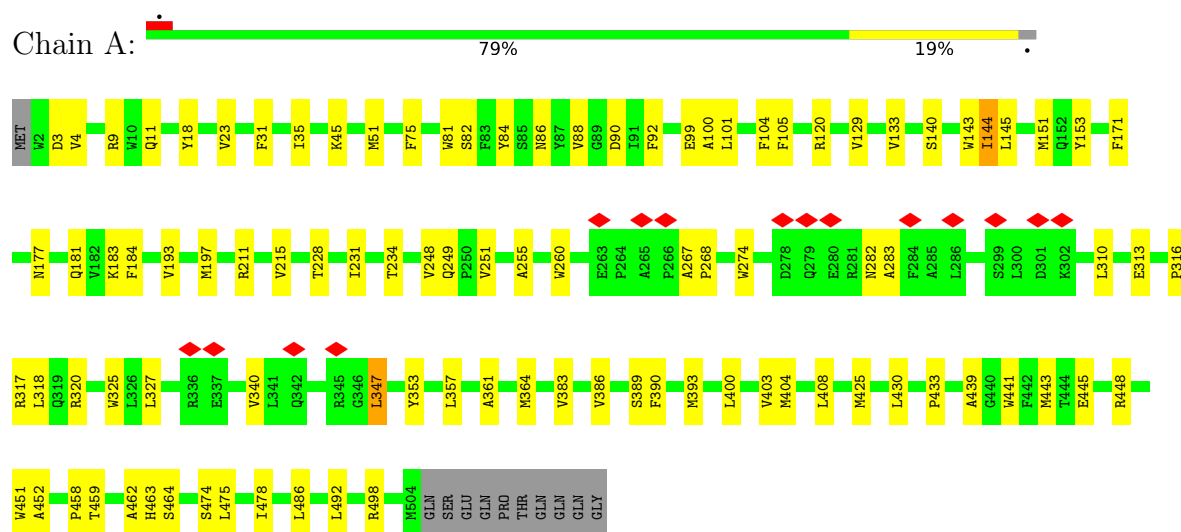
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	1	Total	O	0
			1	1	
8	D	1	Total	O	0
			1	1	

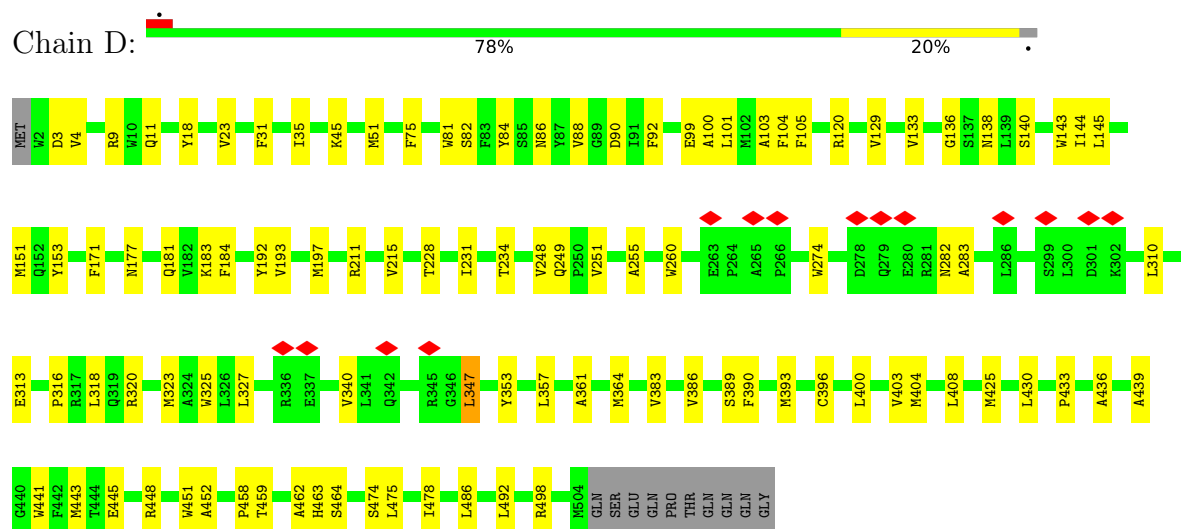
3 Residue-property plots

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

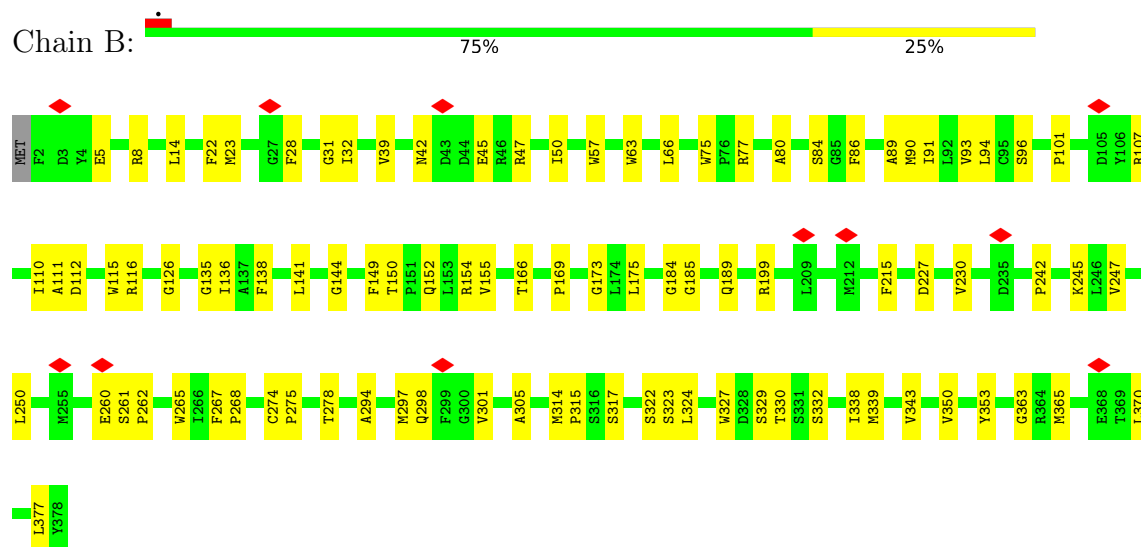
- Molecule 1: Cytochrome bd-II ubiquinol oxidase subunit 1



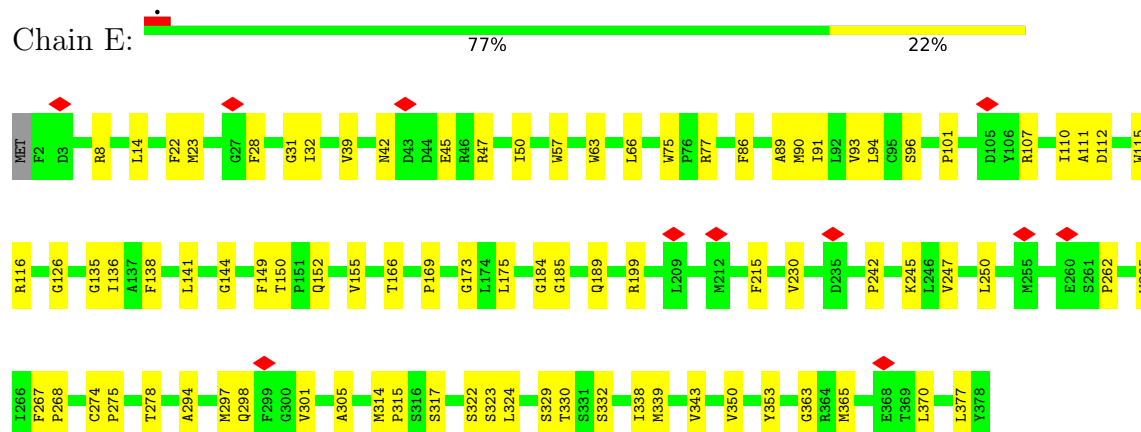
- Molecule 1: Cytochrome bd-II ubiquinol oxidase subunit 1



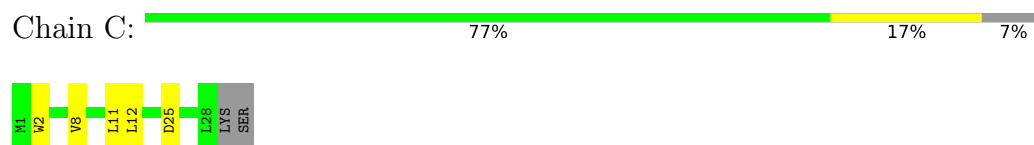
- Molecule 2: Cytochrome bd-II ubiquinol oxidase subunit 2



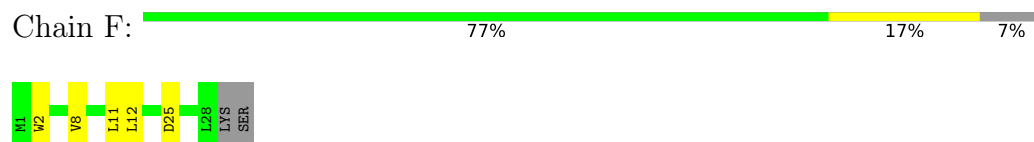
- Molecule 2: Cytochrome bd-II ubiquinol oxidase subunit 2



- Molecule 3: Putative cytochrome bd-II ubiquinol oxidase subunit AppX



- Molecule 3: Putative cytochrome bd-II ubiquinol oxidase subunit AppX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	125497	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 ($e^-/\text{\AA}^2$)	79	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	212.70001, 212.70001, 212.70001	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HDD, UQ8, 0NI, HEB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.13	0/4122	0.26	0/5612
1	D	0.13	0/4122	0.26	0/5612
2	B	0.12	0/3084	0.28	0/4213
2	E	0.12	0/3084	0.28	0/4213
3	C	0.13	0/245	0.26	0/336
3	F	0.13	0/245	0.26	0/336
All	All	0.12	0/14902	0.27	0/20322

