



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:11 PM UTC

PDB ID : 7U6F / pdb_00007u6f
EMDB ID : EMD-24964
Title : Mouse retromer (VPS26/VPS35/VPS29) heterotrimers
Authors : Kendall, A.K.; Chandra, M.; Jackson, L.P.
Deposited on : 2022-03-04
Resolution : 4.90 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:

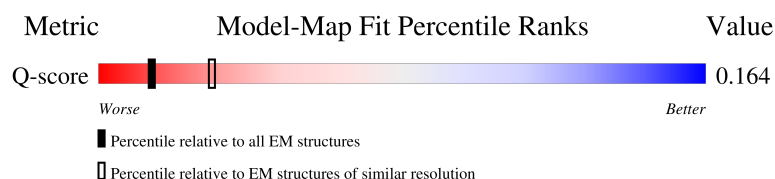
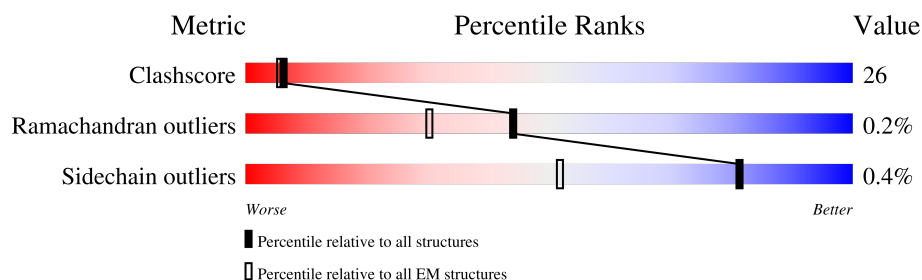
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.90 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	1274 (4.40 - 5.40)

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	D1	796	
2	B3	327	
3	B4	182	

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	GOL	B3	403	-	-	X	-
4	GOL	D1	802	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 10049 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 Vacuolar protein sorting-associated protein 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	D1	733	5949	3797	1020	1099	33	0	0

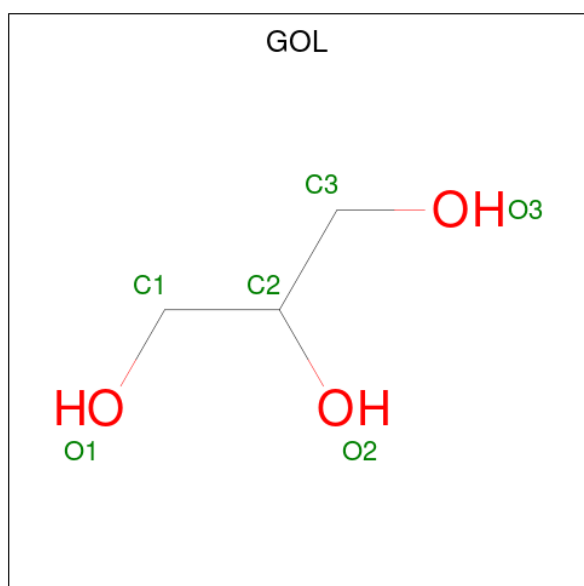
- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 26A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B3	299	2464	1586	415	454	9	0	0

- Molecule 3 is a protein called Vacuolar protein sorting-associated protein 29.

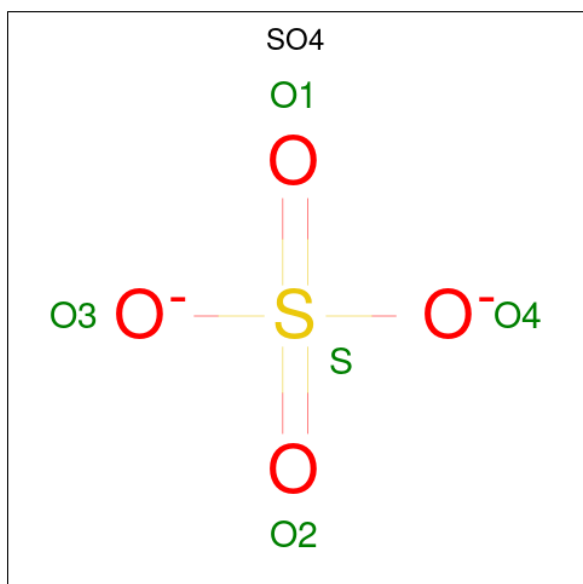
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B4	181	1438	929	241	263	5	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



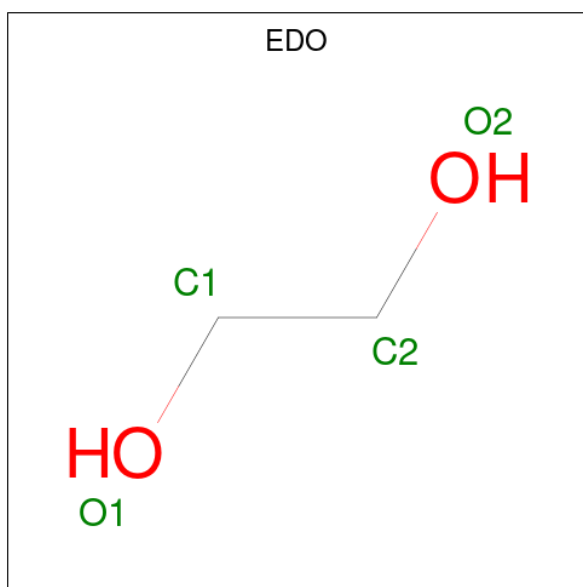
Mol	Chain	Residues	Atoms			AltConf
4	D1	1	Total	C	O	0
			6	3	3	
4	D1	1	Total	C	O	0
			6	3	3	
4	D1	1	Total	C	O	0
			6	3	3	
4	B3	1	Total	C	O	0
			6	3	3	
4	B3	1	Total	C	O	0
			6	3	3	
4	B3	1	Total	C	O	0
			6	3	3	

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	D1	1	Total	O	S	0
			5	4	1	
5	D1	1	Total	O	S	0
			5	4	1	
5	B3	1	Total	O	S	0
			5	4	1	

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	D1	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	

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Mol	Chain	Residues	Atoms			AltConf
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	
6	B3	1	Total	C	O	0
			4	2	2	

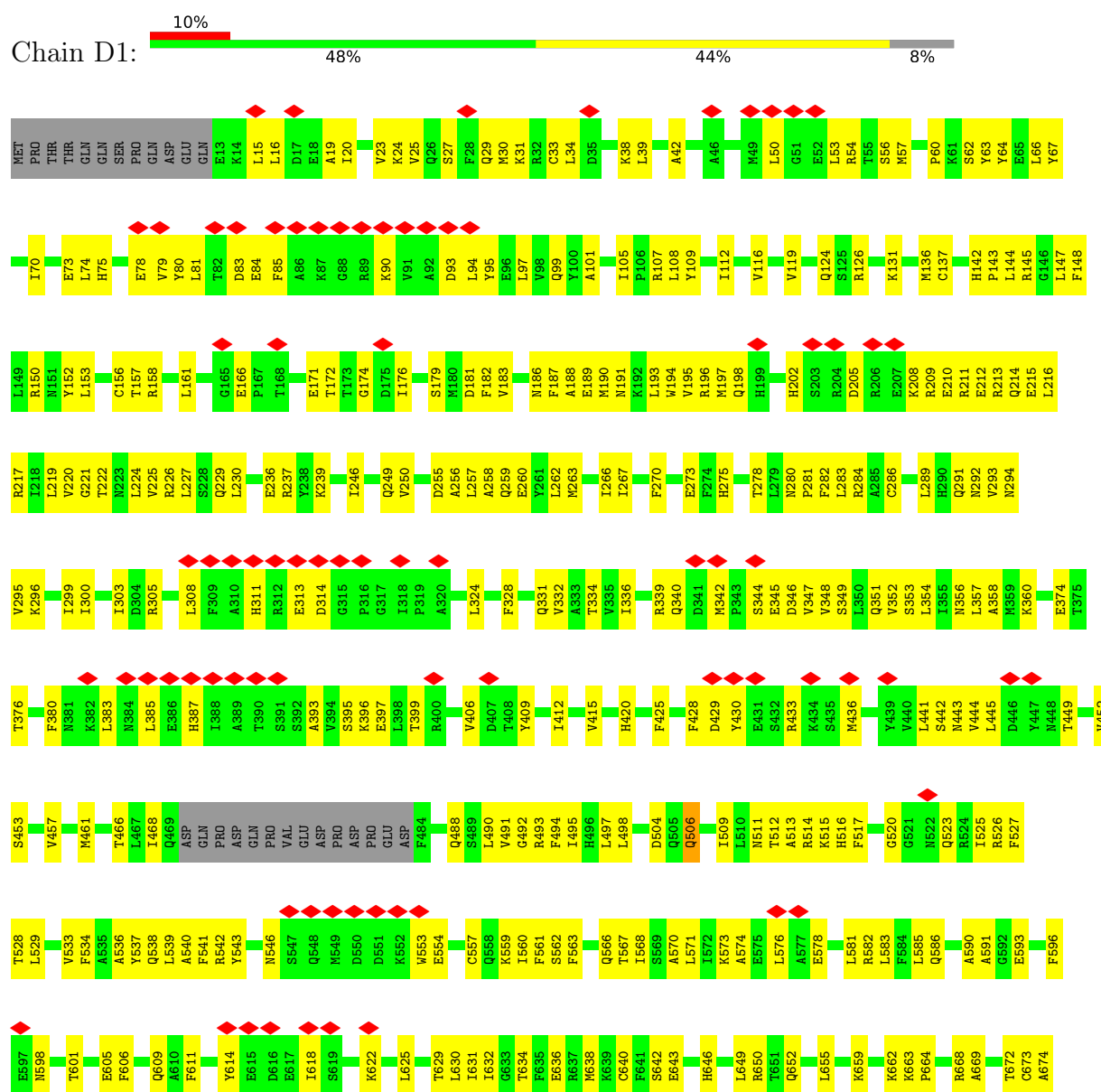
- Molecule 7 is water.

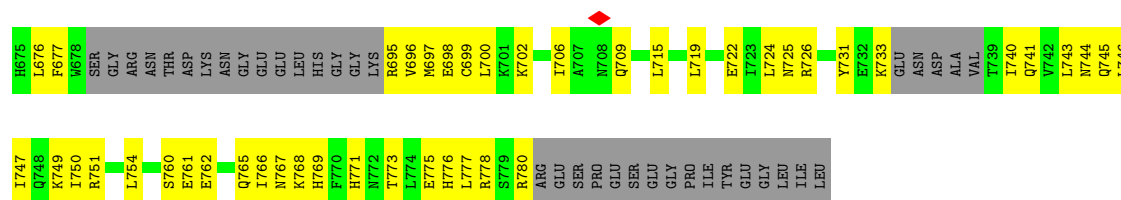
Mol	Chain	Residues	Atoms		AltConf
7	D1	28	Total	O	0
			28	28	
7	B3	38	Total	O	0
			38	38	
7	B4	5	Total	O	0
			5	5	

3 Residue-property plots

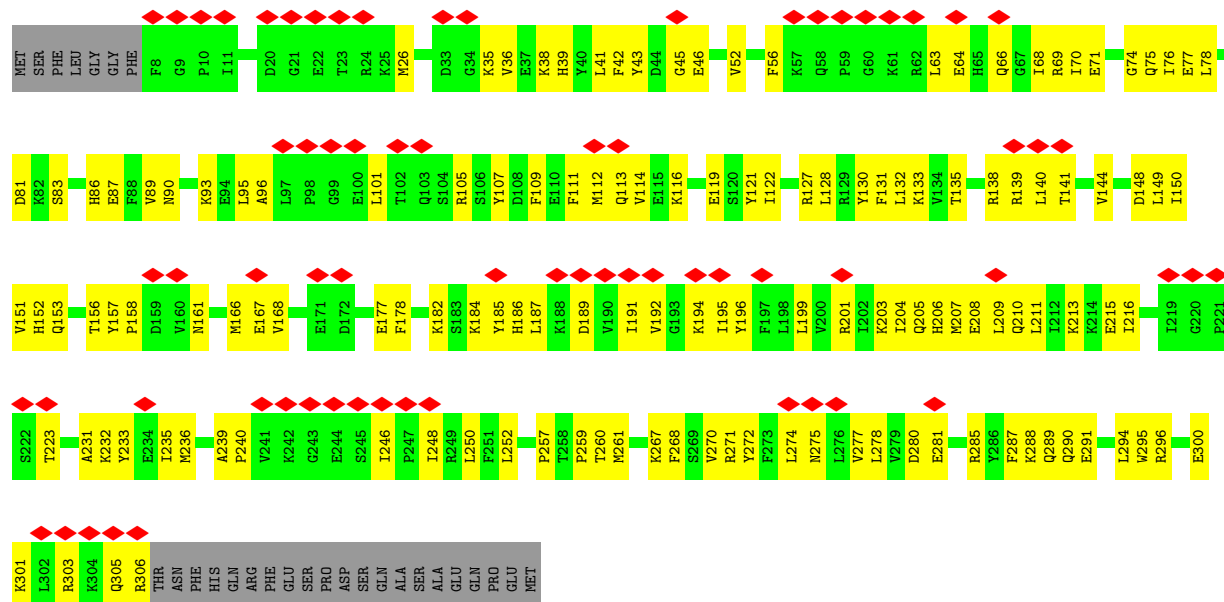
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Vacuolar protein sorting-associated protein 35

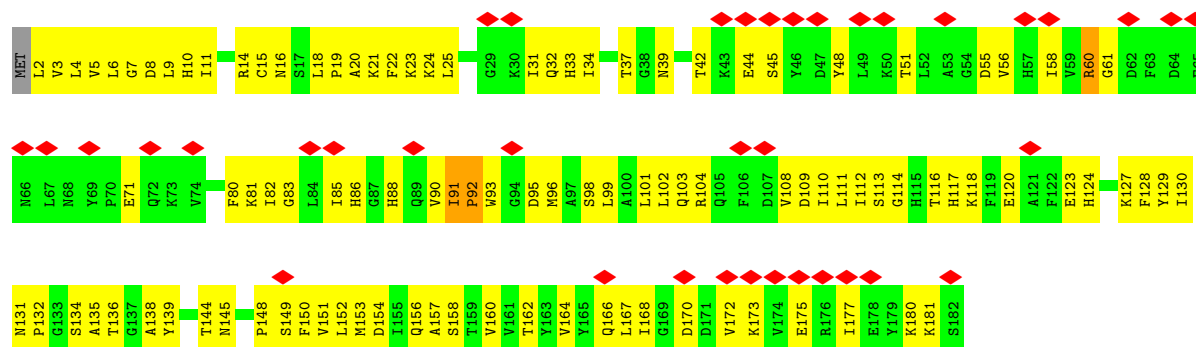




• Molecule 2: Vacuolar protein sorting-associated protein 26A



• Molecule 3: Vacuolar protein sorting-associated protein 29



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43808	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 ($e^-/\text{\AA}^2$)	72	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0119	Depositor
Map size (Å)	241.12, 241.12, 241.12	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.096, 1.096, 1.096	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, GOL

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	D1	0.17	0/6054	0.45	0/8166
2	B3	0.15	0/2513	0.42	0/3383
3	B4	0.22	0/1471	0.51	0/1994
All	All	0.17	0/10038	0.45	0/13543

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	D1	5949	0	6005	305	0
2	B3	2464	0	2501	122	0
3	B4	1438	0	1445	102	0
4	B3	18	0	24	4	0
4	D1	18	0	24	20	0
5	B3	5	0	0	0	0
5	D1	10	0	0	1	0
6	B3	44	0	66	6	0
6	D1	32	0	48	6	0
7	B3	38	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B4	5	0	0	1	0
7	D1	28	0	0	5	0
All	All	10049	0	10113	518	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 26.

