



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 04:46 AM JST

PDB ID : 7W2J
EMDB ID : EMD-32262
Title : Cryo-EM Structure of Membrane-bound Fructose Dehydrogenase from *Gluconobacter japonicus*
Authors : Suzuki, Y.; Makino, F.; Miyata, T.; Tanaka, H.; Namba, K.; Sowa, K.; Kitazumi, Y.; Shirai, O.
Deposited on : 2021-11-24
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

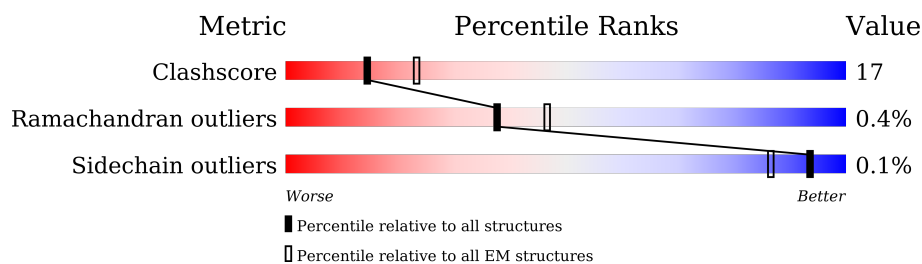
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	544	
1	D	544	
2	B	183	
2	E	183	
3	C	486	
3	F	486	

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
5	F3S	A	602	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16522 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 Fructose dehydrogenase large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4143	2598	733	785	27		
1	D	537	Total	C	N	O	S	0	0
			4143	2598	733	785	27		

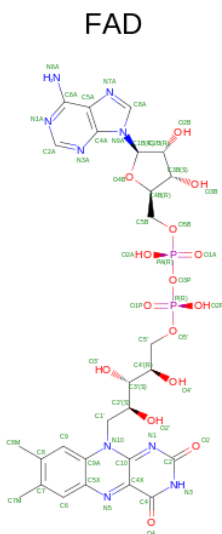
- Molecule 2 is a protein called Fructose dehydrogenase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	97	Total	C	N	O	S	0	0
			780	510	127	141	2		
2	E	97	Total	C	N	O	S	0	0
			780	510	127	141	2		

- Molecule 3 is a protein called Fructose dehydrogenase cytochrome subunit.

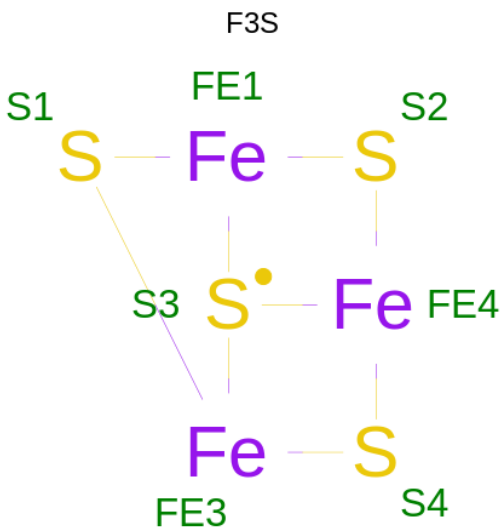
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	418	Total	C	N	O	S	0	0
			3149	1982	547	608	12		
3	F	418	Total	C	N	O	S	0	0
			3149	1982	547	608	12		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



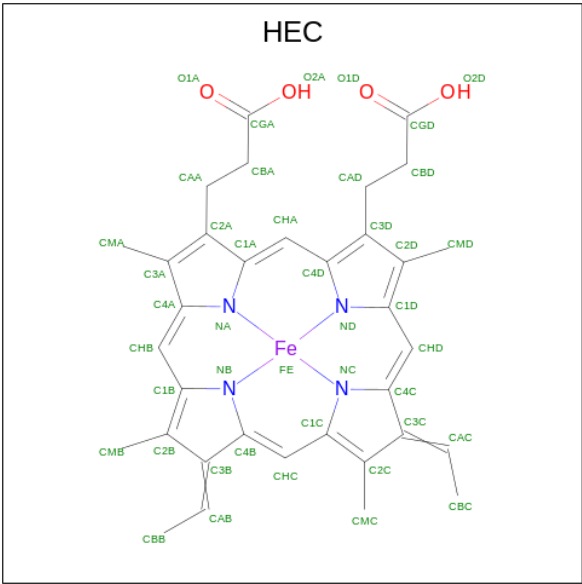
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 7	Fe 3	S 4	0
5	D	1	Total 7	Fe 3	S 4	0

- Molecule 6 is HEME C (three-letter code: HEC) (formula: C₃₄H₃₄FeN₄O₄) (labeled as "Ligand of Interest" by depositor).

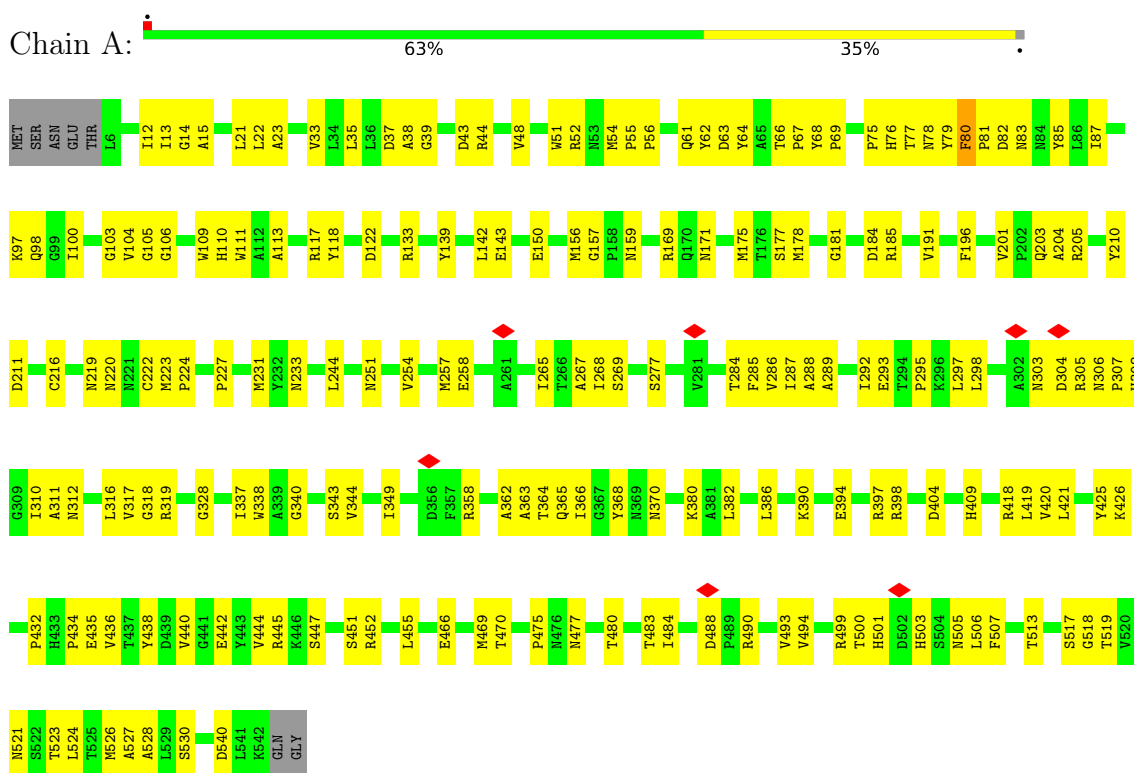


Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	Fe	N	O	0
			129	102	3	12	12	
6	C	1	Total	C	Fe	N	O	0
			129	102	3	12	12	
6	C	1	Total	C	Fe	N	O	0
			129	102	3	12	12	
6	F	1	Total	C	Fe	N	O	0
			129	102	3	12	12	
6	F	1	Total	C	Fe	N	O	0
			129	102	3	12	12	
6	F	1	Total	C	Fe	N	O	0
			129	102	3	12	12	

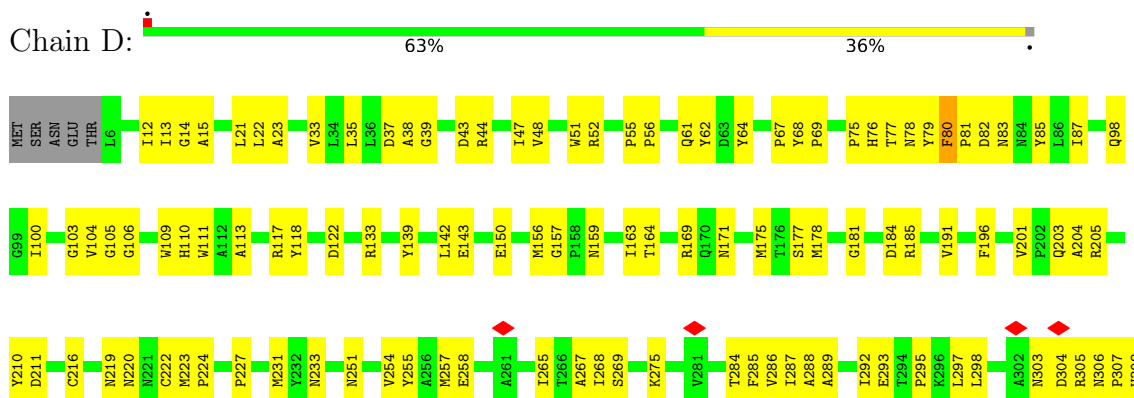
3 Residue-property plots

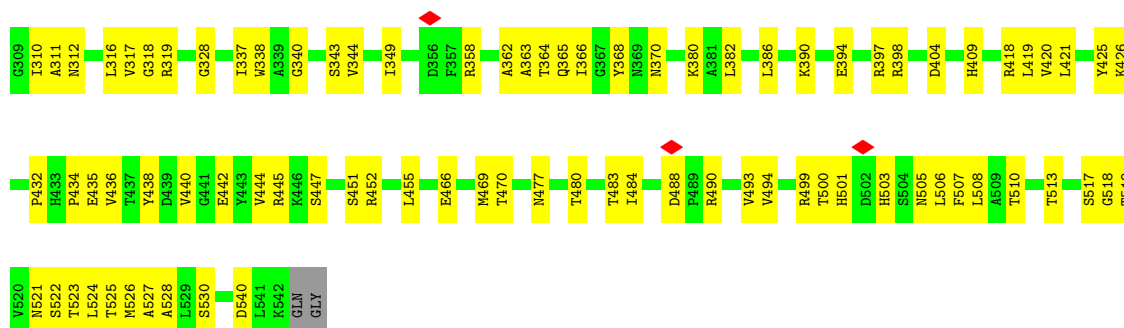
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

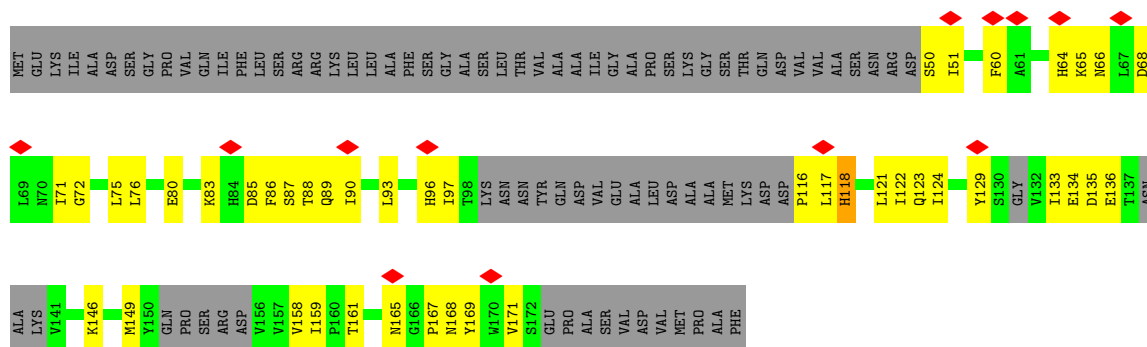
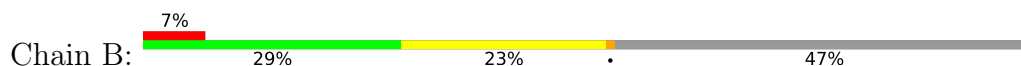


• Molecule 1: Fructose dehydrogenase large subunit

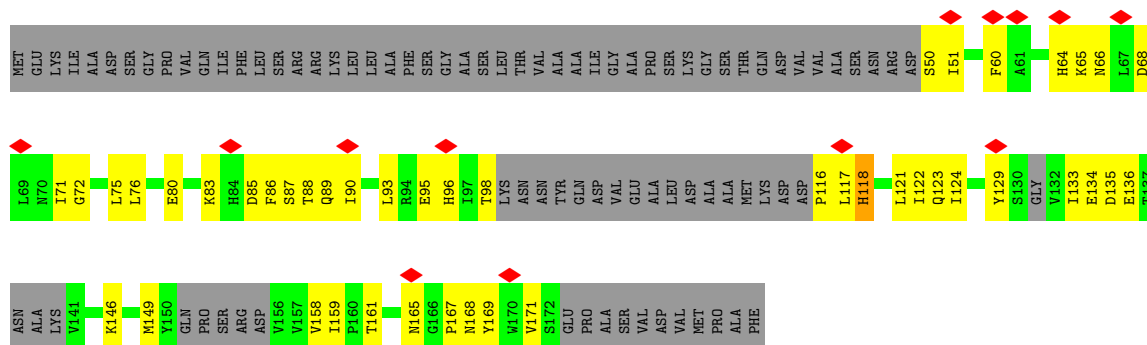
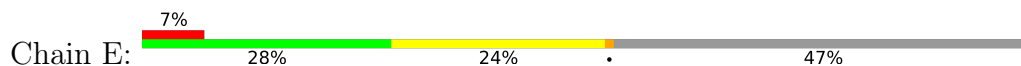




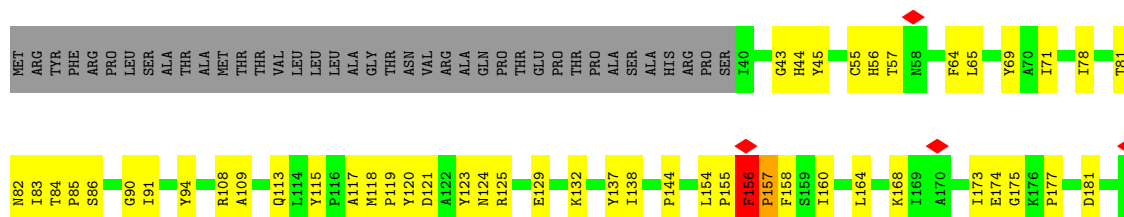
• Molecule 2: Fructose dehydrogenase small subunit

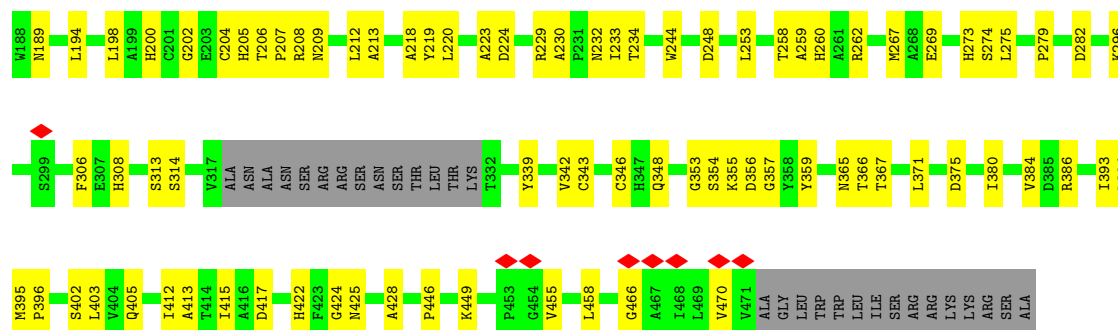


• Molecule 2: Fructose dehydrogenase small subunit

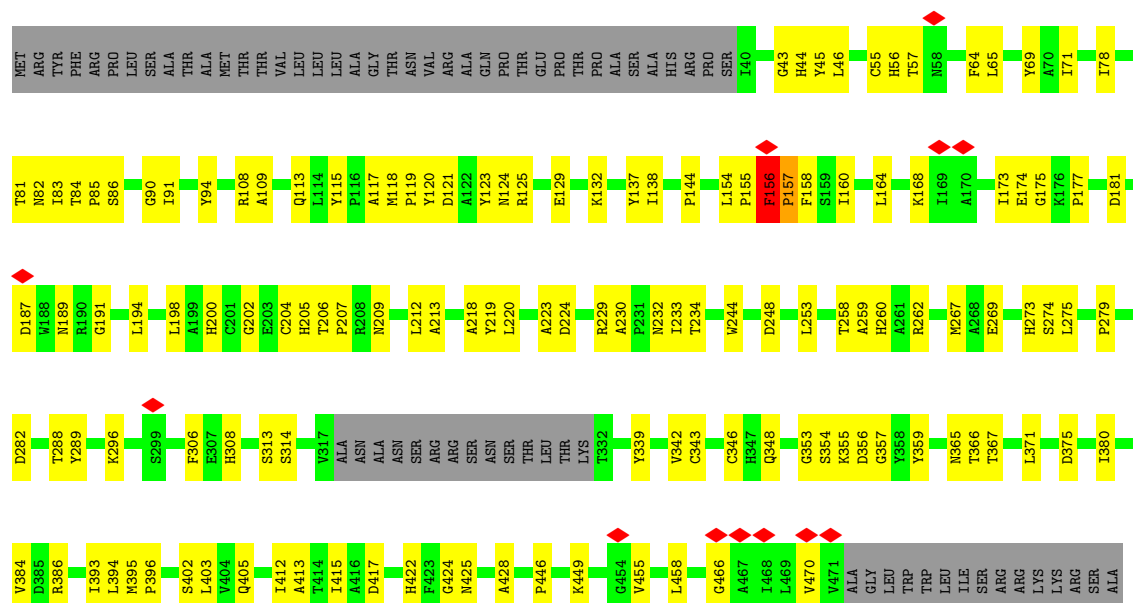


• Molecule 3: Fructose dehydrogenase cytochrome subunit





• Molecule 3: Fructose dehydrogenase cytochrome subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	91745	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	56754	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.168	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	246.68, 246.68, 246.68	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.881, 0.881, 0.881	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, FAD, HEC