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

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	4003	0	4015	72	0
1	D	4003	0	4015	74	0
2	B	2990	0	3075	58	0
2	E	2990	0	3075	54	0
3	C	237	0	254	11	0
3	F	237	0	254	11	0
4	A	86	0	64	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	86	0	64	12	0
5	A	44	0	31	7	0
5	D	44	0	31	7	0
6	A	27	0	0	0	0
6	D	27	0	0	0	0
7	B	53	0	74	8	0
7	E	53	0	74	8	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
All	All	14882	0	15026	260	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 (260) 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:84:TYR:HB2	1:A:462:ALA:HB1	1.71	0.73
1:D:84:TYR:HB2	1:D:462:ALA:HB1	1.71	0.72
3:C:8:VAL:HG13	3:F:12:LEU:HD13	1.72	0.72
1:A:23:VAL:HG11	5:A:603:HDD:HBC1	1.76	0.67
1:A:51:MET:HG2	1:A:215:VAL:HG13	1.77	0.67
1:D:23:VAL:HG11	5:D:603:HDD:HBC1	1.75	0.67
1:D:51:MET:HG2	1:D:215:VAL:HG13	1.77	0.67
1:A:23:VAL:HG22	5:A:603:HDD:HAD1	1.77	0.67
1:A:441:TRP:HB3	4:A:602:HEB:HMB1	1.77	0.67
3:C:12:LEU:HD13	3:F:8:VAL:HG13	1.77	0.67
1:D:181:GLN:HB3	3:F:2:TRP:HB2	1.75	0.67
1:D:23:VAL:HG22	5:D:603:HDD:HAD1	1.77	0.67
1:A:181:GLN:HB3	3:C:2:TRP:HB2	1.77	0.66
1:D:441:TRP:HB3	4:D:602:HEB:HMB1	1.77	0.66
3:C:8:VAL:HG12	3:F:8:VAL:HG12	1.80	0.64
1:D:45:LYS:NZ	3:F:25:ASP:OD2	2.27	0.63
1:A:492:LEU:HD21	2:B:110:ILE:HD11	1.79	0.63
3:C:11:LEU:HB2	3:F:12:LEU:HD11	1.82	0.62
1:D:492:LEU:HD21	2:E:110:ILE:HD11	1.82	0.61
3:C:12:LEU:HD11	3:F:11:LEU:HB2	1.82	0.61
1:A:248:VAL:HG12	1:A:249:GLN:HG3	1.82	0.60
1:D:248:VAL:HG12	1:D:249:GLN:HG3	1.82	0.60
1:D:445:GLU:OE1	1:D:448:ARG:NH2	2.34	0.60
1:A:145:LEU:HD13	1:A:184:PHE:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:PHE:CE1	4:D:601:HEB:HHB	2.37	0.60
1:A:445:GLU:OE1	1:A:448:ARG:NH2	2.34	0.60
3:C:8:VAL:O	3:F:12:LEU:HD12	2.02	0.60
1:D:151:MET:SD	4:D:602:HEB:HHD	2.43	0.59
1:A:45:LYS:NZ	3:C:25:ASP:OD2	2.27	0.59
1:D:386:VAL:HG13	1:D:443:MET:HG2	1.84	0.59
1:A:151:MET:SD	4:A:602:HEB:HHD	2.43	0.58
1:A:390:PHE:CE1	4:A:601:HEB:HHB	2.37	0.58
2:B:150:THR:OG1	2:B:152:GLN:O	2.20	0.58
1:A:386:VAL:HG13	1:A:443:MET:HG2	1.84	0.58
1:D:145:LEU:HD13	1:D:184:PHE:HA	1.84	0.58
1:A:183:LYS:NZ	4:A:601:HEB:O1D	2.36	0.58
1:D:183:LYS:NZ	4:D:601:HEB:O1D	2.36	0.58
2:E:14:LEU:HD21	2:E:343:VAL:HG11	1.86	0.57
1:A:99:GLU:HG3	1:A:140:SER:HA	1.86	0.57
2:B:47:ARG:HD3	2:B:370:LEU:HD21	1.87	0.57
1:A:100:ALA:HA	1:A:104:PHE:HB2	1.87	0.57
1:D:100:ALA:HA	1:D:104:PHE:HB2	1.87	0.56
2:B:14:LEU:HD21	2:B:343:VAL:HG11	1.86	0.56
4:D:602:HEB:CMC	5:D:603:HDD:HAB	2.36	0.56
2:E:47:ARG:HD3	2:E:370:LEU:HD21	1.87	0.56
1:A:120:ARG:HH22	2:B:363:GLY:HA3	1.71	0.56
3:C:12:LEU:HD12	3:F:8:VAL:O	2.06	0.55
1:D:99:GLU:HG3	1:D:140:SER:HA	1.86	0.55
1:A:231:ILE:HA	1:A:234:THR:HG22	1.87	0.55
2:E:22:PHE:HB2	2:E:63:TRP:HB3	1.89	0.55
1:D:231:ILE:HA	1:D:234:THR:HG22	1.87	0.55
1:D:390:PHE:HE1	4:D:601:HEB:HHB	1.71	0.55
4:A:602:HEB:CMC	5:A:603:HDD:HAB	2.36	0.55
2:E:150:THR:OG1	2:E:152:GLN:O	2.20	0.55
7:E:401:UQ8:H15B	7:E:401:UQ8:H21	1.88	0.55
1:A:474:SER:HB2	2:B:91:ILE:HG13	1.89	0.55
1:A:390:PHE:HE1	4:A:601:HEB:HHB	1.71	0.55
1:D:120:ARG:HH22	2:E:363:GLY:HA3	1.72	0.55
7:B:401:UQ8:H15B	7:B:401:UQ8:H21	1.88	0.54
1:A:228:THR:HG21	1:A:408:LEU:HD22	1.87	0.54
1:D:228:THR:HG21	1:D:408:LEU:HD22	1.87	0.54
2:E:47:ARG:NH2	2:E:377:LEU:O	2.41	0.54
2:B:22:PHE:HB2	2:B:63:TRP:HB3	1.89	0.54
1:D:474:SER:HB2	2:E:91:ILE:HG13	1.89	0.54
1:A:211:ARG:NH1	1:A:498:ARG:O	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:433:PRO:HG3	1.90	0.53
2:B:47:ARG:NH2	2:B:377:LEU:O	2.41	0.53
2:B:149:PHE:HD2	2:B:322:SER:HB2	1.73	0.53
2:E:149:PHE:HD2	2:E:322:SER:HB2	1.72	0.53
1:A:403:VAL:HG13	1:A:425:MET:HE3	1.91	0.53
2:B:242:PRO:O	2:B:245:LYS:NZ	2.41	0.53
2:E:42:ASN:HB3	2:E:45:GLU:HG2	1.90	0.53
2:B:42:ASN:HB3	2:B:45:GLU:HG2	1.90	0.53
1:D:400:LEU:HD11	1:D:433:PRO:HG3	1.90	0.53
2:E:57:TRP:HH2	2:E:101:PRO:HG3	1.73	0.53
1:A:251:VAL:HG22	1:A:310:LEU:HD13	1.91	0.52
1:D:441:TRP:HB3	4:D:602:HEB:CMB	2.39	0.52
1:A:177:ASN:OD1	1:A:177:ASN:N	2.42	0.52
2:E:28:PHE:O	2:E:32:ILE:HG12	2.09	0.52
1:A:389:SER:OG	1:A:439:ALA:O	2.28	0.52
1:A:441:TRP:HB3	4:A:602:HEB:CMB	2.39	0.52
2:B:28:PHE:O	2:B:32:ILE:HG12	2.09	0.52
2:B:57:TRP:HH2	2:B:101:PRO:HG3	1.73	0.52
1:D:9:ARG:NE	4:D:602:HEB:O2A	2.43	0.52
1:D:86:ASN:OD1	2:E:77:ARG:NE	2.43	0.52
1:D:403:VAL:HG13	1:D:425:MET:HE3	1.91	0.52
1:D:251:VAL:HG22	1:D:310:LEU:HD13	1.91	0.52
1:A:318:LEU:HD23	1:A:353:TYR:HB3	1.92	0.51
1:A:463:HIS:ND1	1:A:464:SER:O	2.43	0.51
1:D:389:SER:OG	1:D:439:ALA:O	2.28	0.51
1:A:9:ARG:NE	4:A:602:HEB:O2A	2.43	0.51
2:E:31:GLY:HA3	2:E:184:GLY:HA3	1.93	0.51
1:D:105:PHE:HE2	2:E:66:LEU:HD22	1.76	0.51
1:D:255:ALA:HA	1:D:383:VAL:HG13	1.93	0.51
1:A:105:PHE:HE2	2:B:66:LEU:HD22	1.76	0.51
1:A:255:ALA:HA	1:A:383:VAL:HG13	1.93	0.50
1:A:86:ASN:OD1	2:B:77:ARG:NE	2.44	0.50
1:D:318:LEU:HD23	1:D:353:TYR:HB3	1.92	0.50
2:B:31:GLY:HA3	2:B:184:GLY:HA3	1.93	0.50
1:D:463:HIS:ND1	1:D:464:SER:O	2.43	0.50
1:A:320:ARG:HH21	1:A:347:LEU:HA	1.76	0.50
1:D:177:ASN:OD1	1:D:177:ASN:N	2.42	0.50
1:D:320:ARG:HH21	1:D:347:LEU:HA	1.76	0.50
2:E:242:PRO:O	2:E:245:LYS:NZ	2.41	0.50
2:E:305:ALA:HB2	7:E:401:UQ8:H12	1.92	0.50
2:B:305:ALA:HB2	7:B:401:UQ8:H12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:ILE:HD13	2:E:115:TRP:CE2	2.47	0.49
2:B:110:ILE:HD13	2:B:115:TRP:CE2	2.47	0.49
2:E:110:ILE:HG22	2:E:112:ASP:H	1.79	0.48
2:E:90:MET:HA	2:E:93:VAL:HG22	1.95	0.48
2:B:90:MET:HA	2:B:93:VAL:HG22	1.95	0.48
2:B:294:ALA:O	2:B:298:GLN:HG2	2.14	0.48
2:E:294:ALA:O	2:E:298:GLN:HG2	2.14	0.48
2:B:110:ILE:HG22	2:B:112:ASP:H	1.79	0.47
1:A:90:ASP:OD2	2:B:332:SER:N	2.32	0.47
2:B:50:ILE:HD13	2:B:107:ARG:HD3	1.97	0.47
2:E:324:LEU:HD22	2:E:329:SER:HB3	1.95	0.47
1:A:82:SER:H	1:A:464:SER:HB3	1.79	0.47
2:B:324:LEU:HD22	2:B:329:SER:HB3	1.95	0.47
1:A:325:TRP:HE3	1:A:364:MET:HG2	1.80	0.47
1:A:23:VAL:HG13	5:A:603:HDD:HMD2	1.96	0.47
1:D:211:ARG:NH1	1:D:498:ARG:O	2.37	0.47
1:D:101:LEU:HD21	2:E:343:VAL:HA	1.97	0.47
4:D:601:HEB:HHH	4:D:601:HEB:HBC1	1.96	0.46
2:E:365:MET:HE3	2:E:370:LEU:HB2	1.98	0.46
1:D:81:TRP:HB3	1:D:84:TYR:HB3	1.96	0.46
3:C:12:LEU:HD11	3:F:11:LEU:CB	2.46	0.46
1:D:23:VAL:HG13	5:D:603:HDD:HMD2	1.96	0.46
1:D:357:LEU:O	1:D:361:ALA:N	2.49	0.46
2:E:50:ILE:HD13	2:E:107:ARG:HD3	1.96	0.46
1:A:81:TRP:HB3	1:A:84:TYR:HB3	1.96	0.46
2:B:365:MET:HE3	2:B:370:LEU:HB2	1.98	0.46
1:D:90:ASP:OD2	2:E:332:SER:N	2.32	0.46
1:D:82:SER:H	1:D:464:SER:HB3	1.79	0.46
4:A:601:HEB:HHH	4:A:601:HEB:HBC1	1.96	0.46
1:D:325:TRP:HE3	1:D:364:MET:HG2	1.80	0.46
1:A:197:MET:HE2	1:A:404:MET:HE3	1.97	0.45
4:A:602:HEB:HMC1	5:A:603:HDD:HAB	1.98	0.45
1:A:357:LEU:O	1:A:361:ALA:N	2.49	0.45
2:B:144:GLY:HA3	2:B:317:SER:HB3	1.97	0.45
1:A:11:GLN:HB2	1:A:475:LEU:HD13	1.99	0.45
2:B:96:SER:HB3	2:B:126:GLY:HA2	1.98	0.45
1:D:197:MET:HE2	1:D:404:MET:HE3	1.97	0.45
2:E:185:GLY:O	2:E:189:GLN:HG2	2.16	0.45
1:A:99:GLU:HB2	1:A:143:TRP:HB2	1.99	0.45
5:A:603:HDD:HMD2	5:A:603:HDD:HAD2	1.68	0.45
2:E:96:SER:HB3	2:E:126:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD21	2:B:343:VAL:HA	1.98	0.45
2:B:350:VAL:HA	2:B:353:TYR:CE2	2.52	0.45
2:B:185:GLY:O	2:B:189:GLN:HG2	2.17	0.45
1:A:153:TYR:HB2	1:A:248:VAL:HG11	1.99	0.45
4:D:602:HEB:HMC1	5:D:603:HDD:HAB	1.98	0.45
1:A:92:PHE:HZ	4:A:602:HEB:HBC2	1.82	0.45
1:D:153:TYR:HB2	1:D:248:VAL:HG11	1.99	0.45
2:E:86:PHE:HB3	2:E:89:ALA:HB3	1.98	0.45
2:E:144:GLY:HA3	2:E:317:SER:HB3	1.97	0.45
2:B:39:VAL:O	2:B:199:ARG:NH1	2.48	0.45
1:D:18:TYR:HE1	1:D:486:LEU:HB2	1.82	0.45
5:D:603:HDD:HMD2	5:D:603:HDD:HAD2	1.68	0.45
2:E:350:VAL:HA	2:E:353:TYR:CE2	2.52	0.45
2:B:86:PHE:HB3	2:B:89:ALA:HB3	1.98	0.44
1:D:451:TRP:HA	1:D:458:PRO:HA	1.99	0.44
1:D:452:ALA:HB2	1:D:459:THR:HA	1.99	0.44
1:A:18:TYR:CE1	1:A:486:LEU:HB2	2.53	0.44
1:A:452:ALA:HB2	1:A:459:THR:HA	1.99	0.44
2:B:23:MET:HE3	7:B:401:UQ8:H20B	2.00	0.44
1:D:11:GLN:HB2	1:D:475:LEU:HD13	1.98	0.44
2:E:23:MET:HE3	7:E:401:UQ8:H20B	2.00	0.44
1:A:18:TYR:HE1	1:A:486:LEU:HB2	1.82	0.44
1:A:451:TRP:HA	1:A:458:PRO:HA	1.99	0.44
1:A:393:MET:HE2	1:A:393:MET:HB3	1.84	0.44
1:D:99:GLU:HB2	1:D:143:TRP:HB2	1.99	0.44
1:D:18:TYR:CE1	1:D:486:LEU:HB2	2.52	0.44
1:A:31:PHE:O	1:A:35:ILE:HG12	2.18	0.44
2:B:227:ASP:OD1	2:B:227:ASP:N	2.51	0.44
1:D:31:PHE:O	1:D:35:ILE:HG12	2.18	0.44
1:D:92:PHE:HZ	4:D:602:HEB:HBC2	1.82	0.43
1:A:327:LEU:HD13	1:A:340:VAL:HG13	2.00	0.43
1:A:23:VAL:CG1	5:A:603:HDD:HBC1	2.45	0.43
2:B:215:PHE:CE2	7:B:401:UQ8:H4MA	2.54	0.43
2:E:39:VAL:O	2:E:199:ARG:NH1	2.48	0.43
2:E:215:PHE:CE2	7:E:401:UQ8:H4MA	2.54	0.43
1:D:274:TRP:HB3	1:D:283:ALA:HB3	2.00	0.43
1:A:274:TRP:HB3	1:A:283:ALA:HB3	2.00	0.43
1:A:430:LEU:O	1:A:433:PRO:HD2	2.18	0.43
2:B:274:CYS:HB3	2:B:297:MET:HB2	2.00	0.43
1:D:260:TRP:NE1	1:D:282:ASN:OD1	2.40	0.43
2:B:315:PRO:HA	2:B:323:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PRO:HB3	7:B:401:UQ8:H4MB	2.00	0.43
2:B:301:VAL:HG12	7:B:401:UQ8:H13	2.01	0.43
2:E:141:LEU:HG	2:E:314:MET:HA	2.01	0.43
2:B:136:ILE:HG23	2:B:169:PRO:HB2	2.01	0.43
1:D:430:LEU:O	1:D:433:PRO:HD2	2.18	0.42
2:E:8:ARG:HG2	2:E:330:THR:HG21	2.00	0.42
3:C:11:LEU:CB	3:F:12:LEU:HD11	2.48	0.42
1:D:23:VAL:CG1	5:D:603:HDD:HBC1	2.45	0.42
1:D:327:LEU:HD13	1:D:340:VAL:HG13	2.00	0.42
2:B:275:PRO:HA	2:B:278:THR:HG22	2.01	0.42
2:E:275:PRO:HA	2:E:278:THR:HG22	2.02	0.42
1:A:84:TYR:O	1:A:88:VAL:HG22	2.19	0.42
2:E:138:PHE:CE1	2:E:305:ALA:HB1	2.54	0.42
2:E:274:CYS:HB3	2:E:297:MET:HB2	2.00	0.42
1:A:171:PHE:HB2	2:B:338:ILE:HD13	2.00	0.42
1:A:193:VAL:HG13	1:A:404:MET:HE1	2.02	0.42
2:B:135:GLY:HA3	2:B:173:GLY:HA2	2.02	0.42
2:B:138:PHE:CE1	2:B:305:ALA:HB1	2.54	0.42
1:D:171:PHE:HB2	2:E:338:ILE:HD13	2.01	0.42
1:D:393:MET:HB3	1:D:393:MET:HE2	1.83	0.42
2:E:315:PRO:HA	2:E:323:SER:HB3	2.00	0.42
2:B:141:LEU:HG	2:B:314:MET:HA	2.01	0.42
2:B:8:ARG:HG2	2:B:330:THR:HG21	2.00	0.42
2:E:262:PRO:HA	2:E:265:TRP:HD1	1.85	0.42
1:D:84:TYR:O	1:D:88:VAL:HG22	2.19	0.42
2:E:136:ILE:HG23	2:E:169:PRO:HB2	2.01	0.42
2:E:175:LEU:HD11	2:E:215:PHE:HD1	1.85	0.42
2:E:268:PRO:HB3	7:E:401:UQ8:H4MB	2.01	0.42
2:E:267:PHE:HB2	2:E:268:PRO:HD3	2.02	0.42
1:A:75:PHE:HB2	2:B:94:LEU:HD11	2.02	0.41
2:E:135:GLY:HA3	2:E:173:GLY:HA2	2.02	0.41
2:B:230:VAL:HG21	2:B:250:LEU:HD12	2.02	0.41
1:D:3:ASP:OD1	1:D:4:VAL:N	2.53	0.41
2:E:301:VAL:HG12	7:E:401:UQ8:H13	2.01	0.41
2:B:262:PRO:HA	2:B:265:TRP:HD1	1.85	0.41
2:B:111:ALA:HA	2:B:116:ARG:HH22	1.85	0.41
2:B:175:LEU:HD11	2:B:215:PHE:HD1	1.85	0.41
2:B:75:TRP:HZ3	7:B:401:UQ8:H37	1.86	0.41
1:D:138:ASN:OD1	1:D:192:TYR:OH	2.23	0.41
1:D:193:VAL:HG13	1:D:404:MET:HE1	2.02	0.41
7:E:401:UQ8:H27	7:E:401:UQ8:H23	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:ALA:HA	2:E:116:ARG:HH22	1.85	0.41
1:A:267:ALA:HA	1:A:268:PRO:HD3	1.96	0.41
2:B:80:ALA:O	2:B:84:SER:OG	2.29	0.41
2:B:152:GLN:O	2:B:154:ARG:N	2.49	0.41
1:D:183:LYS:HG3	4:D:601:HEB:CGD	2.51	0.41
1:A:11:GLN:HG3	1:A:478:ILE:HD11	2.02	0.41
1:A:183:LYS:HG3	4:A:601:HEB:CGD	2.51	0.41
2:B:267:PHE:HB2	2:B:268:PRO:HD3	2.02	0.41
1:D:396:CYS:HB2	1:D:436:ALA:HB2	2.03	0.41
2:E:75:TRP:HZ3	7:E:401:UQ8:H37	1.86	0.41
1:A:3:ASP:OD1	1:A:4:VAL:N	2.53	0.41
1:A:317:ARG:HH21	1:A:353:TYR:HE1	1.69	0.41
1:D:103:ALA:HB1	1:D:136:GLY:O	2.22	0.40
1:D:105:PHE:CE2	2:E:66:LEU:HD22	2.55	0.40
1:D:313:GLU:O	1:D:316:PRO:HD2	2.21	0.40
2:E:230:VAL:HG21	2:E:250:LEU:HD12	2.02	0.40
2:E:339:MET:HE2	2:E:339:MET:HA	2.03	0.40
1:A:260:TRP:NE1	1:A:282:ASN:OD1	2.40	0.40
1:A:313:GLU:O	1:A:316:PRO:HD2	2.21	0.40
2:B:5:GLU:HG2	2:B:327:TRP:CZ3	2.56	0.40
7:B:401:UQ8:H27	7:B:401:UQ8:H23	1.75	0.40
1:D:492:LEU:HD23	1:D:492:LEU:HA	1.86	0.40
1:A:129:VAL:O	1:A:133:VAL:HG23	2.20	0.40
2:B:260:GLU:OE1	2:B:261:SER:OG	2.33	0.40
2:B:339:MET:HE2	2:B:339:MET:HA	2.03	0.40
1:D:11:GLN:HG3	1:D:478:ILE:HD11	2.02	0.40
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.86	0.40
1:A:144:ILE:HD13	1:A:144:ILE:HA	1.93	0.40
1:D:75:PHE:HB2	2:E:94:LEU:HD11	2.04	0.40
1:D:129:VAL:O	1:D:133:VAL:HG23	2.20	0.40
1:D:323:MET:HA	1:D:323:MET:HE2	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	501/514 (98%)	491 (98%)	10 (2%)	0	100	100
1	D	501/514 (98%)	492 (98%)	9 (2%)	0	100	100
2	B	375/378 (99%)	368 (98%)	7 (2%)	0	100	100
2	E	375/378 (99%)	368 (98%)	7 (2%)	0	100	100
3	C	26/30 (87%)	26 (100%)	0	0	100	100
3	F	26/30 (87%)	26 (100%)	0	0	100	100
All	All	1804/1844 (98%)	1771 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	412/422 (98%)	410 (100%)	2 (0%)	81	89
1	D	412/422 (98%)	410 (100%)	2 (0%)	81	89
2	B	317/318 (100%)	314 (99%)	3 (1%)	70	85
2	E	317/318 (100%)	314 (99%)	3 (1%)	70	85
3	C	27/29 (93%)	27 (100%)	0	100	100
3	F	27/29 (93%)	27 (100%)	0	100	100
All	All	1512/1538 (98%)	1502 (99%)	10 (1%)	73	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	ILE
1	A	347	LEU
2	B	155	VAL
2	B	166	THR