All (518) 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:D1:743:LEU:CD2	4:D1:802:GOL:H11	1.39	1.52
1:D1:747:ILE:HD12	4:D1:802:GOL:C3	1.55	1.34
1:D1:747:ILE:CD1	4:D1:802:GOL:H31	1.67	1.25
1:D1:743:LEU:CD2	4:D1:802:GOL:C1	2.20	1.19
1:D1:743:LEU:HD21	4:D1:802:GOL:H11	1.20	1.12
1:D1:747:ILE:HD12	4:D1:802:GOL:H31	1.19	1.11
1:D1:747:ILE:HD12	4:D1:802:GOL:H32	1.35	1.02
1:D1:743:LEU:HD22	4:D1:802:GOL:H11	1.40	0.99
1:D1:743:LEU:HD22	4:D1:802:GOL:C1	1.95	0.95
1:D1:20:ILE:HG13	1:D1:66:LEU:HD13	1.51	0.91
2:B3:301:LYS:HE2	2:B3:303:ARG:HH12	1.35	0.90
1:D1:747:ILE:CD1	4:D1:802:GOL:C3	2.36	0.88
1:D1:777:LEU:HD21	4:D1:802:GOL:H2	1.57	0.86
1:D1:747:ILE:HD13	4:D1:802:GOL:H31	1.59	0.85
2:B3:42:PHE:HB2	2:B3:151:VAL:HG22	1.58	0.84
3:B4:7:GLY:HA3	3:B4:37:THR:HB	1.58	0.83
3:B4:3:VAL:HG12	3:B4:33:HIS:HB2	1.61	0.83
1:D1:214:GLN:HA	1:D1:217:ARG:HD3	1.61	0.81
1:D1:578:GLU:HB3	1:D1:582:ARG:HH12	1.45	0.81
1:D1:161:LEU:HD11	1:D1:182:PHE:HD2	1.48	0.79
1:D1:534:PHE:HA	1:D1:537:TYR:HD2	1.47	0.78
1:D1:497:LEU:HD12	1:D1:498:LEU:HG	1.66	0.77
1:D1:150:ARG:HE	1:D1:186:ASN:HA	1.50	0.77
2:B3:191:ILE:HG13	2:B3:252:LEU:HD11	1.66	0.76
2:B3:235:ILE:O	2:B3:236:MET:HE2	1.86	0.75
2:B3:235:ILE:HG23	2:B3:236:MET:HG2	1.69	0.74
1:D1:743:LEU:HD23	4:D1:802:GOL:C1	2.16	0.74
2:B3:122:ILE:HD12	2:B3:127:ARG:HG2	1.68	0.74
1:D1:433:ARG:NH1	1:D1:466:THR:O	2.20	0.74
1:D1:267:ILE:O	1:D1:305:ARG:NH1	2.20	0.73
1:D1:270:PHE:O	1:D1:305:ARG:NH1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:103:GLN:NE2	3:B4:108:VAL:O	2.20	0.72
1:D1:150:ARG:HD3	1:D1:190:MET:HE3	1.71	0.72
2:B3:259:PRO:HB3	2:B3:295:TRP:HA	1.72	0.72
1:D1:488:GLN:HG3	1:D1:527:PHE:HB3	1.72	0.72
2:B3:209:LEU:HD11	2:B3:274:LEU:HB3	1.71	0.72
3:B4:8:ASP:HA	3:B4:39:ASN:HB2	1.72	0.72
1:D1:662:LYS:HG2	1:D1:664:PRO:HD2	1.72	0.71
1:D1:214:GLN:O	1:D1:217:ARG:NH1	2.23	0.71
1:D1:202:HIS:O	1:D1:209:ARG:NH1	2.24	0.71
1:D1:433:ARG:HA	1:D1:436:MET:HE2	1.73	0.71
3:B4:130:ILE:HG22	3:B4:132:PRO:HD3	1.71	0.71
3:B4:109:ASP:OD1	3:B4:127:LYS:NZ	2.22	0.70
1:D1:150:ARG:NH1	1:D1:189:GLU:OE1	2.24	0.70
3:B4:91:ILE:O	3:B4:92:PRO:C	2.35	0.70
3:B4:135:ALA:HA	3:B4:149:SER:H	1.56	0.70
3:B4:166:GLN:NE2	3:B4:175:GLU:OE2	2.24	0.70
2:B3:156:THR:HG22	2:B3:157:TYR:H	1.56	0.69
1:D1:409:TYR:HD2	1:D1:415:VAL:HG22	1.57	0.69
2:B3:140:LEU:HG	2:B3:141:THR:HG23	1.74	0.69
2:B3:205:GLN:OE1	2:B3:206:HIS:ND1	2.22	0.69
2:B3:288:LYS:NZ	2:B3:290:GLN:OE1	2.26	0.68
1:D1:743:LEU:HD23	4:D1:802:GOL:H32	1.76	0.68
2:B3:78:LEU:HD11	2:B3:267:LYS:HB3	1.75	0.68
1:D1:741:GLN:O	1:D1:745:GLN:NE2	2.27	0.67
2:B3:177:GLU:HB3	2:B3:196:TYR:HB3	1.76	0.67
1:D1:725:ASN:HD22	3:B4:101:LEU:HD11	1.59	0.67
1:D1:191:ASN:HD22	1:D1:249:GLN:HG3	1.60	0.67
1:D1:695:ARG:N	1:D1:698:GLU:OE1	2.28	0.66
3:B4:42:THR:HG22	3:B4:44:GLU:H	1.60	0.66
2:B3:300:GLU:OE1	2:B3:301:LYS:NZ	2.28	0.66
1:D1:743:LEU:HD23	4:D1:802:GOL:H11	1.63	0.66
1:D1:147:LEU:HA	1:D1:190:MET:HE1	1.77	0.66
3:B4:5:VAL:HB	3:B4:151:VAL:HB	1.77	0.65
1:D1:380:PHE:HA	1:D1:383:LEU:HB2	1.77	0.65
1:D1:525:ILE:HD11	1:D1:574:ALA:HB2	1.77	0.65
1:D1:198:GLN:OE1	1:D1:213:ARG:NH1	2.28	0.65
1:D1:85:PHE:HA	1:D1:90:LYS:HG2	1.79	0.64
3:B4:8:ASP:HB2	3:B4:134:SER:HA	1.79	0.64
3:B4:14:ARG:NH1	3:B4:139:TYR:O	2.30	0.64
2:B3:261:MET:SD	7:B3:502:HOH:O	2.55	0.64
1:D1:498:LEU:HB3	1:D1:509:ILE:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:207:MET:HG3	2:B3:278:LEU:HG	1.80	0.63
1:D1:561:PHE:HD2	1:D1:606:PHE:HE2	1.44	0.63
1:D1:33:CYS:HB3	1:D1:38:LYS:HB2	1.78	0.63
2:B3:101:LEU:HD23	2:B3:105:ARG:HH21	1.63	0.63
1:D1:773:THR:HA	3:B4:104:ARG:HH11	1.64	0.63
2:B3:288:LYS:NZ	2:B3:289:GLN:O	2.32	0.63
1:D1:586:GLN:O	1:D1:590:ALA:N	2.23	0.62
1:D1:638:MET:HE3	1:D1:640:CYS:HB2	1.80	0.62
1:D1:543:TYR:HB3	1:D1:553:TRP:HB2	1.81	0.62
1:D1:582:ARG:O	1:D1:586:GLN:NE2	2.33	0.62
1:D1:332:VAL:HG21	1:D1:354:LEU:HD21	1.82	0.61
2:B3:45:GLY:O	2:B3:113:GLN:NE2	2.33	0.61
2:B3:66:GLN:HE22	2:B3:139:ARG:HG2	1.66	0.61
1:D1:27:SER:OG	1:D1:31:LYS:NZ	2.34	0.61
1:D1:536:ALA:O	1:D1:540:ALA:N	2.32	0.61
2:B3:74:GLY:HA3	2:B3:89:VAL:HB	1.82	0.61
2:B3:207:MET:HB2	2:B3:236:MET:HB2	1.83	0.61
1:D1:119:VAL:HG13	1:D1:126:ARG:HG3	1.82	0.60
2:B3:26:MET:HG3	2:B3:38:LYS:HE3	1.83	0.60
2:B3:236:MET:HE3	2:B3:246:ILE:HG23	1.82	0.60
3:B4:33:HIS:HA	3:B4:55:ASP:HB2	1.83	0.60
1:D1:101:ALA:O	1:D1:107:ARG:NH1	2.34	0.60
1:D1:611:PHE:HE2	1:D1:649:LEU:HD22	1.67	0.60
3:B4:168:ILE:HB	3:B4:173:LYS:HD3	1.84	0.60
1:D1:534:PHE:HA	1:D1:537:TYR:CD2	2.34	0.60
3:B4:109:ASP:HA	3:B4:127:LYS:HD2	1.84	0.60
3:B4:168:ILE:O	3:B4:173:LYS:NZ	2.24	0.60
1:D1:205:ASP:HB3	1:D1:208:LYS:HB3	1.84	0.59
1:D1:126:ARG:NH2	1:D1:174:GLY:O	2.35	0.59
1:D1:674:ALA:HB1	1:D1:696:VAL:HG13	1.85	0.59
1:D1:262:LEU:O	1:D1:266:ILE:HD12	2.03	0.59
2:B3:272:TYR:CD2	2:B3:294:LEU:HD22	2.38	0.59
1:D1:53:LEU:HB2	1:D1:105:ILE:HG21	1.85	0.59
3:B4:2:LEU:HG	3:B4:31:ILE:HG23	1.84	0.59
1:D1:622:LYS:H	1:D1:622:LYS:HD2	1.68	0.58
1:D1:724:LEU:HD11	1:D1:750:ILE:HD13	1.84	0.58
1:D1:743:LEU:CD2	4:D1:802:GOL:H12	2.27	0.58
1:D1:746:LEU:HA	1:D1:749:LYS:HD2	1.85	0.58
3:B4:6:LEU:HD13	3:B4:9:LEU:HD21	1.85	0.58
1:D1:250:VAL:O	1:D1:259:GLN:NE2	2.37	0.58
1:D1:506:GLN:HB3	1:D1:539:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:193:LEU:HD22	1:D1:196:ARG:HH11	1.69	0.57
3:B4:61:GLY:HA2	3:B4:86:HIS:CG	2.38	0.57
3:B4:120:GLU:HB2	3:B4:131:ASN:HB2	1.85	0.57
1:D1:313:GLU:CD	1:D1:314:ASP:H	2.11	0.57
1:D1:194:TRP:HA	1:D1:197:MET:HG2	1.87	0.57
1:D1:559:LYS:O	1:D1:563:PHE:N	2.35	0.57
1:D1:291:GLN:HE22	1:D1:339:ARG:HA	1.69	0.57
3:B4:32:GLN:HG3	3:B4:33:HIS:CD2	2.39	0.57
1:D1:668:ARG:NH2	7:D1:906:HOH:O	2.36	0.57
2:B3:285:ARG:HB2	4:B3:403:GOL:H12	1.87	0.57
3:B4:120:GLU:HB2	3:B4:131:ASN:HD22	1.68	0.57
3:B4:153:MET:HE3	3:B4:162:THR:HG22	1.86	0.57
1:D1:236:GLU:HA	1:D1:239:LYS:HE2	1.87	0.57
1:D1:760:SER:OG	1:D1:761:GLU:N	2.34	0.56
2:B3:76:ILE:HG12	2:B3:128:LEU:HG	1.87	0.56
1:D1:158:ARG:O	1:D1:226:ARG:NE	2.38	0.56
1:D1:488:GLN:NE2	3:B4:42:THR:OG1	2.38	0.56
1:D1:67:TYR:HE1	1:D1:152:TYR:HB2	1.70	0.56
1:D1:523:GLN:HG3	1:D1:526:ARG:HH22	1.71	0.56
3:B4:148:PRO:HD2	3:B4:167:LEU:HB3	1.86	0.56
1:D1:20:ILE:HG22	1:D1:24:LYS:NZ	2.21	0.56
1:D1:387:HIS:NE2	1:D1:428:PHE:O	2.32	0.56
2:B3:168:VAL:HG11	2:B3:288:LYS:HG2	1.87	0.56
1:D1:593:GLU:OE2	3:B4:139:TYR:OH	2.21	0.56
1:D1:766:ILE:HA	1:D1:769:HIS:HB3	1.88	0.56
1:D1:441:LEU:HD21	1:D1:490:LEU:HD22	1.87	0.56
1:D1:585:LEU:HD11	1:D1:631:ILE:HA	1.86	0.56
1:D1:20:ILE:HG22	1:D1:24:LYS:HZ2	1.71	0.56
2:B3:158:PRO:HD3	2:B3:295:TRP:CZ2	2.41	0.56
3:B4:14:ARG:HD2	3:B4:138:ALA:HB1	1.87	0.56
3:B4:103:GLN:CD	3:B4:127:LYS:HG3	2.30	0.56
1:D1:543:TYR:HA	1:D1:546:ASN:HB2	1.87	0.55
1:D1:445:LEU:HD11	1:D1:490:LEU:HA	1.89	0.55
2:B3:161:ASN:ND2	2:B3:184:LYS:O	2.39	0.55
2:B3:182:LYS:HB2	2:B3:185:TYR:CE1	2.42	0.55
3:B4:18:LEU:HB2	3:B4:23:LYS:HE2	1.87	0.55
3:B4:111:LEU:HD12	3:B4:129:TYR:CE1	2.41	0.55
1:D1:743:LEU:HD22	4:D1:802:GOL:H12	1.85	0.55
2:B3:43:TYR:N	2:B3:46:GLU:OE1	2.39	0.55
2:B3:152:HIS:HB3	2:B3:296:ARG:HD2	1.88	0.55
2:B3:199:LEU:HD11	2:B3:201:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B3:272:TYR:HD2	2:B3:294:LEU:HD22	1.71	0.55
2:B3:208:GLU:HG3	2:B3:277:VAL:HB	1.88	0.55
1:D1:27:SER:HA	1:D1:30:MET:HE2	1.89	0.55
1:D1:534:PHE:HZ	3:B4:139:TYR:HB3	1.72	0.55
1:D1:339:ARG:HH22	1:D1:347:VAL:HB	1.71	0.54
1:D1:349:SER:O	6:D1:810:EDO:O1	2.25	0.54
2:B3:42:PHE:HE2	2:B3:149:LEU:HD13	1.73	0.54
1:D1:303:ILE:HD13	1:D1:353:SER:HB2	1.90	0.54
1:D1:395:SER:O	1:D1:399:THR:OG1	2.20	0.54
1:D1:194:TRP:CH2	1:D1:258:ALA:HA	2.43	0.54
1:D1:210:GLU:HG2	1:D1:213:ARG:HH11	1.73	0.54
3:B4:18:LEU:HD23	3:B4:136:THR:HG22	1.89	0.54
1:D1:611:PHE:HE1	1:D1:631:ILE:HG21	1.73	0.54
1:D1:194:TRP:HE1	1:D1:213:ARG:HB3	1.73	0.54
1:D1:762:GLU:O	1:D1:765:GLN:HG2	2.07	0.54
2:B3:39:HIS:HB2	2:B3:150:ILE:HG13	1.90	0.54
2:B3:63:LEU:HD23	2:B3:101:LEU:HD12	1.90	0.54
2:B3:133:LYS:NZ	7:B3:521:HOH:O	2.41	0.54
1:D1:74:LEU:O	1:D1:78:GLU:N	2.40	0.54
1:D1:305:ARG:HA	1:D1:308:LEU:HD12	1.89	0.54
1:D1:706:ILE:O	1:D1:709:GLN:NE2	2.41	0.54
1:D1:33:CYS:HB2	1:D1:42:ALA:HB2	1.90	0.54
1:D1:576:LEU:HG	4:D1:801:GOL:H12	1.90	0.54
1:D1:598:ASN:OD1	1:D1:601:THR:OG1	2.25	0.54
2:B3:186:HIS:N	2:B3:189:ASP:OD2	2.35	0.54
3:B4:156:GLN:HG2	3:B4:157:ALA:H	1.74	0.53
1:D1:773:THR:HA	3:B4:104:ARG:NH1	2.22	0.53
1:D1:142:HIS:CD2	1:D1:145:ARG:HH21	2.26	0.53
1:D1:224:LEU:HD11	1:D1:266:ILE:HG13	1.90	0.53
2:B3:195:ILE:HB	2:B3:246:ILE:HB	1.90	0.53
2:B3:204:ILE:HB	2:B3:239:ALA:HA	1.91	0.53
1:D1:137:CYS:SG	1:D1:150:ARG:NH1	2.81	0.53
1:D1:525:ILE:HA	1:D1:528:THR:HG22	1.89	0.53
1:D1:591:ALA:HA	1:D1:596:PHE:HE1	1.73	0.53
1:D1:634:THR:O	1:D1:638:MET:N	2.42	0.53
1:D1:622:LYS:HA	1:D1:625:LEU:HD12	1.91	0.53
2:B3:112:MET:HE3	2:B3:112:MET:HA	1.90	0.53
1:D1:94:LEU:HA	1:D1:97:LEU:HB2	1.91	0.53
1:D1:311:HIS:CE1	1:D1:360:LYS:HB3	2.43	0.53
1:D1:699:CYS:HA	1:D1:702:LYS:HG3	1.90	0.53
2:B3:275:ASN:HD21	2:B3:289:GLN:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:166:GLN:NE2	7:B4:202:HOH:O	2.42	0.53
1:D1:34:LEU:HD22	1:D1:80:TYR:CD2	2.44	0.53
1:D1:95:TYR:O	1:D1:99:GLN:NE2	2.41	0.53
1:D1:150:ARG:CD	1:D1:190:MET:HE3	2.39	0.53
1:D1:286:CYS:HA	1:D1:289:LEU:HG	1.91	0.53
1:D1:554:GLU:HA	1:D1:596:PHE:HB2	1.91	0.53
2:B3:182:LYS:HB2	2:B3:185:TYR:CZ	2.44	0.53
1:D1:198:GLN:O	1:D1:209:ARG:NE	2.33	0.52
3:B4:158:SER:O	3:B4:180:LYS:HD2	2.09	0.52
1:D1:760:SER:OG	1:D1:761:GLU:OE1	2.26	0.52
3:B4:6:LEU:O	3:B4:37:THR:N	2.42	0.52
2:B3:81:ASP:OD2	2:B3:83:SER:OG	2.27	0.52
1:D1:237:ARG:NH2	7:D1:908:HOH:O	2.43	0.52
2:B3:130:TYR:HD2	2:B3:151:VAL:HG21	1.75	0.52
3:B4:91:ILE:HB	3:B4:92:PRO:HD2	1.92	0.52
2:B3:259:PRO:HG3	2:B3:296:ARG:H	1.75	0.52
1:D1:15:LEU:HD13	1:D1:57:MET:HE2	1.92	0.52
1:D1:263:MET:HE2	1:D1:289:LEU:HD21	1.92	0.52
2:B3:260:THR:N	2:B3:294:LEU:O	2.42	0.51
2:B3:287:PHE:CD1	4:B3:403:GOL:H11	2.44	0.51
1:D1:468:ILE:HD12	1:D1:520:GLY:HA2	1.91	0.51
2:B3:271:ARG:HB3	2:B3:291:GLU:OE1	2.10	0.51
1:D1:191:ASN:O	1:D1:195:VAL:HG23	2.11	0.51
1:D1:741:GLN:OE1	1:D1:745:GLN:NE2	2.44	0.51
2:B3:287:PHE:HB3	4:B3:403:GOL:C1	2.40	0.51
1:D1:409:TYR:CD2	1:D1:415:VAL:HG22	2.41	0.51
1:D1:50:LEU:HD13	1:D1:109:TYR:HB2	1.92	0.51
1:D1:126:ARG:NH1	1:D1:166:GLU:OE2	2.42	0.51
1:D1:695:ARG:HG3	1:D1:697:MET:HE3	1.91	0.51
3:B4:153:MET:HE2	3:B4:160:VAL:HG11	1.91	0.51
3:B4:8:ASP:OD1	3:B4:86:HIS:NE2	2.44	0.51
3:B4:20:ALA:HB1	3:B4:24:LYS:HZ3	1.76	0.51
2:B3:216:ILE:HG23	2:B3:223:THR:HG23	1.92	0.50
3:B4:4:LEU:HD11	3:B4:150:PHE:HD2	1.75	0.50
3:B4:86:HIS:O	3:B4:114:GLY:N	2.44	0.50
1:D1:722:GLU:HA	1:D1:725:ASN:HD21	1.76	0.50
3:B4:4:LEU:HD12	3:B4:151:VAL:O	2.11	0.50
1:D1:514:ARG:HG3	1:D1:515:LYS:HD3	1.93	0.50
3:B4:37:THR:HG22	3:B4:86:HIS:CD2	2.47	0.50
3:B4:128:PHE:CE2	3:B4:130:ILE:HD11	2.46	0.50
3:B4:10:HIS:HB3	3:B4:14:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B4:20:ALA:HB1	3:B4:24:LYS:NZ	2.26	0.50
1:D1:294:ASN:HD22	6:D1:808:EDO:HO2	1.54	0.50
1:D1:442:SER:HA	1:D1:445:LEU:HB2	1.94	0.50
1:D1:514:ARG:HH12	1:D1:529:LEU:HD13	1.77	0.50
2:B3:211:LEU:HB3	2:B3:231:ALA:HB3	1.93	0.50
1:D1:143:PRO:HG3	1:D1:196:ARG:NH1	2.27	0.49
1:D1:197:MET:O	1:D1:209:ARG:HD2	2.12	0.49
3:B4:11:ILE:HG13	3:B4:45:SER:HB3	1.94	0.49
3:B4:134:SER:O	3:B4:148:PRO:HA	2.11	0.49
1:D1:425:PHE:HD1	1:D1:436:MET:HE3	1.77	0.49
1:D1:441:LEU:HD11	1:D1:490:LEU:HD13	1.95	0.49
1:D1:23:VAL:HG21	1:D1:66:LEU:HD11	1.94	0.49
1:D1:194:TRP:HZ3	1:D1:262:LEU:HG	1.76	0.49
1:D1:266:ILE:HG23	1:D1:270:PHE:HD2	1.77	0.49
1:D1:339:ARG:HG3	1:D1:342:MET:HG3	1.94	0.49
1:D1:537:TYR:HB3	1:D1:541:PHE:CE2	2.46	0.49
2:B3:64:GLU:OE1	7:B3:501:HOH:O	2.20	0.49
2:B3:130:TYR:O	2:B3:149:LEU:N	2.39	0.49
3:B4:113:SER:O	3:B4:132:PRO:HD2	2.12	0.49
1:D1:523:GLN:O	1:D1:526:ARG:HG2	2.13	0.49
2:B3:121:TYR:OH	2:B3:213:LYS:NZ	2.36	0.49
1:D1:332:VAL:O	1:D1:336:ILE:HD12	2.13	0.49
1:D1:775:GLU:OE1	1:D1:778:ARG:NE	2.43	0.49
3:B4:5:VAL:N	3:B4:151:VAL:O	2.29	0.49
2:B3:70:ILE:HD11	2:B3:132:LEU:HB3	1.94	0.49
