



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 12:55 PM JST

PDB ID : 6M5G
EMDB ID : EMD-30085
Title : F-actin-Utrophin complex
Authors : Kumari, A.; Ragunath, V.K.; Sirajuddin, M.
Deposited on : 2020-03-10
Resolution : 3.60 Å(reported)
Based on initial model : 5ONV

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) : 2.31.2

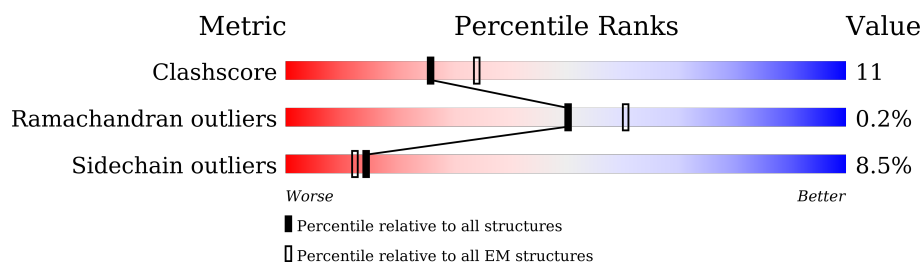
1 Overall quality at a glance

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	377	
1	B	377	
1	C	377	
1	D	377	
1	E	377	
2	F	269	
2	G	269	
2	H	269	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17363 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	370	Total	C	N	O	S	0	0
			2881	1824	488	548	21		
1	B	370	Total	C	N	O	S	0	0
			2879	1823	487	548	21		
1	C	370	Total	C	N	O	S	0	0
			2885	1826	488	550	21		
1	D	370	Total	C	N	O	S	0	0
			2873	1819	487	546	21		
1	E	370	Total	C	N	O	S	0	0
			2876	1821	487	547	21		

- Molecule 2 is a protein called Utrophin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	118	Total	C	N	O	S	0	0
			943	595	173	174	1		
2	G	118	Total	C	N	O	S	0	0
			943	595	173	174	1		
2	H	118	Total	C	N	O	S	0	0
			943	595	173	174	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-7	HIS	-	expression tag	UNP P46939
F	-6	HIS	-	expression tag	UNP P46939
F	-5	HIS	-	expression tag	UNP P46939
F	-4	HIS	-	expression tag	UNP P46939
F	-3	HIS	-	expression tag	UNP P46939
F	-2	HIS	-	expression tag	UNP P46939
F	-1	GLY	-	expression tag	UNP P46939
F	0	SER	-	expression tag	UNP P46939
G	-7	HIS	-	expression tag	UNP P46939

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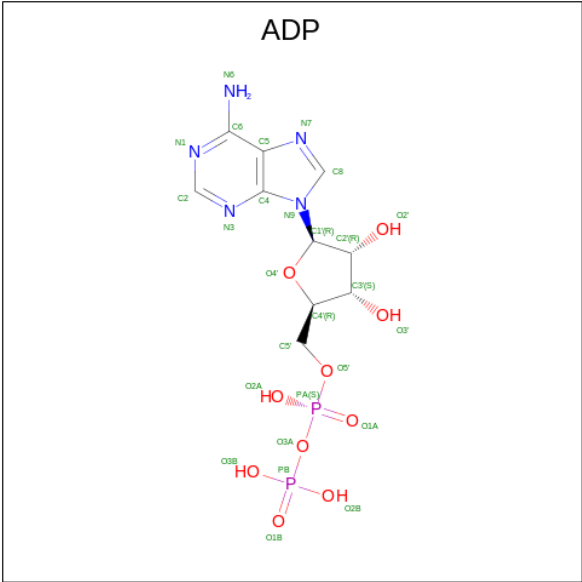
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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	HIS	-	expression tag	UNP P46939
G	-5	HIS	-	expression tag	UNP P46939
G	-4	HIS	-	expression tag	UNP P46939
G	-3	HIS	-	expression tag	UNP P46939
G	-2	HIS	-	expression tag	UNP P46939
G	-1	GLY	-	expression tag	UNP P46939
G	0	SER	-	expression tag	UNP P46939
H	-7	HIS	-	expression tag	UNP P46939
H	-6	HIS	-	expression tag	UNP P46939
H	-5	HIS	-	expression tag	UNP P46939
H	-4	HIS	-	expression tag	UNP P46939
H	-3	HIS	-	expression tag	UNP P46939
H	-2	HIS	-	expression tag	UNP P46939
H	-1	GLY	-	expression tag	UNP P46939
H	0	SER	-	expression tag	UNP P46939

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Mg 1 1	0
3	B	1	Total Mg 1 1	0
3	C	1	Total Mg 1 1	0
3	D	1	Total Mg 1 1	0
3	E	1	Total Mg 1 1	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).