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Mol	Chain	Res	Type
2	B	247	VAL
1	D	144	ILE
1	D	347	LEU
2	E	155	VAL
2	E	166	THR
2	E	247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	125	GLN
1	A	146	ASN
1	A	319	GLN
2	B	60	ASN
1	D	11	GLN
1	D	125	GLN
1	D	146	ASN
1	D	470	GLN
2	E	60	ASN

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](#)

10 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
5	HDD	A	603	1	46,52,52	1.04	3 (6%)	62,89,89	1.20	4 (6%)
4	HEB	D	602	-	50,50,50	2.92	17 (34%)	66,82,82	2.38	20 (30%)
4	HEB	A	602	-	50,50,50	2.92	17 (34%)	66,82,82	2.38	20 (30%)
7	UQ8	B	401	-	53,53,53	0.18	0	66,67,67	0.38	1 (1%)
4	HEB	A	601	1	50,50,50	2.94	17 (34%)	66,82,82	2.42	22 (33%)
6	0NI	D	604	-	28,28,28	0.40	1 (3%)	35,37,37	0.45	0
7	UQ8	E	401	-	53,53,53	0.18	0	66,67,67	0.38	1 (1%)
5	HDD	D	603	1	46,52,52	1.03	3 (6%)	62,89,89	1.20	4 (6%)
6	0NI	A	604	-	28,28,28	0.41	1 (3%)	35,37,37	0.45	0
4	HEB	D	601	1	50,50,50	2.94	17 (34%)	66,82,82	2.42	21 (31%)

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
5	HDD	A	603	1	-	4/9/89/89	0/1/9/9
4	HEB	D	602	-	1/1/3/8	10/14/54/54	-
4	HEB	A	602	-	1/1/3/8	10/14/54/54	-
7	UQ8	B	401	-	-	14/51/75/75	0/1/1/1
4	HEB	A	601	1	1/1/3/8	2/14/54/54	-
6	0NI	D	604	-	-	8/17/17/17	0/2/2/2
7	UQ8	E	401	-	-	14/51/75/75	0/1/1/1
5	HDD	D	603	1	-	4/9/89/89	0/1/9/9
6	0NI	A	604	-	-	8/17/17/17	0/2/2/2
4	HEB	D	601	1	1/1/3/8	2/14/54/54	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	HEB	CHD-C1D	6.56	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEB	CHD-C1D	6.54	1.51	1.38
4	A	602	HEB	CHD-C1D	6.51	1.51	1.38
4	D	601	HEB	CHD-C1D	6.50	1.51	1.38
4	A	601	HEB	CHC-C4B	6.38	1.51	1.38
4	D	601	HEB	CHC-C4B	6.37	1.51	1.38
4	A	602	HEB	CHC-C4B	6.20	1.50	1.38
4	D	602	HEB	CHC-C4B	6.20	1.50	1.38
4	A	602	HEB	CHA-C1A	6.11	1.50	1.38
4	D	602	HEB	CHA-C1A	6.07	1.50	1.38
4	A	601	HEB	CHB-C4A	5.93	1.50	1.38
4	D	601	HEB	CHB-C4A	5.93	1.50	1.38
4	A	601	HEB	CHA-C1A	5.76	1.49	1.38
4	D	601	HEB	CHA-C1A	5.76	1.49	1.38
4	D	601	HEB	FE-ND	5.62	2.12	1.94
4	A	601	HEB	FE-ND	5.61	2.12	1.94
4	A	602	HEB	FE-ND	5.59	2.12	1.94
4	A	602	HEB	CHB-C4A	5.55	1.49	1.38
4	D	602	HEB	FE-ND	5.55	2.12	1.94
4	D	602	HEB	CHB-C4A	5.52	1.49	1.38
4	A	602	HEB	CHA-C4D	5.37	1.51	1.39
4	A	601	HEB	CHB-C1B	5.36	1.51	1.39
4	D	601	HEB	CHB-C1B	5.34	1.51	1.39
4	D	602	HEB	CHA-C4D	5.34	1.51	1.39
4	A	602	HEB	CHB-C1B	5.28	1.51	1.39
4	D	602	HEB	CHB-C1B	5.28	1.51	1.39
4	A	601	HEB	CHA-C4D	5.24	1.51	1.39
4	D	601	HEB	CHA-C4D	5.24	1.51	1.39
4	A	601	HEB	CHD-C4C	4.86	1.50	1.39
4	D	601	HEB	CHD-C4C	4.86	1.50	1.39
4	A	601	HEB	CHC-C1C	4.83	1.50	1.39
4	D	601	HEB	CHC-C1C	4.83	1.50	1.39
4	D	602	HEB	C4D-ND	4.70	1.48	1.38
4	D	601	HEB	C4D-ND	4.69	1.48	1.38
4	A	602	HEB	C4D-ND	4.65	1.48	1.38
4	A	601	HEB	C4D-ND	4.65	1.48	1.38
4	A	602	HEB	CHC-C1C	4.63	1.49	1.39
4	D	602	HEB	CHC-C1C	4.63	1.49	1.39
4	A	602	HEB	CHD-C4C	4.61	1.49	1.39
4	A	601	HEB	C1B-NB	4.58	1.47	1.38
4	D	602	HEB	CHD-C4C	4.56	1.49	1.39
4	D	601	HEB	C1B-NB	4.55	1.47	1.38
4	A	602	HEB	C1B-NB	4.51	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	602	HEB	C1B-NB	4.48	1.47	1.38
4	D	602	HEB	C1D-ND	4.42	1.47	1.40
4	A	602	HEB	C1D-ND	4.40	1.47	1.40
4	A	601	HEB	C1D-ND	4.38	1.47	1.40
4	D	601	HEB	C1D-ND	4.33	1.47	1.40
4	D	602	HEB	C4B-NB	4.24	1.47	1.40
4	D	601	HEB	C4B-NB	4.21	1.47	1.40
4	A	601	HEB	C4B-NB	4.19	1.47	1.40
4	A	602	HEB	C4B-NB	4.19	1.47	1.40
4	A	602	HEB	C4A-C3A	-4.19	1.37	1.45
4	D	602	HEB	C4A-C3A	-4.19	1.37	1.45
4	A	601	HEB	C1A-C2A	-4.05	1.38	1.45
4	D	601	HEB	C1A-C2A	-4.05	1.38	1.45
4	D	602	HEB	C1A-C2A	-3.75	1.38	1.45
4	A	602	HEB	C1A-C2A	-3.74	1.38	1.45
4	A	601	HEB	C4A-C3A	-3.65	1.38	1.45
4	D	601	HEB	C4A-C3A	-3.65	1.38	1.45
5	A	603	HDD	C1A-C2A	-2.74	1.39	1.44
5	D	603	HDD	C1A-C2A	-2.69	1.39	1.44
4	A	601	HEB	FE-NB	2.52	2.02	1.94
4	D	601	HEB	FE-NB	2.52	2.02	1.94
4	D	602	HEB	FE-NB	2.48	2.02	1.94
4	A	602	HEB	FE-NB	2.46	2.02	1.94
5	A	603	HDD	C4C-NC	-2.28	1.35	1.39
5	D	603	HDD	C4C-NC	-2.28	1.35	1.39
4	A	602	HEB	C1C-C2C	-2.27	1.37	1.43
4	D	602	HEB	C1C-C2C	-2.27	1.37	1.43
4	A	601	HEB	C1C-C2C	-2.24	1.37	1.43
4	D	601	HEB	C1C-C2C	-2.24	1.37	1.43
5	A	603	HDD	CHC-C4B	-2.12	1.34	1.38
5	D	603	HDD	CHC-C4B	-2.12	1.34	1.38
6	A	604	0NI	C1-N	2.08	1.38	1.36
6	D	604	0NI	C1-N	2.05	1.38	1.36