1:D1:188:ALA:HA	1:D1:249:GLN:NE2	2.27	0.49
2:B3:68:ILE:HG22	2:B3:95:LEU:HB2	1.95	0.49
2:B3:166:MET:HB3	2:B3:178:PHE:CZ	2.48	0.49
1:D1:219:LEU:O	1:D1:222:THR:OG1	2.25	0.48
2:B3:210:GLN:HG2	2:B3:232:LYS:HG2	1.94	0.48
1:D1:150:ARG:NE	1:D1:186:ASN:HA	2.23	0.48
1:D1:697:MET:HA	1:D1:700:LEU:HD12	1.94	0.48
1:D1:493:ARG:NH2	3:B4:44:GLU:OE2	2.47	0.48
2:B3:76:ILE:HD13	2:B3:268:PHE:HE1	1.78	0.48
1:D1:324:LEU:HD22	1:D1:328:PHE:HE2	1.78	0.48
1:D1:534:PHE:CE1	3:B4:14:ARG:HA	2.49	0.48
3:B4:90:VAL:HG12	3:B4:91:ILE:O	2.13	0.48
1:D1:650:ARG:HE	1:D1:676:LEU:HB3	1.78	0.48
2:B3:87:GLU:OE1	2:B3:90:ASN:ND2	2.47	0.48
3:B4:95:ASP:OD2	3:B4:98:SER:N	2.39	0.48
3:B4:123:GLU:HA	3:B4:128:PHE:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:280:ASN:HB2	1:D1:281:PRO:HD3	1.95	0.48
1:D1:536:ALA:HB1	1:D1:560:ILE:HG23	1.96	0.48
2:B3:161:ASN:CG	2:B3:182:LYS:HB3	2.38	0.48
1:D1:126:ARG:CZ	1:D1:172:THR:HB	2.44	0.48
1:D1:765:GLN:HA	1:D1:768:LYS:NZ	2.29	0.48
1:D1:771:HIS:O	1:D1:775:GLU:HG2	2.13	0.48
2:B3:187:LEU:HD22	2:B3:257:PRO:HG2	1.96	0.47
1:D1:16:LEU:HD13	1:D1:62:SER:OG	2.15	0.47
1:D1:246:ILE:O	1:D1:250:VAL:HG23	2.12	0.47
3:B4:112:ILE:HD13	3:B4:130:ILE:HB	1.96	0.47
1:D1:213:ARG:NH2	1:D1:257:LEU:HB3	2.29	0.47
3:B4:85:ILE:HD13	3:B4:102:LEU:HD21	1.95	0.47
1:D1:339:ARG:CD	1:D1:342:MET:HG3	2.44	0.47
3:B4:60:ARG:HH11	3:B4:71:GLU:HB2	1.78	0.47
1:D1:70:ILE:HA	1:D1:73:GLU:HG2	1.95	0.47
1:D1:208:LYS:HB2	1:D1:208:LYS:HE3	1.66	0.47
1:D1:429:ASP:OD1	1:D1:430:TYR:N	2.47	0.47
1:D1:194:TRP:CZ2	1:D1:258:ALA:HA	2.50	0.47
1:D1:273:GLU:N	1:D1:273:GLU:OE1	2.46	0.47
1:D1:406:VAL:HG11	1:D1:443:ASN:HD22	1.80	0.47
1:D1:642:SER:O	1:D1:646:HIS:N	2.29	0.47
2:B3:69:ARG:NE	2:B3:71:GLU:OE2	2.35	0.47
1:D1:226:ARG:NH1	1:D1:229:GLN:OE1	2.46	0.47
1:D1:488:GLN:HA	1:D1:491:VAL:HG22	1.96	0.47
1:D1:778:ARG:HG3	1:D1:780:ARG:HH11	1.79	0.47
1:D1:194:TRP:O	1:D1:197:MET:HB2	2.15	0.46
1:D1:250:VAL:HG13	1:D1:259:GLN:OE1	2.15	0.46
1:D1:352:VAL:HG12	6:D1:810:EDO:H21	1.97	0.46
1:D1:778:ARG:HG3	1:D1:780:ARG:HD3	1.97	0.46
2:B3:68:ILE:HB	2:B3:96:ALA:HB3	1.97	0.46
2:B3:114:VAL:O	2:B3:116:LYS:NZ	2.40	0.46
2:B3:285:ARG:NH2	7:B3:523:HOH:O	2.44	0.46
3:B4:83:GLY:HA3	3:B4:111:LEU:HD23	1.96	0.46
1:D1:208:LYS:HE2	1:D1:211:ARG:HH21	1.80	0.46
1:D1:513:ALA:O	1:D1:517:PHE:HB2	2.15	0.46
2:B3:35:LYS:HD3	2:B3:36:VAL:N	2.30	0.46
2:B3:93:LYS:HG2	2:B3:111:PHE:CE2	2.51	0.46
1:D1:195:VAL:HG13	1:D1:255:ASP:HB2	1.97	0.46
1:D1:630:LEU:HD11	3:B4:88:HIS:HB2	1.97	0.46
1:D1:158:ARG:HB3	6:D1:813:EDO:H12	1.97	0.46
1:D1:183:VAL:O	1:D1:187:PHE:N	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:311:HIS:NE2	1:D1:360:LYS:HB3	2.30	0.46
1:D1:702:LYS:O	1:D1:706:ILE:HG12	2.16	0.46
2:B3:156:THR:HG22	2:B3:157:TYR:N	2.28	0.46
3:B4:82:ILE:HG23	3:B4:110:ILE:HG22	1.97	0.46
1:D1:30:MET:O	1:D1:34:LEU:HG	2.16	0.46
3:B4:21:LYS:HD3	3:B4:172:VAL:HG23	1.97	0.46
1:D1:189:GLU:OE1	6:D1:807:EDO:H22	2.16	0.46
1:D1:227:LEU:HD13	1:D1:246:ILE:HD11	1.96	0.46
1:D1:669:ALA:O	1:D1:672:THR:OG1	2.33	0.46
1:D1:39:LEU:N	4:D1:805:GOL:O2	2.49	0.46
1:D1:176:ILE:HD11	1:D1:230:LEU:HB3	1.97	0.46
1:D1:494:PHE:CE2	1:D1:498:LEU:HD12	2.50	0.46
2:B3:69:ARG:NH1	6:B3:407:EDO:O1	2.49	0.46
2:B3:204:ILE:HA	2:B3:280:ASP:HA	1.98	0.46
1:D1:374:GLU:HA	1:D1:420:HIS:CE1	2.50	0.46
1:D1:429:ASP:O	1:D1:433:ARG:N	2.35	0.46
1:D1:538:GLN:O	1:D1:542:ARG:N	2.44	0.46
1:D1:715:LEU:O	1:D1:719:LEU:HD23	2.15	0.46
2:B3:287:PHE:HB3	4:B3:403:GOL:H11	1.97	0.46
3:B4:10:HIS:CB	3:B4:14:ARG:HG3	2.46	0.46
1:D1:351:GLN:OE1	1:D1:376:THR:OG1	2.33	0.46
1:D1:492:GLY:O	1:D1:495:ILE:HG22	2.15	0.46
2:B3:86:HIS:C	2:B3:86:HIS:CD2	2.94	0.46
2:B3:116:LYS:HD3	2:B3:151:VAL:HG21	1.98	0.46
2:B3:275:ASN:ND2	2:B3:289:GLN:HG2	2.30	0.46
1:D1:93:ASP:O	1:D1:97:LEU:N	2.39	0.45
1:D1:283:LEU:HD23	1:D1:286:CYS:SG	2.56	0.45
1:D1:646:HIS:O	1:D1:650:ARG:N	2.42	0.45
1:D1:776:HIS:HB3	3:B4:104:ARG:HH12	1.81	0.45
2:B3:187:LEU:HD11	2:B3:259:PRO:HD3	1.98	0.45
3:B4:25:LEU:HD11	3:B4:172:VAL:HG21	1.98	0.45
3:B4:151:VAL:HG22	3:B4:164:VAL:HG23	1.99	0.45
1:D1:142:HIS:CG	1:D1:145:ARG:HH21	2.35	0.45
1:D1:116:VAL:HG11	1:D1:156:CYS:HB3	1.98	0.45
2:B3:39:HIS:HA	6:B3:406:EDO:H21	1.98	0.45
2:B3:233:TYR:CD1	2:B3:250:LEU:HD13	2.51	0.45
1:D1:221:GLY:O	1:D1:225:VAL:HG23	2.17	0.45
1:D1:263:MET:HA	1:D1:266:ILE:HD13	1.98	0.45
2:B3:39:HIS:CG	2:B3:148:ASP:HB2	2.51	0.45
2:B3:203:LYS:O	2:B3:281:GLU:HG2	2.17	0.45
1:D1:54:ARG:NH2	5:D1:803:SO4:O2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:80:TYR:HD2	1:D1:81:LEU:HD22	1.81	0.45
1:D1:108:LEU:HD11	1:D1:136:MET:HG3	1.99	0.45
1:D1:444:VAL:HG13	1:D1:449:THR:HG21	1.98	0.45
1:D1:731:TYR:HD1	1:D1:740:ILE:HG12	1.82	0.45
1:D1:632:ILE:HD11	1:D1:673:CYS:HA	1.99	0.45
2:B3:153:GLN:HG3	6:B3:411:EDO:H12	1.99	0.45
3:B4:10:HIS:CE1	3:B4:14:ARG:HE	2.34	0.45
1:D1:291:GLN:OE1	1:D1:340:GLN:N	2.45	0.45
1:D1:643:GLU:HA	1:D1:646:HIS:HB3	1.98	0.45
1:D1:733:LYS:HD3	1:D1:733:LYS:HA	1.87	0.45
3:B4:83:GLY:N	3:B4:110:ILE:O	2.37	0.45
1:D1:357:LEU:HD12	1:D1:358:ALA:N	2.32	0.45
1:D1:655:LEU:O	1:D1:659:LYS:HG3	2.17	0.45
1:D1:663:LYS:NZ	7:D1:911:HOH:O	2.50	0.45
2:B3:52:VAL:HG23	2:B3:109:PHE:CD1	2.52	0.45
2:B3:132:LEU:HG	2:B3:149:LEU:HD11	1.98	0.45
2:B3:135:THR:N	7:B3:510:HOH:O	2.48	0.45
1:D1:64:TYR:HD1	1:D1:148:PHE:HE1	1.64	0.44
2:B3:131:PHE:HE2	2:B3:133:LYS:HB2	1.81	0.44
3:B4:162:THR:OG1	3:B4:177:ILE:O	2.25	0.44
1:D1:53:LEU:HD22	1:D1:63:TYR:CZ	2.52	0.44
1:D1:124:GLN:HA	1:D1:171:GLU:O	2.18	0.44
1:D1:190:MET:HB3	1:D1:220:VAL:HG22	1.99	0.44
1:D1:289:LEU:HB3	1:D1:293:VAL:HG21	1.98	0.44
3:B4:37:THR:HG22	3:B4:86:HIS:HD2	1.82	0.44
1:D1:754:LEU:HD21	1:D1:767:ASN:HD22	1.81	0.44
3:B4:175:GLU:OE2	3:B4:175:GLU:N	2.51	0.44
1:D1:19:ALA:O	1:D1:23:VAL:HG23	2.18	0.44
1:D1:605:GLU:O	1:D1:609:GLN:HG2	2.17	0.44
3:B4:15:CYS:SG	3:B4:16:ASN:N	2.90	0.44
2:B3:75:GLN:NE2	2:B3:77:GLU:OE2	2.51	0.44
3:B4:144:THR:OG1	3:B4:145:ASN:N	2.51	0.44
2:B3:41:LEU:HA	2:B3:150:ILE:O	2.18	0.44
2:B3:56:PHE:HE1	2:B3:63:LEU:HB2	1.82	0.44
2:B3:93:LYS:HD3	2:B3:93:LYS:HA	1.68	0.44
1:D1:25:VAL:O	1:D1:29:GLN:HG3	2.17	0.44
3:B4:90:VAL:HB	3:B4:93:TRP:HD1	1.82	0.44
3:B4:92:PRO:O	3:B4:93:TRP:C	2.60	0.44
1:D1:494:PHE:CZ	1:D1:513:ALA:HB2	2.53	0.44
3:B4:80:PHE:CZ	3:B4:181:LYS:HB2	2.53	0.44
1:D1:695:ARG:CG	1:D1:697:MET:HE3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:745:GLN:HB3	1:D1:749:LYS:NZ	2.33	0.44
1:D1:142:HIS:CE1	1:D1:145:ARG:HH21	2.35	0.43
1:D1:153:LEU:O	1:D1:157:THR:HG22	2.18	0.43
1:D1:174:GLY:N	7:D1:910:HOH:O	2.50	0.43
1:D1:581:LEU:O	1:D1:585:LEU:HD23	2.18	0.43
2:B3:95:LEU:HD21	2:B3:109:PHE:HB3	2.00	0.43
2:B3:138:ARG:NH1	7:B3:517:HOH:O	2.38	0.43
3:B4:117:HIS:ND1	3:B4:138:ALA:O	2.49	0.43
1:D1:278:THR:C	1:D1:281:PRO:HD2	2.44	0.43
1:D1:636:GLU:CD	3:B4:92:PRO:HG3	2.43	0.43
2:B3:139:ARG:HH12	6:B3:413:EDO:HO1	1.65	0.43
3:B4:81:LYS:HB2	3:B4:109:ASP:H	1.84	0.43
1:D1:294:ASN:ND2	6:D1:808:EDO:O2	2.36	0.43
3:B4:34:ILE:HB	3:B4:56:VAL:HG22	2.01	0.43
1:D1:292:ASN:ND2	7:D1:907:HOH:O	2.38	0.43
1:D1:383:LEU:HB3	1:D1:385:LEU:HG	2.01	0.43
1:D1:778:ARG:HG3	1:D1:780:ARG:NH1	2.34	0.43
2:B3:186:HIS:NE2	2:B3:189:ASP:OD1	2.51	0.43
1:D1:278:THR:OG1	1:D1:282:PHE:HB2	2.19	0.43
1:D1:339:ARG:HD2	1:D1:342:MET:SD	2.58	0.43
1:D1:650:ARG:HD3	1:D1:677:PHE:CZ	2.53	0.43
1:D1:452:VAL:HB	1:D1:498:LEU:HD21	1.99	0.43
1:D1:652:GLN:HA	1:D1:655:LEU:HD12	2.01	0.43
3:B4:56:VAL:HG12	3:B4:58:ILE:HD11	2.00	0.43
1:D1:179:SER:O	1:D1:183:VAL:HG12	2.18	0.43
1:D1:267:ILE:HA	1:D1:275:HIS:NE2	2.33	0.43
3:B4:4:LEU:HD11	3:B4:150:PHE:CD2	2.53	0.43
1:D1:212:GLU:HA	1:D1:215:GLU:CD	2.44	0.43
1:D1:393:ALA:HA	1:D1:396:LYS:HE2	2.01	0.43
1:D1:457:VAL:HG21	1:D1:509:ILE:HD12	1.99	0.43
1:D1:511:ASN:HA	1:D1:514:ARG:HB3	2.00	0.43
2:B3:96:ALA:HB2	2:B3:107:TYR:CE1	2.54	0.43
2:B3:138:ARG:NH2	2:B3:141:THR:OG1	2.52	0.43
3:B4:81:LYS:O	3:B4:110:ILE:N	2.52	0.43
1:D1:246:ILE:O	1:D1:250:VAL:N	2.52	0.43
3:B4:124:HIS:N	3:B4:127:LYS:O	2.43	0.43
1:D1:629:THR:HA	1:D1:632:ILE:HG22	2.01	0.42
2:B3:131:PHE:CE2	2:B3:133:LYS:HB2	2.54	0.42
2:B3:305:GLN:NE2	2:B3:306:ARG:O	2.40	0.42
3:B4:9:LEU:O	3:B4:136:THR:OG1	2.24	0.42
1:D1:571:LEU:HA	1:D1:574:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:725:ASN:OD1	1:D1:726:ARG:N	2.52	0.42
1:D1:63:TYR:CG	1:D1:144:LEU:HD21	2.54	0.42
1:D1:428:PHE:CD1	1:D1:436:MET:HE1	2.54	0.42
1:D1:533:VAL:O	1:D1:536:ALA:HB3	2.20	0.42
2:B3:74:GLY:N	2:B3:89:VAL:O	2.48	0.42
2:B3:133:LYS:HG3	2:B3:144:VAL:HG13	2.01	0.42
2:B3:194:LYS:HA	2:B3:246:ILE:O	2.19	0.42
2:B3:207:MET:HE2	2:B3:236:MET:CB	2.49	0.42
1:D1:295:VAL:O	1:D1:299:ILE:HG13	2.19	0.42
1:D1:345:GLU:HB2	1:D1:397:GLU:OE2	2.20	0.42
1:D1:348:VAL:O	1:D1:352:VAL:HG23	2.19	0.42
3:B4:96:MET:SD	3:B4:96:MET:N	2.85	0.42
1:D1:16:LEU:O	1:D1:20:ILE:HD12	2.20	0.42
1:D1:744:ASN:HA	4:D1:802:GOL:H32	2.01	0.42
2:B3:204:ILE:HD12	2:B3:240:PRO:HD2	2.01	0.42
1:D1:344:SER:O	1:D1:348:VAL:HG23	2.19	0.42
1:D1:412:ILE:HA	1:D1:415:VAL:HG23	2.02	0.42
2:B3:77:GLU:HG2	2:B3:127:ARG:HH21	1.84	0.42
2:B3:161:ASN:ND2	2:B3:182:LYS:HD3	2.35	0.42
1:D1:747:ILE:O	1:D1:751:ARG:HG3	2.19	0.42
1:D1:296:LYS:O	1:D1:300:ILE:HG13	2.19	0.42
1:D1:336:ILE:O	1:D1:339:ARG:HG2	2.20	0.42
2:B3:185:TYR:O	2:B3:294:LEU:HA	2.20	0.42
1:D1:263:MET:O	1:D1:267:ILE:HD12	2.20	0.42
1:D1:491:VAL:HA	1:D1:494:PHE:HB2	2.02	0.42
2:B3:77:GLU:CG	2:B3:127:ARG:HH21	2.33	0.42
2:B3:295:TRP:CD2	6:B3:405:EDO:H22	2.55	0.42
1:D1:83:ASP:OD1	1:D1:84:GLU:N	2.53	0.41
1:D1:331:GLN:O	1:D1:334:THR:OG1	2.36	0.41
1:D1:396:LYS:HE2	1:D1:396:LYS:HB2	1.92	0.41
2:B3:158:PRO:HD3	2:B3:295:TRP:HZ2	1.85	0.41
2:B3:192:VAL:HA	2:B3:248:ILE:O	2.20	0.41
3:B4:82:ILE:HA	3:B4:110:ILE:HB	2.02	0.41
1:D1:108:LEU:O	1:D1:112:ILE:HD12	2.20	0.41
1:D1:461:MET:HB2	1:D1:516:HIS:CE1	2.56	0.41
1:D1:618:ILE:H	1:D1:618:ILE:HD12	1.84	0.41
1:D1:765:GLN:HA	1:D1:768:LYS:HZ3	1.86	0.41
1:D1:131:LYS:NZ	1:D1:181:ASP:OD1	2.52	0.41
3:B4:116:THR:HG23	3:B4:118:LYS:H	1.84	0.41
1:D1:56:SER:HB3	1:D1:145:ARG:NH2	2.36	0.41
1:D1:514:ARG:HD2	1:D1:567:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D1:568:ILE:HG12	1:D1:583:LEU:HD23	2.02	0.41
3:B4:48:TYR:O	3:B4:51:THR:OG1	2.31	0.41
1:D1:60:PRO:HB3	1:D1:216:LEU:HD11	2.02	0.41
1:D1:453:SER:O	1:D1:457:VAL:HG23	2.19	0.41
3:B4:21:LYS:HE2	3:B4:170:ASP:O	2.20	0.41
3:B4:60:ARG:HD2	3:B4:71:GLU:HA	2.03	0.41
1:D1:256:ALA:O	1:D1:260:GLU:HG3	2.20	0.41
1:D1:281:PRO:HA	1:D1:284:ARG:NH1	2.36	0.41
1:D1:498:LEU:HD23	1:D1:498:LEU:HA	1.76	0.41
1:D1:562:SER:O	1:D1:566:GLN:HG3	2.21	0.41
2:B3:26:MET:HE3	2:B3:38:LYS:HG2	2.01	0.41
3:B4:154:ASP:O	3:B4:160:VAL:HA	2.20	0.41
1:D1:356:ASN:O	1:D1:360:LYS:HG2	2.20	0.41
2:B3:69:ARG:HB3	6:B3:407:EDO:H21	2.01	0.41
2:B3:116:LYS:HB3	2:B3:130:TYR:HE2	1.86	0.41
1:D1:75:HIS:O	1:D1:79:VAL:HG13	2.21	0.41
1:D1:557:CYS:O	1:D1:561:PHE:HD1	2.03	0.41
1:D1:775:GLU:HB3	1:D1:778:ARG:HH21	1.86	0.41
2:B3:119:GLU:O	7:B3:502:HOH:O	2.22	0.41
2:B3:167:GLU:OE2	2:B3:177:GLU:HB2	2.21	0.41
3:B4:2:LEU:HD11	3:B4:152:LEU:HD13	2.02	0.41
3:B4:99:LEU:HD12	3:B4:99:LEU:HA	1.91	0.41
1:D1:509:ILE:O	1:D1:512:THR:OG1	2.37	0.41
1:D1:554:GLU:H	1:D1:554:GLU:CD	2.28	0.40
1:D1:769:HIS:CD2	1:D1:769:HIS:C	3.00	0.40
1:D1:296:LYS:NZ	1:D1:346:ASP:HA	2.37	0.40
2:B3:71:GLU:HG3	7:B3:510:HOH:O	2.21	0.40
3:B4:91:ILE:O	3:B4:93:TRP:N	2.54	0.40
1:D1:124:GLN:HB3	1:D1:171:GLU:HB3	2.02	0.40
1:D1:570:ALA:HA	1:D1:573:LYS:HG2	2.04	0.40
3:B4:120:GLU:OE1	3:B4:131:ASN:ND2	2.54	0.40
1:D1:266:ILE:HG23	1:D1:270:PHE:CD2	2.55	0.40
2:B3:215:GLU:OE1	2:B3:270:VAL:HG22	2.22	0.40
3:B4:19:PRO:HG2	3:B4:22:PHE:CG	2.56	0.40
1:D1:731:TYR:CD1	1:D1:740:ILE:HG12	2.57	0.40
2:B3:211:LEU:HD22	2:B3:252:LEU:HD23	2.04	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	D1	725/796 (91%)	691 (95%)	33 (5%)	1 (0%)	48	83
2	B3	297/327 (91%)	277 (93%)	20 (7%)	0	100	100
3	B4	179/182 (98%)	159 (89%)	19 (11%)	1 (1%)	21	58
All	All	1201/1305 (92%)	1127 (94%)	72 (6%)	2 (0%)	44	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B4	92	PRO
1	D1	504	ASP