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	0.45	0/4246	0.54	0/5774
1	D	0.45	0/4246	0.54	0/5774
2	B	0.39	0/798	0.56	0/1081
2	E	0.39	0/798	0.56	0/1081
3	C	0.43	0/3225	0.55	2/4396 (0.0%)
3	F	0.43	0/3225	0.55	2/4396 (0.0%)
All	All	0.43	0/16538	0.55	4/22502 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
2	B	0	1
2	E	0	1
3	C	0	1
3	F	0	1
All	All	0	6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	446	PRO	N-CD-CG	-5.83	94.46	103.20
3	C	446	PRO	N-CD-CG	-5.83	94.46	103.20
3	C	446	PRO	CA-N-CD	-5.31	104.07	111.50
3	F	446	PRO	CA-N-CD	-5.29	104.10	111.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	80	PHE	Peptide
2	B	118	HIS	Peptide
3	C	156	PHE	Peptide
1	D	80	PHE	Peptide
2	E	118	HIS	Peptide
3	F	156	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4143	0	4028	148	0
1	D	4143	0	4028	151	0
2	B	780	0	766	33	0
2	E	780	0	766	35	0
3	C	3149	0	3050	98	0
3	F	3149	0	3050	99	0
4	A	53	0	27	9	0
4	D	53	0	27	9	0
5	A	7	0	0	2	0
5	D	7	0	0	1	0
6	C	129	0	90	11	0
6	F	129	0	90	11	0
All	All	16522	0	15922	556	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 17.