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEB	CHB-C1B-NB	-6.91	116.99	124.42
4	D	601	HEB	CHB-C1B-NB	-6.86	117.04	124.42
4	A	601	HEB	CHA-C4D-ND	-6.82	117.08	124.42
4	D	601	HEB	CHA-C4D-ND	-6.80	117.10	124.42
4	A	602	HEB	CHB-C1B-NB	-6.49	117.44	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	HEB	CHB-C1B-NB	-6.49	117.44	124.42
4	D	602	HEB	CHA-C4D-ND	-6.44	117.49	124.42
4	A	602	HEB	CHA-C4D-ND	-6.37	117.56	124.42
4	D	601	HEB	CHC-C4B-NB	-6.28	116.59	124.37
4	A	601	HEB	CHC-C4B-NB	-6.28	116.60	124.37
4	A	602	HEB	CHD-C1D-ND	-6.15	116.76	124.37
4	D	602	HEB	CHD-C1D-ND	-6.15	116.76	124.37
4	A	601	HEB	CHD-C1D-ND	-6.15	116.76	124.37
4	D	601	HEB	CHD-C1D-ND	-6.12	116.80	124.37
4	A	602	HEB	CHC-C4B-NB	-5.95	117.01	124.37
4	D	602	HEB	CHC-C4B-NB	-5.94	117.02	124.37
5	A	603	HDD	O1D-CGD-O2D	5.10	125.11	120.81
5	D	603	HDD	O1D-CGD-O2D	5.07	125.08	120.81
4	A	602	HEB	C4B-NB-C1B	-4.78	99.55	105.21
4	D	602	HEB	C4B-NB-C1B	-4.77	99.56	105.21
4	A	601	HEB	C4B-NB-C1B	-4.68	99.66	105.21
4	D	601	HEB	C4B-NB-C1B	-4.66	99.68	105.21
4	A	601	HEB	C1D-ND-C4D	-4.51	99.87	105.21
4	D	601	HEB	C1D-ND-C4D	-4.47	99.91	105.21
4	D	602	HEB	C1D-ND-C4D	-4.36	100.04	105.21
4	A	601	HEB	CHA-C1A-NA	4.34	129.17	124.45
4	D	601	HEB	CHA-C1A-NA	4.34	129.17	124.45
4	A	602	HEB	C1D-ND-C4D	-4.31	100.10	105.21
4	D	602	HEB	CHA-C1A-NA	4.27	129.10	124.45
4	A	602	HEB	CHA-C1A-NA	4.24	129.07	124.45
4	A	601	HEB	CHB-C1B-C2B	4.16	131.60	125.03
4	D	601	HEB	CHB-C1B-C2B	4.13	131.55	125.03
4	D	601	HEB	CHA-C4D-C3D	4.00	130.61	124.77
4	A	601	HEB	CHA-C4D-C3D	3.98	130.57	124.77
4	A	602	HEB	CHB-C1B-C2B	3.91	131.21	125.03
4	D	602	HEB	CHB-C1B-C2B	3.90	131.18	125.03
4	D	602	HEB	CHA-C4D-C3D	3.90	130.45	124.77
4	A	602	HEB	CHA-C4D-C3D	3.87	130.42	124.77
4	A	602	HEB	CHB-C4A-NA	3.61	128.39	124.45
4	D	602	HEB	CHB-C4A-NA	3.57	128.34	124.45
5	A	603	HDD	C1C-CHC-C4B	-3.31	114.43	124.66
5	D	603	HDD	C1C-CHC-C4B	-3.31	114.43	124.66
4	D	601	HEB	C3C-C4C-NC	-3.25	107.06	109.80
4	A	601	HEB	C3C-C4C-NC	-3.22	107.08	109.80
4	A	602	HEB	C4A-CHB-C1B	-3.19	119.24	126.02
4	D	602	HEB	C4A-CHB-C1B	-3.18	119.27	126.02
4	D	601	HEB	CHC-C4B-C3B	3.17	131.08	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEB	CHC-C4B-C3B	3.14	131.02	125.23
5	D	603	HDD	CHA-C4D-ND	-3.03	120.11	124.28
5	A	603	HDD	CHA-C4D-ND	-3.00	120.15	124.28
4	D	601	HEB	C4A-CHB-C1B	-2.82	120.02	126.02
4	D	602	HEB	CHC-C4B-C3B	2.82	130.43	125.23
4	A	602	HEB	CHC-C4B-C3B	2.81	130.41	125.23
4	A	601	HEB	C4A-CHB-C1B	-2.81	120.05	126.02
4	D	601	HEB	CHA-C1A-C2A	-2.79	120.47	124.86
4	A	601	HEB	CHA-C1A-C2A	-2.78	120.47	124.86
4	D	602	HEB	C3C-C4C-NC	-2.74	107.49	109.80
4	A	602	HEB	C3C-C4C-NC	-2.72	107.51	109.80
4	A	601	HEB	CHB-C4A-NA	2.69	127.39	124.45
4	D	601	HEB	CHB-C4A-NA	2.69	127.38	124.45
4	D	602	HEB	C4C-CHD-C1D	-2.60	120.12	126.25
4	A	602	HEB	C4C-CHD-C1D	-2.58	120.17	126.25
4	D	601	HEB	C4C-CHD-C1D	-2.54	120.28	126.25
4	A	601	HEB	C4C-CHD-C1D	-2.53	120.29	126.25
4	D	602	HEB	CHA-C1A-C2A	-2.51	120.89	124.86
4	A	602	HEB	CHA-C1A-C2A	-2.49	120.93	124.86
4	D	602	HEB	CHD-C4C-NC	2.45	128.31	123.86
4	A	602	HEB	CHD-C4C-NC	2.42	128.24	123.86
4	A	602	HEB	CHC-C1C-NC	2.32	128.06	123.86
4	D	602	HEB	CHC-C1C-NC	2.32	128.06	123.86
5	D	603	HDD	C2D-C1D-CHD	2.30	127.85	124.27
4	A	601	HEB	C1A-CHA-C4D	-2.29	121.14	126.02
4	D	601	HEB	C1A-CHA-C4D	-2.29	121.14	126.02
4	A	601	HEB	CHC-C1C-NC	2.26	127.97	123.86
4	D	601	HEB	CHC-C1C-NC	2.25	127.95	123.86
5	A	603	HDD	C2D-C1D-CHD	2.25	127.77	124.27
4	A	602	HEB	C1A-CHA-C4D	-2.24	121.26	126.02
4	D	602	HEB	C1A-CHA-C4D	-2.22	121.31	126.02
4	A	602	HEB	C3B-C4B-NB	2.20	112.58	110.17
4	A	602	HEB	CHC-C1C-C2C	-2.18	121.09	127.43
4	D	602	HEB	C3B-C4B-NB	2.17	112.55	110.17
4	D	602	HEB	CHC-C1C-C2C	-2.17	121.13	127.43
4	D	601	HEB	CHD-C4C-NC	2.13	127.72	123.86
4	A	601	HEB	CHD-C4C-NC	2.12	127.70	123.86
4	A	601	HEB	C1D-C2D-C3D	2.09	109.18	106.98
4	D	601	HEB	C1D-C2D-C3D	2.08	109.17	106.98
7	B	401	UQ8	C7-C6-C5	-2.08	116.10	118.52
7	E	401	UQ8	C7-C6-C5	-2.07	116.10	118.52
4	A	601	HEB	C3D-C4D-ND	2.06	112.35	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEB	CHC-C1C-C2C	-2.04	121.49	127.43
4	D	601	HEB	CHC-C1C-C2C	-2.04	121.49	127.43
4	A	601	HEB	C3B-C4B-NB	2.01	112.38	110.17
4	D	601	HEB	C3D-C4D-ND	2.00	112.29	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	601	HEB	NA
4	A	602	HEB	NA
4	D	601	HEB	NA
4	D	602	HEB	NA

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	604	0NI	C10-C11-C12-C13
6	A	604	0NI	C10-C11-C12-C14
6	D	604	0NI	C10-C11-C12-C13
6	D	604	0NI	C10-C11-C12-C14
6	A	604	0NI	C20-C21-C22-C24
6	D	604	0NI	C20-C21-C22-C24
6	A	604	0NI	C13-C12-C14-C15
6	D	604	0NI	C13-C12-C14-C15
7	B	401	UQ8	C20-C19-C21-C22
7	E	401	UQ8	C20-C19-C21-C22
6	A	604	0NI	C11-C12-C14-C15
6	D	604	0NI	C11-C12-C14-C15
6	A	604	0NI	C20-C21-C22-C23
6	D	604	0NI	C20-C21-C22-C23
7	B	401	UQ8	C35-C34-C36-C37
7	E	401	UQ8	C35-C34-C36-C37
7	B	401	UQ8	C18-C19-C21-C22
7	E	401	UQ8	C18-C19-C21-C22
6	D	604	0NI	C15-C16-C17-C18
6	A	604	0NI	C15-C16-C17-C18
7	B	401	UQ8	C33-C34-C36-C37
7	E	401	UQ8	C33-C34-C36-C37
4	A	602	HEB	C4C-C3C-CAC-CBC
4	D	602	HEB	C4C-C3C-CAC-CBC
5	A	603	HDD	C4C-C3C-CAC-CBC
5	D	603	HDD	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	A	603	HDD	C2C-C3C-CAC-CBC
5	D	603	HDD	C2C-C3C-CAC-CBC
7	B	401	UQ8	C23-C24-C26-C27
7	E	401	UQ8	C23-C24-C26-C27
4	A	602	HEB	C1A-C2A-CAA-CBA
4	D	602	HEB	C1A-C2A-CAA-CBA
7	B	401	UQ8	C25-C24-C26-C27
7	E	401	UQ8	C25-C24-C26-C27
7	B	401	UQ8	C30-C29-C31-C32
7	E	401	UQ8	C30-C29-C31-C32
4	A	602	HEB	C3A-C2A-CAA-CBA
4	D	602	HEB	C3A-C2A-CAA-CBA
7	B	401	UQ8	C28-C29-C31-C32
7	E	401	UQ8	C28-C29-C31-C32
7	B	401	UQ8	C5-C4-O4-C4M
7	E	401	UQ8	C5-C4-O4-C4M
4	A	602	HEB	C2C-C3C-CAC-CBC
4	D	602	HEB	C2C-C3C-CAC-CBC
7	B	401	UQ8	C14-C16-C17-C18
7	E	401	UQ8	C14-C16-C17-C18
7	B	401	UQ8	C2-C3-O3-C3M
7	E	401	UQ8	C2-C3-O3-C3M
6	D	604	0NI	C15-C16-C17-C19
6	A	604	0NI	C15-C16-C17-C19
4	A	601	HEB	CAD-CBD-CGD-O1D
4	D	601	HEB	CAD-CBD-CGD-O1D
7	B	401	UQ8	C19-C21-C22-C23
7	E	401	UQ8	C19-C21-C22-C23
4	A	601	HEB	CAD-CBD-CGD-O2D
4	D	601	HEB	CAD-CBD-CGD-O2D
4	A	602	HEB	CAA-CBA-CGA-O2A
4	D	602	HEB	CAA-CBA-CGA-O2A
5	A	603	HDD	CAA-CBA-CGA-O1A
5	D	603	HDD	CAA-CBA-CGA-O1A
4	A	602	HEB	CAA-CBA-CGA-O1A
4	D	602	HEB	CAA-CBA-CGA-O1A
7	B	401	UQ8	C29-C31-C32-C33
7	E	401	UQ8	C29-C31-C32-C33
4	A	602	HEB	CAD-CBD-CGD-O1D
4	D	602	HEB	CAD-CBD-CGD-O1D
5	A	603	HDD	CAA-CBA-CGA-O2A
5	D	603	HDD	CAA-CBA-CGA-O2A