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	D1	664/720 (92%)	662 (100%)	2 (0%)	86	84
2	B3	272/296 (92%)	272 (100%)	0	100	100
3	B4	159/160 (99%)	157 (99%)	2 (1%)	61	72
All	All	1095/1176 (93%)	1091 (100%)	4 (0%)	81	83

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D1	506	GLN

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Mol	Chain	Res	Type
1	D1	614	TYR
3	B4	60	ARG
3	B4	91	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	D1	191	ASN
1	D1	223	ASN
1	D1	443	ASN
1	D1	488	GLN
1	D1	511	ASN
1	D1	586	GLN
1	D1	609	GLN
1	D1	646	HIS
1	D1	675	HIS
1	D1	745	GLN
1	D1	769	HIS
2	B3	75	GLN
2	B3	152	HIS
2	B3	153	GLN
2	B3	275	ASN
3	B4	39	ASN
3	B4	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

28 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	$\# Z > 2$
4	GOL	B3	402	-	5,5,5	0.08	0	5,5,5	0.32	0
4	GOL	D1	802	-	5,5,5	0.09	0	5,5,5	0.34	0
4	GOL	D1	801	-	5,5,5	0.08	0	5,5,5	0.32	0
6	EDO	D1	809	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	B3	414	-	3,3,3	0.42	0	2,2,2	0.39	0
6	EDO	B3	415	-	3,3,3	0.43	0	2,2,2	0.39	0
6	EDO	D1	810	-	3,3,3	0.42	0	2,2,2	0.38	0
4	GOL	D1	805	-	5,5,5	0.96	0	5,5,5	1.07	0
6	EDO	B3	410	-	3,3,3	0.42	0	2,2,2	0.37	0
6	EDO	B3	407	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	B3	409	-	3,3,3	0.41	0	2,2,2	0.40	0
6	EDO	B3	411	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	B3	408	-	3,3,3	0.43	0	2,2,2	0.37	0
6	EDO	D1	808	-	3,3,3	0.42	0	2,2,2	0.38	0
4	GOL	B3	403	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	B3	404	-	5,5,5	0.09	0	5,5,5	0.33	0
6	EDO	B3	412	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	B3	413	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	D1	806	-	3,3,3	0.43	0	2,2,2	0.38	0
5	SO4	B3	401	-	4,4,4	0.23	0	6,6,6	0.07	0
6	EDO	B3	406	-	3,3,3	0.42	0	2,2,2	0.38	0
6	EDO	D1	813	-	3,3,3	0.42	0	2,2,2	0.40	0
5	SO4	D1	803	-	4,4,4	0.23	0	6,6,6	0.08	0
6	EDO	D1	811	-	3,3,3	0.43	0	2,2,2	0.38	0
6	EDO	D1	812	-	3,3,3	0.42	0	2,2,2	0.40	0
6	EDO	D1	807	-	3,3,3	0.42	0	2,2,2	0.36	0
5	SO4	D1	804	-	4,4,4	0.23	0	6,6,6	0.08	0
6	EDO	B3	405	-	3,3,3	0.42	0	2,2,2	0.39	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	GOL	B3	402	-	-	2/4/4/4	-
4	GOL	D1	802	-	-	2/4/4/4	-
6	EDO	D1	809	-	-	0/1/1/1	-
6	EDO	B3	414	-	-	0/1/1/1	-
6	EDO	B3	415	-	-	0/1/1/1	-
6	EDO	D1	810	-	-	0/1/1/1	-
4	GOL	D1	805	-	-	2/4/4/4	-
6	EDO	B3	410	-	-	0/1/1/1	-
6	EDO	B3	407	-	-	0/1/1/1	-
6	EDO	B3	409	-	-	0/1/1/1	-
6	EDO	B3	411	-	-	0/1/1/1	-
6	EDO	B3	408	-	-	0/1/1/1	-
6	EDO	D1	808	-	-	0/1/1/1	-
4	GOL	B3	403	-	-	2/4/4/4	-
4	GOL	B3	404	-	-	0/4/4/4	-
6	EDO	B3	412	-	-	0/1/1/1	-
6	EDO	B3	413	-	-	0/1/1/1	-
6	EDO	D1	806	-	-	0/1/1/1	-
6	EDO	B3	406	-	-	0/1/1/1	-
6	EDO	D1	813	-	-	0/1/1/1	-
6	EDO	D1	811	-	-	0/1/1/1	-
6	EDO	D1	812	-	-	0/1/1/1	-
6	EDO	D1	807	-	-	0/1/1/1	-
4	GOL	D1	801	-	-	4/4/4/4	-
6	EDO	B3	405	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D1	801	GOL	O1-C1-C2-C3
4	D1	801	GOL	C1-C2-C3-O3
4	D1	801	GOL	O2-C2-C3-O3
4	D1	802	GOL	C1-C2-C3-O3
4	D1	805	GOL	C1-C2-C3-O3
4	B3	402	GOL	C1-C2-C3-O3
4	D1	802	GOL	O2-C2-C3-O3

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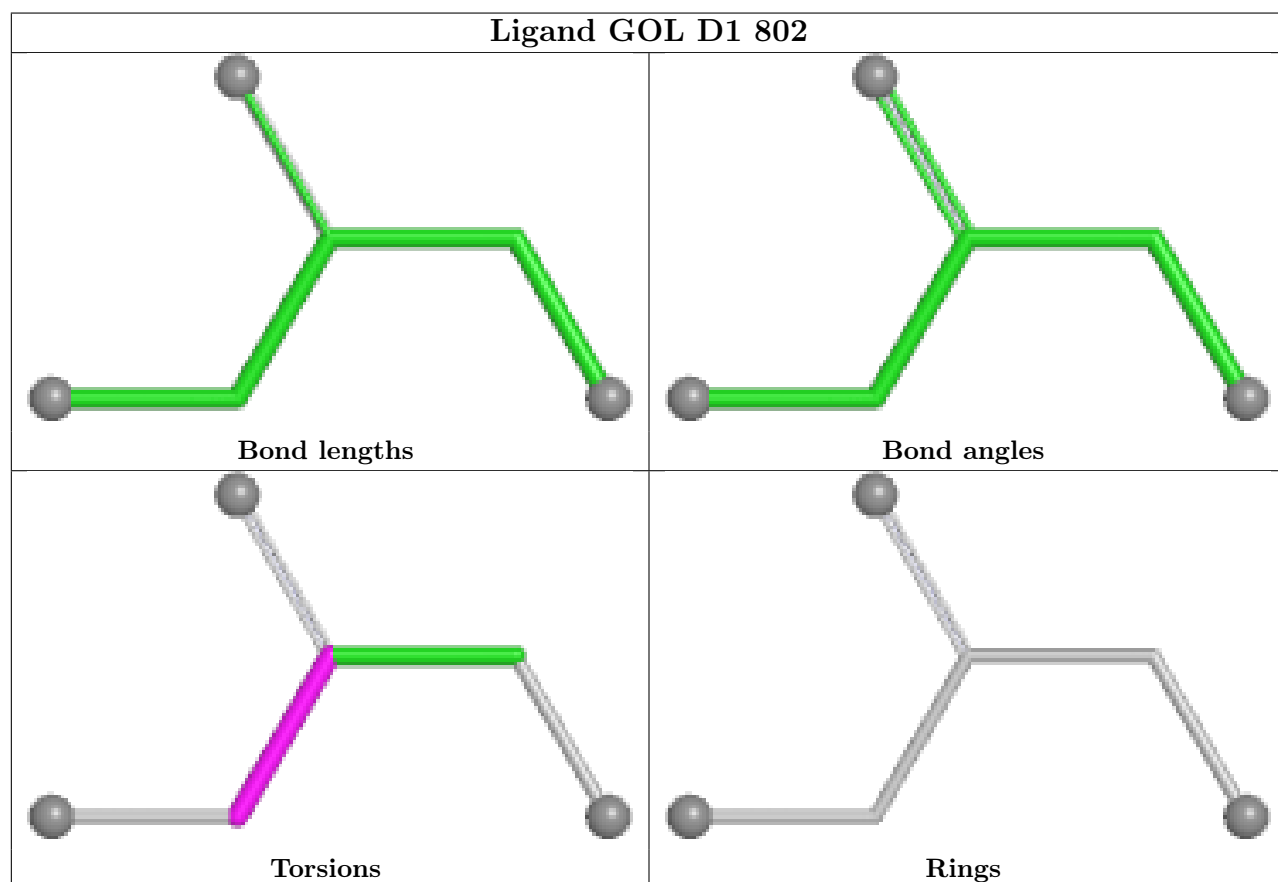
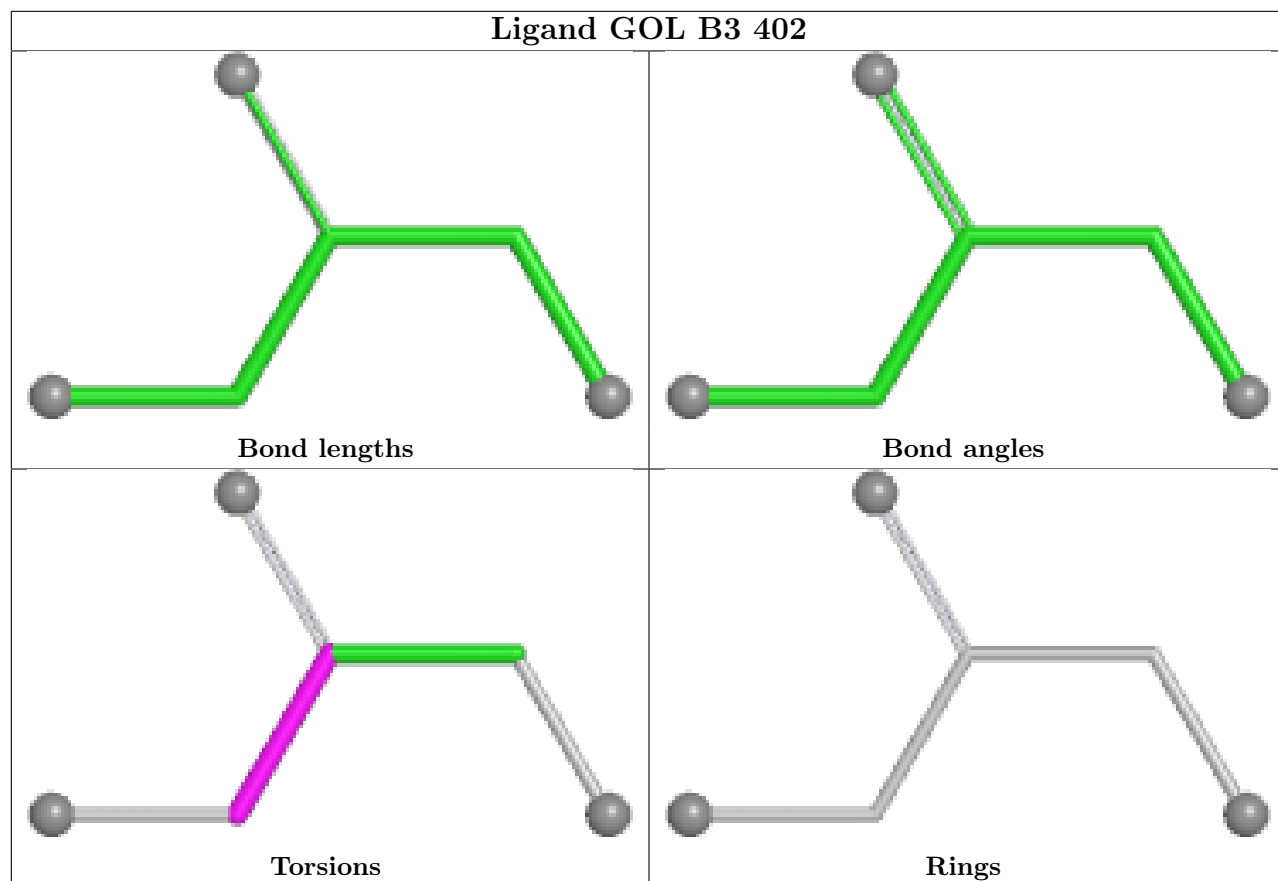
Mol	Chain	Res	Type	Atoms
4	B3	403	GOL	C1-C2-C3-O3
4	D1	801	GOL	O1-C1-C2-O2
4	D1	805	GOL	O2-C2-C3-O3
4	B3	402	GOL	O2-C2-C3-O3
4	B3	403	GOL	O2-C2-C3-O3

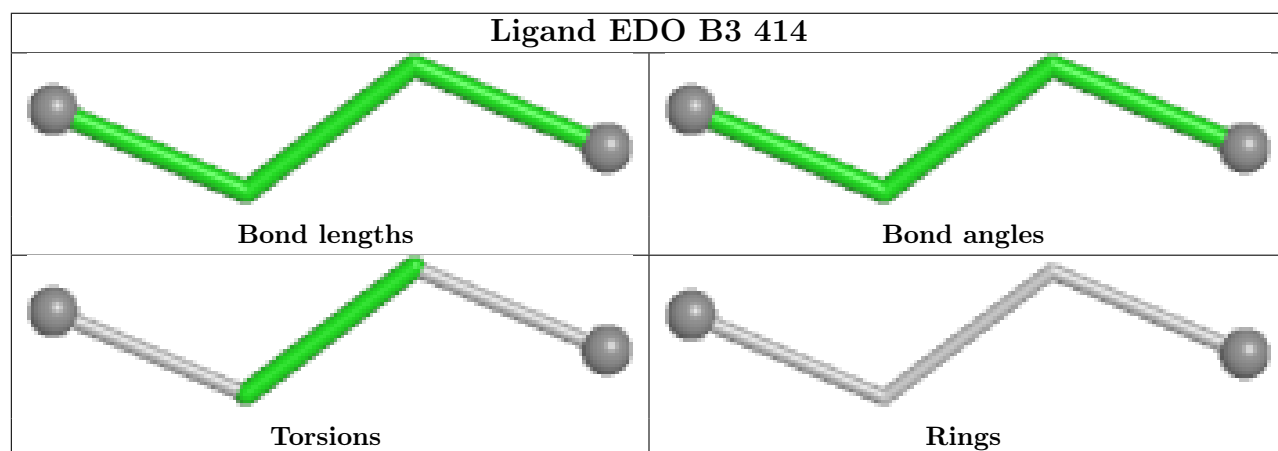
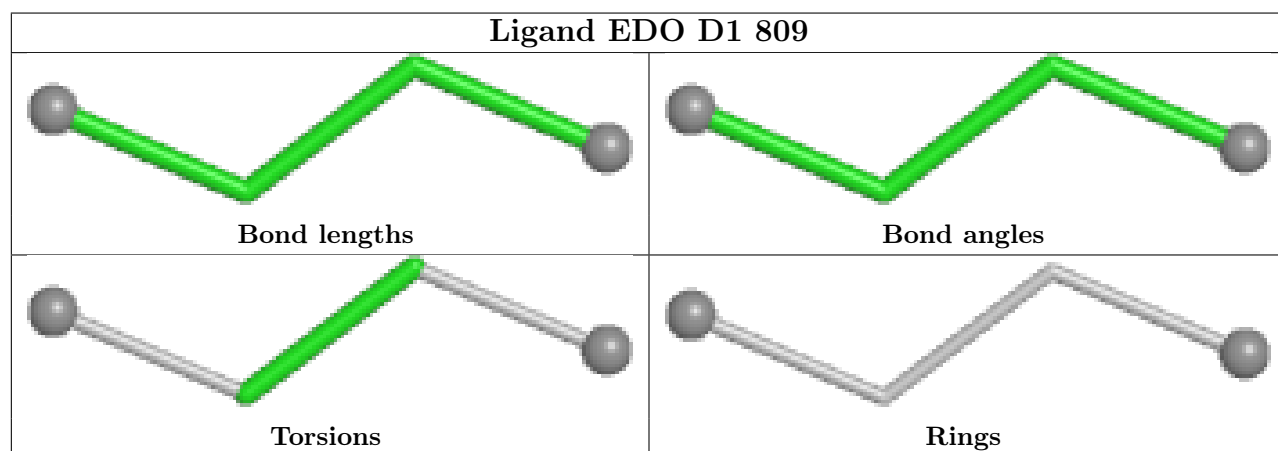
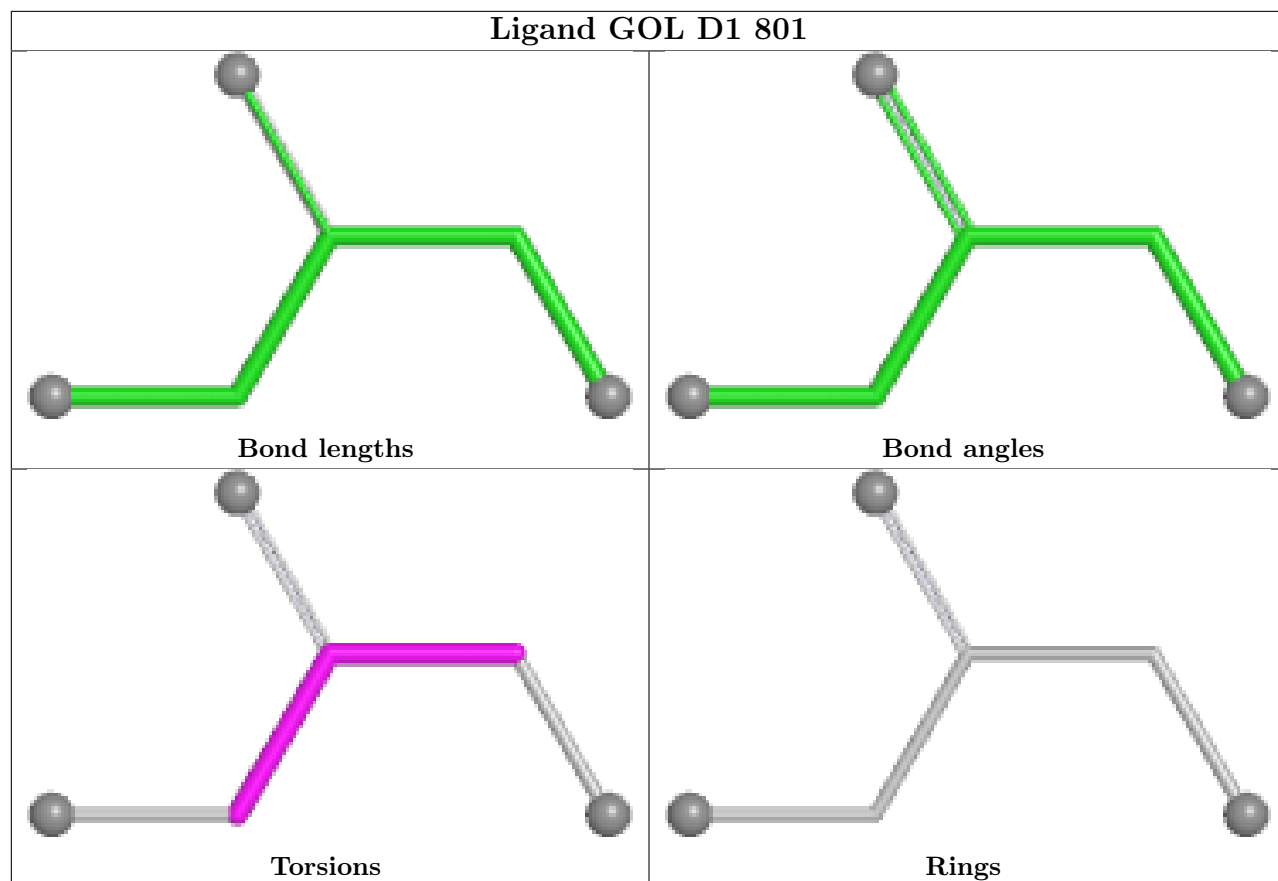
There are no ring outliers.