All (556) 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:D:56:PRO:HG2	2:E:133:ILE:HB	1.59	0.84
1:A:56:PRO:HG2	2:B:133:ILE:HB	1.59	0.82
1:D:521:ASN:HB3	4:D:601:FAD:HN3	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASN:HB3	4:A:601:FAD:HN3	1.42	0.82
1:D:118:TYR:HE1	1:D:518:GLY:HA3	1.45	0.81
3:C:470:VAL:HG22	3:F:470:VAL:HG22	1.61	0.81
1:A:118:TYR:HE1	1:A:518:GLY:HA3	1.45	0.79
3:C:156:PHE:O	3:C:158:PHE:N	2.16	0.79
3:F:156:PHE:O	3:F:158:PHE:N	2.16	0.79
3:C:466:GLY:HA3	3:F:466:GLY:HA3	1.65	0.78
1:D:380:LYS:HD2	1:D:398:ARG:HE	1.51	0.76
1:A:380:LYS:HD2	1:A:398:ARG:HE	1.50	0.75
1:D:122:ASP:OD1	1:D:358:ARG:NH2	2.19	0.74
2:B:60:PHE:HB3	2:B:65:LYS:HD2	1.70	0.73
1:A:122:ASP:OD1	1:A:358:ARG:NH2	2.19	0.73
1:D:295:PRO:HB2	1:D:419:LEU:HD23	1.70	0.72
1:A:295:PRO:HB2	1:A:419:LEU:HD23	1.70	0.72
2:E:60:PHE:HB3	2:E:65:LYS:HD2	1.70	0.72
3:C:71:ILE:HD11	3:C:117:ALA:HB1	1.72	0.71
1:D:499:ARG:NH2	1:D:540:ASP:OD2	2.24	0.71
1:A:499:ARG:NH2	1:A:540:ASP:OD2	2.24	0.70
1:D:493:VAL:O	1:D:501:HIS:ND1	2.24	0.70
3:F:65:LEU:HD12	3:F:83:ILE:HB	1.73	0.70
1:A:493:VAL:O	1:A:501:HIS:ND1	2.24	0.70
1:D:205:ARG:NH2	1:D:343:SER:OG	2.24	0.70
3:C:65:LEU:HD12	3:C:83:ILE:HB	1.73	0.69
2:E:64:HIS:ND1	2:E:66:ASN:O	2.19	0.69
1:A:205:ARG:NH2	1:A:343:SER:OG	2.24	0.69
3:F:71:ILE:HD11	3:F:117:ALA:HB1	1.72	0.69
3:F:308:HIS:CE1	3:F:425:ASN:HA	2.28	0.69
3:C:308:HIS:CE1	3:C:425:ASN:HA	2.28	0.68
1:D:328:GLY:H	1:D:470:THR:HG22	1.59	0.68
1:A:68:TYR:OH	1:A:224:PRO:O	2.09	0.68
1:A:133:ARG:HE	1:A:484:ILE:HG21	1.59	0.67
3:F:365:ASN:HD21	6:F:501:HEC:HBA2	1.59	0.67
2:B:64:HIS:ND1	2:B:66:ASN:O	2.19	0.67
3:C:365:ASN:HD21	6:C:501:HEC:HBA2	1.59	0.67
3:F:64:PHE:HD2	3:F:65:LEU:HD23	1.60	0.67
1:D:133:ARG:HE	1:D:484:ILE:HG21	1.59	0.67
1:D:418:ARG:HD2	1:D:420:VAL:HG13	1.78	0.66
3:C:64:PHE:HD2	3:C:65:LEU:HD23	1.60	0.66
3:C:124:ASN:ND2	3:C:173:ILE:O	2.29	0.66
6:C:501:HEC:HMD1	6:C:501:HEC:HBD2	1.78	0.66
1:A:328:GLY:H	1:A:470:THR:HG22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:380:ILE:HG12	6:F:501:HEC:HMB2	1.77	0.66
3:F:224:ASP:HA	3:F:229:ARG:HA	1.78	0.65
3:C:380:ILE:HG12	6:C:501:HEC:HMB2	1.78	0.65
1:A:418:ARG:HD2	1:A:420:VAL:HG13	1.78	0.65
3:C:253:LEU:HD11	6:C:502:HEC:HMB2	1.78	0.65
3:F:253:LEU:HD11	6:F:502:HEC:HMB2	1.78	0.65
1:A:117:ARG:NH1	1:A:139:TYR:OH	2.31	0.64
3:F:124:ASN:ND2	3:F:173:ILE:O	2.29	0.64
6:F:501:HEC:HBD2	6:F:501:HEC:HMD1	1.78	0.64
3:F:413:ALA:O	3:F:417:ASP:N	2.29	0.64
3:C:224:ASP:HA	3:C:229:ARG:HA	1.78	0.64
6:F:501:HEC:HBA1	6:F:501:HEC:HHA	1.80	0.63
6:C:501:HEC:HHA	6:C:501:HEC:HBA1	1.80	0.63
1:D:117:ARG:NH1	1:D:139:TYR:OH	2.31	0.63
1:D:178:MET:HE1	1:D:216:CYS:HB3	1.81	0.63
1:D:292:ILE:HG23	1:D:293:GLU:HG2	1.80	0.63
1:A:292:ILE:HG23	1:A:293:GLU:HG2	1.80	0.62
1:A:419:LEU:HD11	1:A:434:PRO:HB2	1.82	0.62
3:C:413:ALA:O	3:C:417:ASP:N	2.29	0.62
2:B:89:GLN:OE1	2:B:123:GLN:NE2	2.33	0.62
1:D:398:ARG:NH2	1:D:466:GLU:OE1	2.33	0.62
1:D:419:LEU:HD13	1:D:436:VAL:HG22	1.82	0.62
2:B:168:ASN:OD1	2:B:169:TYR:N	2.32	0.61
2:E:168:ASN:OD1	2:E:169:TYR:N	2.32	0.61
1:A:178:MET:HE1	1:A:216:CYS:HB3	1.81	0.61
1:A:269:SER:HG	1:A:277:SER:HG	1.45	0.61
1:D:419:LEU:HD11	1:D:434:PRO:HB2	1.82	0.61
1:A:494:VAL:HG21	1:A:513:THR:HG23	1.82	0.61
1:D:494:VAL:HG21	1:D:513:THR:HG23	1.82	0.61
3:F:181:ASP:O	3:F:189:ASN:ND2	2.32	0.61
2:E:89:GLN:OE1	2:E:123:GLN:NE2	2.33	0.61
2:E:146:LYS:NZ	2:E:171:VAL:O	2.34	0.61
1:D:523:THR:HG22	4:D:601:FAD:O2	2.01	0.60
1:A:419:LEU:HD13	1:A:436:VAL:HG22	1.82	0.60
2:B:72:GLY:HA2	2:B:75:LEU:HB2	1.83	0.60
3:F:248:ASP:OD1	3:F:258:THR:HG21	2.01	0.60
1:A:398:ARG:NH2	1:A:466:GLU:OE1	2.33	0.60
1:A:523:THR:HG22	4:A:601:FAD:O2	2.01	0.60
2:B:146:LYS:NZ	2:B:171:VAL:O	2.34	0.60
1:D:523:THR:N	4:D:601:FAD:O2	2.30	0.59
2:B:68:ASP:O	2:B:71:ILE:HG12	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:MET:HE2	6:C:503:HEC:NA	2.18	0.59
3:C:248:ASP:OD1	3:C:258:THR:HG21	2.01	0.59
1:A:523:THR:N	4:A:601:FAD:O2	2.31	0.59
1:D:44:ARG:NH2	1:D:233:ASN:OD1	2.35	0.59
2:E:68:ASP:O	2:E:71:ILE:HG12	2.03	0.59
2:E:72:GLY:HA2	2:E:75:LEU:HB2	1.83	0.59
3:F:118:MET:HE2	6:F:503:HEC:NA	2.17	0.59
1:A:62:TYR:OH	1:A:404:ASP:OD2	2.21	0.59
1:D:68:TYR:OH	1:D:224:PRO:O	2.09	0.59
3:F:86:SER:HB3	3:F:90:GLY:H	1.68	0.58
3:C:209:ASN:HD21	3:C:213:ALA:HB3	1.68	0.58
3:C:86:SER:HB3	3:C:90:GLY:H	1.68	0.58
1:D:12:ILE:HD12	1:D:33:VAL:HG13	1.86	0.58
1:A:12:ILE:HD12	1:A:33:VAL:HG13	1.86	0.57
1:D:39:GLY:HA3	1:D:103:GLY:HA2	1.86	0.57
3:C:181:ASP:O	3:C:189:ASN:ND2	2.32	0.57
1:A:44:ARG:NH2	1:A:233:ASN:OD1	2.35	0.57
3:C:65:LEU:O	3:C:84:THR:HG23	2.04	0.57
3:C:91:ILE:HD11	3:C:138:ILE:HG21	1.86	0.57
1:D:110:HIS:CE1	4:D:601:FAD:HM71	2.40	0.57
3:F:209:ASN:HD21	3:F:213:ALA:HB3	1.68	0.57
1:D:62:TYR:OH	1:D:404:ASP:OD2	2.21	0.57
1:D:219:ASN:HD22	1:D:227:PRO:HG2	1.70	0.57
1:A:219:ASN:HD22	1:A:227:PRO:HG2	1.70	0.56
3:C:85:PRO:HG2	3:C:144:PRO:HG3	1.86	0.56
3:F:91:ILE:HD11	3:F:138:ILE:HG21	1.86	0.56
3:F:65:LEU:O	3:F:84:THR:HG23	2.04	0.56
3:F:313:SER:HB3	3:F:422:HIS:CD2	2.41	0.56
2:B:129:TYR:O	2:B:134:GLU:HB3	2.06	0.56
3:F:85:PRO:HG2	3:F:144:PRO:HG3	1.86	0.56
1:A:39:GLY:HA3	1:A:103:GLY:HA2	1.86	0.56
3:C:313:SER:HB3	3:C:422:HIS:CD2	2.41	0.56
3:C:455:VAL:HG13	3:F:458:LEU:HD21	1.88	0.56
1:D:23:ALA:HB2	1:D:35:LEU:HD11	1.87	0.55
1:D:440:VAL:HB	1:D:444:VAL:HG21	1.88	0.55
1:D:488:ASP:OD2	1:D:490:ARG:NH1	2.38	0.55
1:A:365:GLN:HG2	1:A:519:THR:O	2.06	0.55
2:E:134:GLU:O	2:E:136:GLU:N	2.39	0.55
1:A:440:VAL:HB	1:A:444:VAL:HG21	1.88	0.55
1:A:488:ASP:OD2	1:A:490:ARG:NH1	2.38	0.55
1:A:23:ALA:HB2	1:A:35:LEU:HD11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:HH12	1:D:143:GLU:HG2	1.72	0.55
2:E:129:TYR:O	2:E:134:GLU:HB3	2.06	0.55
1:A:82:ASP:OD1	1:A:83:ASN:N	2.40	0.55
1:A:358:ARG:HD3	1:A:363:ALA:HB2	1.89	0.55
1:D:358:ARG:HD3	1:D:363:ALA:HB2	1.89	0.55
1:A:110:HIS:CE1	4:A:601:FAD:HM71	2.40	0.55
1:A:191:VAL:CG1	1:A:196:PHE:HB2	2.37	0.55
3:F:260:HIS:HB3	3:F:306:PHE:HB2	1.90	0.54
1:A:117:ARG:HH12	1:A:143:GLU:HG2	1.72	0.54
1:D:310:ILE:HG23	1:D:503:HIS:CE1	2.43	0.54
1:A:311:ALA:H	1:A:503:HIS:HE1	1.55	0.54
1:D:365:GLN:HG2	1:D:519:THR:O	2.06	0.54
1:A:289:ALA:HA	4:A:601:FAD:H4B	1.90	0.54
1:D:480:THR:HG21	1:D:517:SER:HA	1.88	0.54
3:F:119:PRO:O	3:F:123:TYR:N	2.40	0.54
1:D:311:ALA:H	1:D:503:HIS:HE1	1.55	0.54
1:D:191:VAL:CG1	1:D:196:PHE:HB2	2.37	0.54
2:B:134:GLU:O	2:B:136:GLU:N	2.38	0.54
1:D:82:ASP:OD1	1:D:83:ASN:N	2.40	0.54
3:F:386:ARG:NH2	3:F:393:ILE:HD11	2.23	0.54
1:A:310:ILE:HG23	1:A:503:HIS:CE1	2.43	0.54
3:C:260:HIS:HB3	3:C:306:PHE:HB2	1.90	0.54
1:A:480:THR:HG21	1:A:517:SER:HA	1.88	0.53
1:D:289:ALA:HA	4:D:601:FAD:H4B	1.90	0.53
3:C:458:LEU:HD21	3:F:455:VAL:HG13	1.89	0.53
1:D:13:ILE:HD11	1:D:287:ILE:HG23	1.90	0.53
3:F:207:PRO:HB3	3:F:223:ALA:HB2	1.90	0.53
3:C:157:PRO:O	3:C:160:ILE:HG12	2.09	0.53
1:A:150:GLU:OE1	1:A:169:ARG:NH1	2.38	0.53
3:C:386:ARG:NH2	3:C:393:ILE:HD11	2.23	0.53
1:D:394:GLU:OE1	1:D:397:ARG:NH2	2.41	0.53
1:A:13:ILE:HD11	1:A:287:ILE:HG23	1.90	0.53
1:A:265:ILE:HG21	1:A:285:PHE:HB2	1.91	0.53
1:D:349:ILE:HB	1:D:366:ILE:HB	1.91	0.53
1:A:257:MET:HE1	1:A:310:ILE:HG21	1.91	0.53
1:D:265:ILE:HG21	1:D:285:PHE:HB2	1.91	0.53
3:C:207:PRO:HB3	3:C:223:ALA:HB2	1.90	0.53
3:F:219:TYR:HB3	3:F:296:LYS:HZ2	1.74	0.53
1:A:394:GLU:OE1	1:A:397:ARG:NH2	2.41	0.52
1:D:62:TYR:HB3	1:D:64:TYR:CZ	2.44	0.52
1:D:150:GLU:OE1	1:D:169:ARG:NH1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:157:PRO:O	3:F:160:ILE:HG12	2.09	0.52
1:D:500:THR:OG1	1:D:503:HIS:HB2	2.09	0.52
1:A:349:ILE:HB	1:A:366:ILE:HB	1.91	0.52
1:A:500:THR:OG1	1:A:503:HIS:HB2	2.09	0.52
1:A:159:ASN:ND2	1:A:175:MET:O	2.42	0.52
1:D:159:ASN:ND2	1:D:175:MET:O	2.42	0.52
1:A:524:LEU:O	1:A:528:ALA:N	2.42	0.52
1:A:43:ASP:HB3	3:C:405:GLN:HE22	1.74	0.52
1:A:62:TYR:HB3	1:A:64:TYR:CZ	2.44	0.52
3:C:308:HIS:ND1	3:C:425:ASN:OD1	2.43	0.52
3:C:313:SER:OG	3:C:314:SER:N	2.43	0.52
1:D:231:MET:HB3	5:D:602:F3S:S3	2.50	0.52
1:D:303:ASN:N	1:D:306:ASN:O	2.43	0.52
3:F:308:HIS:ND1	3:F:425:ASN:OD1	2.43	0.52
3:F:354:SER:OG	3:F:355:LYS:N	2.43	0.52
3:C:45:TYR:OH	3:C:282:ASP:OD2	2.26	0.51
1:D:524:LEU:O	1:D:528:ALA:N	2.42	0.51
1:A:51:TRP:HD1	1:A:67:PRO:HG2	1.75	0.51
1:A:67:PRO:O	1:A:69:PRO:HD3	2.10	0.51
1:A:303:ASN:N	1:A:306:ASN:O	2.43	0.51
1:D:483:THR:O	1:D:513:THR:HA	2.11	0.51
1:A:110:HIS:CG	1:A:110:HIS:O	2.64	0.51
1:D:43:ASP:HB3	3:F:405:GLN:HE22	1.75	0.51
1:D:257:MET:HE1	1:D:310:ILE:HG21	1.91	0.51
3:F:313:SER:OG	3:F:314:SER:N	2.43	0.51
1:A:483:THR:O	1:A:513:THR:HA	2.11	0.51
1:A:210:TYR:CD1	1:A:211:ASP:HB2	2.46	0.51
1:A:231:MET:HB3	5:A:602:F3S:S3	2.50	0.51
3:C:354:SER:OG	3:C:355:LYS:N	2.43	0.51
1:D:210:TYR:CD1	1:D:211:ASP:HB2	2.46	0.51
3:F:45:TYR:OH	3:F:282:ASP:OD2	2.26	0.51
1:D:67:PRO:O	1:D:69:PRO:HD3	2.10	0.51
1:D:110:HIS:O	1:D:110:HIS:CG	2.64	0.50
1:D:78:ASN:OD1	1:D:79:TYR:N	2.44	0.50
1:D:223:MET:HB2	1:D:224:PRO:HD3	1.93	0.50
1:D:191:VAL:HG12	1:D:196:PHE:HB2	1.93	0.50
1:A:191:VAL:HG12	1:A:196:PHE:HB2	1.92	0.50
1:D:307:PRO:HG2	1:D:308:HIS:ND1	2.27	0.50
1:A:78:ASN:OD1	1:A:79:TYR:N	2.44	0.50
1:A:111:TRP:CD2	1:A:113:ALA:HA	2.47	0.50
1:A:307:PRO:HG2	1:A:308:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:CYS:HA	3:C:69:TYR:HD2	1.77	0.50
3:C:119:PRO:O	3:C:123:TYR:N	2.39	0.50
3:F:55:CYS:HA	3:F:69:TYR:HD2	1.77	0.50
3:F:56:HIS:CD2	3:F:83:ILE:HG13	2.47	0.50
1:A:319:ARG:HH21	1:A:418:ARG:NH1	2.10	0.49
1:D:104:VAL:O	1:D:109:TRP:NE1	2.39	0.49
3:F:262:ARG:NH2	3:F:357:GLY:O	2.39	0.49
3:C:342:VAL:HG23	3:C:343:CYS:SG	2.53	0.49
1:D:319:ARG:HH21	1:D:418:ARG:NH1	2.10	0.49
3:F:200:HIS:O	3:F:200:HIS:ND1	2.42	0.49
1:A:111:TRP:CE3	1:A:113:ALA:HA	2.47	0.49
3:F:279:PRO:HD2	3:F:282:ASP:OD2	2.13	0.49
1:A:223:MET:HB2	1:A:224:PRO:HD3	1.93	0.49
3:F:129:GLU:O	3:F:132:LYS:HG2	2.13	0.49
3:C:220:LEU:O	3:C:234:THR:HG23	2.12	0.49
2:B:85:ASP:O	2:B:88:THR:OG1	2.27	0.49
2:E:51:ILE:HG22	2:E:76:LEU:HD13	1.95	0.49
3:F:220:LEU:O	3:F:234:THR:HG23	2.12	0.49
3:F:371:LEU:HD12	3:F:428:ALA:HB2	1.95	0.49
1:D:75:PRO:HD2	1:D:85:TYR:HE2	1.78	0.49
1:A:75:PRO:HD2	1:A:85:TYR:HE2	1.78	0.49
3:C:279:PRO:HD2	3:C:282:ASP:OD2	2.13	0.49
3:C:371:LEU:HD12	3:C:428:ALA:HB2	1.95	0.49
3:C:56:HIS:CD2	3:C:83:ILE:HG13	2.47	0.49
3:C:129:GLU:O	3:C:132:LYS:HG2	2.12	0.49
3:C:262:ARG:NH2	3:C:357:GLY:O	2.39	0.49
3:F:342:VAL:HG23	3:F:343:CYS:SG	2.53	0.49
1:A:76:HIS:HB2	1:A:100:ILE:O	2.13	0.49
2:B:51:ILE:HG22	2:B:76:LEU:HD13	1.95	0.49
3:C:219:TYR:HB3	3:C:296:LYS:HZ2	1.77	0.49
1:D:113:ALA:HB1	1:D:204:ALA:HB3	1.95	0.49
1:A:113:ALA:HB1	1:A:204:ALA:HB3	1.95	0.48
1:D:51:TRP:HD1	1:D:67:PRO:HG2	1.75	0.48
1:D:111:TRP:CE3	1:D:113:ALA:HA	2.47	0.48
1:A:286:VAL:HG22	1:A:507:PHE:HB2	1.94	0.48
2:B:76:LEU:O	2:B:80:GLU:HG2	2.13	0.48
1:D:111:TRP:CD2	1:D:113:ALA:HA	2.47	0.48
2:E:85:ASP:O	2:E:88:THR:OG1	2.28	0.48
1:A:438:TYR:HE2	1:A:440:VAL:HG12	1.78	0.48
3:C:267:MET:HG3	6:C:502:HEC:C4D	2.44	0.48
1:D:286:VAL:HG22	1:D:507:PHE:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:SER:OG	1:D:344:VAL:N	2.46	0.48
2:E:95:GLU:O	2:E:98:THR:OG1	2.24	0.48
1:A:133:ARG:HH21	1:A:484:ILE:HG22	1.79	0.48
1:A:328:GLY:H	1:A:470:THR:CG2	2.25	0.48
1:D:438:TYR:HE2	1:D:440:VAL:HG12	1.78	0.48
3:F:267:MET:HG3	6:F:502:HEC:C4D	2.44	0.48
2:E:76:LEU:O	2:E:80:GLU:HG2	2.13	0.48
1:D:133:ARG:HH21	1:D:484:ILE:HG22	1.79	0.48
1:D:22:LEU:HD13	1:D:530:SER:O	2.14	0.48
1:D:87:ILE:O	1:D:435:GLU:HA	2.14	0.48
2:E:158:VAL:HG21	3:F:356:ASP:OD1	2.13	0.48
3:C:200:HIS:O	3:C:200:HIS:ND1	2.42	0.48
1:D:118:TYR:CE1	1:D:518:GLY:HA3	2.37	0.48
2:E:96:HIS:ND1	2:E:117:LEU:HD12	2.29	0.48
2:E:118:HIS:CG	2:E:118:HIS:O	2.67	0.48
2:E:146:LYS:HE2	2:E:167:PRO:HG2	1.96	0.48
3:F:396:PRO:CD	6:F:501:HEC:HBC2	2.44	0.48
1:D:181:GLY:O	1:D:185:ARG:NH1	2.47	0.48
1:A:181:GLY:O	1:A:185:ARG:NH1	2.47	0.48
1:A:257:MET:HG2	1:A:268:ILE:HG12	1.95	0.48
1:A:343:SER:OG	1:A:344:VAL:N	2.46	0.48
3:C:308:HIS:NE2	3:C:424:GLY:O	2.47	0.48
1:D:76:HIS:HB2	1:D:100:ILE:O	2.13	0.48
1:D:142:LEU:HD11	1:D:528:ALA:O	2.14	0.48
3:C:396:PRO:CD	6:C:501:HEC:HBC2	2.44	0.47
3:F:346:CYS:HB3	3:F:359:TYR:CD1	2.49	0.47
1:A:22:LEU:HD13	1:A:530:SER:O	2.14	0.47
1:A:104:VAL:O	1:A:109:TRP:NE1	2.39	0.47
3:C:205:HIS:CE1	3:C:230:ALA:HB1	2.49	0.47
1:D:257:MET:HG2	1:D:268:ILE:HG12	1.95	0.47
1:D:328:GLY:H	1:D:470:THR:CG2	2.25	0.47
3:F:156:PHE:HB3	3:F:157:PRO:HD2	1.96	0.47
3:F:308:HIS:NE2	3:F:424:GLY:O	2.47	0.47
1:A:210:TYR:HD1	1:A:211:ASP:HB2	1.80	0.47
2:B:118:HIS:CG	2:B:118:HIS:O	2.67	0.47
3:C:269:GLU:O	3:C:273:HIS:ND1	2.45	0.47
1:D:184:ASP:OD2	1:D:370:ASN:ND2	2.48	0.47
1:D:254:VAL:HG12	1:D:297:LEU:HD11	1.95	0.47
3:F:339:TYR:HB2	3:F:415:ILE:HG23	1.96	0.47
2:B:96:HIS:ND1	2:B:117:LEU:HD12	2.29	0.47
2:B:146:LYS:HE2	2:B:167:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:274:SER:OG	3:C:275:LEU:HD12	2.15	0.47
3:C:346:CYS:HB3	3:C:359:TYR:CD1	2.49	0.47
3:F:205:HIS:CE1	3:F:230:ALA:HB1	2.49	0.47
1:A:308:HIS:HD2	1:A:312:ASN:ND2	2.13	0.47
1:A:421:LEU:HD12	1:A:432:PRO:HG2	1.96	0.47
3:C:117:ALA:HB3	6:C:503:HEC:HMD2	1.97	0.47
1:A:87:ILE:O	1:A:435:GLU:HA	2.14	0.47
1:A:142:LEU:HD11	1:A:528:ALA:O	2.14	0.47
1:A:220:ASN:HD21	1:A:340:GLY:HA2	1.80	0.47
1:A:257:MET:HB3	1:A:265:ILE:HD11	1.96	0.47
1:A:338:TRP:CD1	2:B:165:ASN:HB2	2.49	0.47
1:A:440:VAL:HB	1:A:444:VAL:CG2	2.45	0.47
1:D:15:ALA:O	1:D:105:GLY:N	2.44	0.47
1:D:191:VAL:HG11	1:D:349:ILE:HD11	1.96	0.47
1:D:210:TYR:HD1	1:D:211:ASP:HB2	1.80	0.47
1:D:257:MET:HB3	1:D:265:ILE:HD11	1.96	0.47
3:F:218:ALA:HA	3:F:296:LYS:HD3	1.97	0.47
1:A:254:VAL:HG12	1:A:297:LEU:HD11	1.95	0.47
1:A:15:ALA:O	1:A:105:GLY:N	2.44	0.47
1:A:184:ASP:OD2	1:A:370:ASN:ND2	2.48	0.47
2:B:133:ILE:HG23	2:B:134:GLU:N	2.30	0.47
3:C:218:ALA:HA	3:C:296:LYS:HD3	1.97	0.47
1:A:118:TYR:CE1	1:A:518:GLY:HA3	2.37	0.47
3:C:339:TYR:HB2	3:C:415:ILE:HG23	1.96	0.47
1:D:316:LEU:HD23	1:D:319:ARG:HD2	1.97	0.47
1:D:421:LEU:HD12	1:D:432:PRO:HG2	1.96	0.47
1:A:62:TYR:HB3	1:A:64:TYR:CE1	2.51	0.46
1:A:156:MET:CE	1:A:205:ARG:HB2	2.45	0.46
3:C:206:THR:HB	3:C:220:LEU:H	1.79	0.46
1:D:220:ASN:HD21	1:D:340:GLY:HA2	1.80	0.46
3:F:117:ALA:HB3	6:F:503:HEC:HMD2	1.97	0.46
1:D:338:TRP:CD1	2:E:165:ASN:HB2	2.51	0.46
3:F:206:THR:HB	3:F:220:LEU:H	1.79	0.46
6:F:502:HEC:HBC3	6:F:502:HEC:HMC1	1.97	0.46
1:D:22:LEU:HD12	1:D:22:LEU:HA	1.76	0.46
1:D:62:TYR:HB3	1:D:64:TYR:CE1	2.50	0.46
1:D:308:HIS:HD2	1:D:312:ASN:ND2	2.13	0.46
1:D:442:GLU:HA	1:D:445:ARG:HB2	1.98	0.46
1:A:191:VAL:HG11	1:A:349:ILE:HD11	1.96	0.46
1:A:442:GLU:HA	1:A:445:ARG:HB2	1.98	0.46
3:C:156:PHE:HB3	3:C:157:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:ALA:H	1:D:447:SER:HB2	1.80	0.46
3:F:121:ASP:N	3:F:121:ASP:OD1	2.49	0.46
3:F:274:SER:OG	3:F:275:LEU:HD12	2.15	0.46
1:A:222:CYS:HB2	1:A:344:VAL:HG22	1.98	0.46
1:A:362:ALA:H	1:A:447:SER:HB2	1.81	0.46
3:F:115:TYR:CZ	3:F:154:LEU:HD12	2.51	0.46
1:A:98:GLN:HB2	1:A:477:ASN:HA	1.98	0.46
1:D:364:THR:HG22	1:D:409:HIS:CD2	2.51	0.46
3:F:124:ASN:HD21	3:F:175:GLY:H	1.64	0.46
1:A:169:ARG:NH2	1:A:171:ASN:O	2.49	0.46
3:C:44:HIS:ND1	3:C:137:TYR:HE1	2.14	0.46
1:D:223:MET:HG3	1:D:344:VAL:HG21	1.98	0.46
2:E:133:ILE:HG23	2:E:134:GLU:N	2.30	0.46
1:A:316:LEU:HD23	1:A:319:ARG:HD2	1.97	0.46
1:A:425:TYR:O	1:A:426:LYS:HE2	2.16	0.46
3:C:124:ASN:HD21	3:C:175:GLY:H	1.64	0.46
1:D:61:GLN:HB2	1:D:80:PHE:HZ	1.81	0.46
1:D:118:TYR:HD2	1:D:525:THR:HG1	1.63	0.46
3:F:64:PHE:CD2	3:F:65:LEU:HD23	2.46	0.46
3:C:43:GLY:HA3	3:C:137:TYR:HB2	1.97	0.45
6:C:502:HEC:HMC1	6:C:502:HEC:HBC3	1.97	0.45
1:D:425:TYR:O	1:D:426:LYS:HE2	2.16	0.45
1:A:364:THR:HG22	1:A:409:HIS:CD2	2.51	0.45
3:F:43:GLY:HA3	3:F:137:TYR:HB2	1.97	0.45
3:F:269:GLU:O	3:F:273:HIS:ND1	2.45	0.45
1:D:156:MET:CE	1:D:205:ARG:HB2	2.45	0.45
1:D:451:SER:O	1:D:455:LEU:HG	2.17	0.45
1:D:508:LEU:HD23	1:D:508:LEU:HA	1.78	0.45
3:F:44:HIS:ND1	3:F:137:TYR:HE1	2.14	0.45
2:B:158:VAL:HG22	2:B:159:ILE:N	2.32	0.45
2:B:159:ILE:HD12	2:B:159:ILE:H	1.81	0.45
3:C:115:TYR:CZ	3:C:154:LEU:HD12	2.51	0.45
1:D:169:ARG:NH2	1:D:171:ASN:O	2.49	0.45
1:D:222:CYS:HB2	1:D:344:VAL:HG22	1.98	0.45
2:E:83:LYS:HB2	2:E:86:PHE:HB2	1.98	0.45
1:A:220:ASN:ND2	1:A:340:GLY:O	2.50	0.45
1:D:440:VAL:HB	1:D:444:VAL:CG2	2.45	0.45
3:F:207:PRO:HD2	3:F:218:ALA:O	2.17	0.45
1:A:219:ASN:ND2	1:A:227:PRO:HG2	2.31	0.45
3:C:253:LEU:HD12	3:C:275:LEU:CD2	2.47	0.45
1:A:319:ARG:HH21	1:A:418:ARG:CZ	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:253:LEU:HD12	3:F:275:LEU:CD2	2.47	0.45
1:A:451:SER:O	1:A:455:LEU:HG	2.17	0.45
3:C:82:ASN:OD1	3:C:83:ILE:N	2.49	0.45
3:C:244:TRP:HZ2	3:C:366:THR:HG21	1.82	0.45
1:D:304:ASP:OD1	1:D:305:ARG:N	2.50	0.45
3:F:46:LEU:HD23	3:F:46:LEU:HA	1.77	0.45
3:F:244:TRP:HZ2	3:F:366:THR:HG21	1.81	0.45
1:A:61:GLN:HB2	1:A:80:PHE:HZ	1.81	0.45
1:A:499:ARG:HB2	1:A:507:PHE:CE1	2.52	0.45
2:B:83:LYS:HB2	2:B:86:PHE:HB2	1.98	0.45
2:E:159:ILE:HD12	2:E:159:ILE:H	1.81	0.45
1:A:298:LEU:HB2	1:A:317:VAL:HG21	1.99	0.45
3:C:125:ARG:HA	3:C:177:PRO:HA	1.99	0.45
3:C:207:PRO:HD2	3:C:218:ALA:O	2.17	0.45
1:A:223:MET:HG3	1:A:344:VAL:HG21	1.98	0.44
2:B:158:VAL:HG21	3:C:356:ASP:OD1	2.16	0.44
3:F:82:ASN:OD1	3:F:83:ILE:N	2.49	0.44
3:F:113:GLN:HB2	3:F:164:LEU:HD12	2.00	0.44
3:F:380:ILE:HG21	3:F:412:ILE:HG23	1.99	0.44
1:A:14:GLY:HA3	1:A:288:ALA:O	2.17	0.44
1:A:386:LEU:HD12	1:A:390:LYS:HG3	2.00	0.44
2:B:118:HIS:ND1	2:B:122:ILE:HA	2.32	0.44
1:D:14:GLY:HA3	1:D:288:ALA:O	2.17	0.44
1:D:98:GLN:HB2	1:D:477:ASN:HA	1.98	0.44
1:A:38:ALA:O	1:A:251:ASN:HA	2.18	0.44
1:D:298:LEU:HB2	1:D:317:VAL:HG21	1.99	0.44
1:D:319:ARG:HH21	1:D:418:ARG:CZ	2.30	0.44
1:D:382:LEU:HD11	2:E:135:ASP:HA	1.99	0.44
2:E:158:VAL:HG22	2:E:159:ILE:N	2.32	0.44
1:A:382:LEU:HD11	2:B:135:ASP:HA	2.00	0.44
3:C:258:THR:HG22	3:C:259:ALA:H	1.82	0.44
1:D:37:ASP:OD1	4:D:601:FAD:H51A	2.18	0.44
1:D:499:ARG:HB2	1:D:507:PHE:CE1	2.52	0.44
3:F:258:THR:HG22	3:F:259:ALA:H	1.82	0.44
1:D:219:ASN:ND2	1:D:227:PRO:HG2	2.31	0.44
1:D:220:ASN:ND2	1:D:340:GLY:O	2.50	0.44
1:D:421:LEU:HD23	1:D:421:LEU:H	1.83	0.44
1:A:304:ASP:OD1	1:A:305:ARG:N	2.50	0.44
1:A:421:LEU:HD23	1:A:421:LEU:H	1.83	0.44
3:F:125:ARG:HA	3:F:177:PRO:HA	1.99	0.44
3:C:113:GLN:HB2	3:C:164:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:380:ILE:HG21	3:C:412:ILE:HG23	1.99	0.44
1:D:295:PRO:HB3	1:D:318:GLY:HA2	1.99	0.44
1:D:312:ASN:OD1	1:D:317:VAL:HG12	2.18	0.44
1:A:37:ASP:OD1	4:A:601:FAD:H51A	2.18	0.43
1:A:106:GLY:HA2	4:A:601:FAD:O2A	2.17	0.43
2:B:89:GLN:O	2:B:93:LEU:HG	2.18	0.43
1:D:106:GLY:HA2	4:D:601:FAD:O2A	2.17	0.43
3:C:64:PHE:CD2	3:C:65:LEU:HD23	2.46	0.43
3:C:124:ASN:HD21	3:C:174:GLU:HA	1.84	0.43
1:D:38:ALA:O	1:D:251:ASN:HA	2.18	0.43
1:D:311:ALA:H	1:D:503:HIS:CE1	2.36	0.43
3:C:121:ASP:N	3:C:121:ASP:OD1	2.49	0.43
1:A:295:PRO:HB3	1:A:318:GLY:HA2	1.99	0.43
2:B:149:MET:SD	2:B:161:THR:HG21	2.59	0.43
1:D:21:LEU:HD12	1:D:527:ALA:HB1	2.00	0.43
1:D:255:TYR:HH	1:D:269:SER:HG	1.62	0.43
3:C:258:THR:HG22	3:C:259:ALA:N	2.33	0.43
3:F:94:TYR:CE1	3:F:109:ALA:HB2	2.54	0.43
3:F:258:THR:HG22	3:F:259:ALA:N	2.33	0.43
1:D:55:PRO:HA	1:D:56:PRO:HD3	1.88	0.43
3:C:94:TYR:CE1	3:C:109:ALA:HB2	2.54	0.43
3:C:120:TYR:HA	3:C:123:TYR:HB2	2.00	0.43
3:C:348:GLN:HG2	3:C:353:GLY:O	2.18	0.43
1:D:175:MET:HE2	1:D:210:TYR:HB2	2.01	0.43
2:E:118:HIS:ND1	2:E:122:ILE:HA	2.32	0.43
2:E:158:VAL:HG22	2:E:159:ILE:H	1.84	0.43
1:A:175:MET:HE2	1:A:210:TYR:HB2	2.01	0.43
3:F:124:ASN:HD21	3:F:174:GLU:HA	1.84	0.43
3:F:348:GLN:HG2	3:F:353:GLY:O	2.18	0.43
1:A:156:MET:SD	1:A:177:SER:HA	2.59	0.43
1:A:521:ASN:CB	4:A:601:FAD:HN3	2.22	0.43
2:B:158:VAL:HG22	2:B:159:ILE:H	1.84	0.43
3:C:164:LEU:O	3:C:168:LYS:N	2.43	0.43
3:C:402:SER:OG	3:C:403:LEU:N	2.52	0.43
3:F:120:TYR:HA	3:F:123:TYR:HB2	2.01	0.43
3:F:187:ASP:OD2	3:F:288:THR:OG1	2.35	0.43
1:A:21:LEU:HD12	1:A:527:ALA:HB1	2.00	0.42
1:A:258:GLU:HB2	1:A:267:ALA:HB3	2.01	0.42
3:C:118:MET:HB3	3:C:120:TYR:H	1.83	0.42
3:F:118:MET:HB3	3:F:120:TYR:H	1.83	0.42
3:F:160:ILE:HG13	3:F:160:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:402:SER:OG	3:F:403:LEU:N	2.52	0.42
1:A:312:ASN:OD1	1:A:317:VAL:HG12	2.18	0.42
1:A:368:TYR:HB2	1:A:404:ASP:O	2.19	0.42
3:C:194:LEU:HD23	3:C:198:LEU:HB2	2.01	0.42
1:D:386:LEU:HD12	1:D:390:LYS:HG3	2.00	0.42
2:E:89:GLN:O	2:E:93:LEU:HG	2.19	0.42
3:F:394:LEU:HD23	3:F:395:MET:N	2.34	0.42
1:A:13:ILE:HG12	1:A:286:VAL:O	2.19	0.42
1:D:13:ILE:HG12	1:D:286:VAL:O	2.19	0.42
1:D:38:ALA:HB2	4:D:601:FAD:H2B	2.01	0.42
3:F:57:THR:HB	3:F:64:PHE:HA	2.02	0.42
3:F:224:ASP:OD1	3:F:224:ASP:N	2.51	0.42
3:C:202:GLY:O	3:C:204:CYS:N	2.52	0.42
1:D:156:MET:SD	1:D:177:SER:HA	2.59	0.42
3:F:232:ASN:OD1	3:F:234:THR:OG1	2.23	0.42
3:F:384:VAL:HG22	3:F:395:MET:HB3	2.01	0.42
1:D:201:VAL:O	1:D:203:GLN:HG3	2.20	0.42
1:D:284:THR:HA	1:D:505:ASN:OD1	2.20	0.42
2:E:149:MET:SD	2:E:161:THR:HG21	2.59	0.42
3:F:82:ASN:OD1	3:F:84:THR:N	2.51	0.42
1:A:77:THR:HG22	1:A:78:ASN:H	1.85	0.42
3:C:232:ASN:OD1	3:C:234:THR:OG1	2.23	0.42
3:C:384:VAL:HG22	3:C:395:MET:HB3	2.01	0.42
3:C:394:LEU:HD23	3:C:395:MET:N	2.34	0.42
1:D:368:TYR:HB2	1:D:404:ASP:O	2.20	0.42
1:D:522:SER:O	1:D:522:SER:OG	2.29	0.42
1:A:500:THR:OG1	1:A:506:LEU:HB3	2.20	0.42
3:C:212:LEU:HD23	3:C:212:LEU:HA	1.82	0.42
3:F:202:GLY:O	3:F:204:CYS:N	2.52	0.42
3:C:367:THR:HG23	3:C:375:ASP:HB3	2.02	0.42
3:F:194:LEU:HD23	3:F:198:LEU:HB2	2.01	0.42
3:F:220:LEU:HD22	3:F:233:ILE:HD11	2.01	0.42
2:B:97:ILE:HD12	2:B:97:ILE:HA	1.92	0.42
1:A:523:THR:HA	1:A:526:MET:HB2	2.02	0.42
3:C:81:THR:HB	6:C:503:HEC:O2A	2.20	0.42
1:D:500:THR:OG1	1:D:506:LEU:HB3	2.20	0.42
1:D:523:THR:HA	1:D:526:MET:HB2	2.02	0.42
1:A:244:LEU:HD12	1:A:244:LEU:HA	1.93	0.41
3:F:94:TYR:CZ	3:F:109:ALA:HB2	2.55	0.41
1:A:452:ARG:HG2	1:A:469:MET:SD	2.60	0.41
3:C:56:HIS:CE1	3:C:83:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:HIS:HE1	4:D:601:FAD:HM71	1.84	0.41
2:E:116:PRO:O	2:E:121:LEU:HD13	2.21	0.41
2:B:50:SER:O	2:B:76:LEU:HD11	2.20	0.41
3:C:57:THR:HB	3:C:64:PHE:HA	2.02	0.41
3:C:371:LEU:HD12	3:C:371:LEU:HA	1.95	0.41
1:D:258:GLU:HB2	1:D:267:ALA:HB3	2.01	0.41
1:D:288:ALA:HA	1:D:510:THR:HG1	1.85	0.41
1:D:469:MET:HB2	1:D:469:MET:HE3	1.98	0.41
2:E:50:SER:O	2:E:76:LEU:HD11	2.20	0.41
1:A:201:VAL:O	1:A:203:GLN:HG3	2.20	0.41
2:B:124:ILE:O	2:B:124:ILE:HG13	2.20	0.41
2:E:118:HIS:H	2:E:121:LEU:HB2	1.86	0.41
3:F:78:ILE:HD12	3:F:78:ILE:H	1.85	0.41
1:A:38:ALA:HB2	4:A:601:FAD:H2B	2.02	0.41
1:A:284:THR:HA	1:A:505:ASN:OD1	2.20	0.41
2:B:118:HIS:H	2:B:121:LEU:HB2	1.86	0.41
3:F:81:THR:HB	6:F:503:HEC:O2A	2.20	0.41
1:D:77:THR:HG22	1:D:78:ASN:H	1.85	0.41
3:F:56:HIS:CE1	3:F:83:ILE:HD11	2.55	0.41
1:A:337:ILE:HD13	1:A:337:ILE:HA	1.90	0.41
1:D:337:ILE:HD13	1:D:337:ILE:HA	1.90	0.41
3:F:367:THR:HG23	3:F:375:ASP:HB3	2.02	0.41
1:A:48:VAL:HG12	1:A:52:ARG:HE	1.86	0.41
1:A:63:ASP:OD2	1:A:66:THR:OG1	2.18	0.41
3:C:78:ILE:HD12	3:C:78:ILE:H	1.85	0.41
3:C:94:TYR:CZ	3:C:109:ALA:HB2	2.55	0.41
3:C:220:LEU:HD22	3:C:233:ILE:HD11	2.01	0.41
1:D:43:ASP:O	1:D:47:ILE:HG12	2.21	0.41
1:D:48:VAL:HG12	1:D:52:ARG:HE	1.86	0.41
1:D:77:THR:HG22	1:D:78:ASN:N	2.36	0.41
1:D:163:ILE:HG13	1:D:164:THR:N	2.36	0.41
1:D:452:ARG:HG2	1:D:469:MET:SD	2.60	0.41
2:E:124:ILE:HG13	2:E:124:ILE:O	2.20	0.41
1:A:13:ILE:CG1	1:A:287:ILE:HA	2.51	0.41
1:A:133:ARG:HG2	1:A:133:ARG:HH11	1.86	0.41
2:B:116:PRO:O	2:B:121:LEU:HD13	2.20	0.41
3:F:164:LEU:O	3:F:168:LYS:N	2.43	0.41
1:A:157:GLY:O	1:A:177:SER:N	2.55	0.40
2:E:133:ILE:HG23	2:E:134:GLU:H	1.86	0.40
1:A:97:LYS:O	1:A:475:PRO:HG3	2.21	0.40
1:A:380:LYS:HD2	1:A:398:ARG:NE	2.28	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:ARG:HD2	3:C:213:ALA:O	2.22	0.40
3:C:224:ASP:N	3:C:224:ASP:OD1	2.51	0.40
3:F:108:ARG:HG2	3:F:109:ALA:H	1.86	0.40
3:F:191:GLY:HA3	3:F:289:TYR:HB2	2.04	0.40
1:A:54:MET:HA	1:A:55:PRO:HD3	1.96	0.40
1:A:77:THR:HG22	1:A:78:ASN:N	2.36	0.40
1:D:157:GLY:O	1:D:177:SER:N	2.55	0.40
1:D:275:LYS:HG3	1:D:275:LYS:O	2.22	0.40
2:E:87:SER:HA	2:E:90:ILE:HG12	2.03	0.40
1:A:68:TYR:CE2	1:A:109:TRP:HB3	2.57	0.40
2:B:87:SER:HA	2:B:90:ILE:HG12	2.04	0.40
3:C:160:ILE:O	3:C:160:ILE:HG13	2.20	0.40
1:D:13:ILE:CG1	1:D:287:ILE:HA	2.51	0.40
1:D:133:ARG:HH11	1:D:133:ARG:HG2	1.86	0.40
2:E:86:PHE:O	2:E:90:ILE:HG23	2.21	0.40
1:A:219:ASN:HB2	5:A:602:F3S:S1	2.62	0.40
1:A:311:ALA:H	1:A:503:HIS:CE1	2.36	0.40
3:C:108:ARG:HG2	3:C:109:ALA:H	1.86	0.40
3:C:205:HIS:ND1	3:C:230:ALA:HB1	2.36	0.40
3:F:212:LEU:HD23	3:F:212:LEU:HA	1.82	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	535/544 (98%)	473 (88%)	61 (11%)	1 (0%)	47	79
1	D	535/544 (98%)	473 (88%)	61 (11%)	1 (0%)	47	79
2	B	87/183 (48%)	68 (78%)	19 (22%)	0	100	100
2	E	87/183 (48%)	68 (78%)	19 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	414/486 (85%)	377 (91%)	34 (8%)	3 (1%)	22	61
3	F	414/486 (85%)	378 (91%)	33 (8%)	3 (1%)	22	61
All	All	2072/2426 (85%)	1837 (89%)	227 (11%)	8 (0%)	38	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	157	PRO
3	F	157	PRO
3	C	155	PRO
3	F	155	PRO
3	C	156	PHE
3	F	156	PHE
1	A	81	PRO
1	D	81	PRO