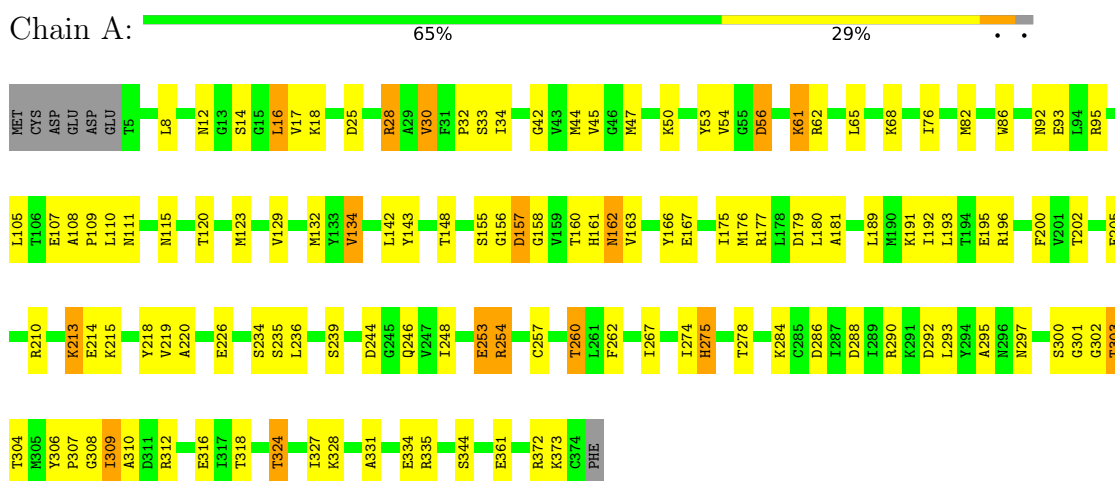


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

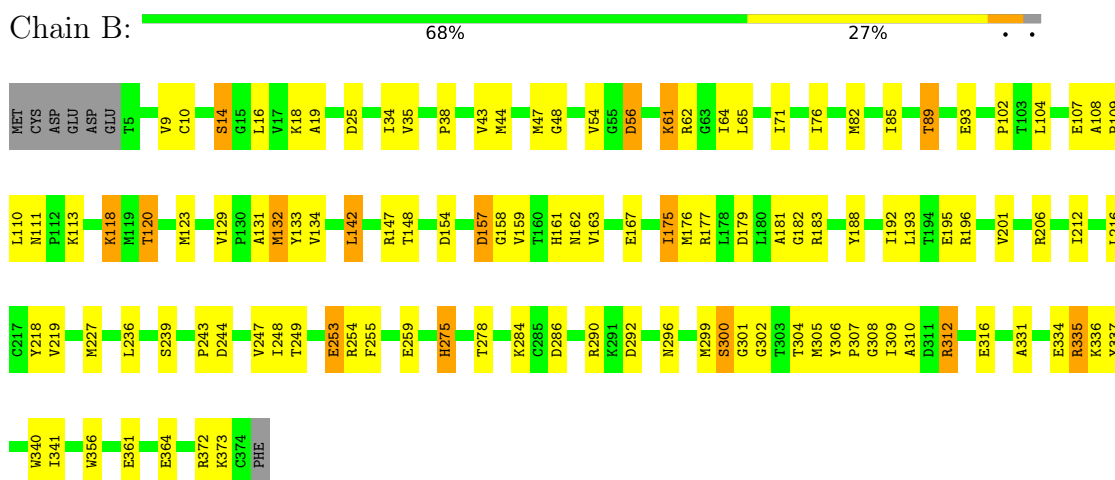
3 Residue-property plots

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: Actin, alpha skeletal muscle

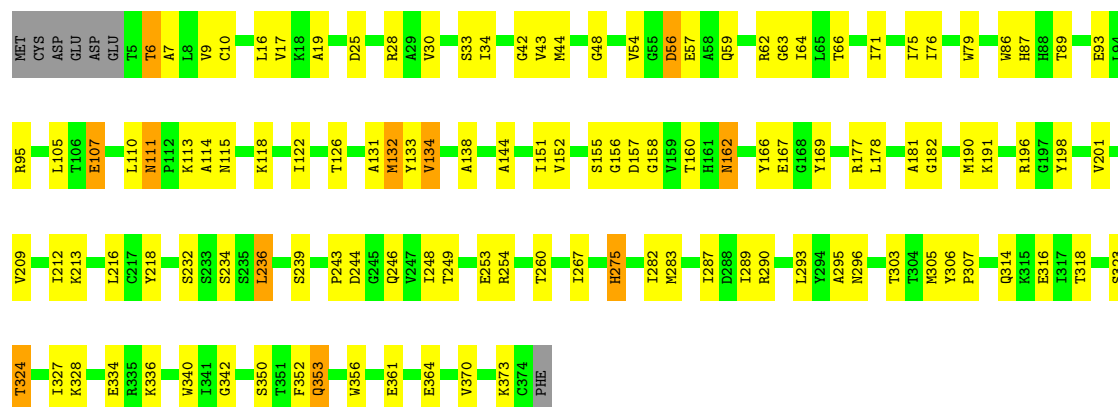


- Molecule 1: Actin, alpha skeletal muscle



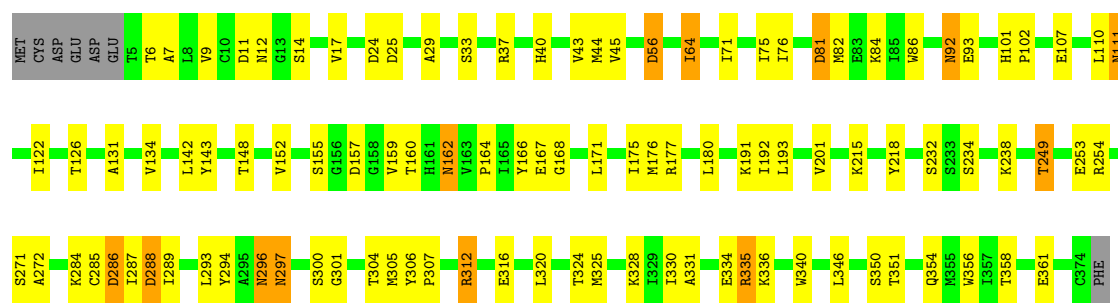
- Molecule 1: Actin, alpha skeletal muscle





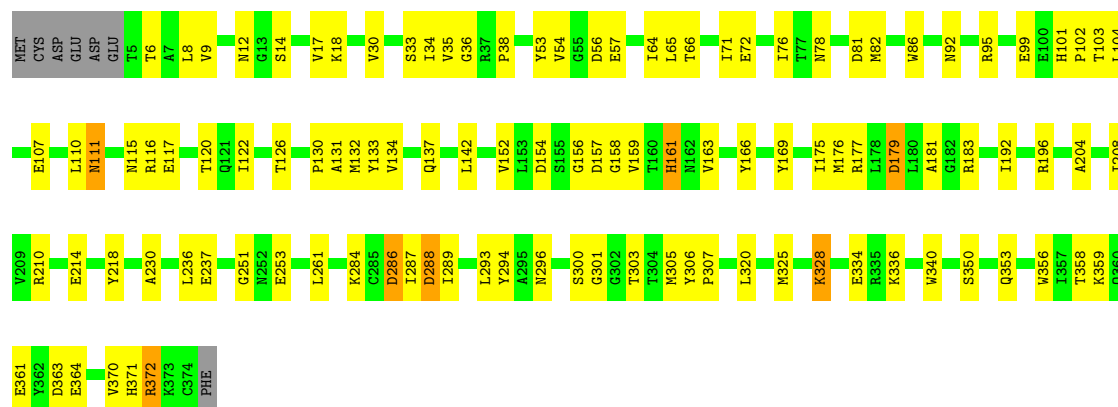
• Molecule 1: Actin, alpha skeletal muscle

Chain D: 71% 24% . .