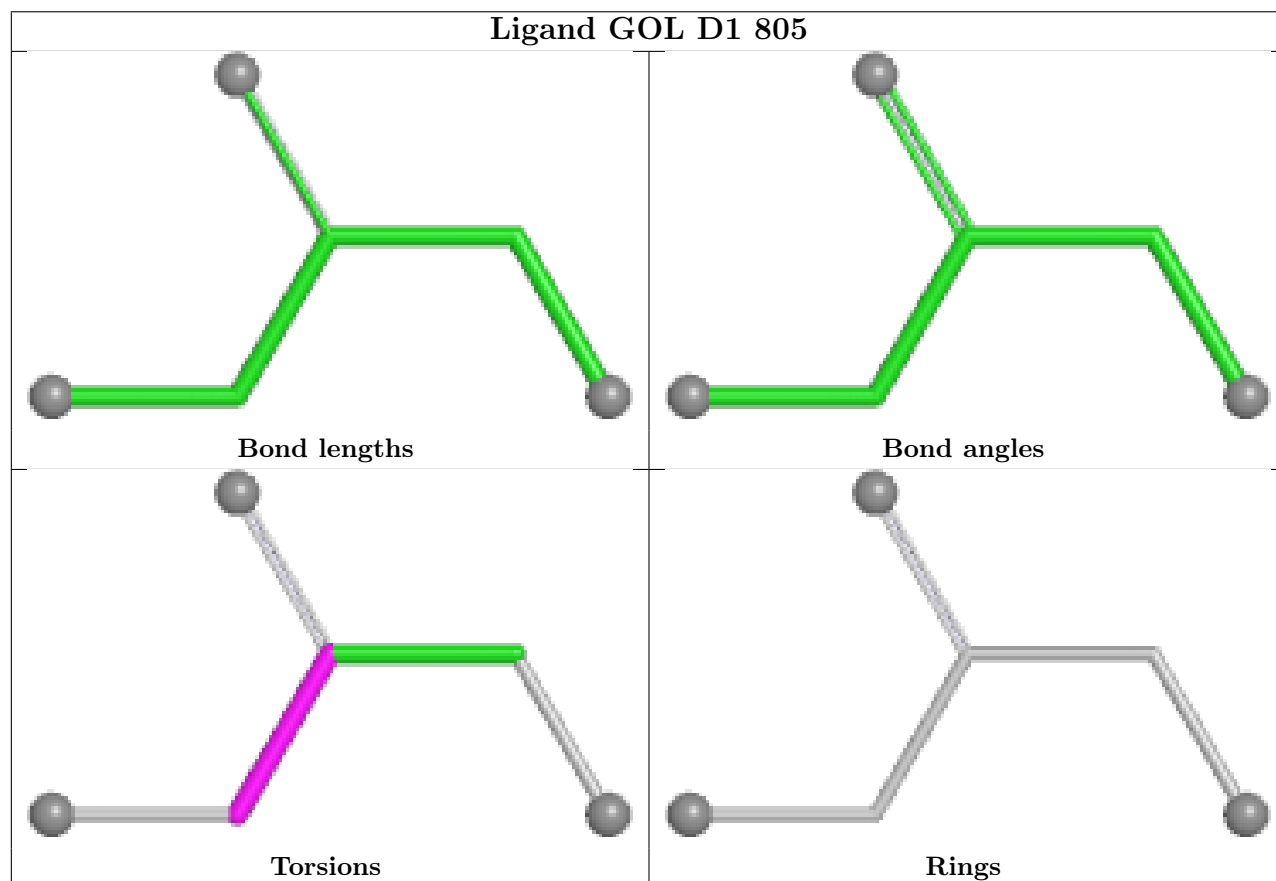
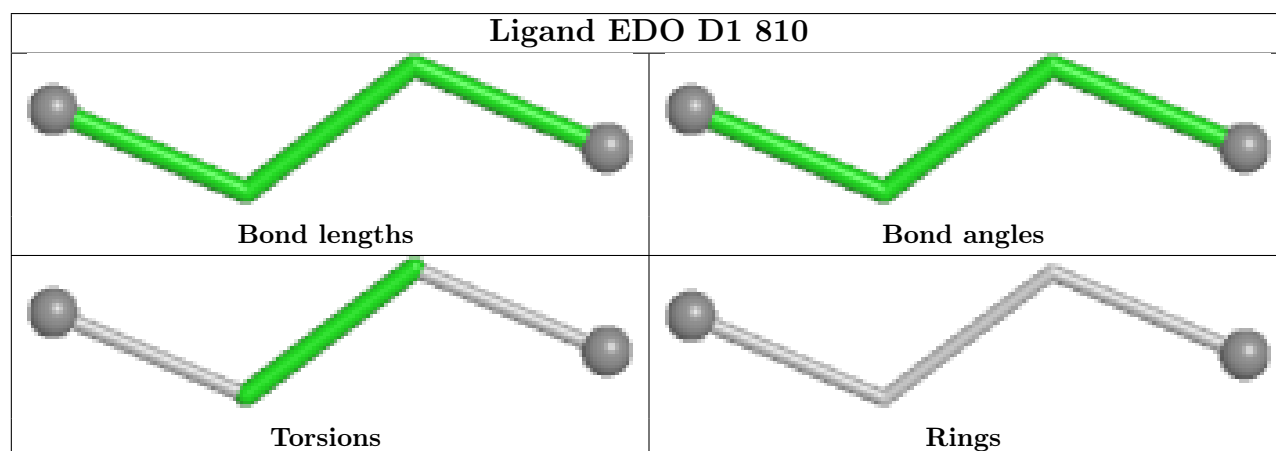
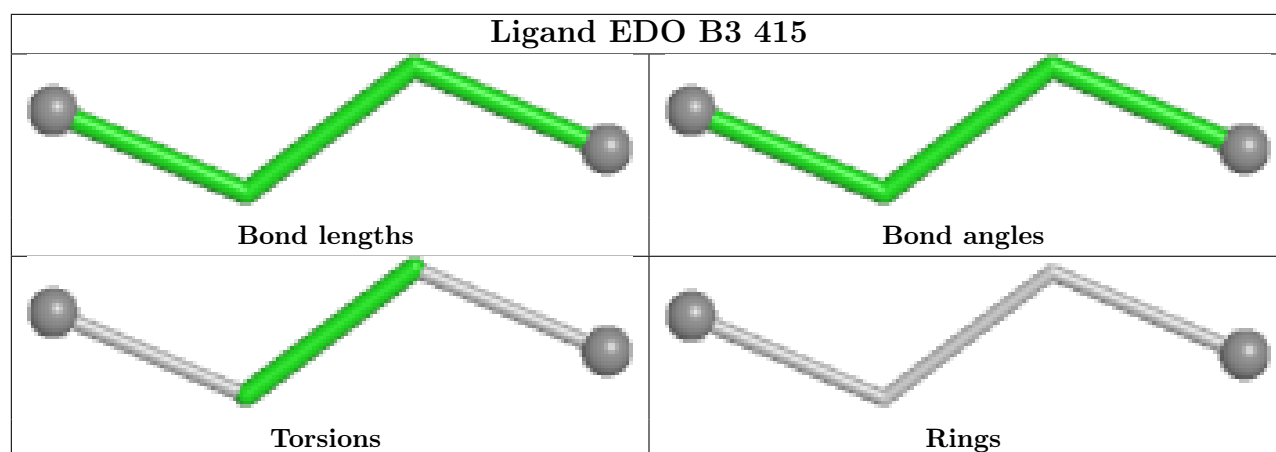
14 monomers are involved in 37 short contacts:

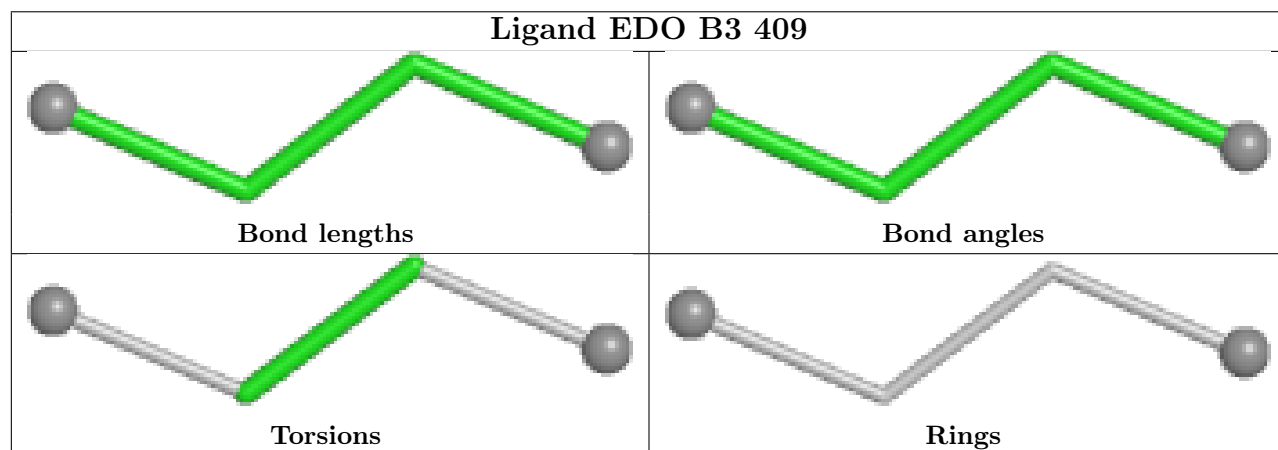
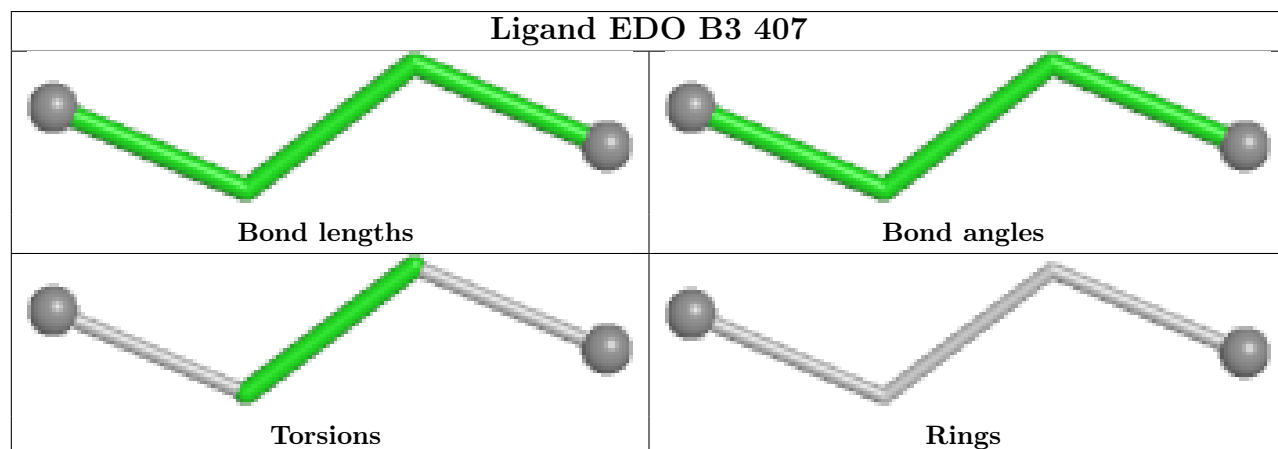
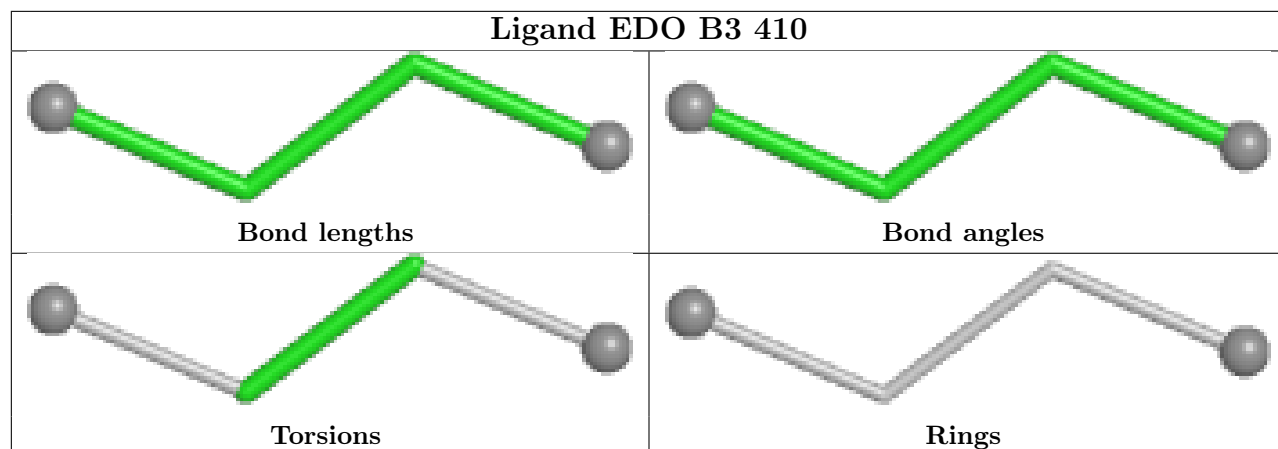
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D1	802	GOL	18	0
4	D1	801	GOL	1	0
6	D1	810	EDO	2	0
4	D1	805	GOL	1	0
6	B3	407	EDO	2	0
6	B3	411	EDO	1	0
6	D1	808	EDO	2	0
4	B3	403	GOL	4	0
6	B3	413	EDO	1	0
6	B3	406	EDO	1	0
6	D1	813	EDO	1	0
5	D1	803	SO4	1	0
6	D1	807	EDO	1	0
6	B3	405	EDO	1	0

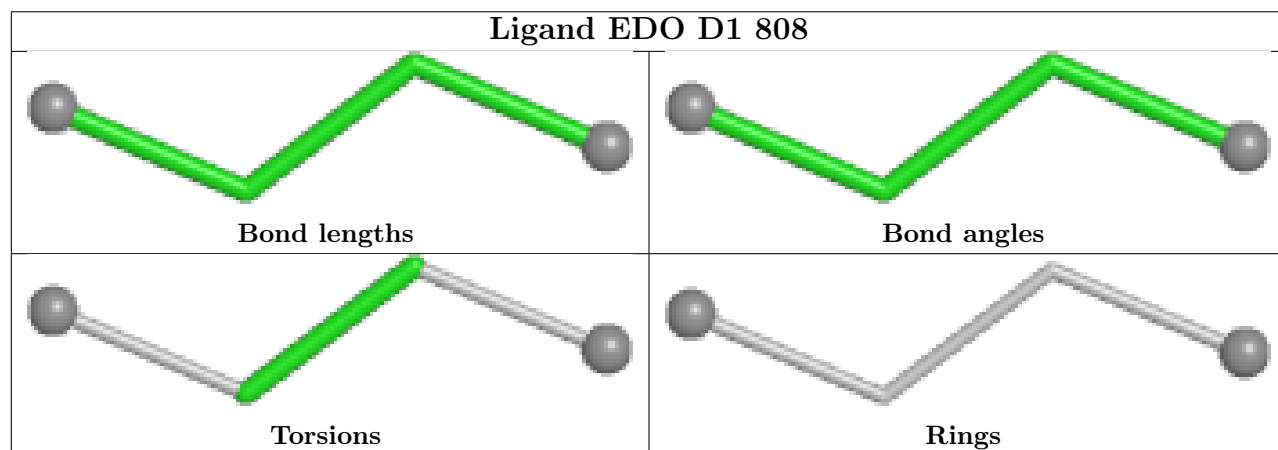
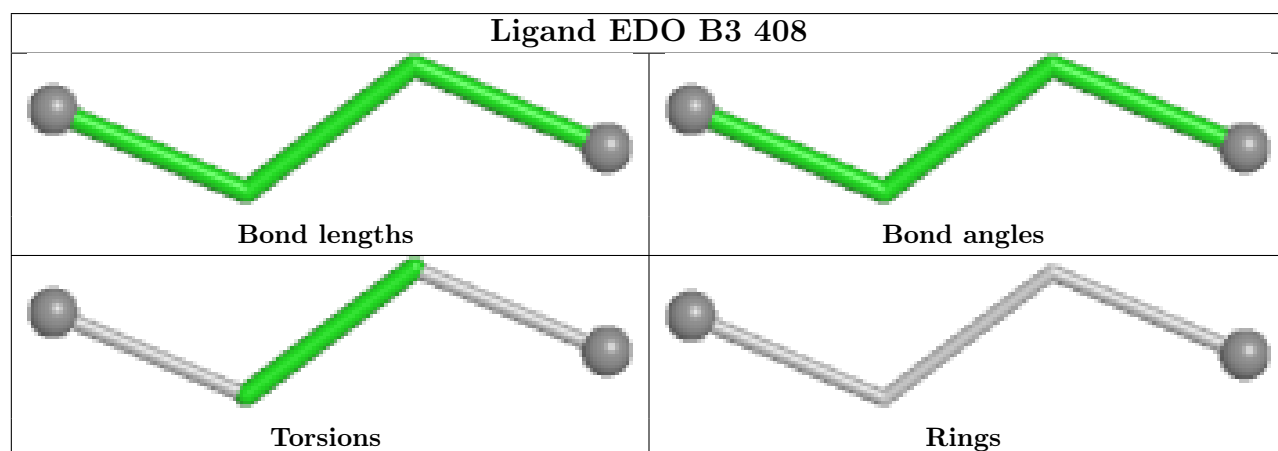
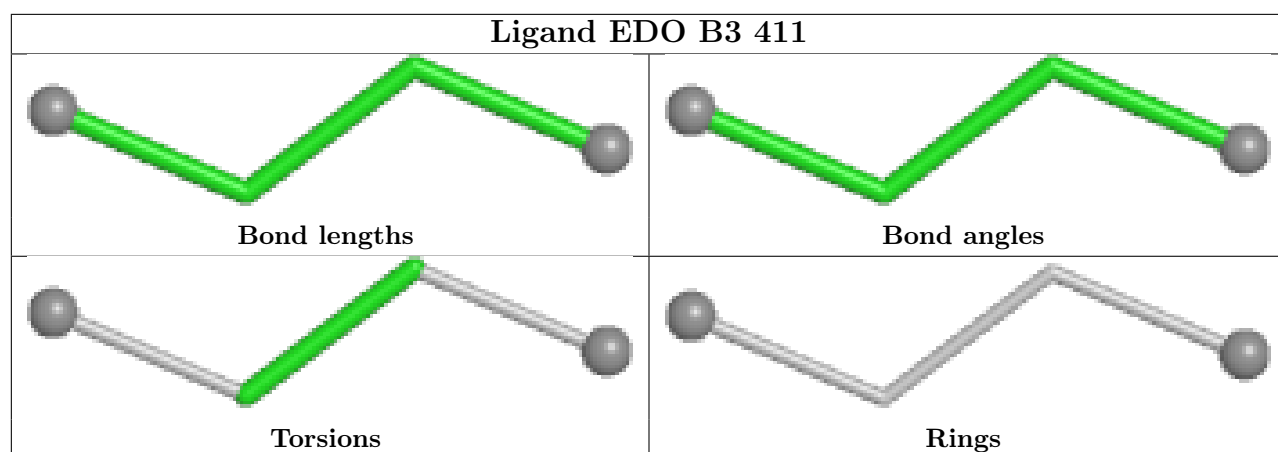
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