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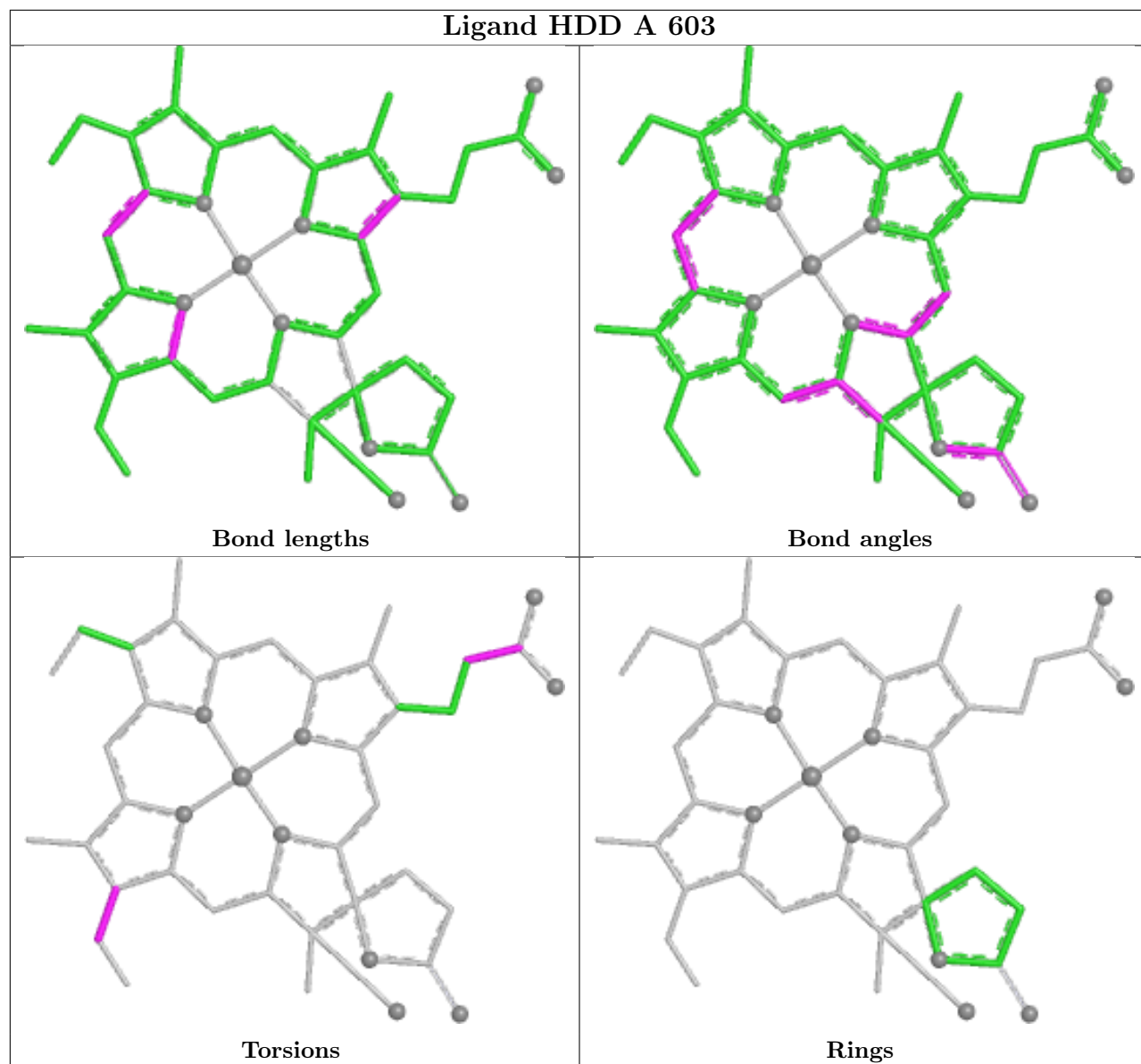
Mol	Chain	Res	Type	Atoms
7	B	401	UQ8	C40-C39-C41-C42
7	E	401	UQ8	C40-C39-C41-C42
4	A	602	HEB	C2A-CAA-CBA-CGA
4	D	602	HEB	C2B-C3B-CAB-CBB
4	A	602	HEB	C2B-C3B-CAB-CBB
4	A	602	HEB	CAD-CBD-CGD-O2D
4	D	602	HEB	C2A-CAA-CBA-CGA
4	D	602	HEB	CAD-CBD-CGD-O2D

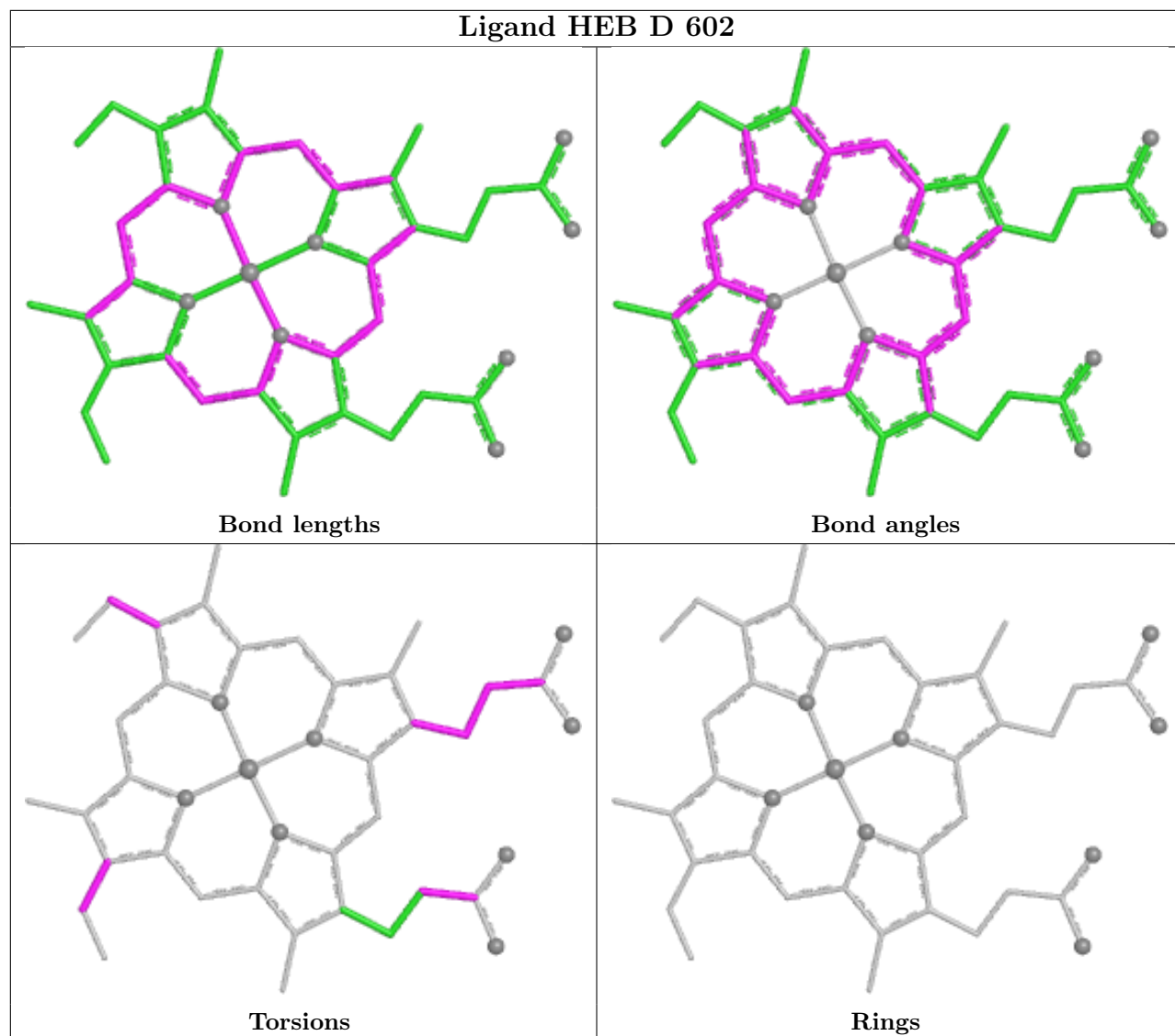
There are no ring outliers.

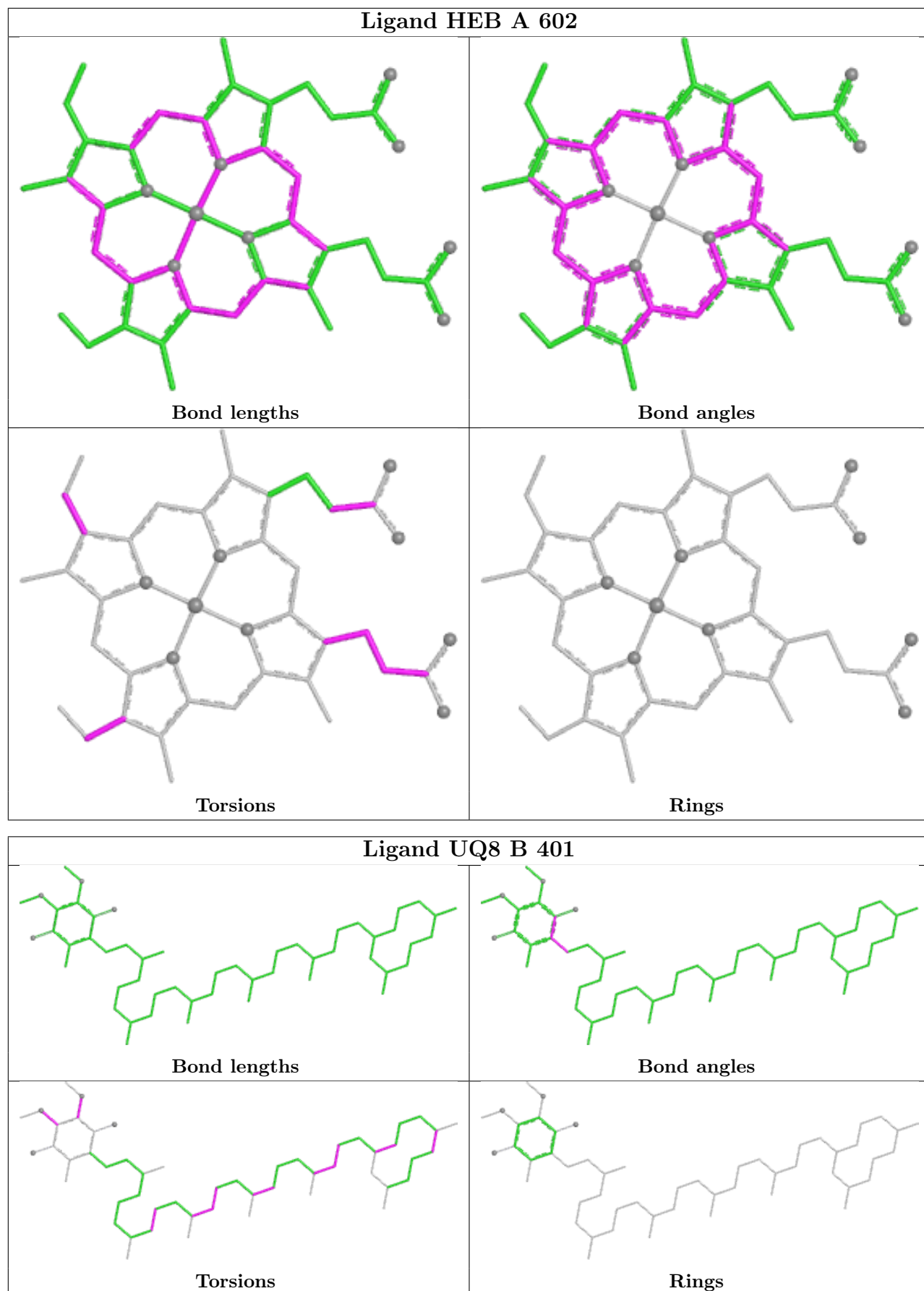
8 monomers are involved in 50 short contacts:

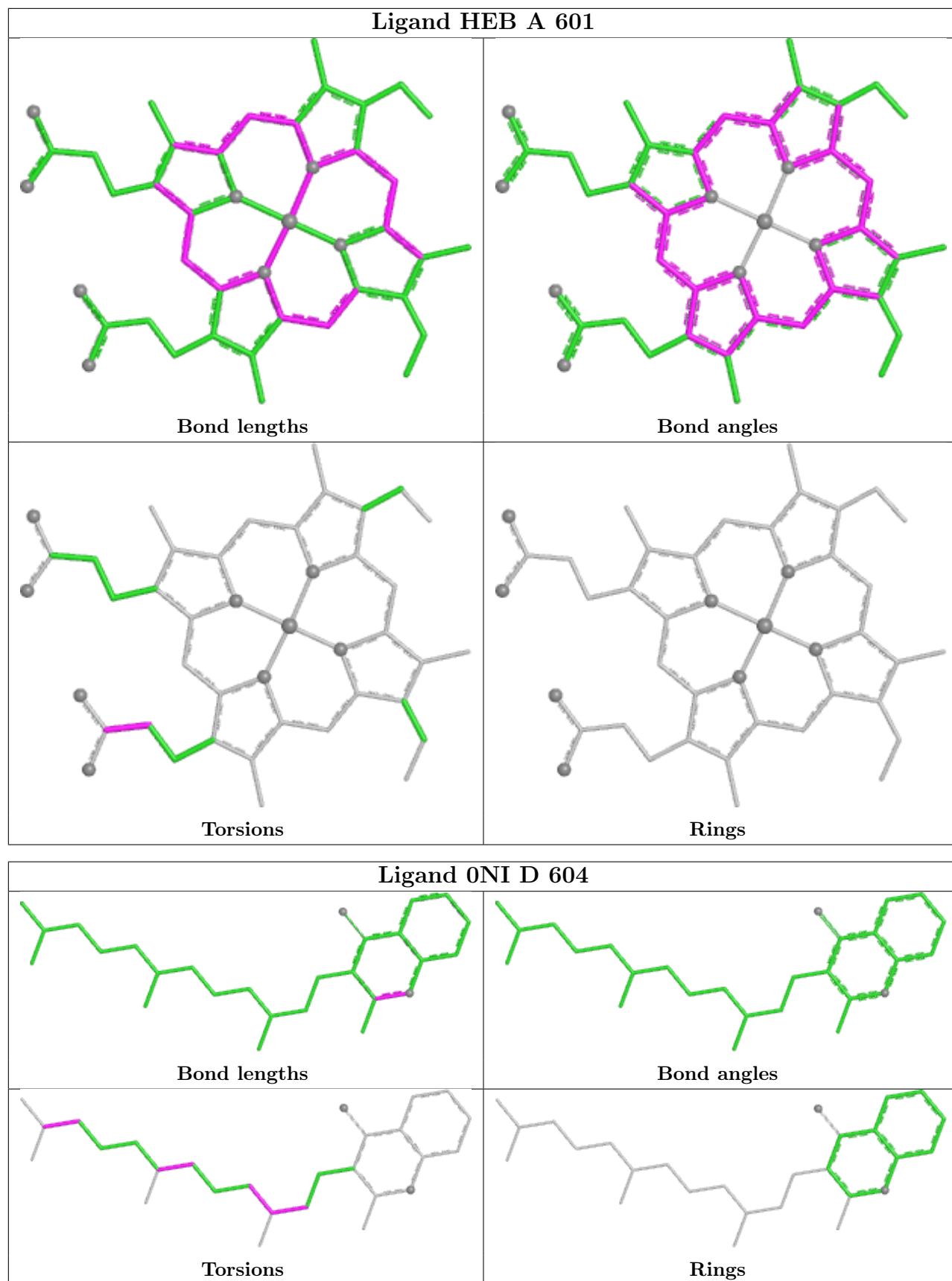
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	HDD	7	0
4	D	602	HEB	7	0
4	A	602	HEB	7	0
7	B	401	UQ8	8	0
4	A	601	HEB	5	0
7	E	401	UQ8	8	0
5	D	603	HDD	7	0
4	D	601	HEB	5	0