• Molecule 1: Actin, alpha skeletal muscle

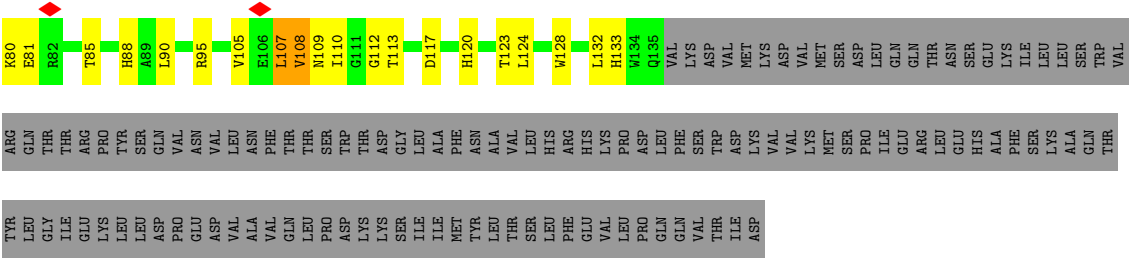
Chain E: 69% 27% . .



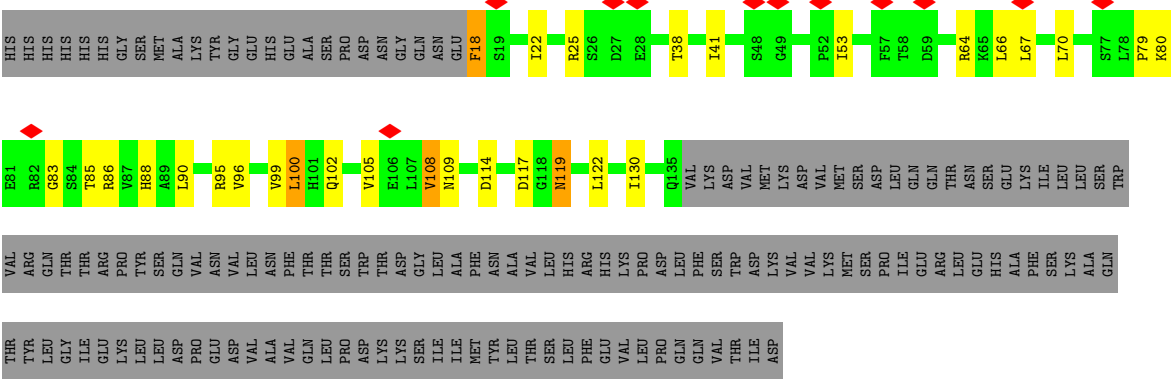
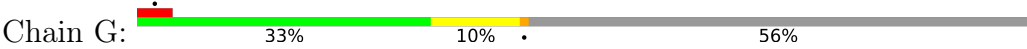
• Molecule 2: Utrophin

Chain F: 32% 10% 56%

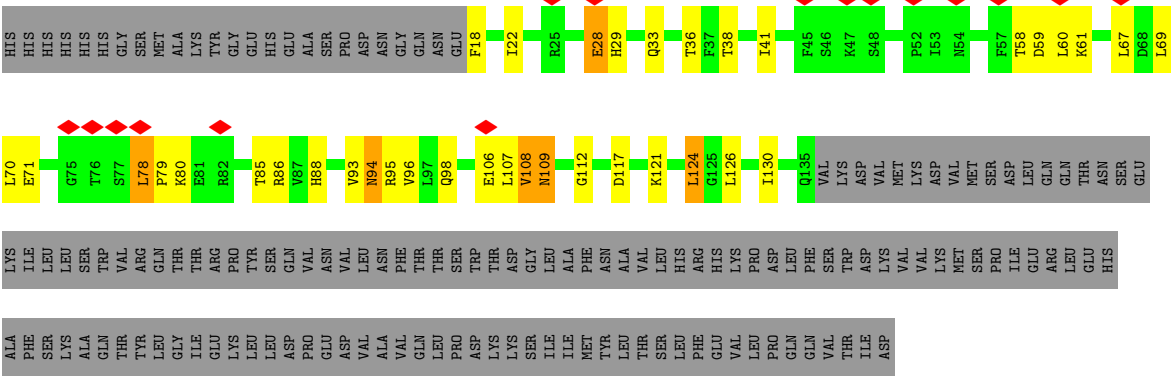




• Molecule 2: Utrophin



• Molecule 2: Utrophin



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-166.6°, rise=27.5 Å, axial sym=C1	Depositor
Number of segments used	149660	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; GCTF for CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.6	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	4735	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.284	Depositor
Minimum map value	-0.116	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.0464	Depositor
Map size (Å)	353.28, 353.28, 353.28	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG

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	0.54	0/2943	0.52	0/3988
1	B	0.56	0/2941	0.53	0/3985
1	C	0.56	0/2947	0.52	0/3993
1	D	0.54	0/2935	0.51	0/3979
1	E	0.49	0/2938	0.49	0/3983
2	F	0.28	0/960	0.46	0/1297
2	G	0.29	0/960	0.44	0/1297
2	H	0.28	0/960	0.45	0/1297
All	All	0.51	0/17584	0.51	0/23819

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2881	0	2853	77	0
1	B	2879	0	2846	78	0
1	C	2885	0	2857	74	0
1	D	2873	0	2838	61	0
1	E	2876	0	2839	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	943	0	959	17	0
2	G	943	0	959	21	0
2	H	943	0	959	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	3	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
4	E	27	0	12	1	0
All	All	17363	0	17170	391	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 11.