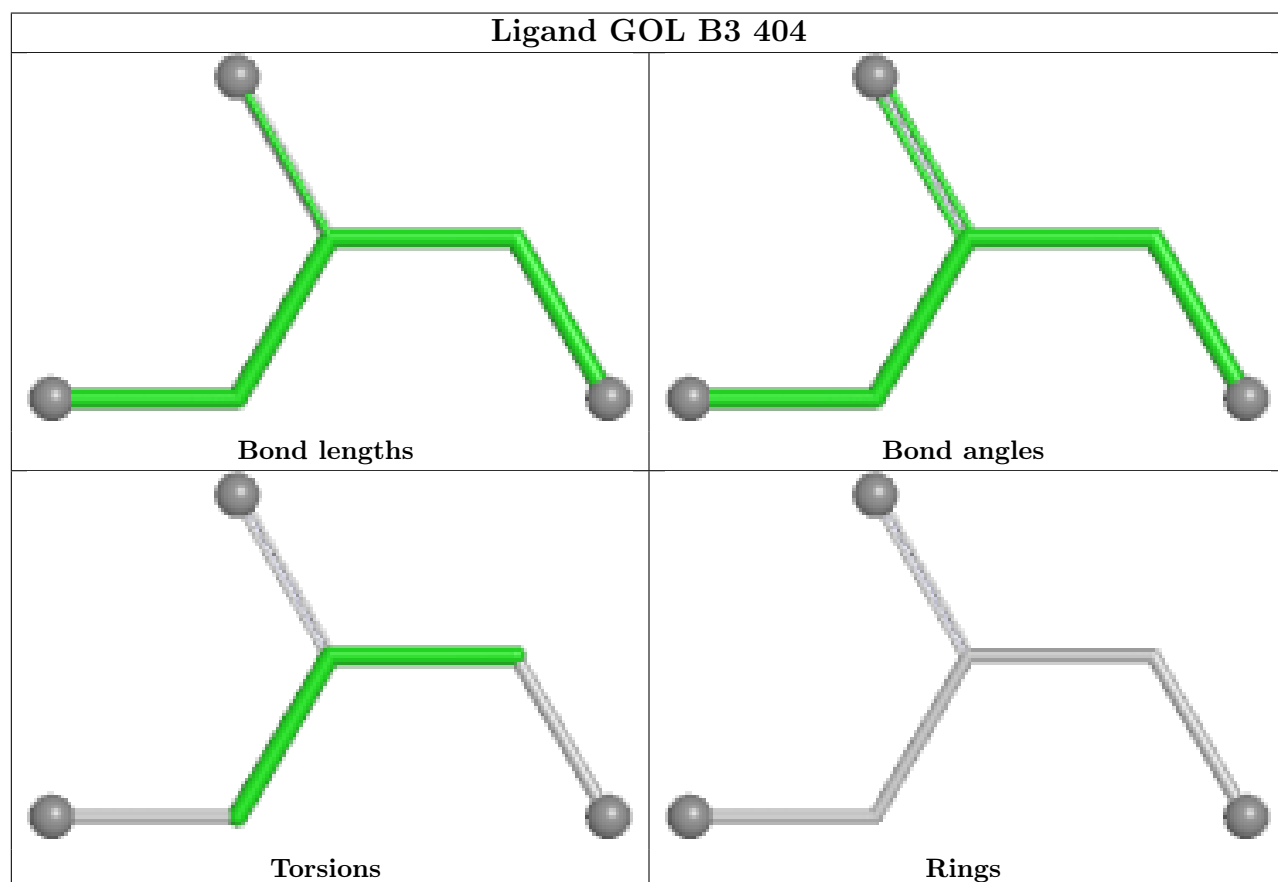
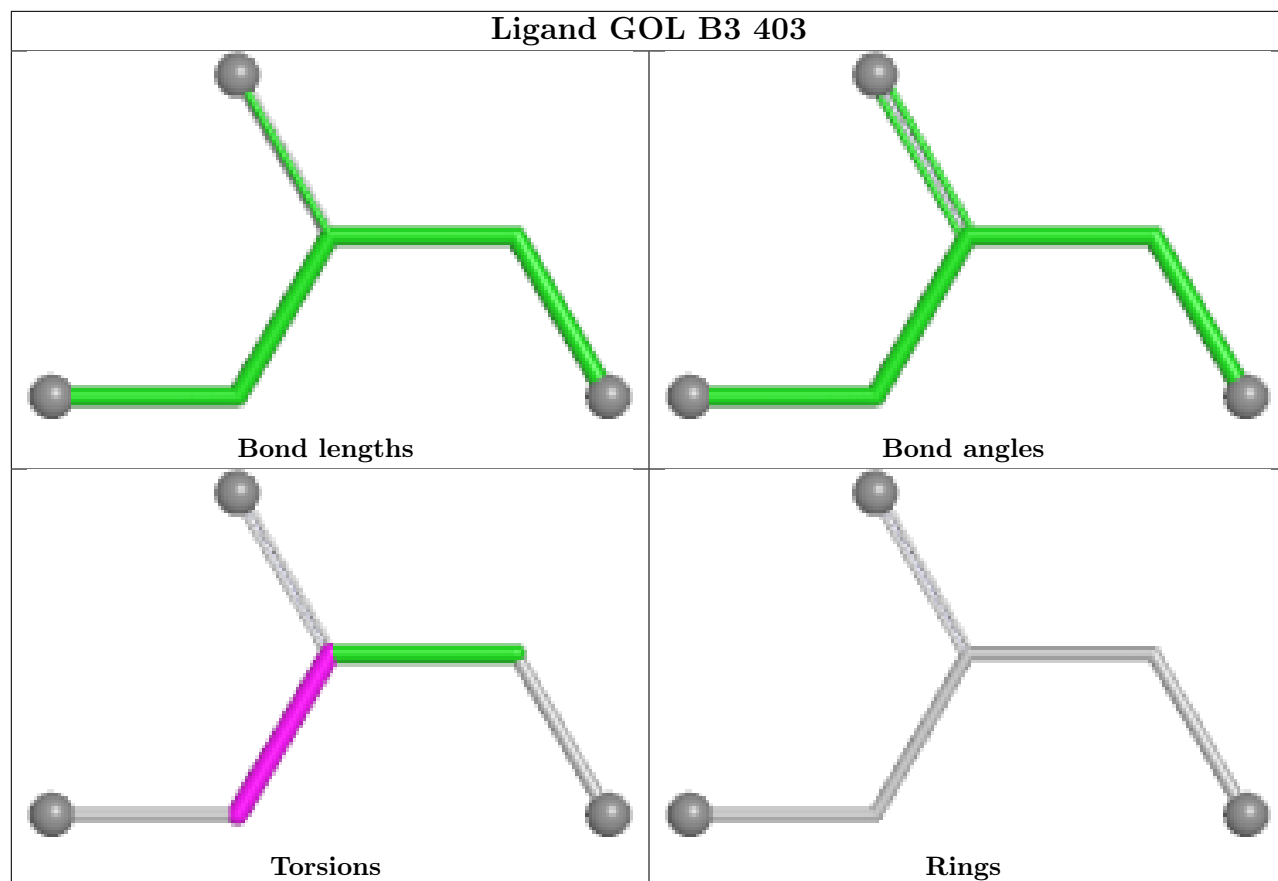


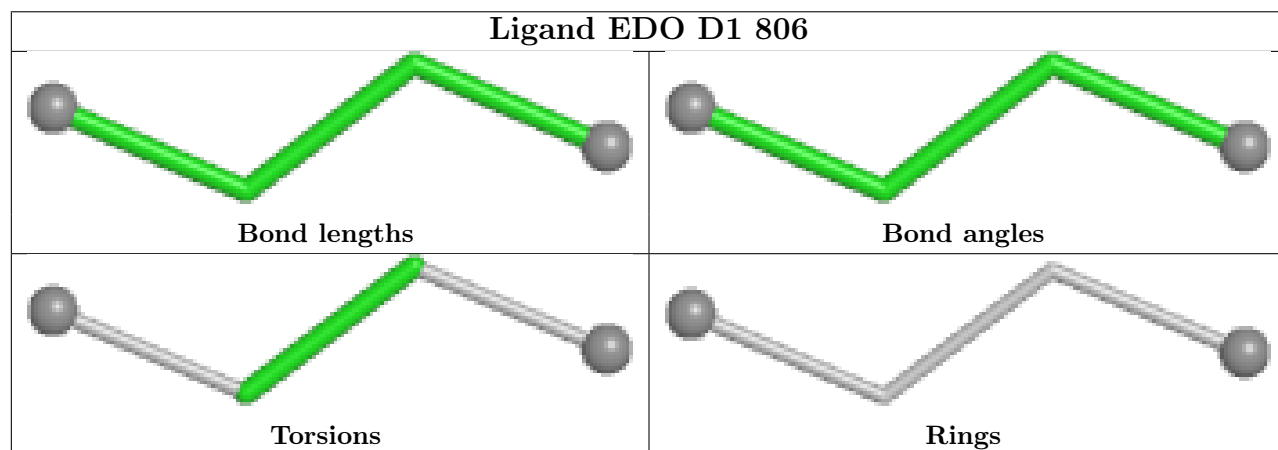
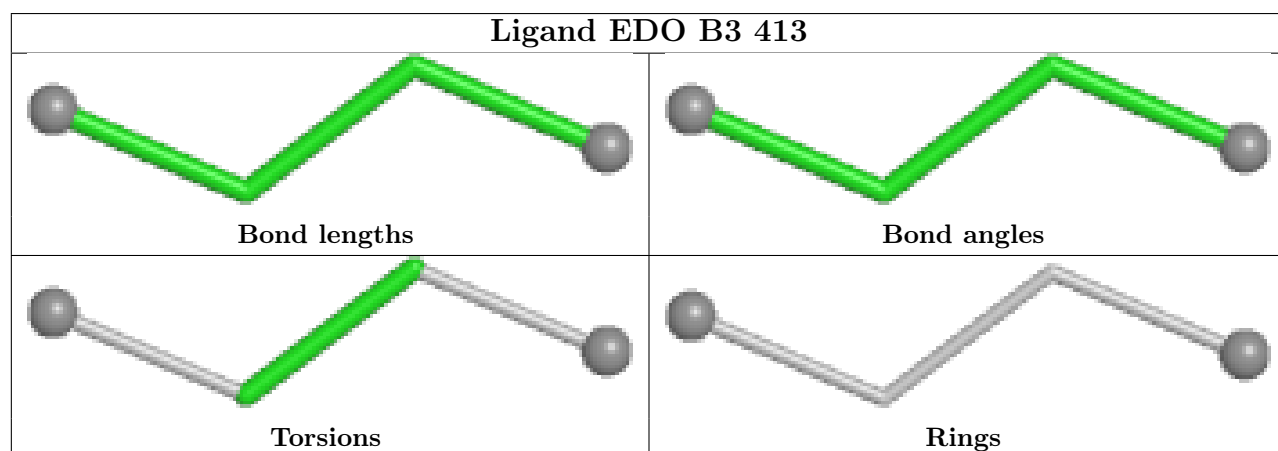
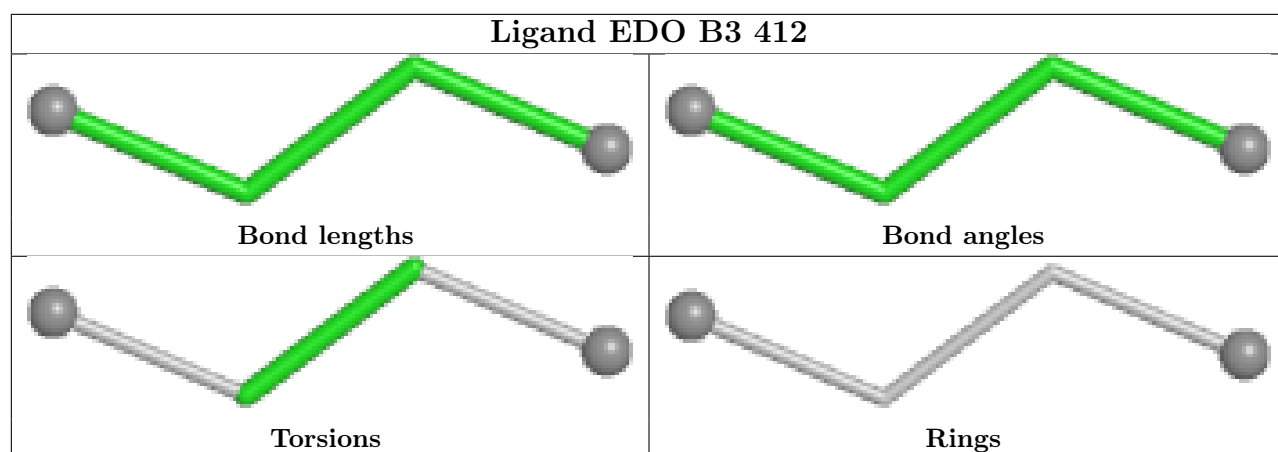


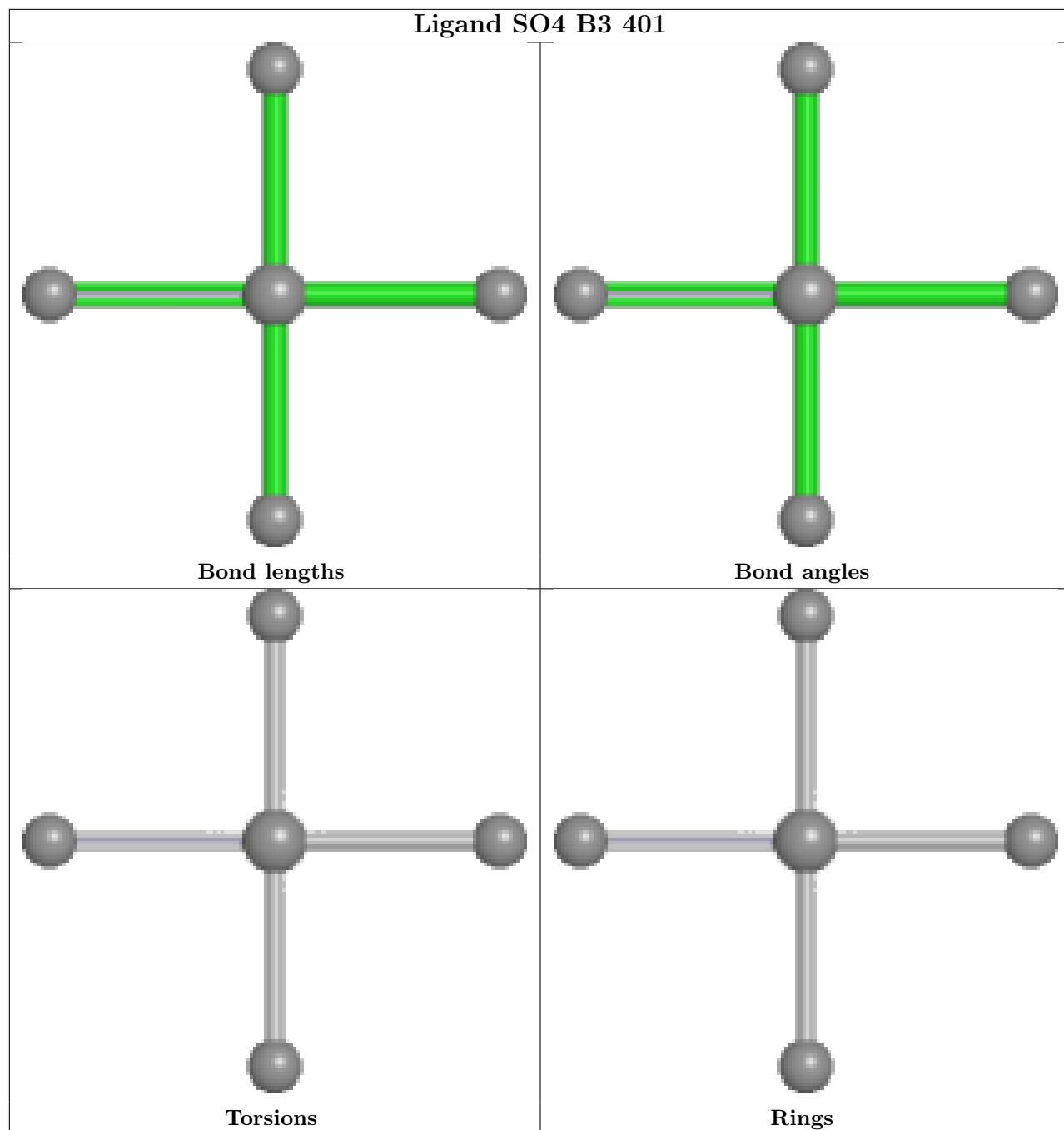


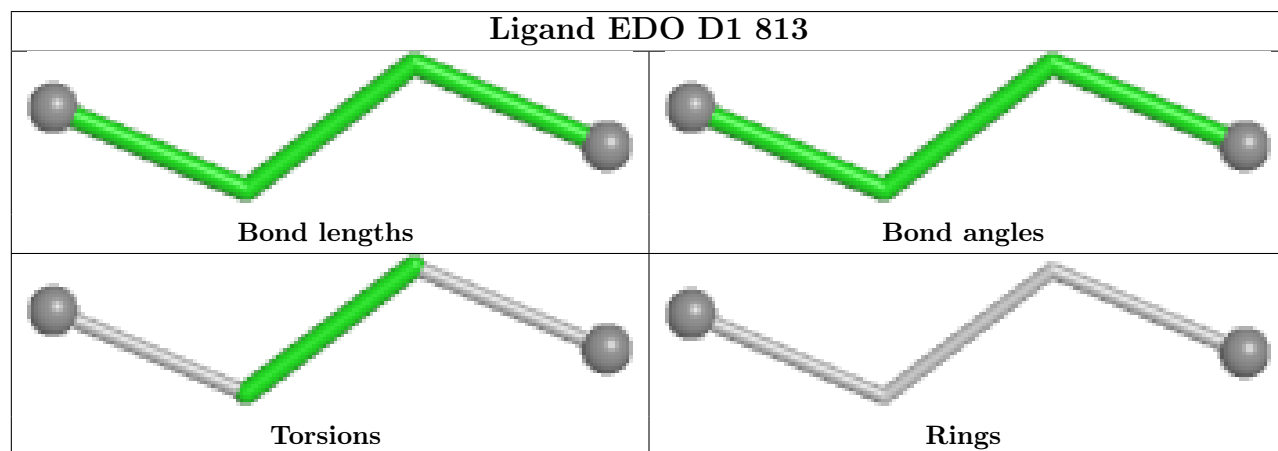
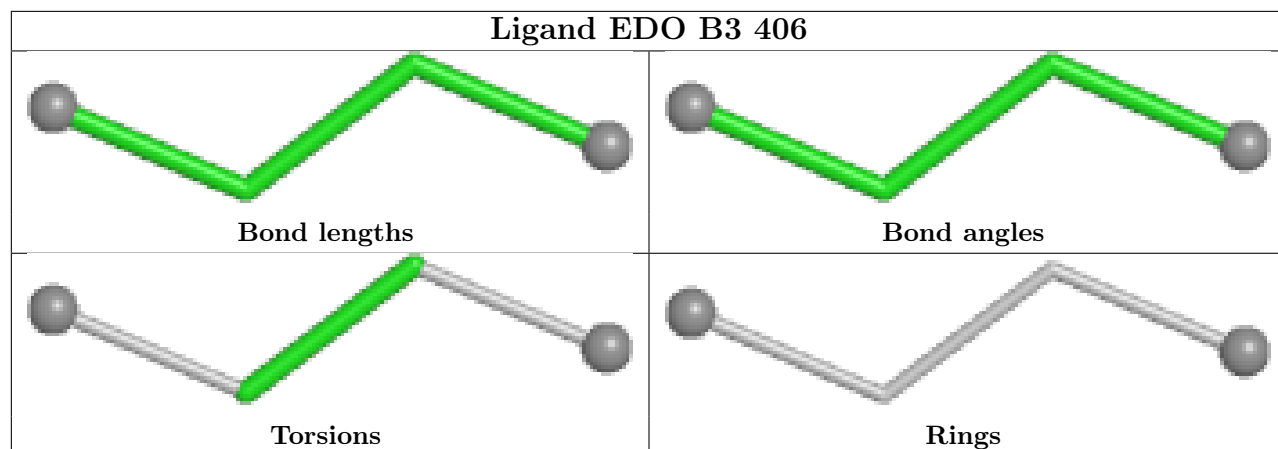