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	440/446 (99%)	440 (100%)	0	100	100
1	D	440/446 (99%)	440 (100%)	0	100	100
2	B	84/152 (55%)	84 (100%)	0	100	100
2	E	84/152 (55%)	84 (100%)	0	100	100
3	C	328/384 (85%)	327 (100%)	1 (0%)	92	97
3	F	328/384 (85%)	327 (100%)	1 (0%)	92	97
All	All	1704/1964 (87%)	1702 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	449	LYS
3	F	449	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	HIS
1	A	220	ASN
1	A	308	HIS
1	A	503	HIS
3	C	124	ASN
3	C	365	ASN
1	D	110	HIS
1	D	220	ASN
1	D	308	HIS
1	D	503	HIS
2	E	89	GLN
2	E	123	GLN
3	F	124	ASN
3	F	365	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 monosaccharides 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
6	HEC	F	501	3	32,50,50	2.21	4 (12%)	24,82,82	2.02	8 (33%)
6	HEC	F	502	3	32,50,50	2.37	4 (12%)	24,82,82	1.70	6 (25%)
4	FAD	A	601	-	53,58,58	0.71	1 (1%)	68,89,89	0.80	3 (4%)
5	F3S	D	602	1	0,9,9	-	-	-	-	-
6	HEC	C	502	3	32,50,50	2.38	4 (12%)	24,82,82	1.71	6 (25%)
6	HEC	F	503	3	32,50,50	2.26	4 (12%)	24,82,82	1.61	3 (12%)
4	FAD	D	601	-	53,58,58	0.71	1 (1%)	68,89,89	0.81	3 (4%)
6	HEC	C	503	3	32,50,50	2.25	4 (12%)	24,82,82	1.61	3 (12%)
6	HEC	C	501	3	32,50,50	2.21	4 (12%)	24,82,82	2.03	8 (33%)
5	F3S	A	602	1	0,9,9	-	-	-	-	-