All (391) 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:B:158:GLY:H	1:B:181:ALA:HB3	1.32	0.94
1:A:158:GLY:H	1:A:181:ALA:HB3	1.38	0.88
1:A:219:VAL:HB	1:A:308:GLY:HA3	1.62	0.81
1:B:56:ASP:OD1	1:B:56:ASP:N	2.13	0.76
1:B:244:ASP:HB2	1:D:287:ILE:HG23	1.69	0.75
1:A:56:ASP:OD1	1:A:56:ASP:N	2.19	0.74
1:C:236:LEU:O	1:C:254:ARG:NH1	2.21	0.73
1:B:163:VAL:HA	1:B:175:ILE:HG22	1.71	0.73
1:B:219:VAL:HB	1:B:308:GLY:HA3	1.68	0.73
1:D:110:LEU:O	1:D:177:ARG:NH1	2.23	0.71
1:A:244:ASP:HB2	1:C:287:ILE:HG23	1.70	0.71
1:A:244:ASP:OD2	1:A:246:GLN:NE2	2.24	0.70
1:C:162:ASN:OD1	1:C:162:ASN:N	2.24	0.70
2:H:71:GLU:HB2	2:H:78:LEU:HD11	1.74	0.70
1:A:236:LEU:O	1:A:254:ARG:NH1	2.25	0.69
1:B:300:SER:OG	1:B:301:GLY:N	2.26	0.68
1:B:331:ALA:HB1	1:B:335:ARG:HH12	1.59	0.68
1:E:288:ASP:OD1	1:E:288:ASP:N	2.25	0.67
1:E:350:SER:O	1:E:353:GLN:NE2	2.24	0.67
1:D:9:VAL:O	1:D:340:TRP:NE1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:GLU:HB3	2:F:18:PHE:HB3	1.77	0.66
1:C:95:ARG:HD3	2:H:124:LEU:HD13	1.77	0.66
1:E:17:VAL:HG23	1:E:33:SER:HB3	1.78	0.66
1:C:9:VAL:O	1:C:340:TRP:NE1	2.29	0.65
1:D:71:ILE:HG12	1:D:76:ILE:HG12	1.78	0.65
1:A:162:ASN:HD21	1:A:278:THR:HG22	1.62	0.65
1:B:236:LEU:O	1:B:254:ARG:NH1	2.29	0.65
1:C:213:LYS:NZ	4:C:402:ADP:O2'	2.25	0.65
1:D:354:GLN:N	1:D:354:GLN:OE1	2.30	0.64
1:E:210:ARG:NH1	1:E:214:GLU:OE2	2.29	0.64
1:A:28:ARG:HH11	2:G:25:ARG:HD2	1.61	0.64
1:C:158:GLY:H	1:C:181:ALA:HB3	1.63	0.64
1:C:318:THR:HG22	1:C:327:ILE:HG13	1.78	0.64
1:D:56:ASP:N	1:D:56:ASP:OD1	2.31	0.63
1:B:334:GLU:OE1	1:B:334:GLU:N	2.29	0.63
1:E:72:GLU:OE2	1:E:183:ARG:NH1	2.31	0.63
1:C:212:ILE:HG23	1:C:216:LEU:HD12	1.80	0.63
1:C:111:ASN:ND2	1:C:177:ARG:HH12	1.96	0.63
1:C:107:GLU:OE2	1:C:115:ASN:ND2	2.28	0.62
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.80	0.62
1:D:312:ARG:NH1	1:D:316:GLU:OE2	2.33	0.62
1:C:87:HIS:NE2	2:H:106:GLU:OE1	2.33	0.62
1:C:196:ARG:NH2	1:C:249:THR:O	2.33	0.62
1:C:244:ASP:HB2	1:E:287:ILE:HG23	1.81	0.61
1:B:111:ASN:OD1	1:B:177:ARG:NH1	2.32	0.61
1:D:331:ALA:HB1	1:D:335:ARG:HH12	1.64	0.61
1:B:14:SER:HB2	1:B:157:ASP:O	2.01	0.61
1:C:361:GLU:OE1	1:C:373:LYS:NZ	2.32	0.61
1:E:12:ASN:HD22	1:E:86:TRP:HE1	1.48	0.61
1:C:25:ASP:N	1:C:25:ASP:OD1	2.33	0.61
1:A:12:ASN:HD21	1:A:86:TRP:HE1	1.46	0.61
1:A:25:ASP:N	1:A:25:ASP:OD1	2.33	0.60
1:E:328:LYS:HZ2	1:E:328:LYS:HB2	1.66	0.60
1:A:318:THR:HG22	1:A:327:ILE:HD13	1.82	0.60
1:C:283:MET:SD	1:C:290:ARG:NH1	2.74	0.60
1:D:328:LYS:HE3	1:D:330:ILE:HD11	1.83	0.60
1:D:358:THR:N	1:D:361:GLU:OE1	2.34	0.60
1:E:14:SER:HB2	1:E:157:ASP:HB3	1.84	0.60
1:C:114:ALA:HB1	1:C:118:LYS:HE3	1.84	0.60
1:E:230:ALA:HB2	1:E:236:LEU:HD23	1.83	0.60
1:D:176:MET:SD	1:D:284:LYS:NZ	2.74	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:GLY:N	1:E:181:ALA:HB3	2.17	0.59
1:E:289:ILE:HG22	1:E:293:LEU:HG	1.84	0.59
1:D:286:ASP:N	1:D:286:ASP:OD1	2.34	0.59
1:D:300:SER:OG	1:D:301:GLY:N	2.35	0.59
2:G:64:ARG:HG2	2:G:80:LYS:HD3	1.84	0.59
1:D:297:ASN:N	1:D:297:ASN:OD1	2.35	0.59
1:B:227:MET:HG2	1:B:255:PHE:HE1	1.67	0.59
1:E:158:GLY:H	1:E:181:ALA:HB3	1.67	0.59
1:C:275:HIS:HD2	1:C:316:GLU:HB3	1.68	0.58
1:D:12:ASN:HD22	1:D:86:TRP:HE1	1.49	0.58
1:D:162:ASN:OD1	1:D:162:ASN:N	2.37	0.58
1:A:50:LYS:HE2	1:A:53:TYR:CD2	2.38	0.58
1:B:259:GLU:OE2	1:B:312:ARG:NH1	2.33	0.58
1:E:92:ASN:O	1:E:95:ARG:NH1	2.37	0.58
2:H:85:THR:H	2:H:88:HIS:HD2	1.52	0.57
2:G:79:PRO:HG2	2:G:95:ARG:HH12	1.69	0.57
1:C:56:ASP:OD1	1:C:56:ASP:N	2.36	0.57