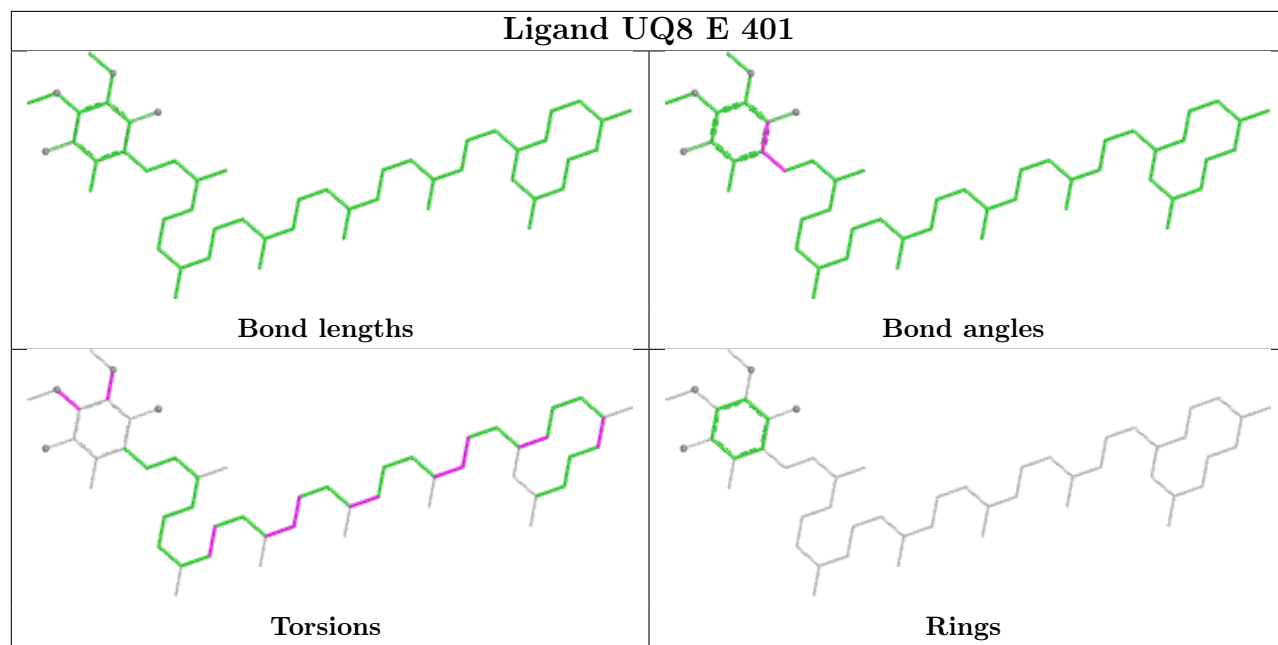
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

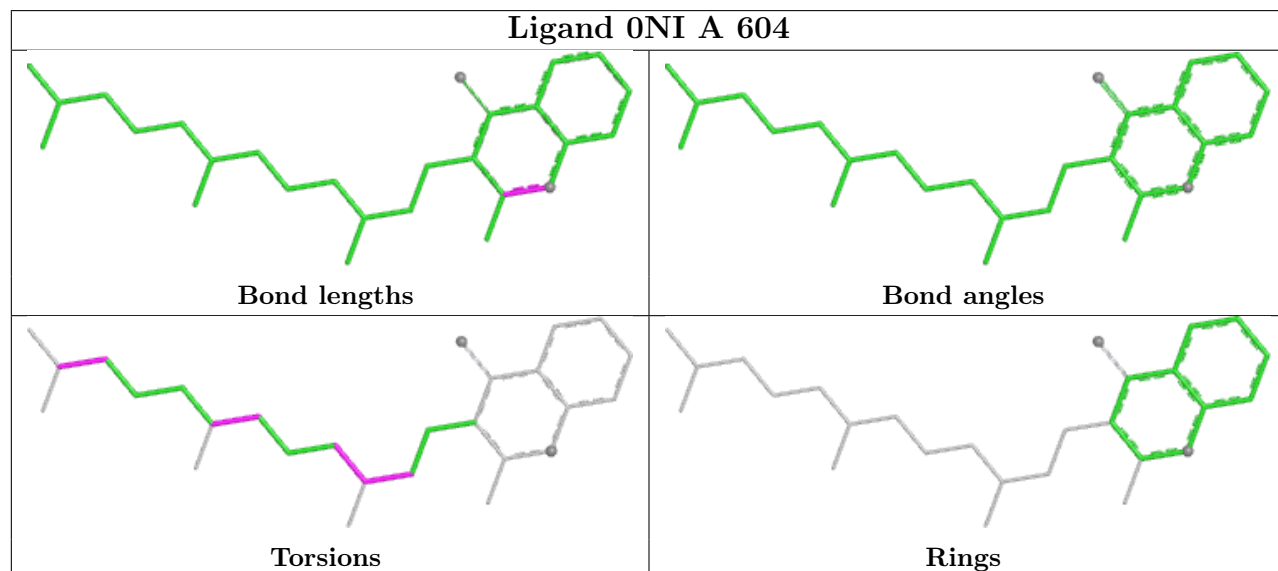
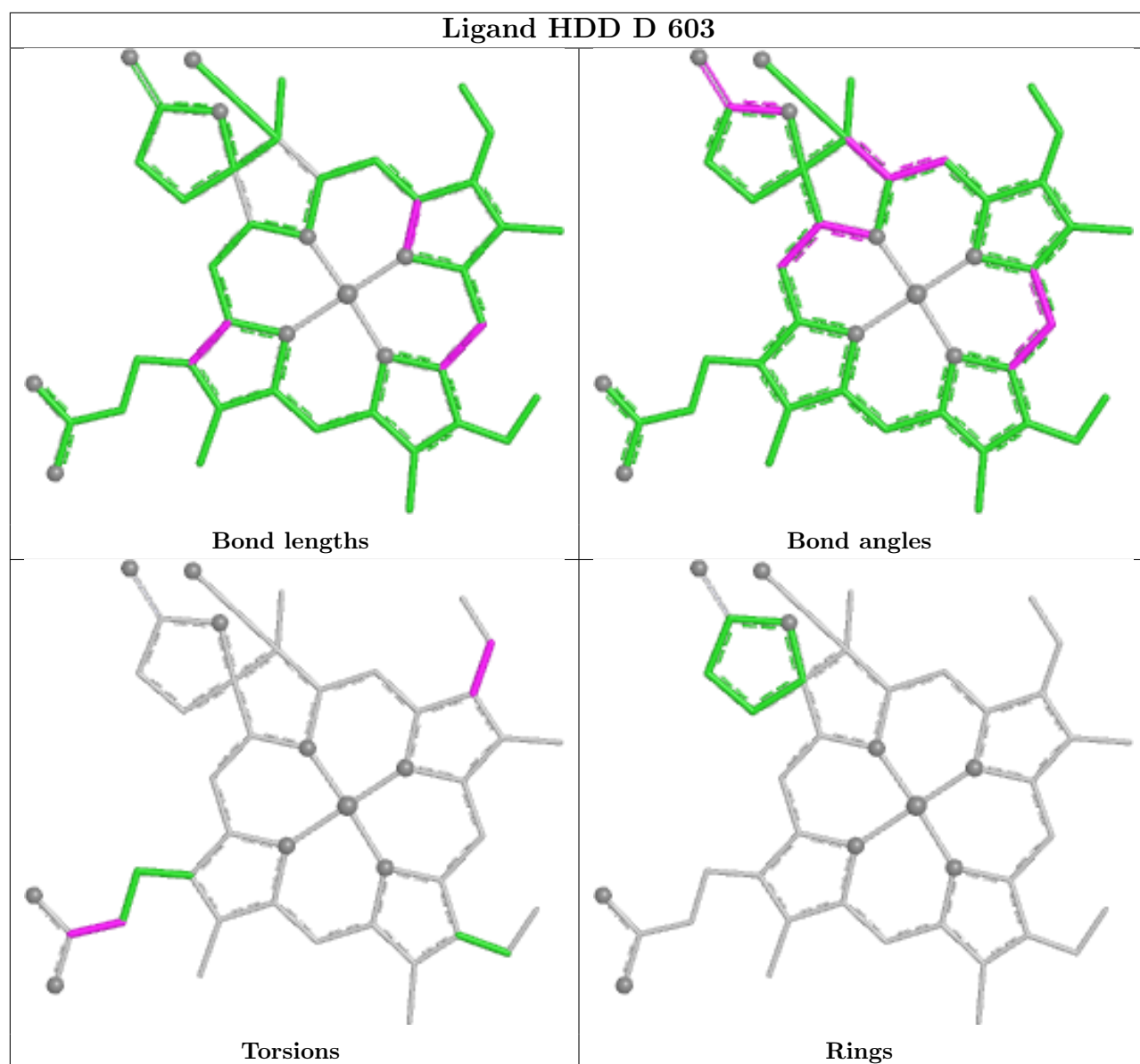


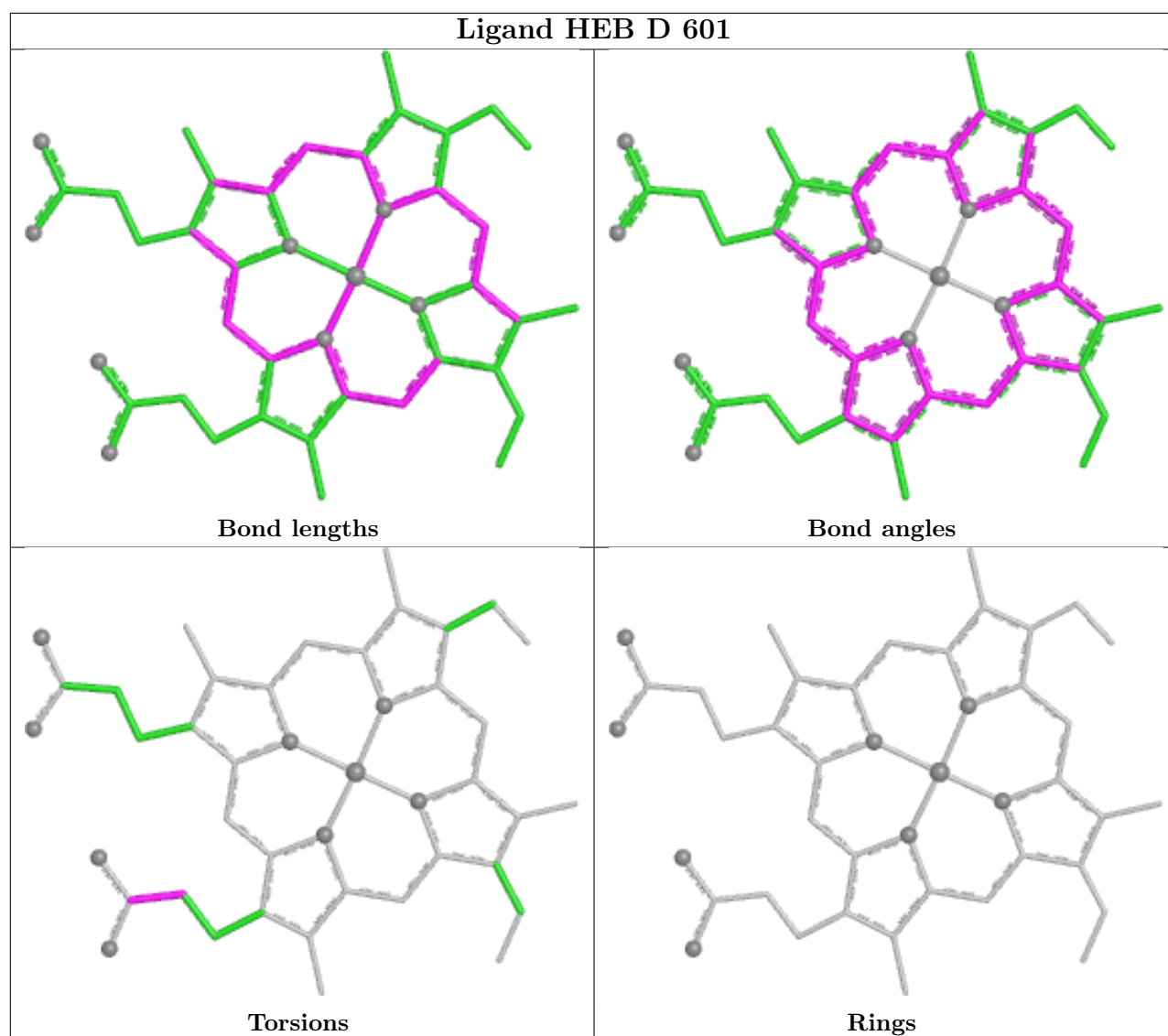












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

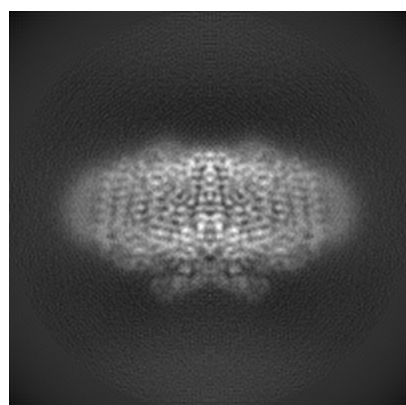
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13048. These allow visual inspection of the internal detail of the map and identification of artifacts.