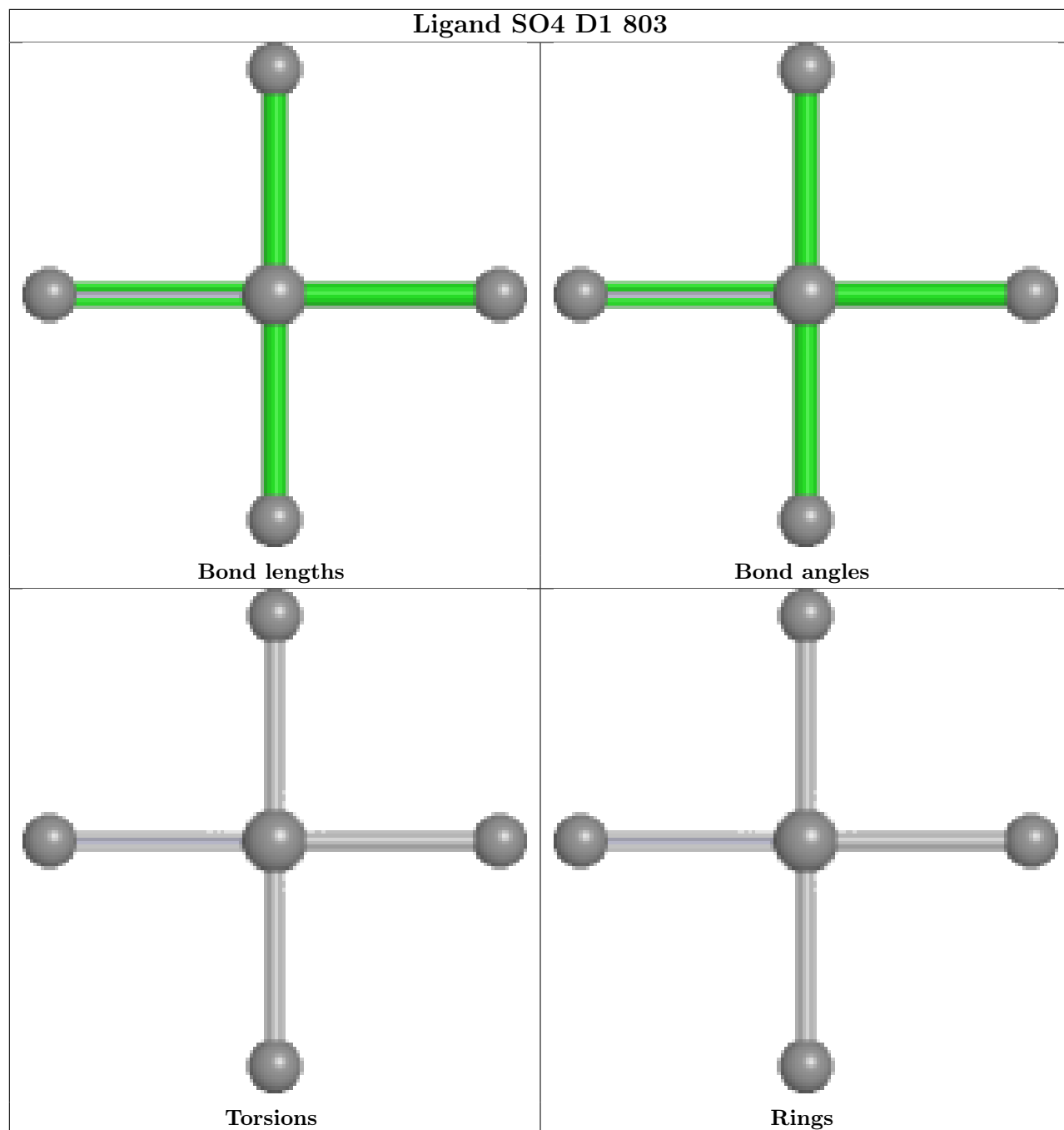


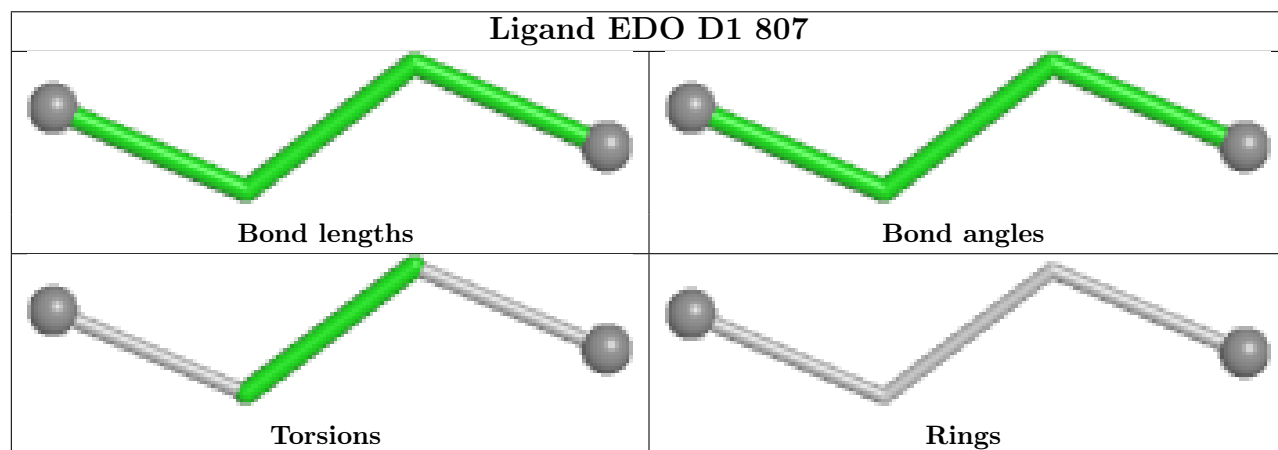
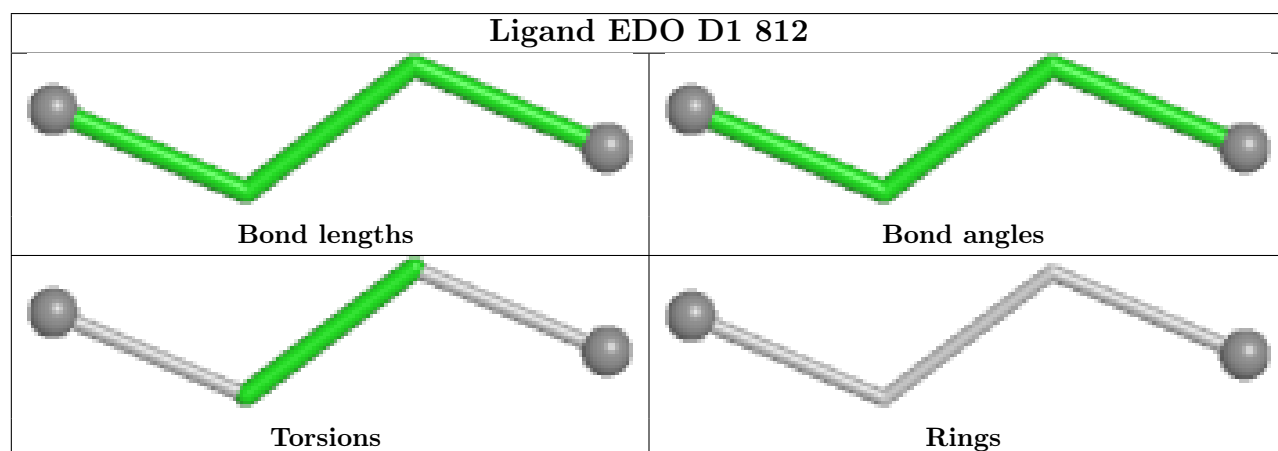
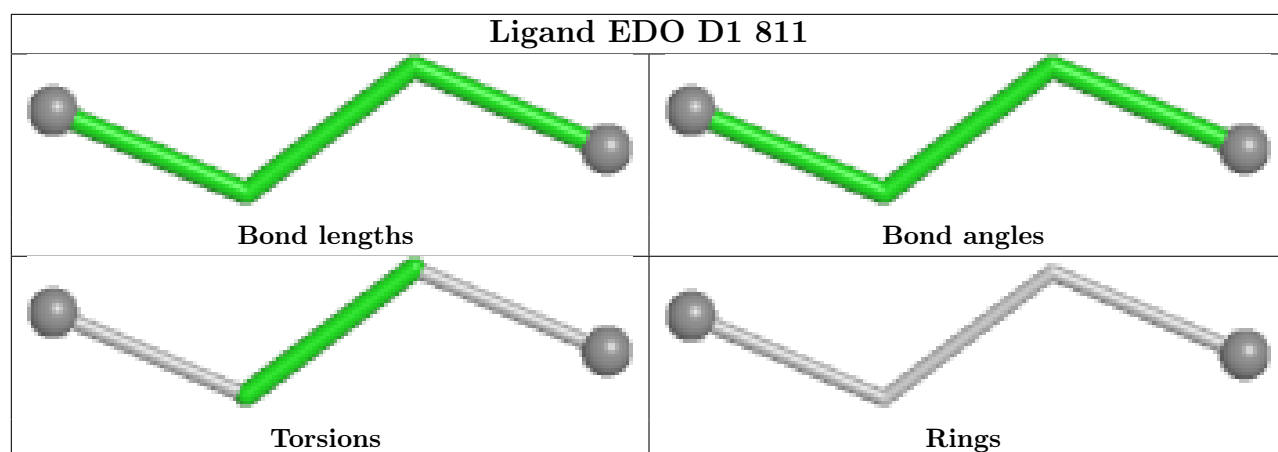


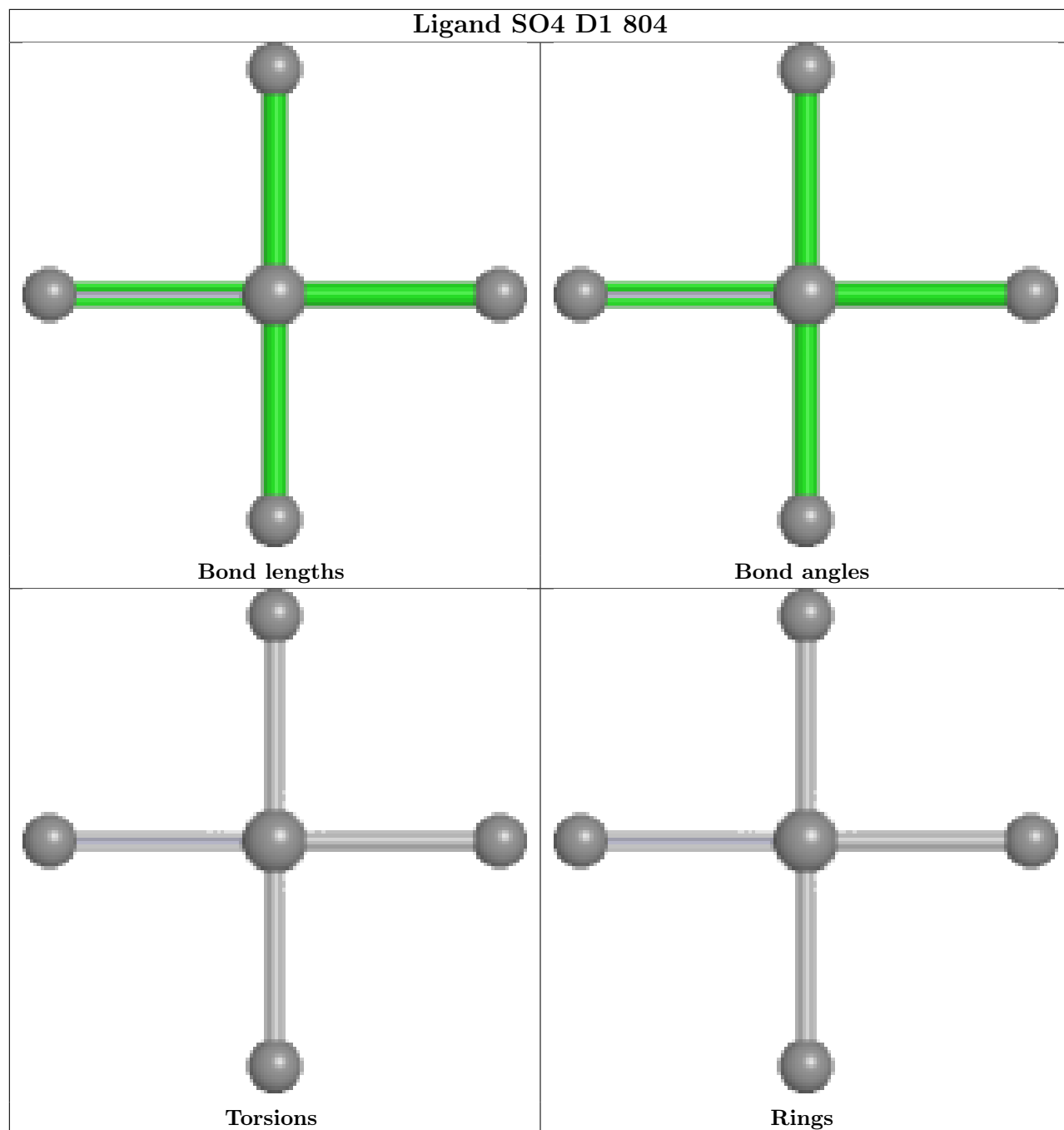


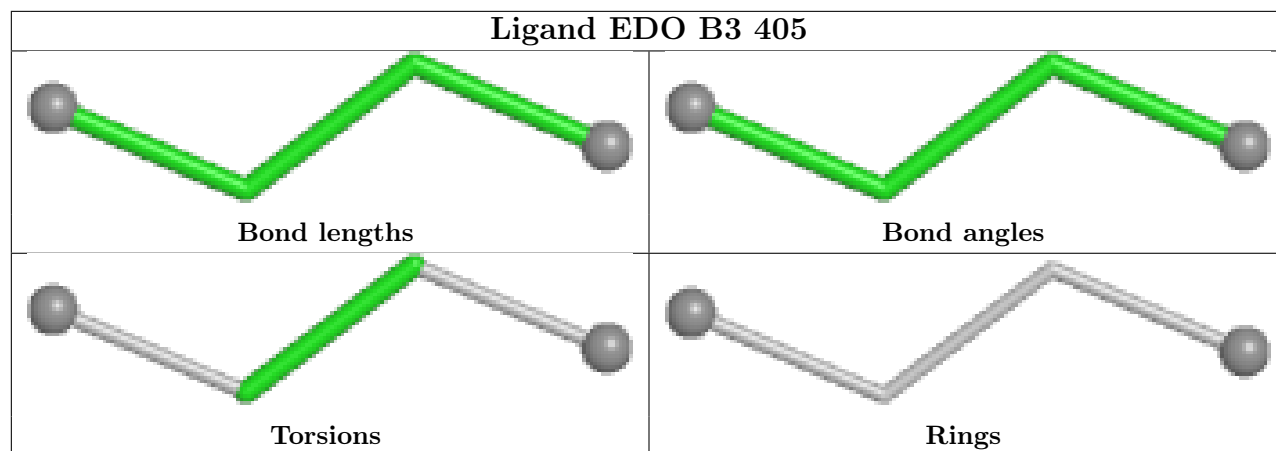












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

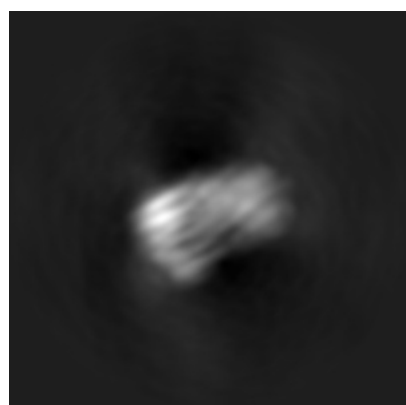
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24964. 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](#)

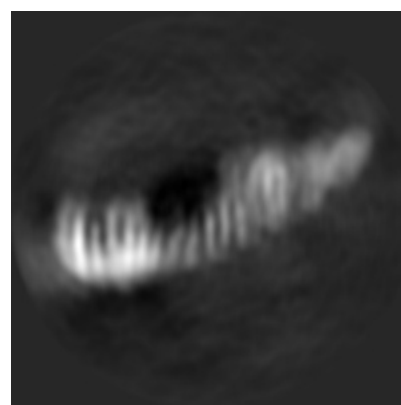
6.1.1 Primary map



X



Y

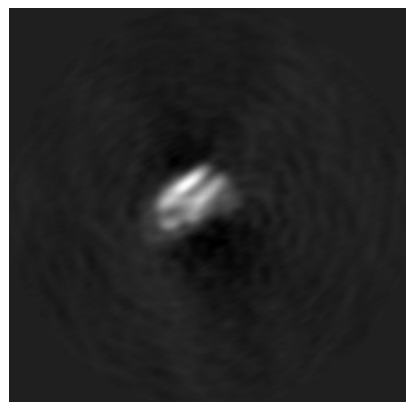


Z

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

6.2 Central slices [i](#)

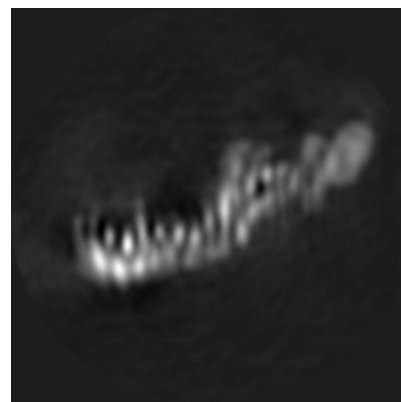
6.2.1 Primary map



X Index: 110



Y Index: 110



Z Index: 110

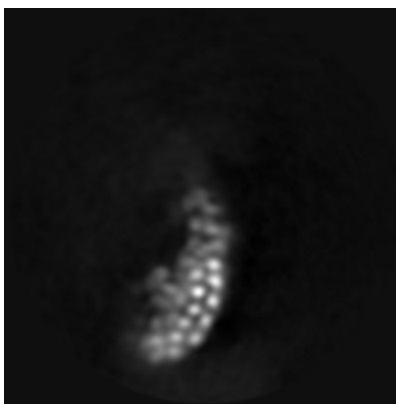
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

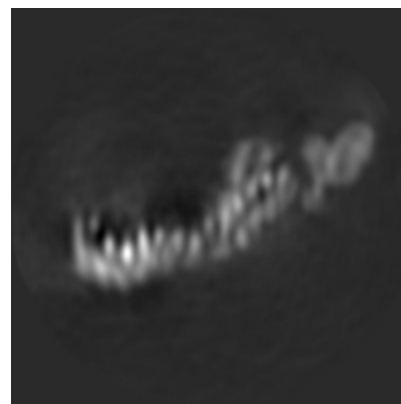
6.3.1 Primary map



X Index: 37



Y Index: 84

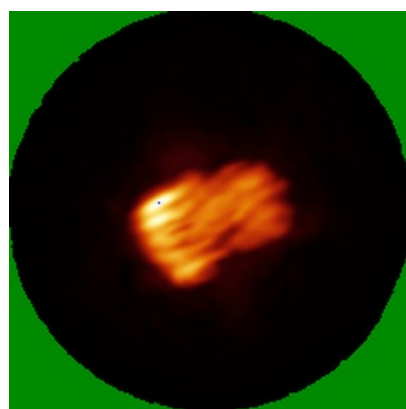


Z Index: 107

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

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

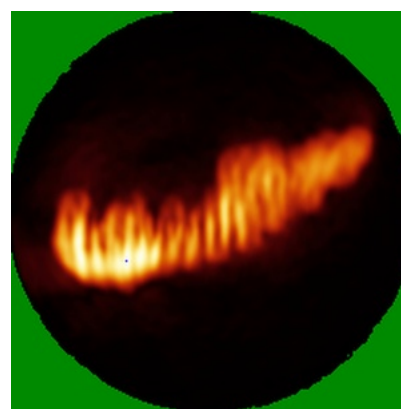
6.4.1 Primary map



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.