1:E:111:ASN:ND2	1:E:177:ARG:HH12	2.02	0.57
1:C:48:GLY:O	2:H:112:GLY:N	2.36	0.57
1:B:110:LEU:O	1:B:177:ARG:NH1	2.37	0.57
1:C:155:SER:HB3	1:C:160:THR:HG23	1.86	0.57
1:B:25:ASP:OD1	1:B:25:ASP:N	2.35	0.57
2:F:79:PRO:HG2	2:F:95:ARG:HH12	1.68	0.57
1:C:244:ASP:OD2	1:C:246:GLN:NE2	2.37	0.57
1:B:176:MET:SD	1:B:284:LYS:NZ	2.78	0.57
2:G:67:LEU:HD23	2:G:80:LYS:HG2	1.86	0.57
1:D:218:TYR:HA	1:D:307:PRO:HD2	1.86	0.56
1:A:158:GLY:H	1:A:181:ALA:CB	2.15	0.56
1:E:131:ALA:HB1	1:E:356:TRP:HB3	1.87	0.56
1:E:176:MET:SD	1:E:284:LYS:NZ	2.77	0.56
1:B:43:VAL:O	1:B:44:MET:HG2	2.06	0.56
1:C:350:SER:O	1:C:353:GLN:NE2	2.38	0.56
1:E:102:PRO:HB3	1:E:131:ALA:HB3	1.86	0.56
1:E:36:GLY:HA3	1:E:65:LEU:HD23	1.86	0.56
1:A:200:PHE:HB3	1:A:205:GLU:HB3	1.88	0.55
1:E:286:ASP:OD1	1:E:286:ASP:N	2.39	0.55
1:A:107:GLU:HG2	1:A:108:ALA:H	1.70	0.55
1:A:17:VAL:HG23	1:A:33:SER:HB3	1.89	0.55
1:A:195:GLU:HB2	1:B:113:LYS:HG2	1.88	0.55
1:C:334:GLU:N	1:C:334:GLU:OE1	2.36	0.55
1:E:110:LEU:O	1:E:177:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LEU:HD11	1:A:267:ILE:HD12	1.88	0.55
1:B:120:THR:OG1	1:B:132:MET:SD	2.62	0.55
1:D:288:ASP:OD1	1:D:288:ASP:N	2.36	0.55
2:H:86:ARG:NH2	2:H:117:ASP:OD1	2.39	0.55
1:A:334:GLU:OE1	1:A:334:GLU:N	2.39	0.54
1:E:359:LYS:NZ	1:E:363:ASP:OD1	2.40	0.54
1:C:166:TYR:CD1	1:C:289:ILE:HG23	2.43	0.54
1:D:296:ASN:OD1	1:D:296:ASN:N	2.41	0.54
1:C:43:VAL:O	1:C:44:MET:HG2	2.07	0.54
1:A:76:ILE:HD13	1:A:82:MET:HG2	1.90	0.54
1:E:350:SER:OG	2:H:95:ARG:NH2	2.41	0.54
1:A:25:ASP:OD1	2:G:25:ARG:NH1	2.37	0.54
1:C:17:VAL:HG23	1:C:33:SER:HB3	1.89	0.54
1:D:271:SER:OG	1:D:272:ALA:N	2.41	0.54
1:A:156:GLY:HA2	1:A:303:THR:OG1	2.07	0.54
1:B:195:GLU:HB2	1:C:113:LYS:HG2	1.89	0.53
1:D:232:SER:O	1:D:234:SER:OG	2.26	0.53
2:H:67:LEU:HB3	2:H:80:LYS:HZ1	1.72	0.53
1:B:76:ILE:HD13	1:B:82:MET:HG2	1.89	0.53
1:C:260:THR:HG21	1:C:267:ILE:HD11	1.89	0.53
2:H:79:PRO:O	2:H:95:ARG:NH1	2.41	0.53
1:A:334:GLU:HB3	2:G:18:PHE:HB3	1.90	0.53
1:E:300:SER:OG	1:E:301:GLY:N	2.41	0.53
1:A:50:LYS:NZ	2:G:114:ASP:OD2	2.29	0.53
1:B:9:VAL:O	1:B:340:TRP:NE1	2.36	0.53
1:D:33:SER:O	1:D:33:SER:OG	2.26	0.53
1:A:300:SER:OG	1:A:301:GLY:N	2.42	0.53
1:B:361:GLU:HA	1:B:364:GLU:HG2	1.91	0.53
1:C:42:GLY:HA2	1:E:169:TYR:HA	1.90	0.53
1:C:324:THR:O	1:C:324:THR:OG1	2.22	0.53
2:G:83:GLY:HA3	2:G:88:HIS:CD2	2.43	0.53
1:A:275:HIS:HD2	1:A:316:GLU:HB3	1.74	0.53
1:A:234:SER:OG	1:A:235:SER:N	2.41	0.52
1:C:138:ALA:O	1:C:152:VAL:HG21	2.10	0.52
1:A:158:GLY:N	1:A:181:ALA:HB3	2.18	0.52
1:A:155:SER:HB3	1:A:160:THR:HG23	1.91	0.52
1:A:361:GLU:OE1	1:A:373:LYS:NZ	2.37	0.52
2:F:38:THR:HA	2:F:41:ILE:HG12	1.92	0.52
1:C:71:ILE:HG12	1:C:76:ILE:HG12	1.91	0.52
1:C:314:GLN:O	1:C:318:THR:HG23	2.10	0.52
1:B:331:ALA:HB1	1:B:335:ARG:NH1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:O	1:E:340:TRP:NE1	2.40	0.52
1:B:212:ILE:HG23	1:B:216:LEU:HD12	1.91	0.52
2:G:86:ARG:NH2	2:G:117:ASP:OD1	2.42	0.52
1:B:48:GLY:O	2:F:112:GLY:N	2.38	0.51
1:E:76:ILE:HD13	1:E:82:MET:HG2	1.92	0.51
1:E:163:VAL:HA	1:E:175:ILE:HG22	1.91	0.51
1:B:18:LYS:NZ	4:B:402:ADP:O2B	2.44	0.51
1:C:305:MET:SD	1:C:336:LYS:HB2	2.51	0.51
1:B:10:CYS:HA	1:B:19:ALA:HA	1.92	0.51
1:C:190:MET:HB3	1:C:209:VAL:HG11	1.93	0.51
2:H:67:LEU:HB3	2:H:80:LYS:NZ	2.26	0.51
1:C:275:HIS:CD2	1:C:316:GLU:HB3	2.45	0.51
1:D:305:MET:SD	1:D:336:LYS:HB2	2.50	0.51
1:E:56:ASP:OD1	1:E:56:ASP:N	2.42	0.51
1:A:28:ARG:HE	2:G:25:ARG:HG3	1.75	0.51
1:D:6:THR:O	1:D:101:HIS:ND1	2.41	0.50
2:H:38:THR:HA	2:H:41:ILE:HG12	1.92	0.50