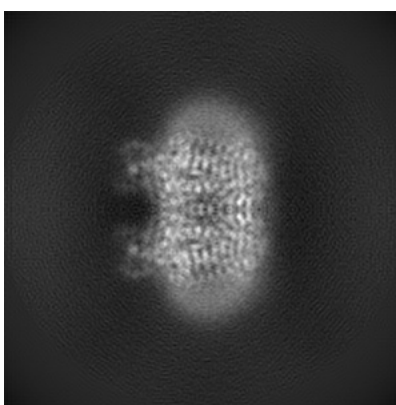
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

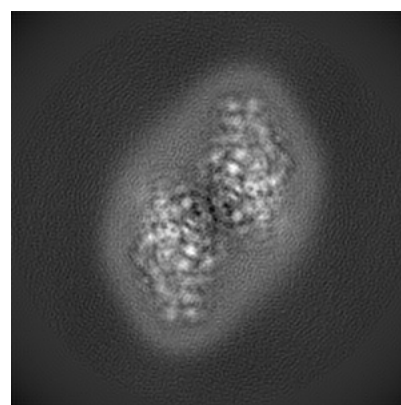
6.1.1 Primary map



X



Y

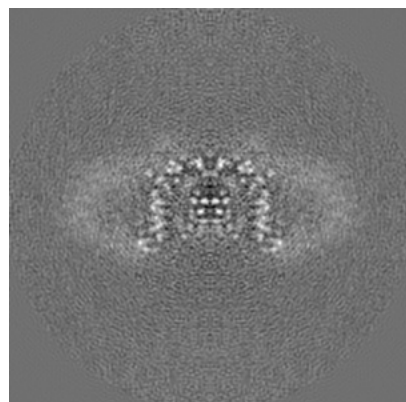


Z

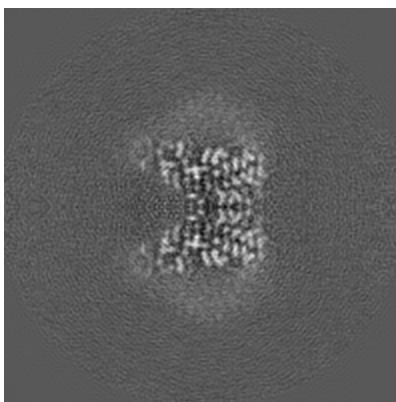
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

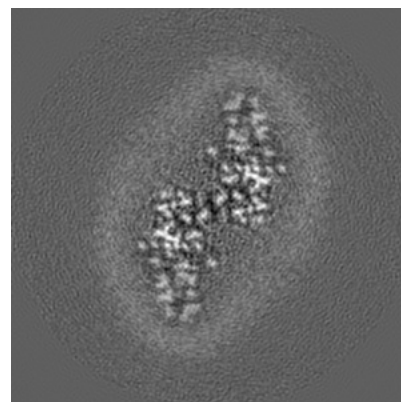
6.2.1 Primary map



X Index: 100



Y Index: 100

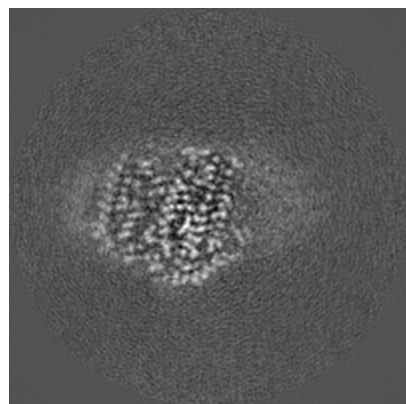


Z Index: 100

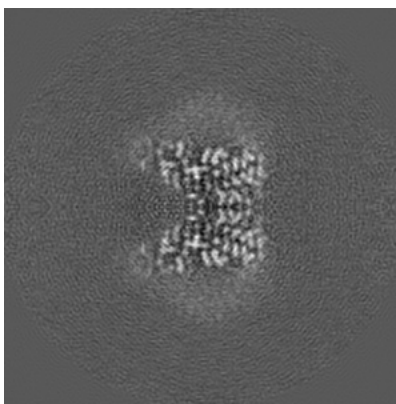
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

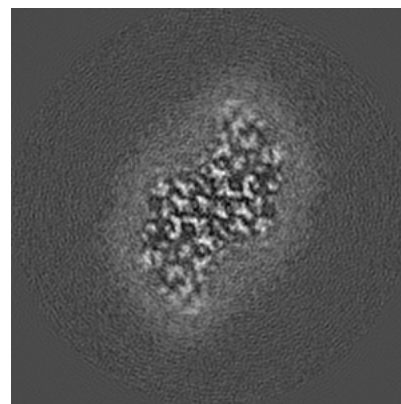
6.3.1 Primary map



X Index: 78



Y Index: 100

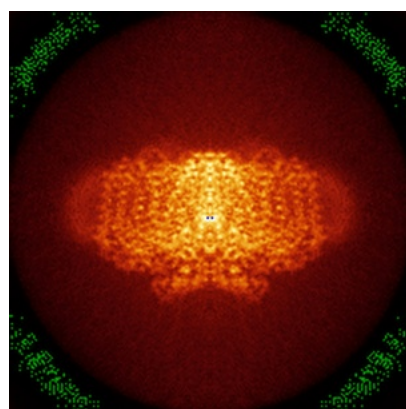


Z Index: 118

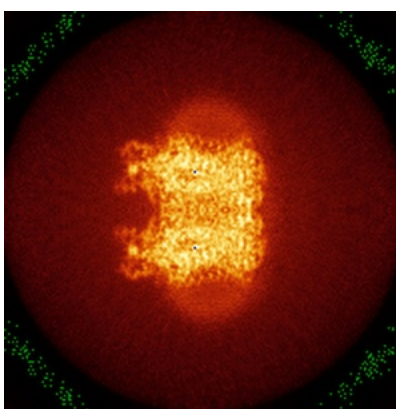
The images above show the largest variance slices of the map in three orthogonal directions.

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

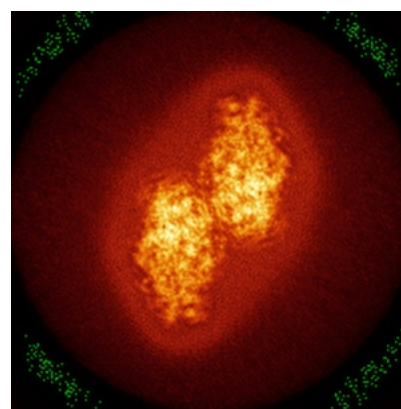
6.4.1 Primary map



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

This section was not generated.