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
6	HEC	F	502	3	-	4/10/54/54	-
4	FAD	A	601	-	-	8/30/50/50	0/6/6/6
5	F3S	D	602	1	-	-	0/3/3/3
6	HEC	C	502	3	-	4/10/54/54	-
5	F3S	A	602	1	-	-	0/3/3/3
6	HEC	F	503	3	-	3/10/54/54	-
4	FAD	D	601	-	-	8/30/50/50	0/6/6/6
6	HEC	C	501	3	-	5/10/54/54	-
6	HEC	C	503	3	-	3/10/54/54	-
6	HEC	F	501	3	-	5/10/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	HEC	C2B-C3B	-8.05	1.32	1.40
6	F	502	HEC	C2B-C3B	-7.98	1.32	1.40
6	F	503	HEC	C3C-C2C	-7.07	1.33	1.40
6	C	503	HEC	C3C-C2C	-7.06	1.33	1.40
6	F	501	HEC	C3C-C2C	-6.98	1.33	1.40
6	C	501	HEC	C3C-C2C	-6.96	1.33	1.40
6	C	502	HEC	C3C-C2C	-6.89	1.33	1.40
6	F	502	HEC	C3C-C2C	-6.82	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	501	HEC	C2B-C3B	-6.75	1.33	1.40
6	C	501	HEC	C2B-C3B	-6.74	1.33	1.40
6	F	503	HEC	C2B-C3B	-6.37	1.34	1.40
6	C	503	HEC	C2B-C3B	-6.36	1.34	1.40
6	F	503	HEC	C3D-C2D	5.42	1.53	1.37
6	C	503	HEC	C3D-C2D	5.42	1.53	1.37
6	F	502	HEC	C3D-C2D	5.40	1.53	1.37
6	C	502	HEC	C3D-C2D	5.39	1.53	1.37
6	C	501	HEC	C3D-C2D	5.15	1.52	1.37
6	F	501	HEC	C3D-C2D	5.15	1.52	1.37
6	F	503	HEC	CAD-C3D	2.46	1.55	1.52
6	C	503	HEC	CAD-C3D	2.39	1.55	1.52
6	F	501	HEC	CAD-C3D	2.31	1.55	1.52
6	C	501	HEC	CAD-C3D	2.28	1.55	1.52
4	A	601	FAD	C4-N3	-2.12	1.34	1.38
4	D	601	FAD	C4-N3	-2.11	1.34	1.38
6	C	502	HEC	CAD-C3D	2.02	1.55	1.52
6	F	502	HEC	CAD-C3D	2.02	1.55	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	501	HEC	CMB-C2B-C1B	-4.12	122.14	128.46
6	C	501	HEC	CMB-C2B-C1B	-4.10	122.16	128.46
6	C	503	HEC	CMB-C2B-C1B	-3.75	122.70	128.46
6	F	503	HEC	CMB-C2B-C1B	-3.74	122.71	128.46
6	C	502	HEC	CMC-C2C-C1C	-3.55	123.00	128.46
6	C	501	HEC	CAA-CBA-CGA	-3.53	103.85	113.76
6	F	501	HEC	CAA-CBA-CGA	-3.53	103.86	113.76
6	F	502	HEC	CMC-C2C-C1C	-3.52	123.06	128.46
6	F	501	HEC	CMB-C2B-C3B	3.43	129.85	125.82
6	C	501	HEC	CMB-C2B-C3B	3.41	129.83	125.82
6	C	502	HEC	CMD-C2D-C1D	-3.19	123.56	128.46
6	F	502	HEC	CMD-C2D-C1D	-3.19	123.56	128.46
4	A	601	FAD	P-O3P-PA	-3.16	121.98	132.83
4	D	601	FAD	P-O3P-PA	-3.15	122.03	132.83
6	C	503	HEC	CMC-C2C-C1C	-3.14	123.64	128.46
6	F	503	HEC	CMC-C2C-C1C	-3.11	123.69	128.46
6	F	502	HEC	CMD-C2D-C3D	3.04	130.67	124.94
6	C	502	HEC	CMD-C2D-C3D	3.04	130.67	124.94
6	C	502	HEC	CBA-CAA-C2A	-2.97	107.60	112.60
6	F	501	HEC	CMC-C2C-C1C	-2.97	123.91	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	502	HEC	CBA-CAA-C2A	-2.96	107.62	112.60
6	C	501	HEC	CMC-C2C-C1C	-2.95	123.92	128.46
6	F	503	HEC	CMB-C2B-C3B	2.73	129.03	125.82
6	C	503	HEC	CMB-C2B-C3B	2.72	129.02	125.82
6	C	501	HEC	CMD-C2D-C3D	2.57	129.79	124.94
6	F	501	HEC	CMD-C2D-C3D	2.56	129.76	124.94
4	D	601	FAD	C4'-C3'-C2'	2.48	118.52	113.36
4	A	601	FAD	C4'-C3'-C2'	2.48	118.51	113.36
6	F	501	HEC	CMD-C2D-C1D	-2.38	124.81	128.46
6	C	501	HEC	CMD-C2D-C1D	-2.36	124.83	128.46
4	A	601	FAD	C5A-C6A-N6A	2.32	123.88	120.35
6	C	501	HEC	C1D-C2D-C3D	-2.32	105.38	107.00
4	D	601	FAD	C5A-C6A-N6A	2.31	123.87	120.35
6	F	501	HEC	C1D-C2D-C3D	-2.26	105.42	107.00
6	C	501	HEC	CBD-CAD-C3D	2.10	116.20	112.62
6	F	501	HEC	CBD-CAD-C3D	2.09	116.19	112.62
6	C	502	HEC	CMB-C2B-C1B	-2.08	125.27	128.46
6	F	502	HEC	CMB-C2B-C1B	-2.06	125.30	128.46
6	C	502	HEC	CAA-CBA-CGA	-2.04	108.03	113.76
6	F	502	HEC	CAA-CBA-CGA	-2.03	108.05	113.76

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	FAD	C5B-O5B-PA-O1A
4	A	601	FAD	C3'-C4'-C5'-O5'
4	A	601	FAD	O4'-C4'-C5'-O5'
4	A	601	FAD	C5'-O5'-P-O1P
4	A	601	FAD	C5'-O5'-P-O3P
4	D	601	FAD	C5B-O5B-PA-O1A
4	D	601	FAD	C3'-C4'-C5'-O5'
4	D	601	FAD	O4'-C4'-C5'-O5'
4	D	601	FAD	C5'-O5'-P-O1P
4	D	601	FAD	C5'-O5'-P-O3P
6	C	501	HEC	C1A-C2A-CAA-CBA
6	C	501	HEC	C3A-C2A-CAA-CBA
6	C	501	HEC	C2D-C3D-CAD-CBD
6	C	501	HEC	C4D-C3D-CAD-CBD
6	C	502	HEC	C2D-C3D-CAD-CBD
6	C	502	HEC	C4D-C3D-CAD-CBD
6	F	501	HEC	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
6	F	501	HEC	C3A-C2A-CAA-CBA
6	F	501	HEC	C2D-C3D-CAD-CBD
6	F	501	HEC	C4D-C3D-CAD-CBD
6	F	502	HEC	C2D-C3D-CAD-CBD
6	F	502	HEC	C4D-C3D-CAD-CBD
4	A	601	FAD	C3B-C4B-C5B-O5B
4	D	601	FAD	C3B-C4B-C5B-O5B
6	C	503	HEC	C3D-CAD-CBD-CGD
6	F	503	HEC	C3D-CAD-CBD-CGD
4	A	601	FAD	O4B-C4B-C5B-O5B
4	D	601	FAD	O4B-C4B-C5B-O5B
6	C	503	HEC	C2D-C3D-CAD-CBD
6	C	503	HEC	C4D-C3D-CAD-CBD
6	F	503	HEC	C2D-C3D-CAD-CBD
6	F	503	HEC	C4D-C3D-CAD-CBD
6	C	501	HEC	C3D-CAD-CBD-CGD
6	F	501	HEC	C3D-CAD-CBD-CGD
6	C	502	HEC	CAA-CBA-CGA-O1A
6	F	502	HEC	CAA-CBA-CGA-O1A
4	A	601	FAD	C5B-O5B-PA-O3P
4	D	601	FAD	C5B-O5B-PA-O3P
6	F	502	HEC	CAA-CBA-CGA-O2A
6	C	502	HEC	CAA-CBA-CGA-O2A

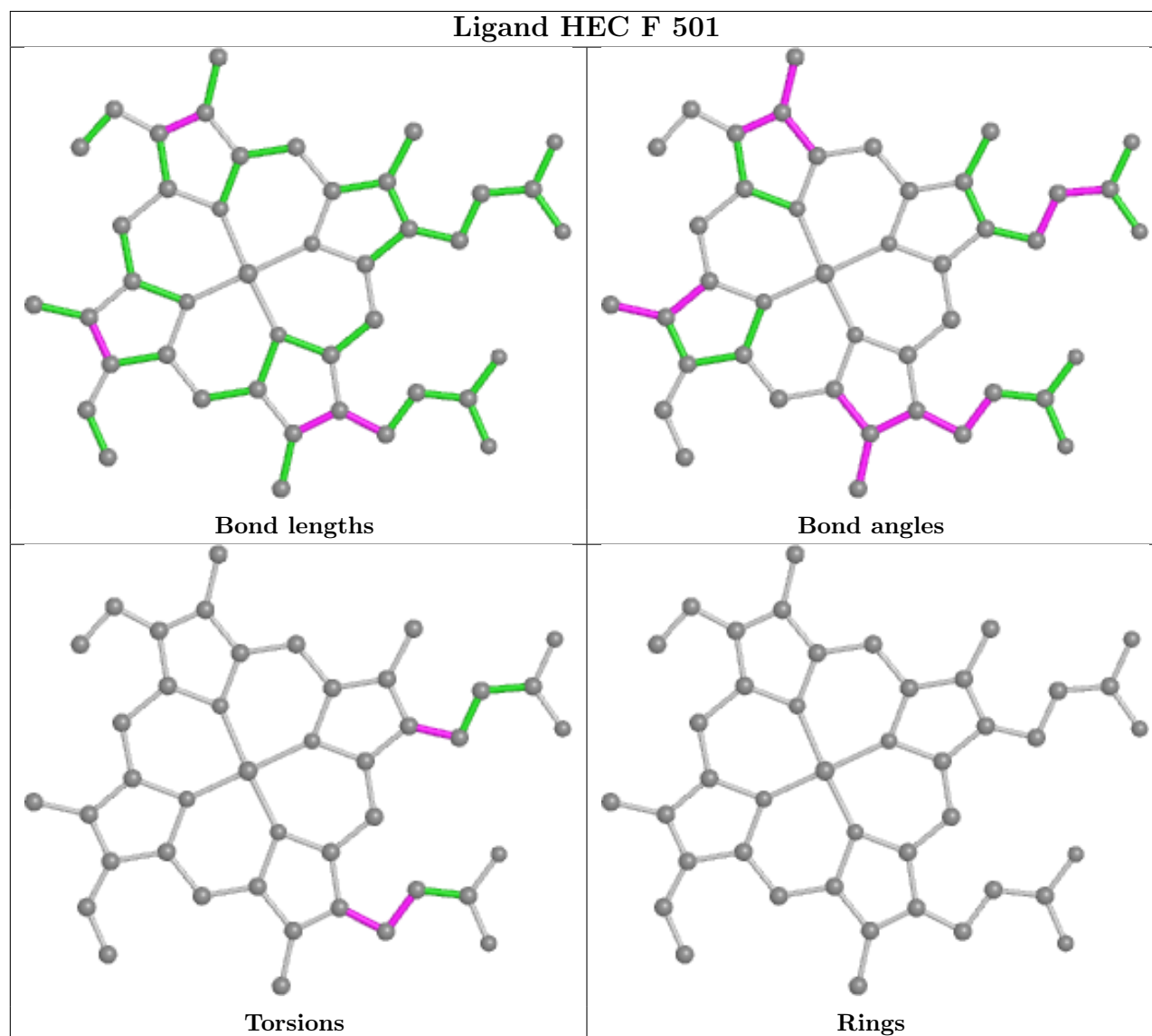
There are no ring outliers.