1:B:85:ILE:O	1:B:89:THR:OG1	2.28	0.50
1:A:16:LEU:HA	1:A:32:PRO:HA	1.93	0.50
1:B:157:ASP:H	1:B:182:GLY:H	1.59	0.50
1:C:306:TYR:CE1	4:C:402:ADP:H2	2.29	0.50
1:D:350:SER:OG	2:F:81:GLU:OE2	2.20	0.50
1:E:158:GLY:CA	1:E:181:ALA:HB3	2.41	0.50
1:A:274:ILE:HD11	1:A:309:ILE:HD11	1.93	0.50
1:E:179:ASP:N	1:E:179:ASP:OD1	2.44	0.50
1:D:37:ARG:HH12	1:D:84:LYS:NZ	2.09	0.50
1:B:243:PRO:HG2	1:D:287:ILE:HG22	1.93	0.50
2:G:38:THR:HA	2:G:41:ILE:HG12	1.93	0.50
1:B:306:TYR:CE1	4:B:402:ADP:H2	2.30	0.49
1:E:358:THR:HB	1:E:361:GLU:HG3	1.94	0.49
1:C:95:ARG:HH21	2:H:33:GLN:HG3	1.77	0.49
1:E:196:ARG:HD2	1:E:253:GLU:OE2	2.12	0.49
2:H:59:ASP:O	2:H:60:LEU:HD12	2.13	0.49
1:C:289:ILE:HG22	1:C:293:LEU:HG	1.93	0.49
1:A:42:GLY:HA2	1:C:169:TYR:HA	1.94	0.49
1:A:163:VAL:HA	1:A:175:ILE:HG22	1.94	0.49
2:G:66:LEU:HD21	2:G:96:VAL:HG11	1.94	0.49
1:A:110:LEU:O	1:A:177:ARG:NH1	2.45	0.49
2:F:71:GLU:O	2:F:75:GLY:N	2.43	0.49
1:E:117:GLU:OE2	1:E:371:HIS:NE2	2.46	0.49
1:C:132:MET:HG2	1:C:133:TYR:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:NH2	1:B:249:THR:O	2.46	0.48
2:G:85:THR:OG1	2:G:86:ARG:N	2.46	0.48
2:G:108:VAL:HG23	2:G:109:ASN:H	1.77	0.48
1:C:62:ARG:O	1:C:64:ILE:N	2.46	0.48
1:C:152:VAL:O	1:C:162:ASN:HA	2.13	0.48
1:D:24:ASP:OD1	1:D:25:ASP:N	2.43	0.48
1:D:92:ASN:OD1	1:D:92:ASN:N	2.44	0.48
1:D:122:ILE:O	1:D:126:THR:OG1	2.27	0.48
2:F:105:VAL:HG22	2:F:133:HIS:CD2	2.48	0.48
1:D:43:VAL:O	1:D:44:MET:HG2	2.14	0.48
1:E:158:GLY:HA2	1:E:181:ALA:HB3	1.95	0.48
2:F:107:LEU:HD22	2:F:110:ILE:HG21	1.96	0.48
2:F:108:VAL:HG23	2:F:109:ASN:H	1.78	0.48
1:A:92:ASN:O	1:A:95:ARG:NH1	2.47	0.47
1:B:38:PRO:HA	1:B:64:ILE:O	2.14	0.47
1:E:120:THR:HG22	1:E:132:MET:SD	2.55	0.47
1:C:86:TRP:HA	1:C:89:THR:HG22	1.97	0.47
1:D:131:ALA:HB1	1:D:356:TRP:HB3	1.97	0.47
1:A:47:MET:SD	2:G:90:LEU:HD13	2.55	0.47
1:A:308:GLY:O	1:A:310:ALA:N	2.47	0.47
1:B:142:LEU:HA	1:B:142:LEU:HD12	1.69	0.47
1:D:7:ALA:HA	1:D:102:PRO:HD2	1.96	0.47
1:D:81:ASP:OD1	1:D:81:ASP:N	2.44	0.47
1:E:305:MET:SD	1:E:336:LYS:HB2	2.55	0.47
2:H:108:VAL:HG23	2:H:109:ASN:H	1.80	0.47
2:F:64:ARG:HG2	2:F:80:LYS:HD3	1.97	0.47
1:B:14:SER:N	4:B:402:ADP:O3B	2.48	0.47
1:E:8:LEU:HB2	1:E:103:THR:HG22	1.97	0.47
1:A:295:ALA:O	1:A:328:LYS:HB3	2.15	0.47
1:A:262:PHE:HZ	1:A:309:ILE:HG13	1.80	0.46
1:B:275:HIS:HD2	1:B:316:GLU:HB3	1.81	0.46
1:C:243:PRO:HG2	1:E:287:ILE:HG22	1.97	0.46
1:E:218:TYR:HA	1:E:307:PRO:HD2	1.96	0.46
1:A:213:LYS:NZ	4:A:402:ADP:O2'	2.29	0.46
1:C:105:LEU:O	1:C:134:VAL:HA	2.15	0.46
1:C:361:GLU:HA	1:C:364:GLU:HG2	1.97	0.46
1:E:120:THR:HG21	1:E:370:VAL:HG21	1.95	0.46
1:B:35:VAL:HG22	1:B:54:VAL:HB	1.97	0.46
1:D:40:HIS:HD2	1:D:64:ILE:HG22	1.80	0.46
1:B:162:ASN:O	1:B:175:ILE:HA	2.16	0.46
1:D:17:VAL:HG23	1:D:33:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LYS:HG2	1:E:30:VAL:HG22	1.97	0.46
1:E:35:VAL:HG22	1:E:54:VAL:HG12	1.96	0.46
1:A:50:LYS:HE3	2:G:109:ASN:OD1	2.16	0.46
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.77	0.46
1:D:152:VAL:O	1:D:162:ASN:HA	2.15	0.46
1:B:71:ILE:HG12	1:B:76:ILE:HG12	1.96	0.46
1:C:110:LEU:O	1:C:177:ARG:NH1	2.49	0.46
1:E:192:ILE:HD12	1:E:192:ILE:HA	1.76	0.46
1:C:6:THR:OG1	1:C:7:ALA:N	2.48	0.46
1:C:190:MET:HB2	1:C:209:VAL:HG21	1.97	0.46
1:E:122:ILE:O	1:E:126:THR:OG1	2.27	0.46
1:E:361:GLU:HA	1:E:364:GLU:HG2	1.97	0.46
1:A:306:TYR:C	1:A:308:GLY:H	2.19	0.46
1:B:109:PRO:HD2	1:B:161:HIS:CE1	2.51	0.46
1:B:299:MET:HE2	1:B:304:THR:HB	1.97	0.46
1:A:14:SER:HB2	1:A:157:ASP:O	2.16	0.45