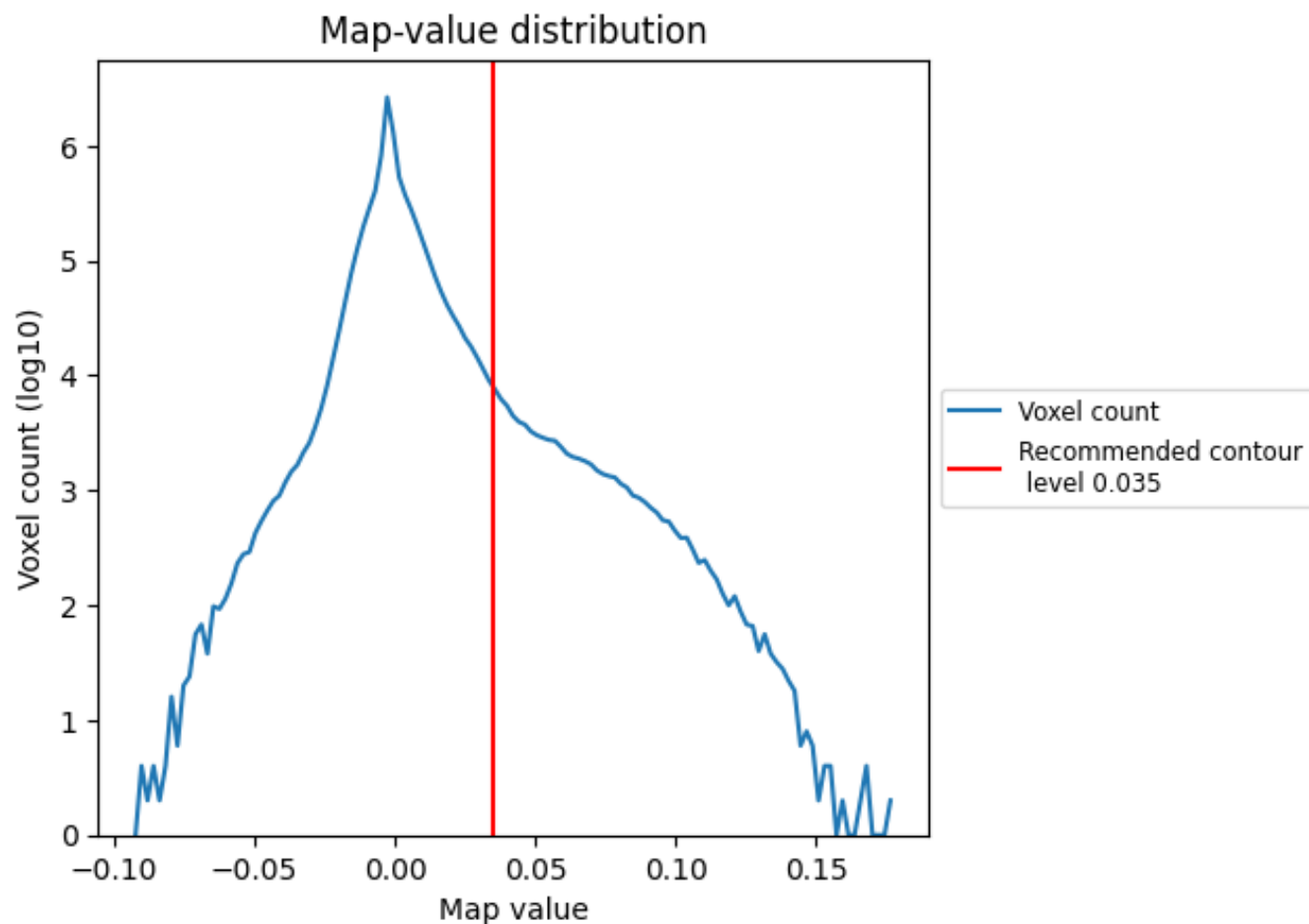
6.6 Mask visualisation

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

7 Map analysis [i](#)

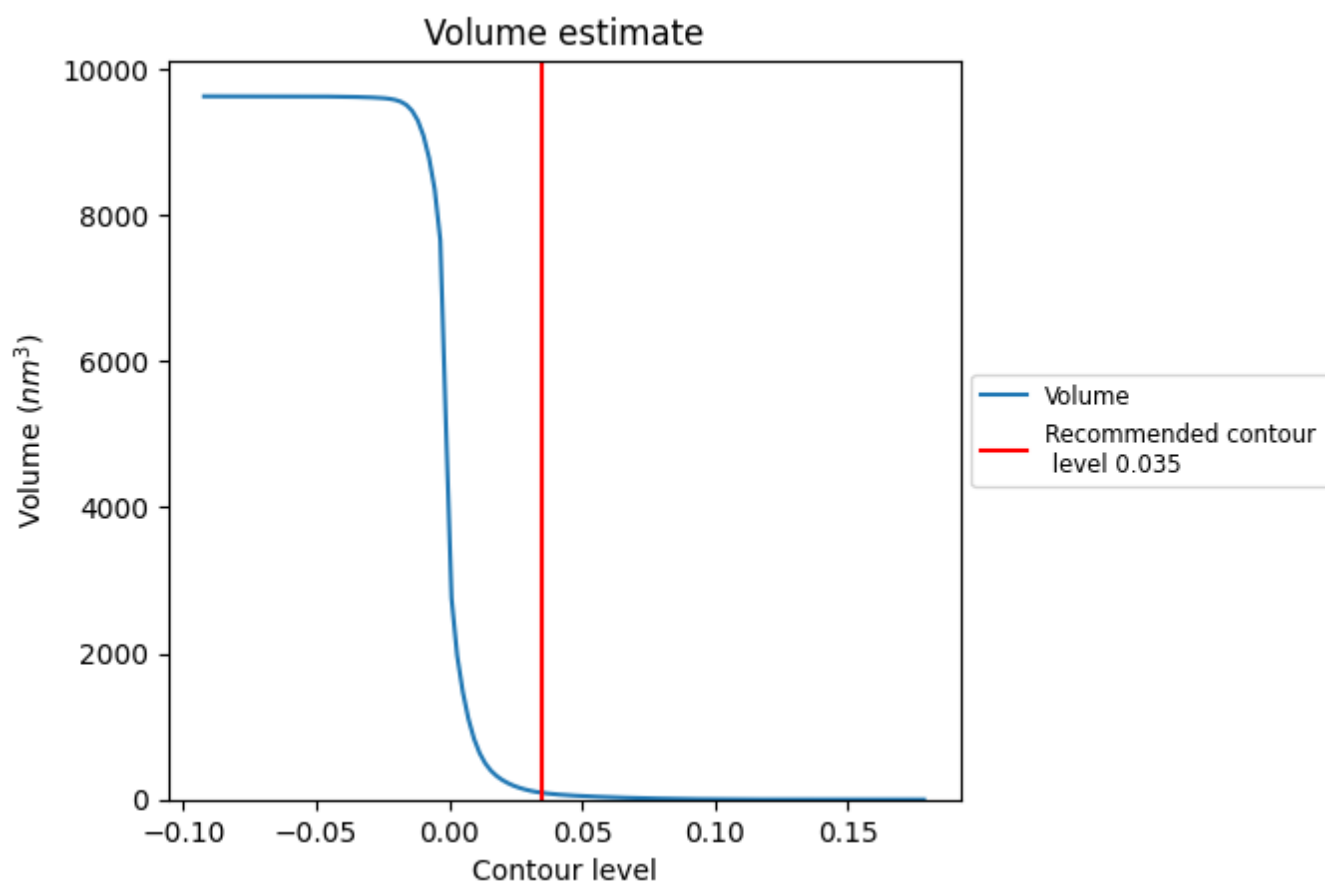
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

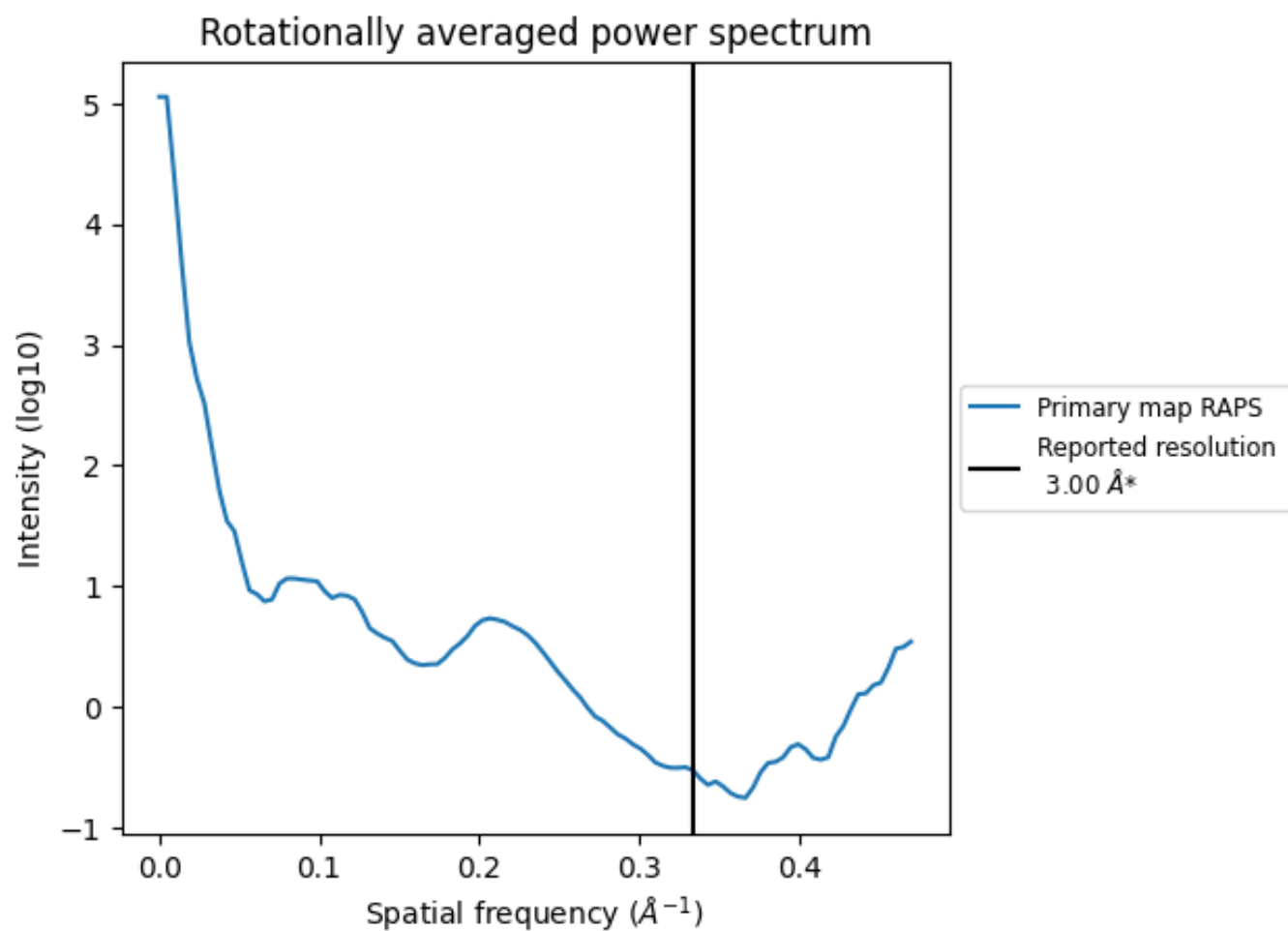
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm³; this corresponds to an approximate mass of 84 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.

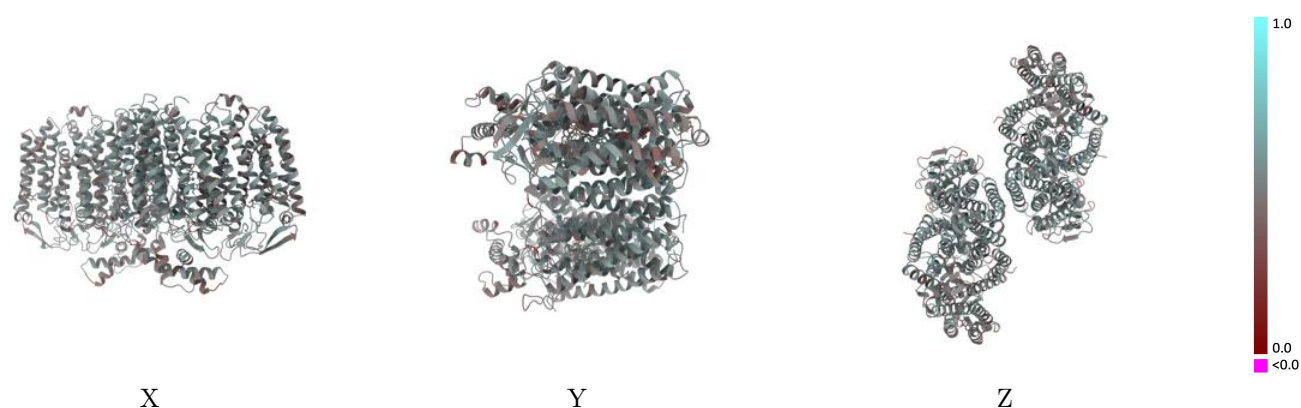
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13048 and PDB model 7OSE. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

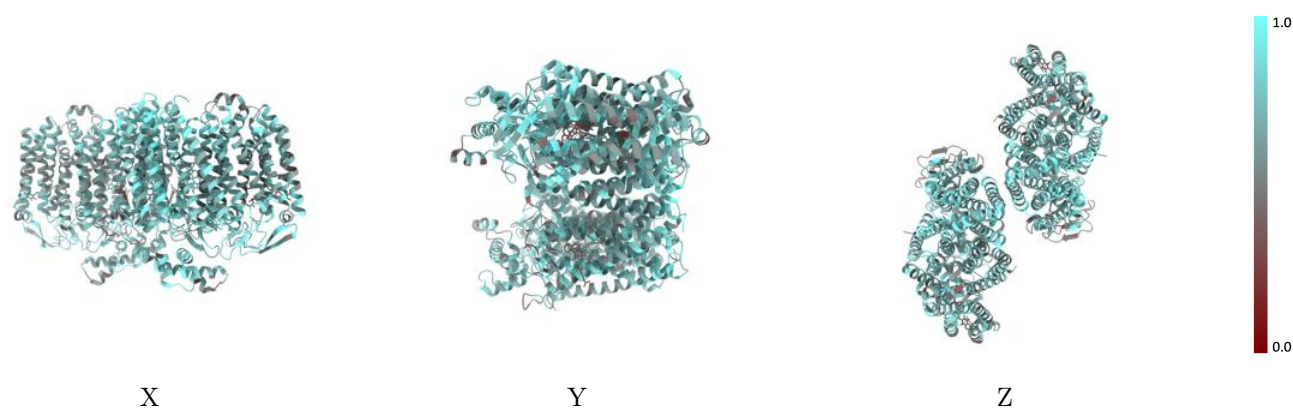
This section was not generated.

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



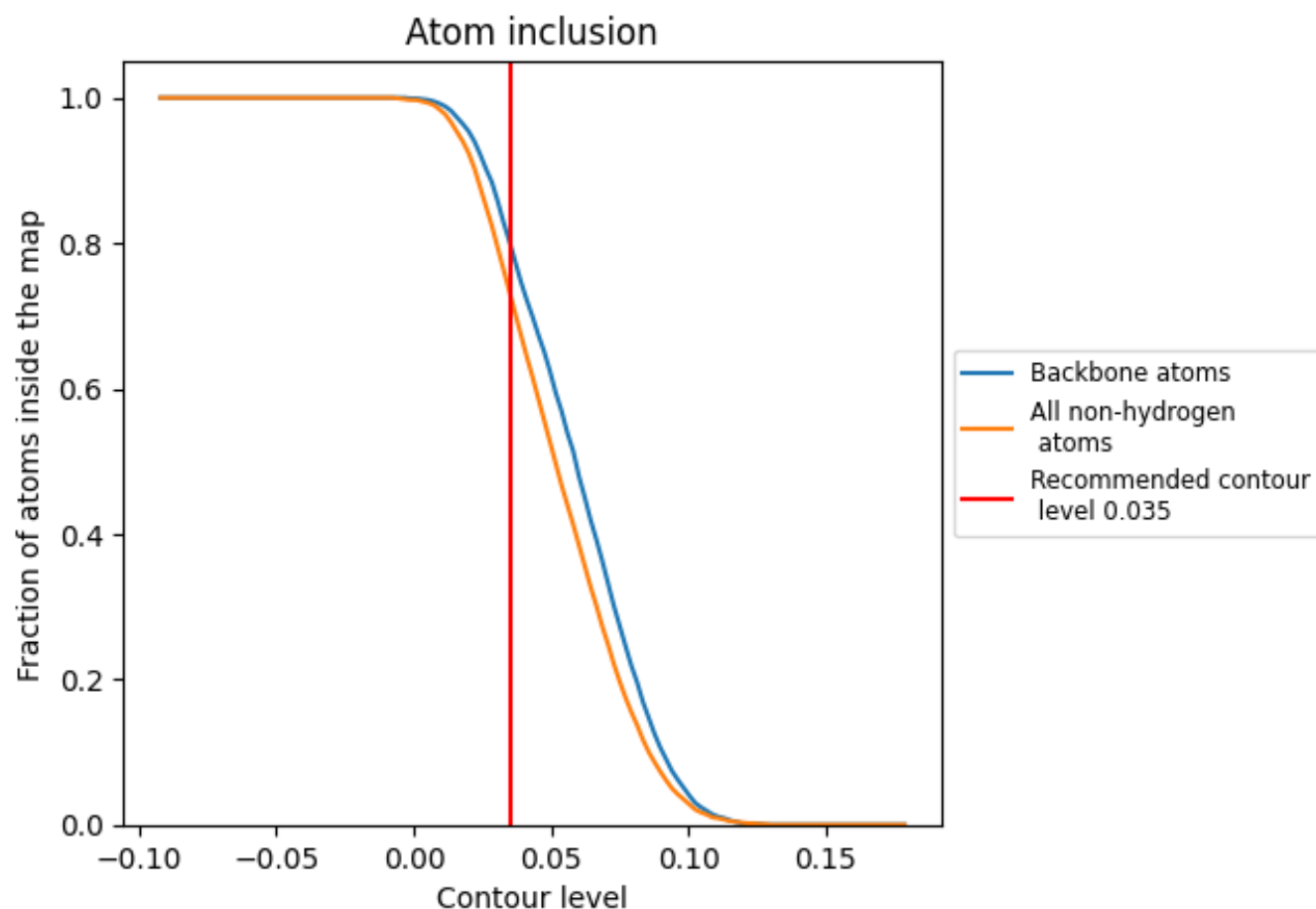
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 73% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7300	0.5060
A	0.7560	0.5090
B	0.7070	0.4980
C	0.8010	0.5630
D	0.7570	0.5090
E	0.7070	0.4970
F	0.8050	0.5620

1.0

0.0

<0.0