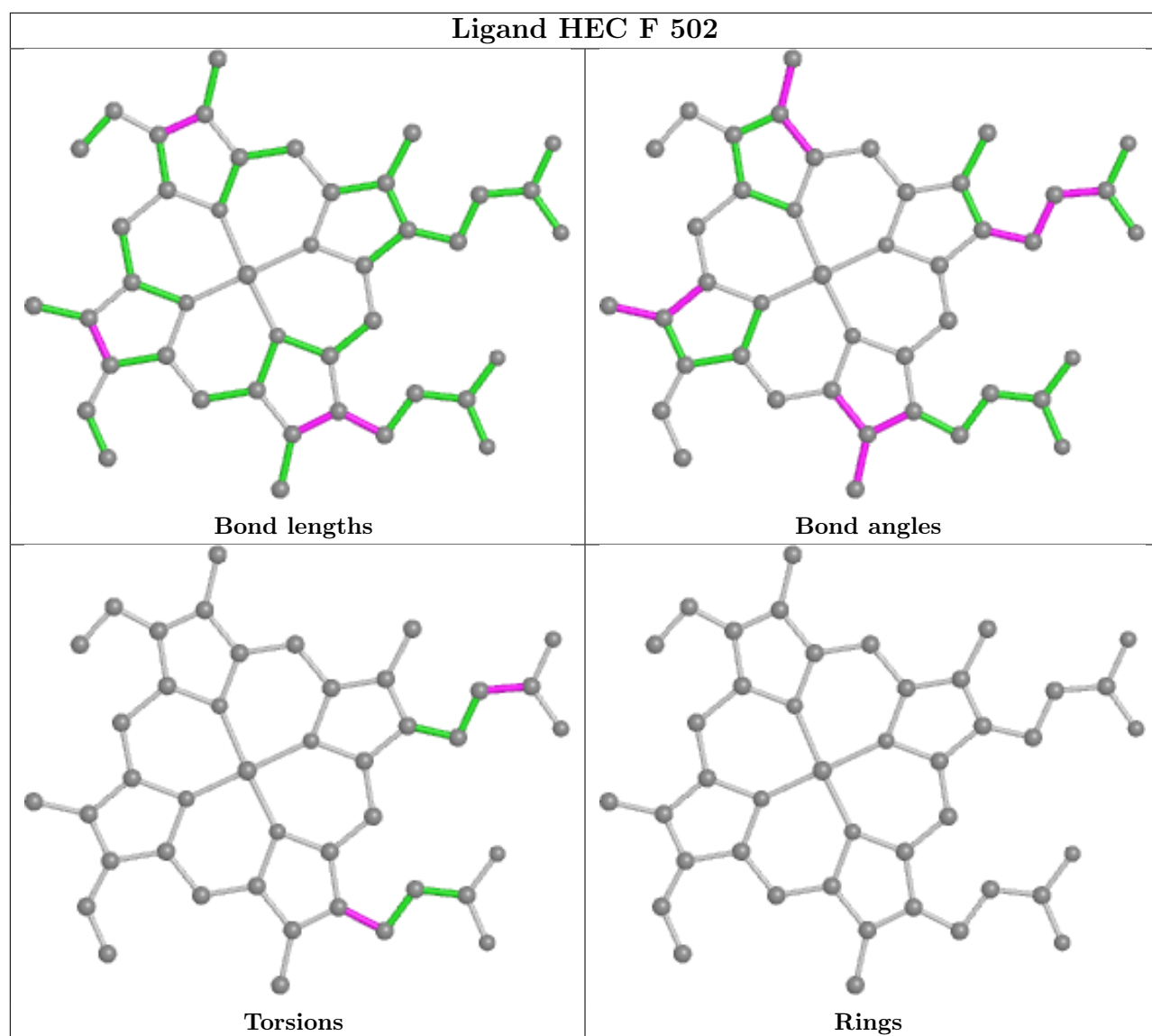
10 monomers are involved in 43 short contacts:

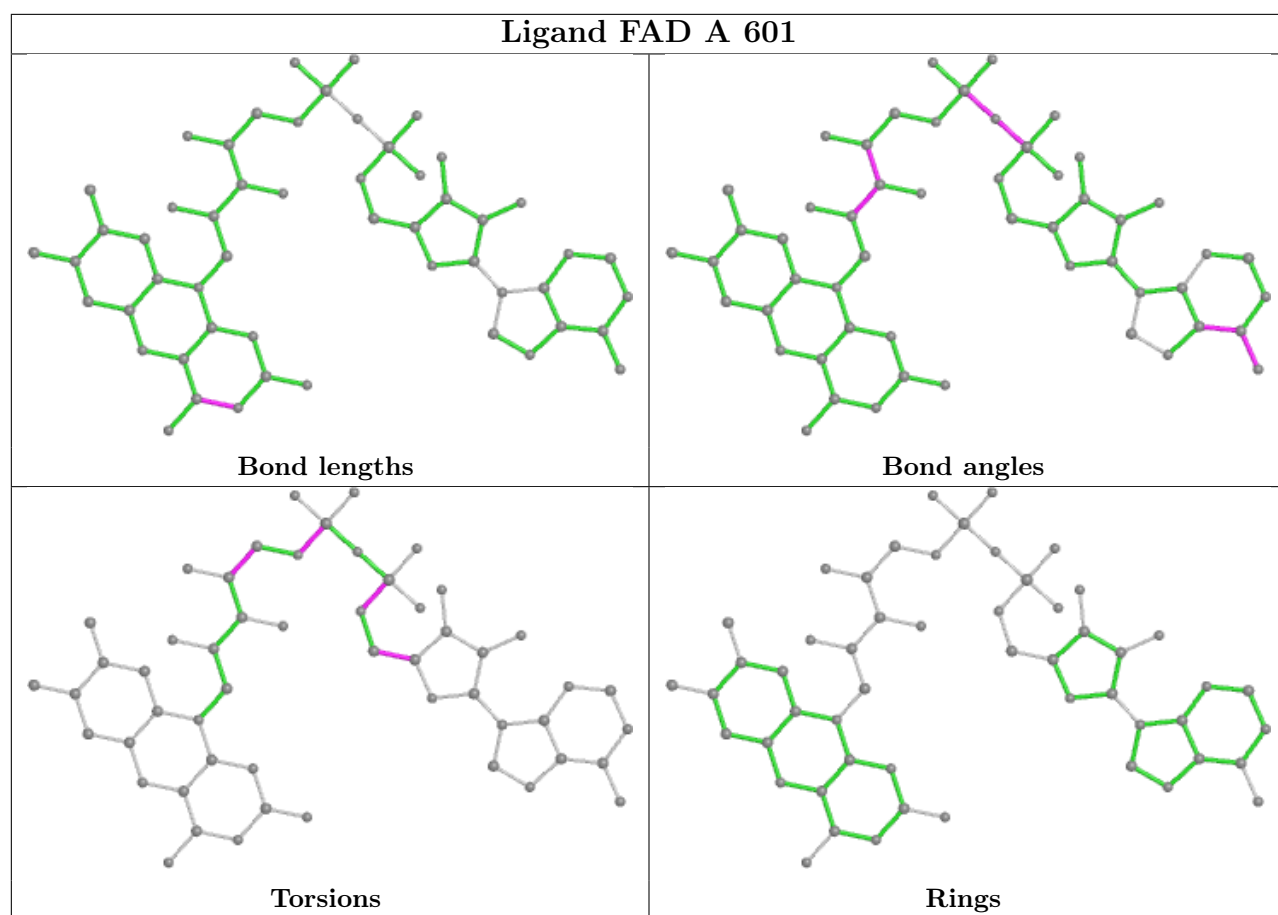
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	501	HEC	5	0
6	F	502	HEC	3	0
4	A	601	FAD	9	0
5	D	602	F3S	1	0
6	C	502	HEC	3	0
6	F	503	HEC	3	0
4	D	601	FAD	9	0
6	C	503	HEC	3	0
6	C	501	HEC	5	0
5	A	602	F3S	2	0

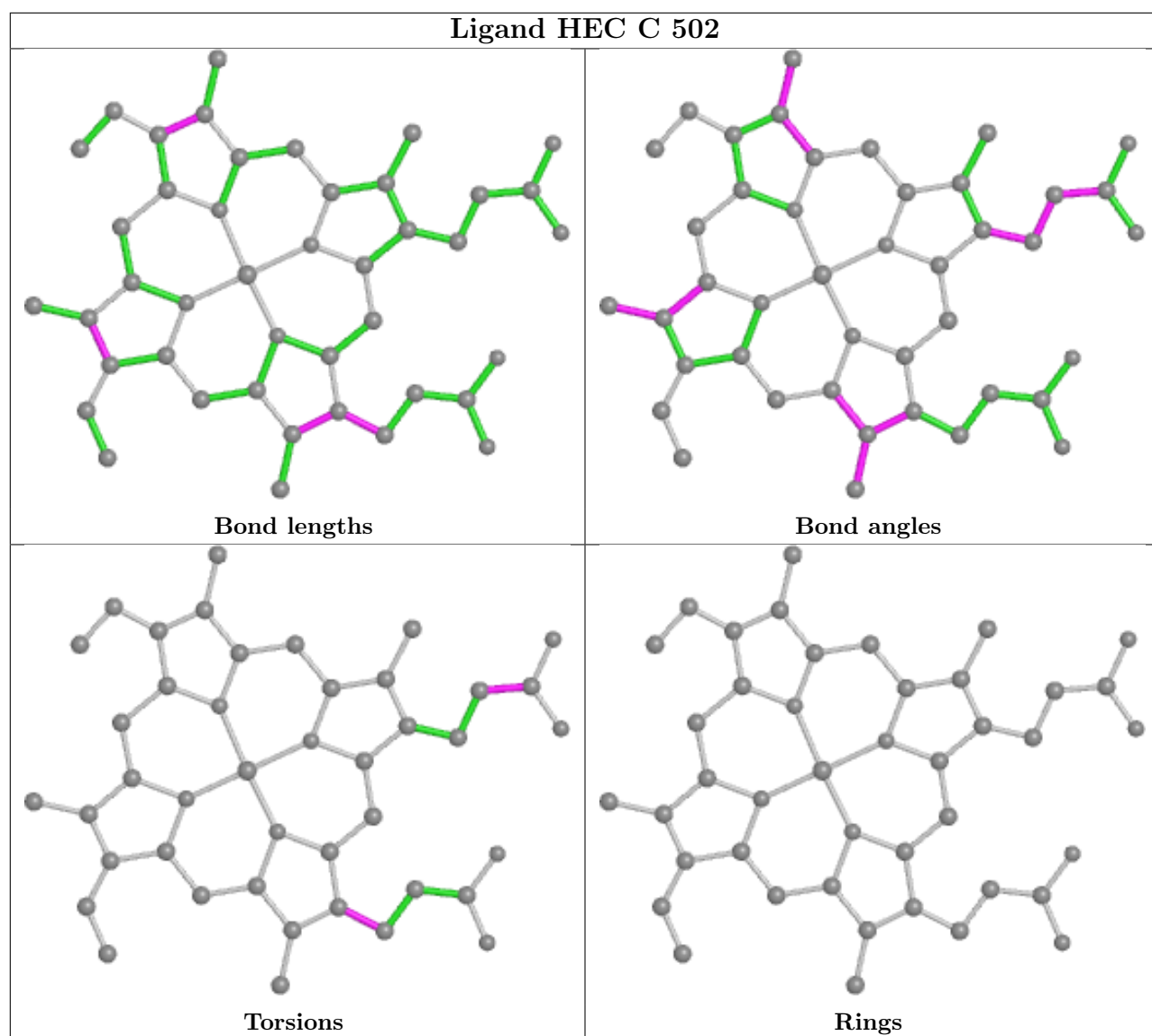
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

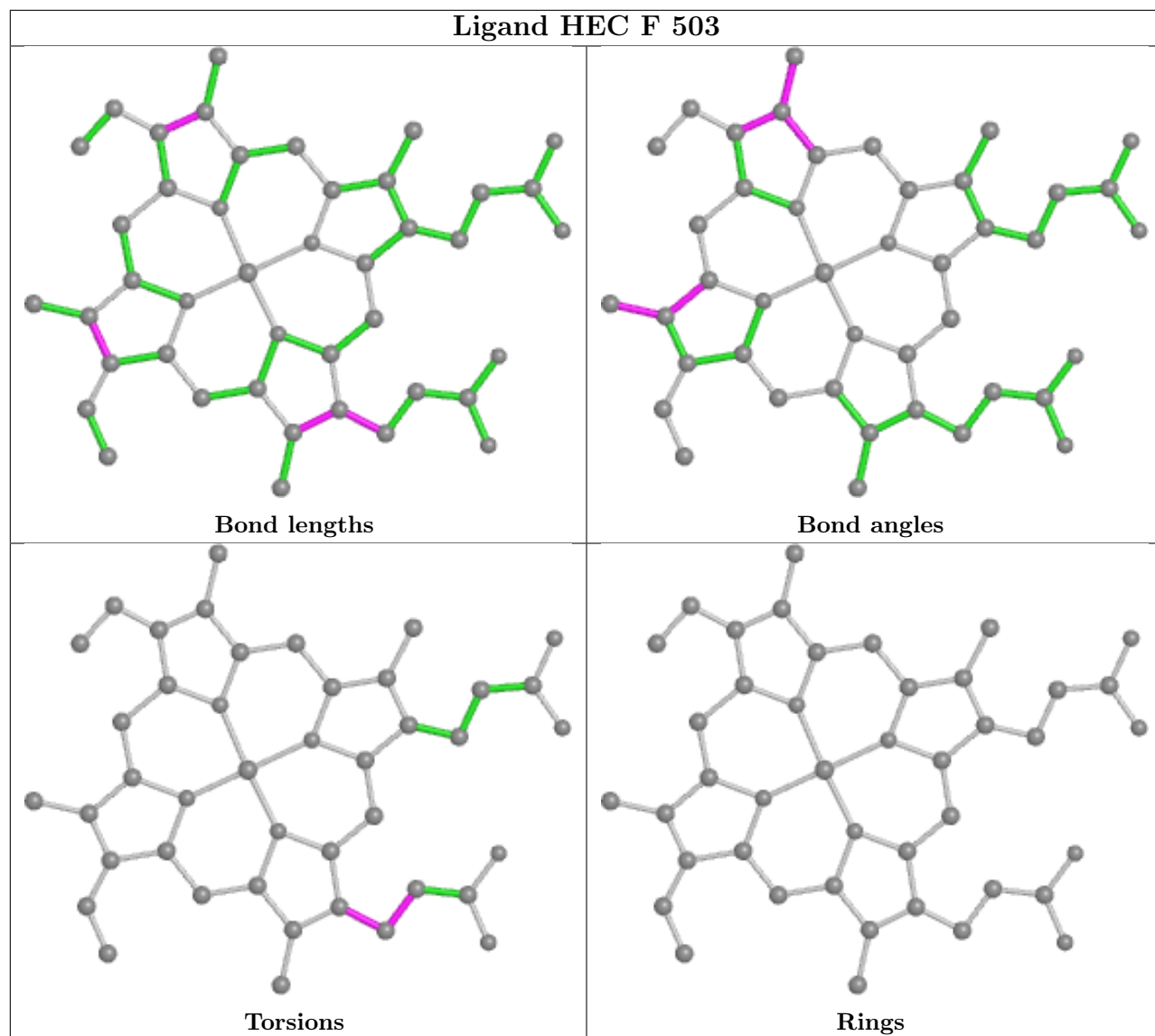
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