1:E:142:LEU:HD13	1:E:152:VAL:HG23	1.97	0.45
1:B:236:LEU:HD13	1:B:236:LEU:HA	1.70	0.45
1:E:353:GLN:HA	1:E:356:TRP:HE1	1.81	0.45
1:B:157:ASP:H	1:B:182:GLY:N	2.15	0.45
1:C:138:ALA:HB1	1:C:152:VAL:HB	1.98	0.45
1:D:155:SER:O	1:D:155:SER:OG	2.35	0.45
1:D:164:PRO:HD2	1:D:175:ILE:HG22	1.98	0.45
1:E:53:TYR:HB3	1:E:57:GLU:OE1	2.16	0.45
1:C:10:CYS:HA	1:C:19:ALA:HA	1.99	0.45
2:G:119:ASN:HD22	2:G:122:LEU:H	1.65	0.45
1:A:302:GLY:O	1:A:304:THR:N	2.49	0.45
1:A:109:PRO:HD2	1:A:161:HIS:CD2	2.51	0.45
1:A:202:THR:OG1	1:A:205:GLU:OE1	2.33	0.45
1:A:306:TYR:CE1	4:A:402:ADP:H2	2.34	0.45
1:B:54:VAL:H	2:F:109:ASN:ND2	2.15	0.45
1:B:62:ARG:NE	1:D:288:ASP:OD2	2.50	0.45
1:B:286:ASP:OD1	1:B:286:ASP:N	2.48	0.45
1:D:306:TYR:CE1	4:D:402:ADP:H2	2.34	0.45
1:A:123:MET:O	1:A:129:VAL:HG22	2.17	0.45
2:F:85:THR:H	2:F:88:HIS:HD2	1.64	0.45
1:D:294:TYR:CD2	1:D:325:MET:HG2	2.52	0.45
1:B:147:ARG:NE	1:B:296:ASN:OD1	2.48	0.45
1:B:123:MET:O	1:B:129:VAL:HG22	2.17	0.45
1:E:6:THR:O	1:E:101:HIS:ND1	2.50	0.45
1:A:257:CYS:O	1:A:260:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:HIS:CD2	1:A:316:GLU:HB3	2.52	0.44
1:B:286:ASP:O	1:B:290:ARG:HG3	2.17	0.44
2:G:99:VAL:HA	2:G:102:GLN:OE1	2.18	0.44
1:D:171:LEU:HD12	1:D:285:CYS:SG	2.57	0.44
1:E:353:GLN:HA	1:E:356:TRP:NE1	2.33	0.44
1:A:196:ARG:HD2	1:A:253:GLU:OE2	2.18	0.44
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.81	0.44
1:B:44:MET:HG3	1:D:168:GLY:HA2	1.99	0.44
1:C:157:ASP:H	1:C:182:GLY:H	1.64	0.44
1:B:192:ILE:HD12	1:B:253:GLU:HB3	1.99	0.44
1:D:166:TYR:CD1	1:D:289:ILE:HG23	2.53	0.44
1:E:35:VAL:HG21	1:E:81:ASP:HB2	2.00	0.44
1:D:111:ASN:HD22	1:D:111:ASN:HA	1.54	0.44
1:E:204:ALA:O	1:E:208:ILE:HG13	2.18	0.43
1:E:237:GLU:OE1	1:E:237:GLU:N	2.45	0.43
2:H:28:GLU:HG3	2:H:29:HIS:N	2.32	0.43
2:H:126:LEU:HD23	2:H:126:LEU:H	1.82	0.43
1:A:210:ARG:O	1:A:214:GLU:HG3	2.17	0.43
1:B:132:MET:HE3	1:B:132:MET:HB3	1.91	0.43
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.84	0.43
1:B:118:LYS:HB2	1:B:118:LYS:HE3	1.70	0.43
1:E:107:GLU:C	1:E:137:GLN:HE21	2.21	0.43
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.88	0.43
1:A:12:ASN:ND2	1:A:86:TRP:HE1	2.16	0.43
1:B:102:PRO:HB3	1:B:131:ALA:HB3	2.00	0.43
1:C:144:ALA:HB2	1:C:342:GLY:N	2.33	0.43
1:D:157:ASP:HB2	4:D:402:ADP:H4'	1.99	0.43
1:E:107:GLU:OE1	1:E:116:ARG:NE	2.52	0.43
1:C:28:ARG:HD3	1:C:28:ARG:HA	1.82	0.43
2:G:100:LEU:HD21	2:G:130:ILE:HG22	2.00	0.43
1:B:255:PHE:O	1:B:259:GLU:HB2	2.19	0.43
1:E:294:TYR:CD2	1:E:325:MET:HG2	2.54	0.43
1:A:189:LEU:HA	1:A:192:ILE:HG22	2.01	0.43
1:C:93:GLU:OE2	2:H:121:LYS:HD3	2.18	0.43
1:A:220:ALA:HB1	1:A:226:GLU:HG3	2.01	0.42
1:C:218:TYR:HA	1:C:307:PRO:HD2	2.01	0.42
1:A:120:THR:HG22	1:A:132:MET:SD	2.59	0.42
1:B:9:VAL:HG13	1:B:104:LEU:HD23	1.99	0.42
1:D:238:LYS:O	1:D:249:THR:HA	2.19	0.42
1:D:331:ALA:HB1	1:D:335:ARG:NH1	2.34	0.42
2:H:58:THR:HA	2:H:61:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLY:O	1:B:310:ALA:N	2.52	0.42
1:C:151:ILE:HD12	1:C:282:ILE:HG13	2.00	0.42
1:D:155:SER:HB2	1:D:160:THR:OG1	2.20	0.42
1:A:68:LYS:HB3	1:A:68:LYS:HE3	1.77	0.42
1:A:176:MET:SD	1:A:284:LYS:NZ	2.87	0.42
1:B:188:TYR:O	1:B:192:ILE:HG12	2.19	0.42
1:B:227:MET:HG2	1:B:255:PHE:CE1	2.53	0.42
1:D:76:ILE:HD13	1:D:82:MET:HG2	2.01	0.42
1:C:334:GLU:HB3	2:H:18:PHE:CB	2.49	0.42
1:E:81:ASP:OD1	1:E:81:ASP:N	2.44	0.42
1:A:331:ALA:HB1	1:A:335:ARG:NH1	2.34	0.42
1:D:192:ILE:HD12	1:D:192:ILE:HA	1.76	0.42
1:E:237:GLU:HA	1:E:251:GLY:HA2	2.02	0.42
2:H:94:ASN:O	2:H:98:GLN:HG2	2.19	0.42