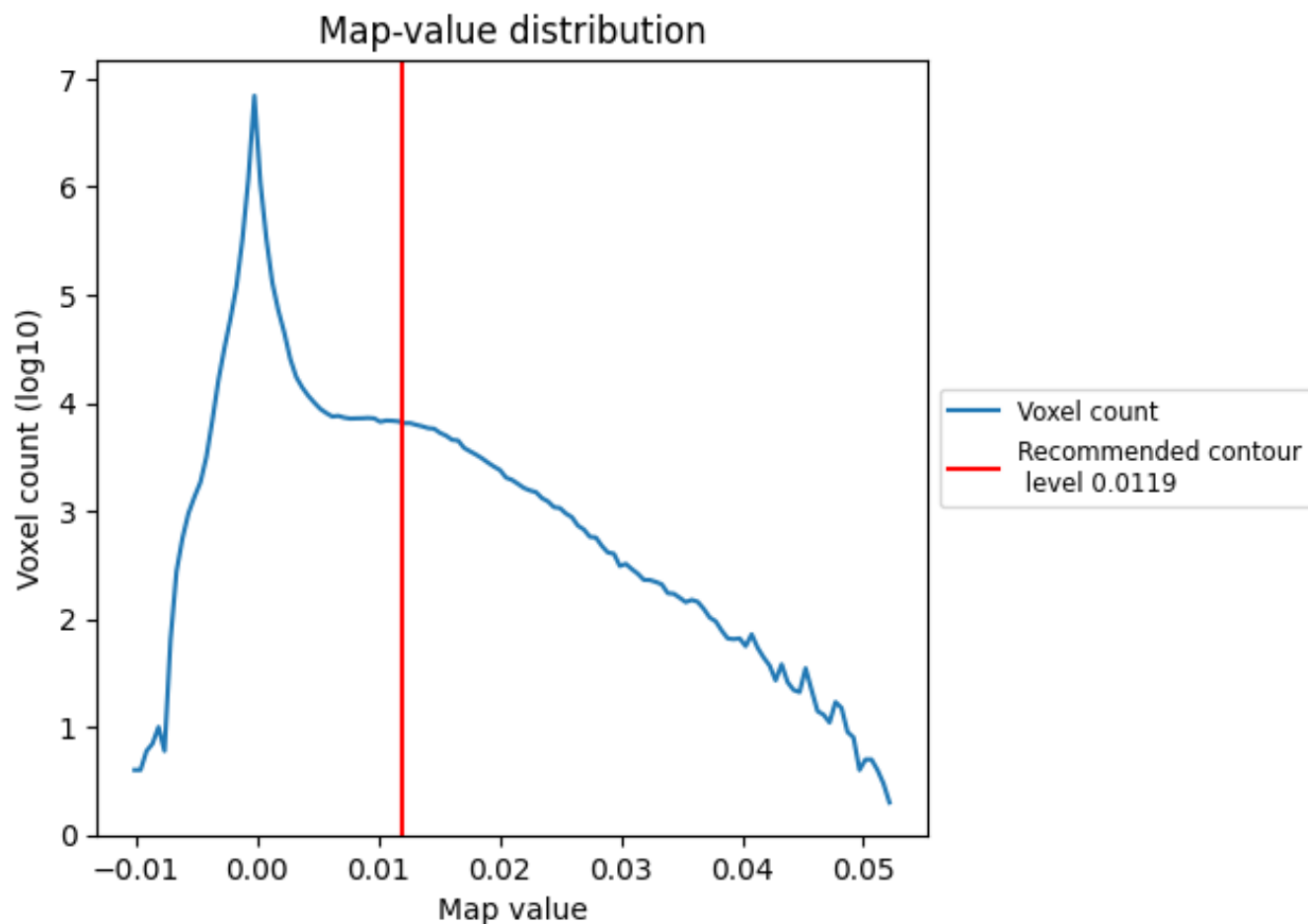
6.6 Mask visualisation

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

7 Map analysis [i](#)

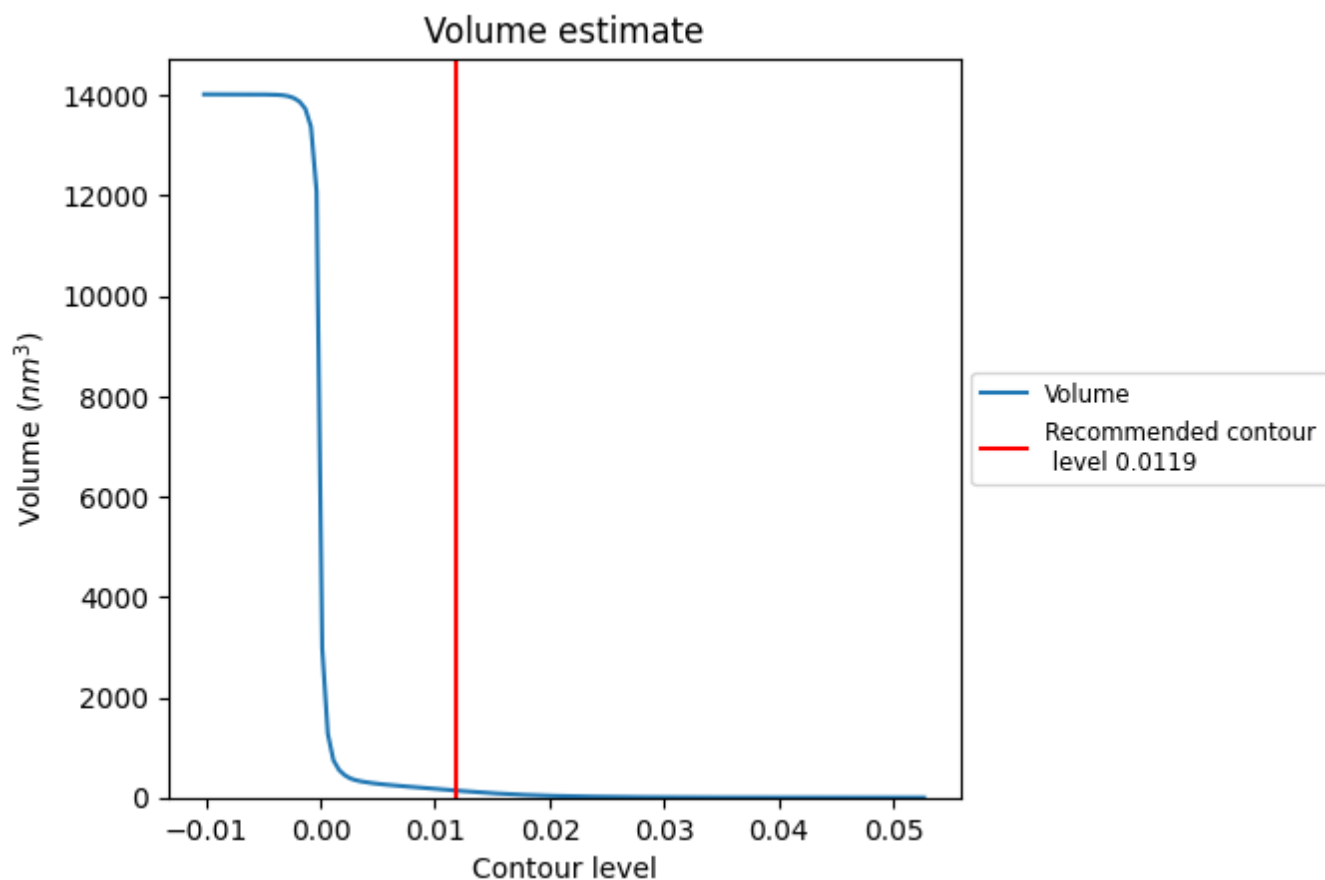
This section contains the results of statistical analysis of the map.

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.

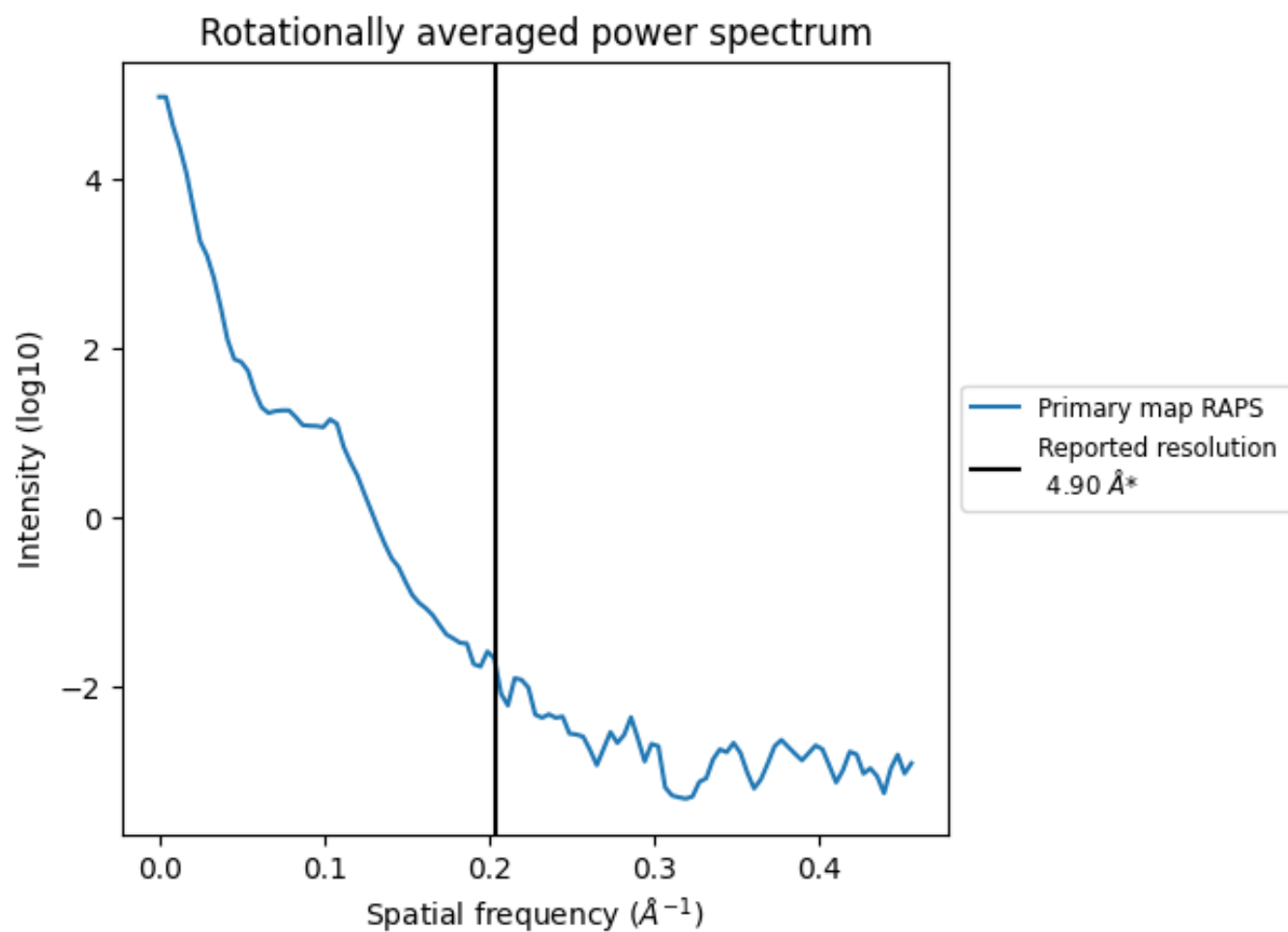
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 125 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 0.204 Å⁻¹

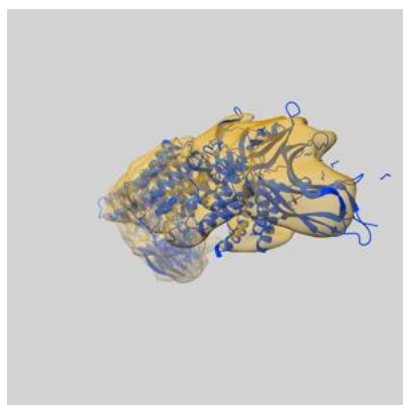
8 Fourier-Shell correlation ⓘ

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

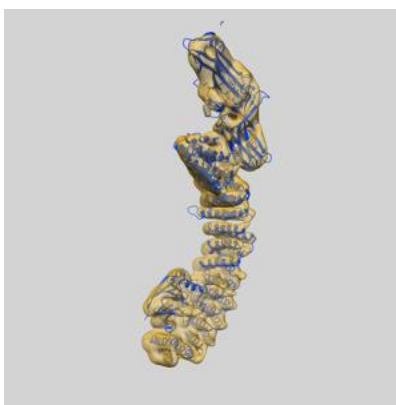
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24964 and PDB model 7U6F. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



X



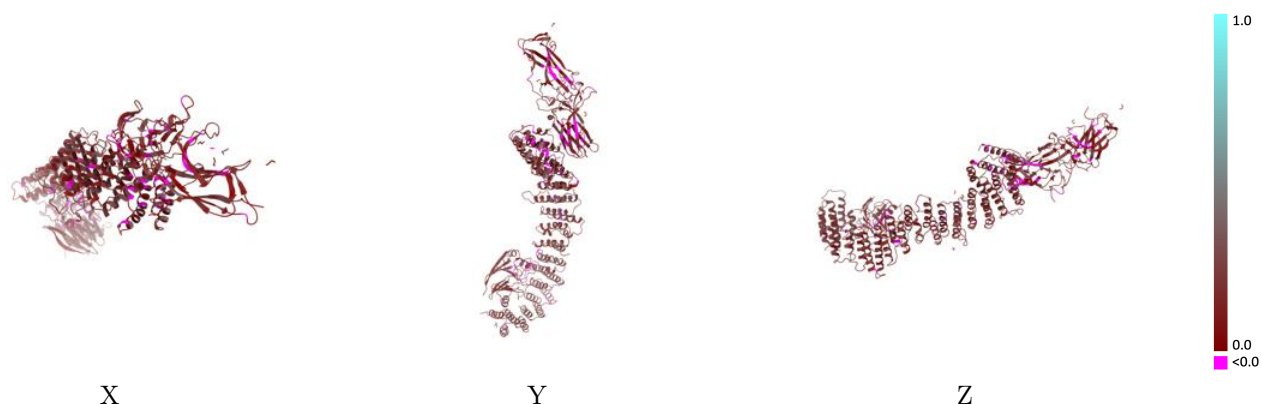
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0119 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

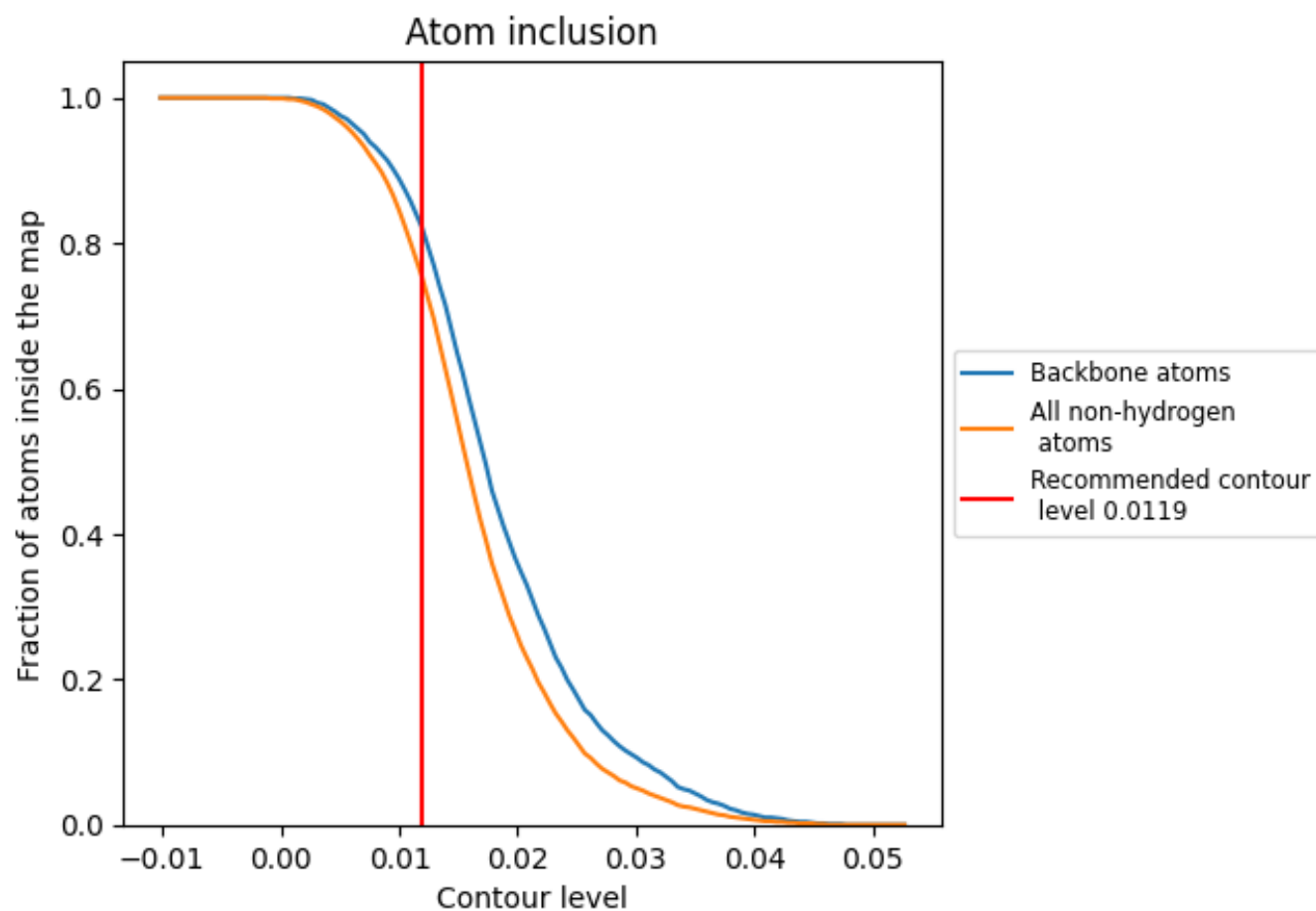


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0119) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7550	0.1640
B3	0.6980	0.1420
B4	0.6980	0.1630
D1	0.7960	0.1740