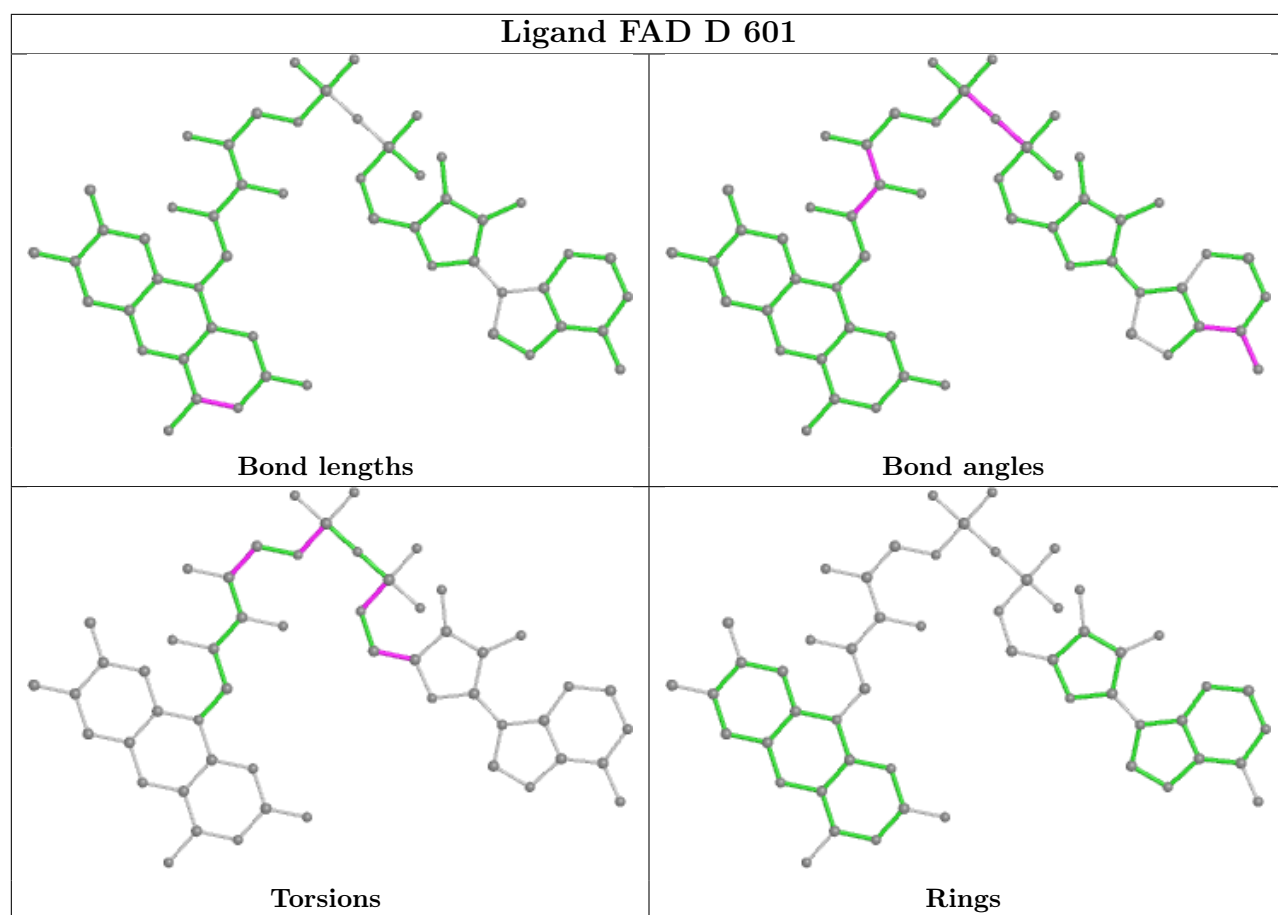


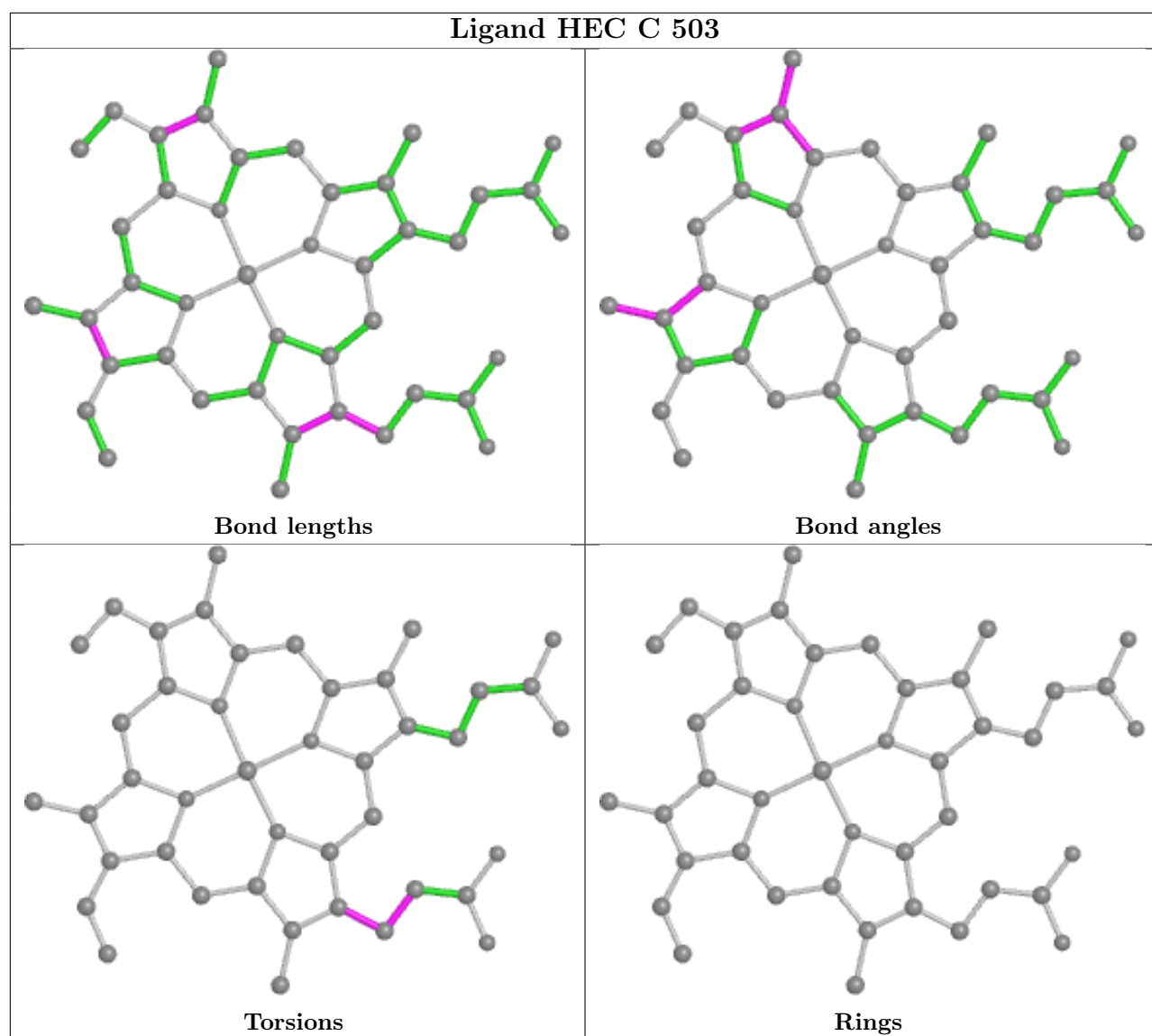


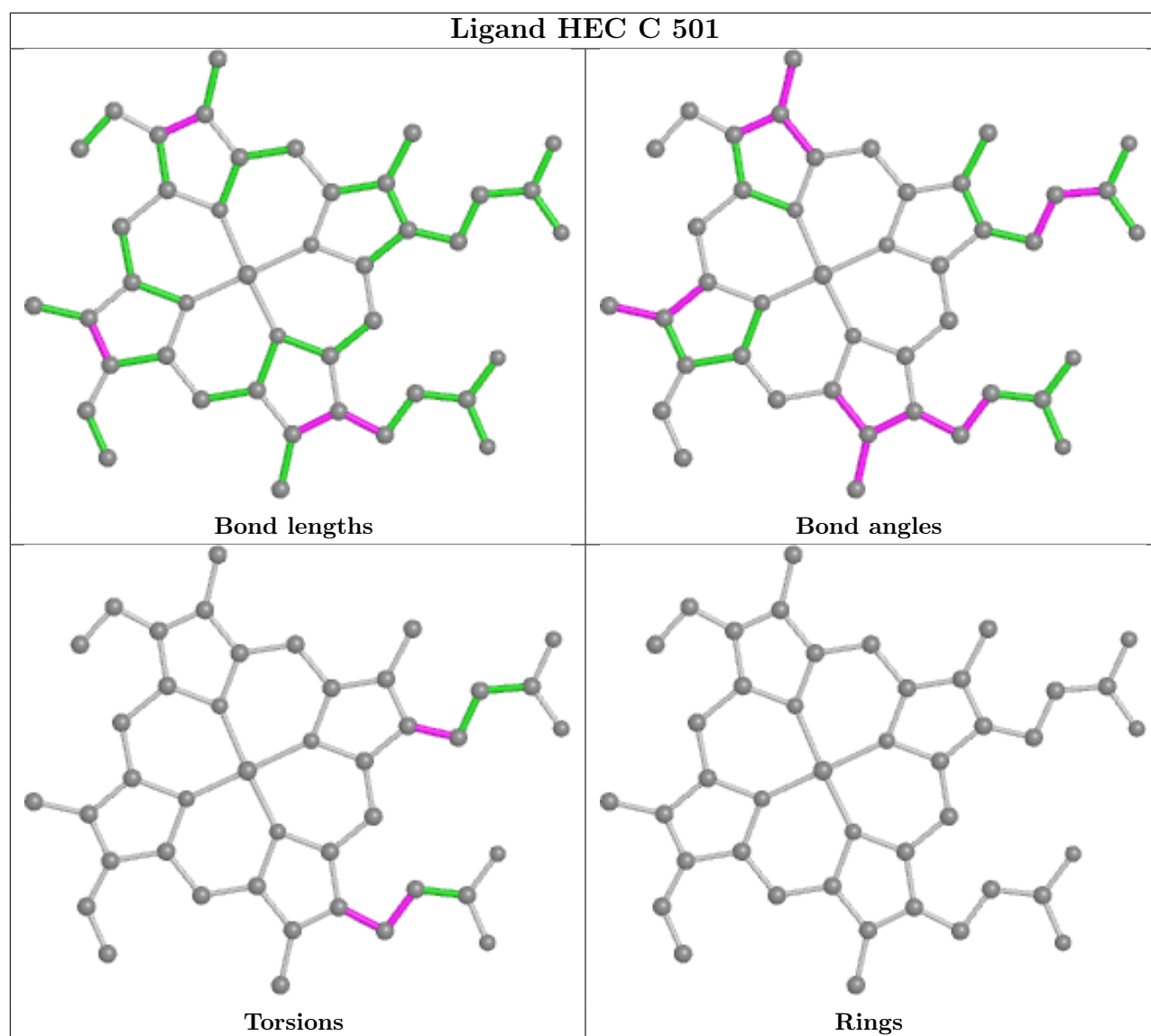












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

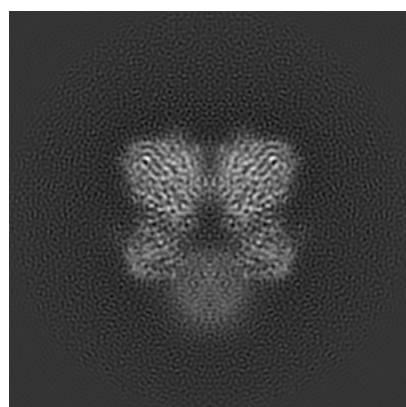
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32262. These allow visual inspection of the internal detail of the map and identification of artifacts.

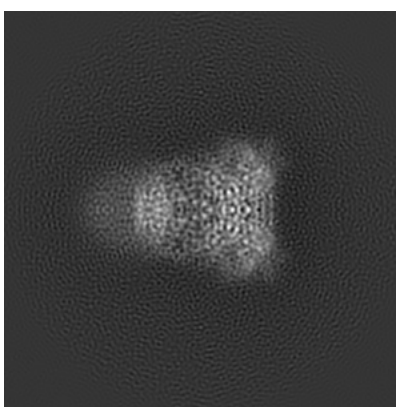
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

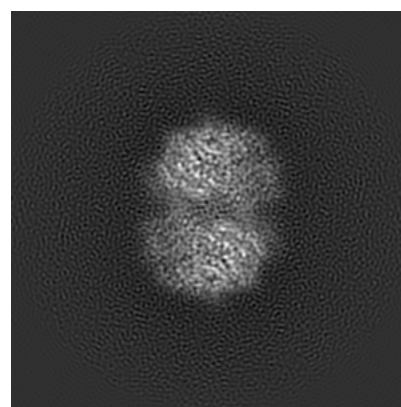
6.1.1 Primary map



X



Y

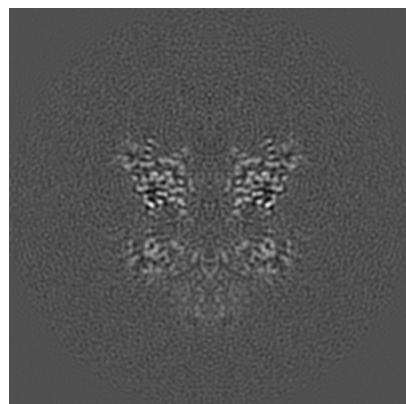


Z

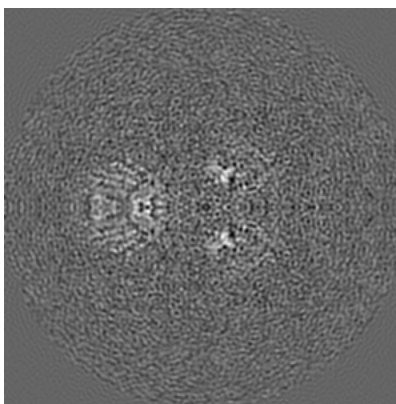
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

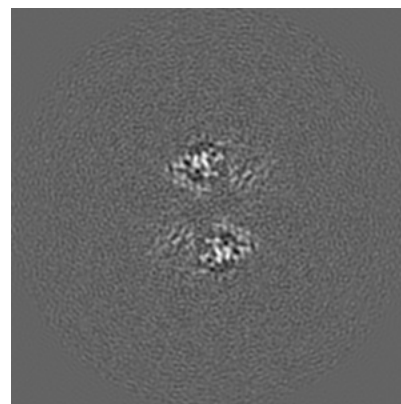
6.2.1 Primary map



X Index: 140



Y Index: 140

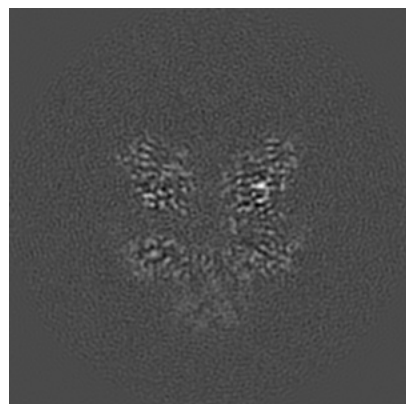


Z Index: 140

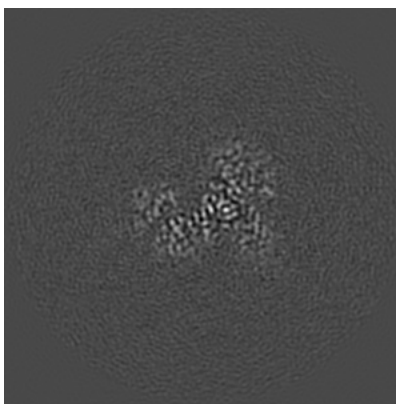
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

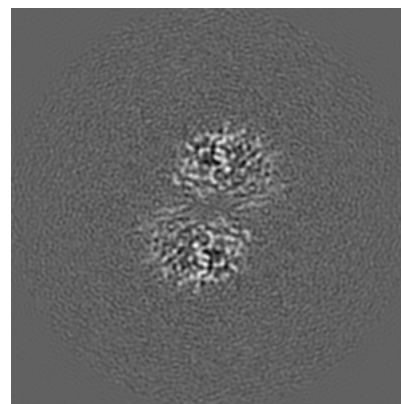
6.3.1 Primary map



X Index: 138



Y Index: 175

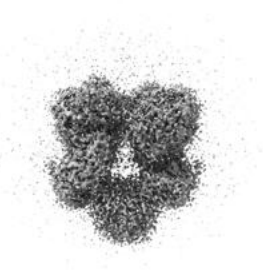


Z Index: 152

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

6.4 Orthogonal surface views [i](#)

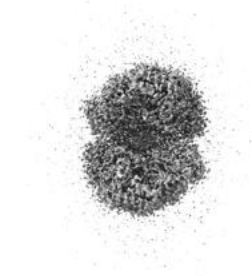
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

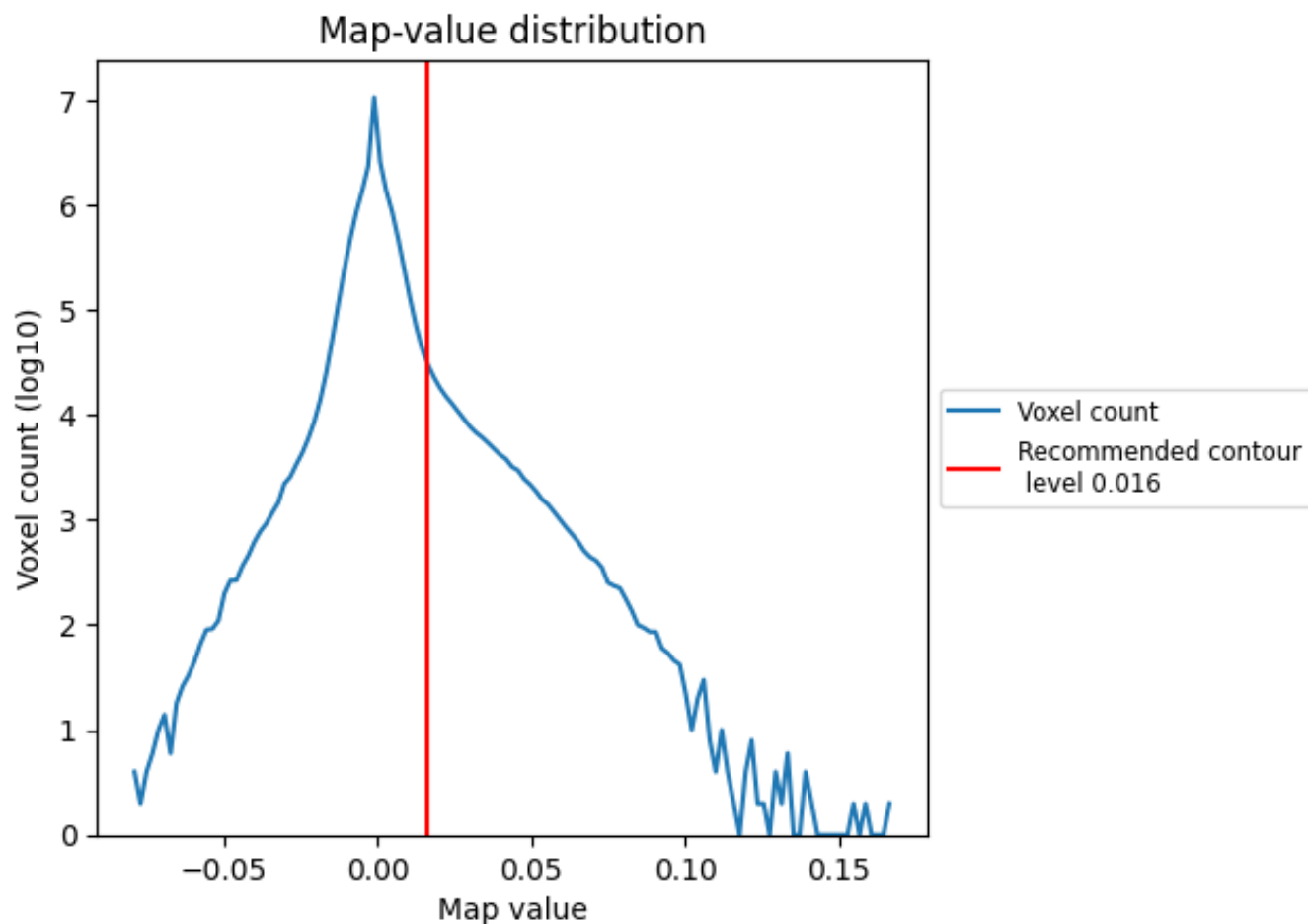
6.5 Mask visualisation

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

7 Map analysis [i](#)

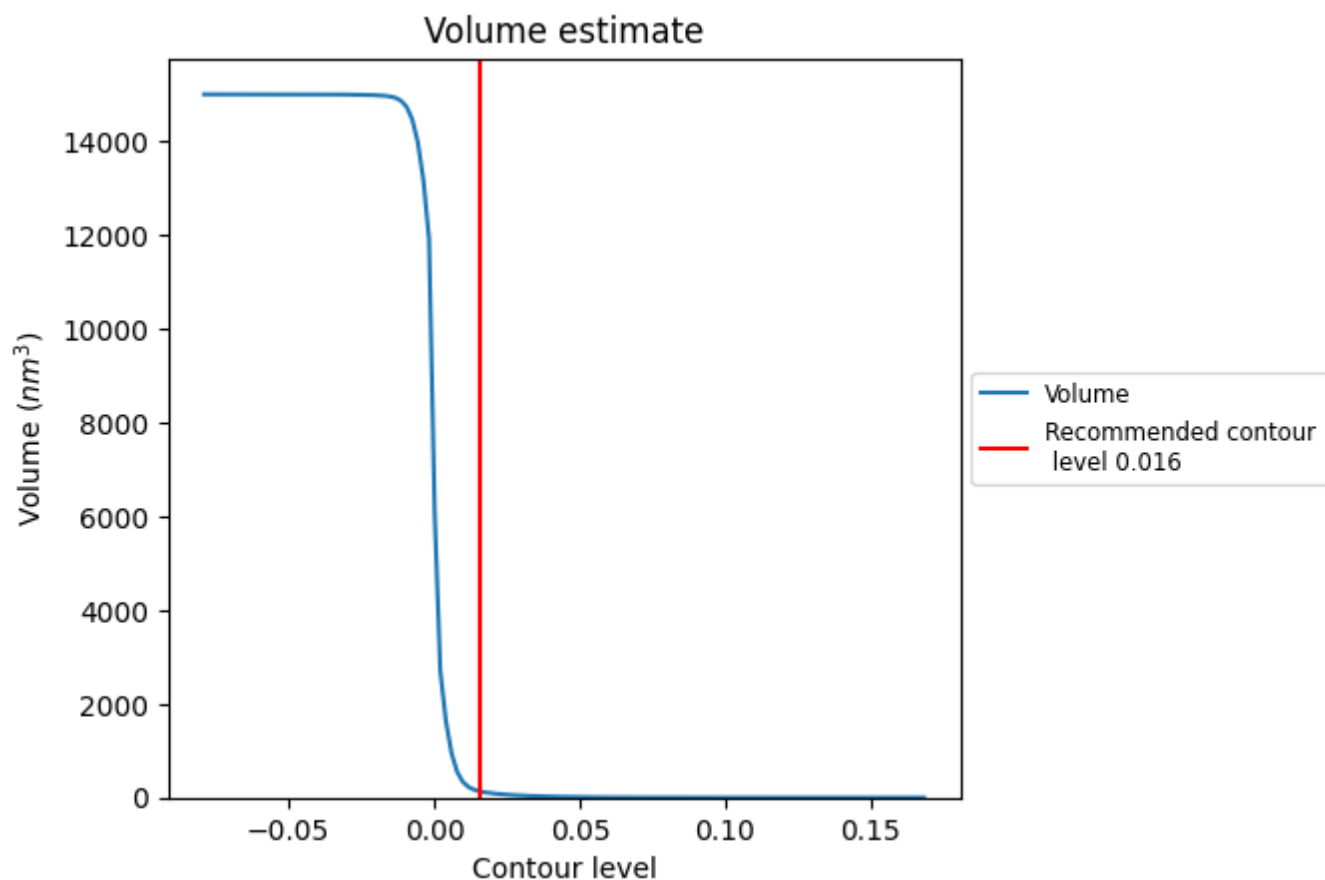
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

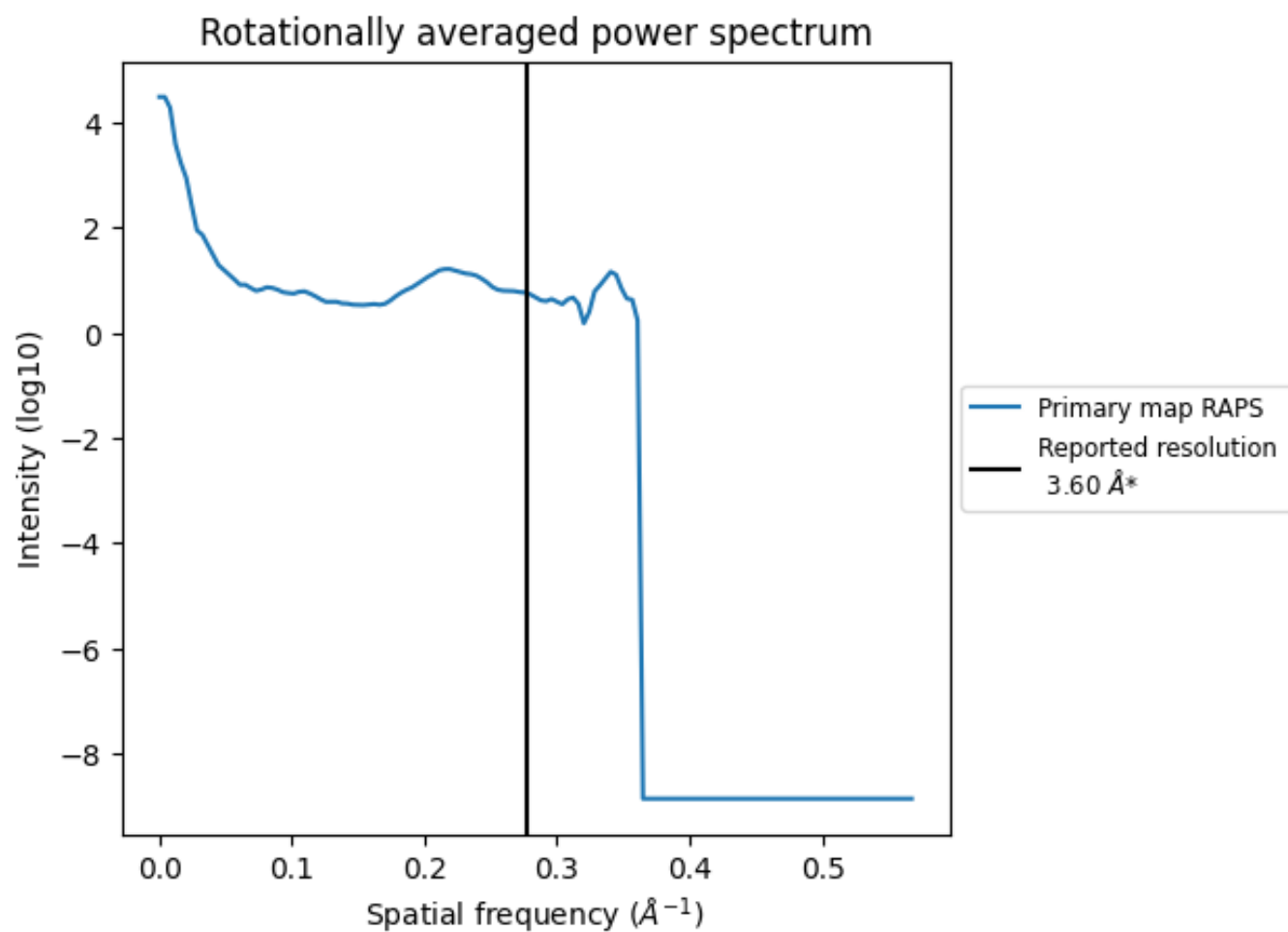
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 129 nm³; this corresponds to an approximate mass of 117 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 0.278 Å⁻¹

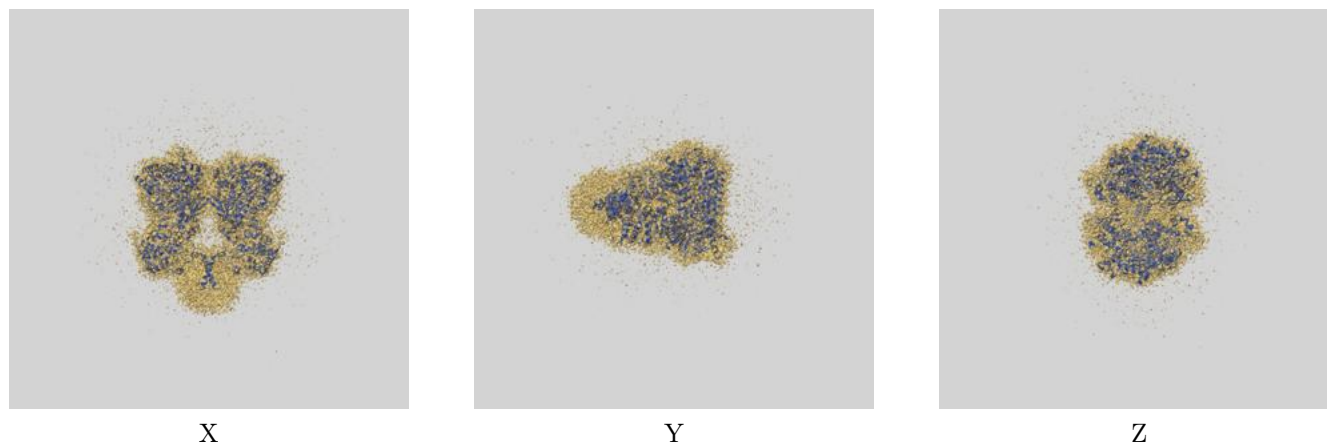
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

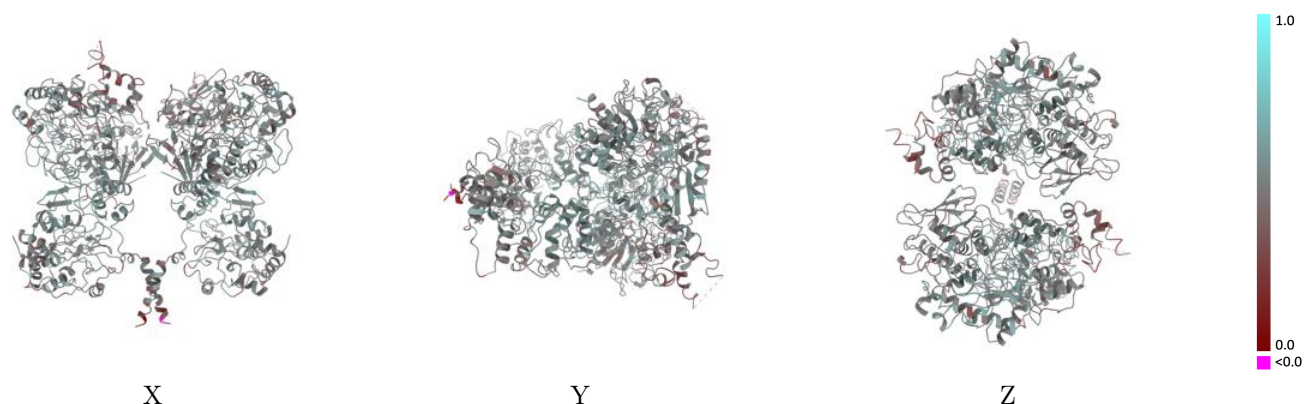
This section contains information regarding the fit between EMDB map EMD-32262 and PDB model 7W2J. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



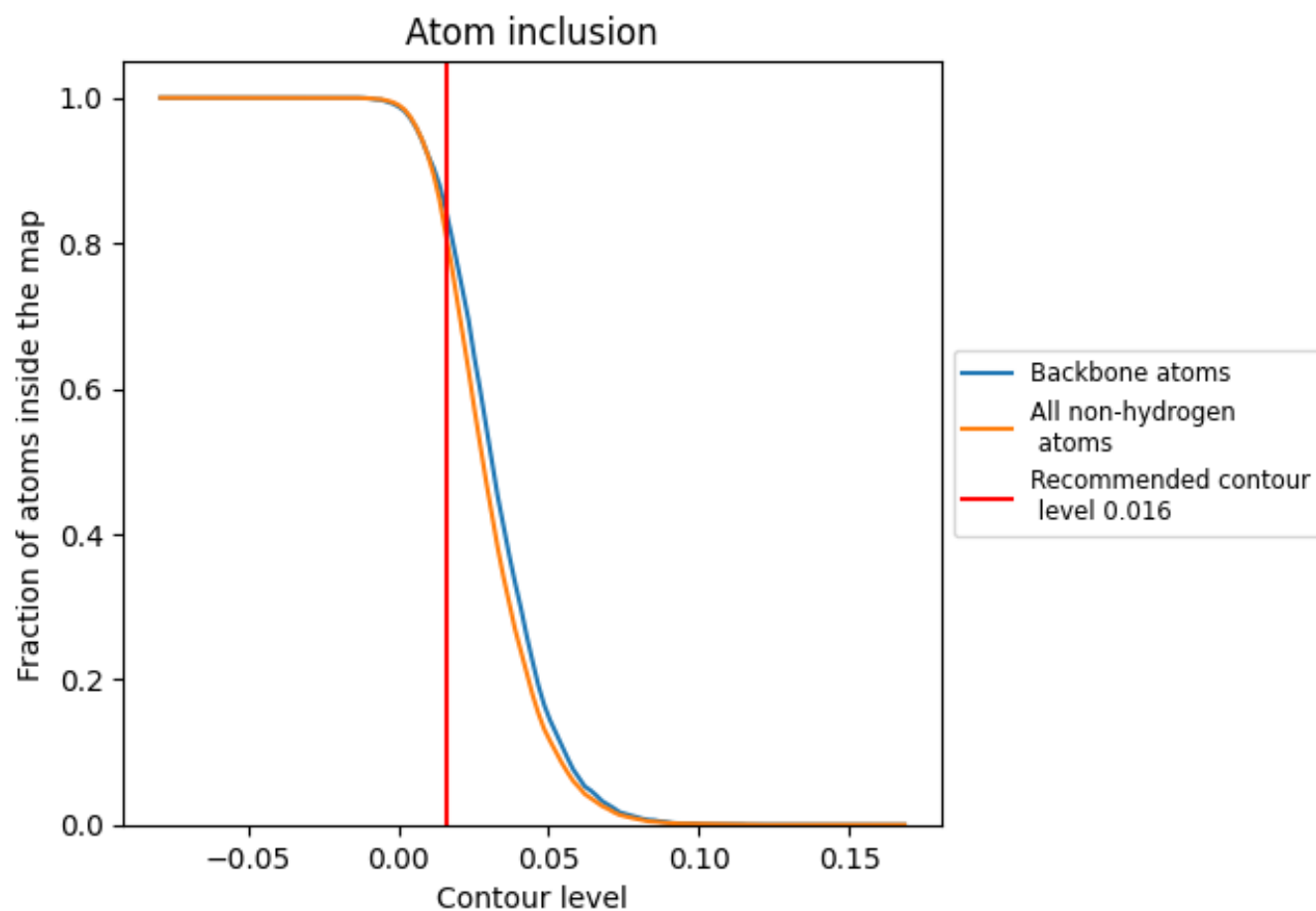
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 81% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8092	<div></div> 0.4930
A	<div></div> 0.8252	<div></div> 0.5030
B	<div></div> 0.6554	<div></div> 0.4020
C	<div></div> 0.8264	<div></div> 0.5010
D	<div></div> 0.8250	<div></div> 0.5050
E	<div></div> 0.6554	<div></div> 0.4020
F	<div></div> 0.8252	<div></div> 0.5010