1:A:105:LEU:O	1:A:134:VAL:HA	2.20	0.42
1:A:166:TYR:O	1:A:167:GLU:HG3	2.20	0.42
1:C:334:GLU:HB3	2:H:18:PHE:HB3	2.02	0.42
1:C:76:ILE:HD12	1:C:79:TRP:CH2	2.54	0.42
1:C:156:GLY:HA2	1:C:303:THR:OG1	2.20	0.42
1:C:239:SER:HA	1:C:248:ILE:O	2.19	0.42
1:D:142:LEU:HA	1:D:142:LEU:HD12	1.65	0.42
1:E:99:GLU:H	1:E:99:GLU:CD	2.19	0.42
1:E:101:HIS:O	1:E:130:PRO:HD2	2.20	0.42
1:B:107:GLU:HG2	1:B:108:ALA:H	1.84	0.42
1:A:192:ILE:HD12	1:A:192:ILE:HA	1.83	0.42
1:A:218:TYR:HA	1:A:307:PRO:HD2	2.02	0.42
1:B:361:GLU:OE1	1:B:373:LYS:NZ	2.50	0.42
1:E:71:ILE:HG12	1:E:76:ILE:HG12	2.02	0.42
1:A:324:THR:O	1:A:324:THR:OG1	2.38	0.41
1:B:120:THR:HG23	1:B:132:MET:HE1	2.01	0.41
1:C:122:ILE:O	1:C:126:THR:HB	2.20	0.41
2:F:107:LEU:HD12	2:F:107:LEU:H	1.84	0.41
2:H:93:VAL:O	2:H:96:VAL:HG12	2.19	0.41
1:D:215:LYS:HE2	1:D:215:LYS:HB3	1.81	0.41
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.78	0.41
1:A:286:ASP:O	1:A:290:ARG:HG3	2.20	0.41
1:B:302:GLY:O	1:B:305:MET:HG3	2.20	0.41
2:G:100:LEU:HD22	2:G:105:VAL:HB	2.03	0.41
1:B:302:GLY:O	1:B:304:THR:N	2.53	0.41
1:C:295:ALA:O	1:C:328:LYS:HB2	2.21	0.41
2:F:120:HIS:HA	2:F:123:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE2	1:A:61:LYS:HB3	1.92	0.41
1:A:215:LYS:HB3	1:A:215:LYS:HE2	1.78	0.41
1:B:218:TYR:HA	1:B:307:PRO:HD2	2.02	0.41
1:B:334:GLU:C	1:B:336:LYS:H	2.24	0.41
1:E:161:HIS:CD2	1:E:161:HIS:N	2.88	0.41
1:E:306:TYR:CE1	4:E:402:ADP:H2	2.39	0.41
1:A:239:SER:HA	1:A:248:ILE:O	2.21	0.41
1:E:78:ASN:ND2	1:E:81:ASP:OD2	2.54	0.41
1:D:293:LEU:HD23	1:D:293:LEU:HA	1.90	0.41
1:C:232:SER:O	1:C:234:SER:OG	2.33	0.41
1:D:300:SER:O	1:D:304:THR:OG1	2.26	0.41
1:D:304:THR:O	1:D:335:ARG:NH2	2.50	0.41
1:E:166:TYR:CD1	1:E:289:ILE:HG23	2.56	0.41
1:B:47:MET:SD	2:F:90:LEU:HD13	2.61	0.41
1:B:61:LYS:O	1:B:65:LEU:HD22	2.21	0.41
1:B:239:SER:HA	1:B:248:ILE:O	2.21	0.41
1:B:306:TYR:C	1:B:308:GLY:H	2.23	0.41
1:C:131:ALA:HB1	1:C:356:TRP:HB3	2.02	0.41
1:D:14:SER:N	4:D:402:ADP:O3B	2.54	0.41
1:D:29:ALA:HB1	1:D:93:GLU:HG2	2.02	0.41
2:H:58:THR:O	2:H:61:LYS:HG2	2.21	0.41
1:C:56:ASP:HA	1:C:59:GLN:HB3	2.03	0.41
1:C:158:GLY:N	1:C:181:ALA:HB3	2.32	0.41
1:E:156:GLY:HA2	1:E:303:THR:OG1	2.21	0.41
1:B:337:TYR:O	1:B:341:ILE:HG13	2.21	0.40
1:A:202:THR:N	1:A:205:GLU:OE1	2.51	0.40
1:C:151:ILE:HG23	1:C:151:ILE:O	2.21	0.40
1:D:143:TYR:CZ	1:D:346:LEU:HD13	2.56	0.40
1:E:38:PRO:HA	1:E:64:ILE:O	2.22	0.40
1:E:372:ARG:HE	1:E:372:ARG:HB3	1.70	0.40
2:F:113:THR:HG22	2:F:117:ASP:OD2	2.21	0.40
1:A:45:VAL:HG21	1:C:352:PHE:HB2	2.03	0.40
1:D:289:ILE:HG22	1:D:293:LEU:HG	2.04	0.40
2:G:70:LEU:HD23	2:G:99:VAL:HG23	2.03	0.40
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.90	0.40
1:A:107:GLU:OE2	1:A:115:ASN:ND2	2.54	0.40
1:B:132:MET:HG2	1:B:133:TYR:N	2.37	0.40
2:H:126:LEU:O	2:H:130:ILE:HG13	2.22	0.40
1:A:18:LYS:HG2	1:A:30:VAL:HB	2.03	0.40
1:B:183:ARG:HD3	1:B:206:ARG:NH2	2.36	0.40
1:E:104:LEU:HD12	1:E:133:TYR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:296:ASN:OD1	1:E:296:ASN:N	2.54	0.40
2:F:128:TRP:CZ2	2:F:132:LEU:HD13	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/377 (98%)	328 (89%)	39 (11%)	1 (0%)	41	75
1	B	368/377 (98%)	324 (88%)	43 (12%)	1 (0%)	41	75
1	C	368/377 (98%)	329 (89%)	38 (10%)	1 (0%)	41	75
1	D	368/377 (98%)	335 (91%)	33 (9%)	0	100	100
1	E	368/377 (98%)	340 (92%)	27 (7%)	1 (0%)	41	75
2	F	116/269 (43%)	105 (90%)	11 (10%)	0	100	100
2	G	116/269 (43%)	108 (93%)	8 (7%)	0	100	100
2	H	116/269 (43%)	109 (94%)	7 (6%)	0	100	100
All	All	2188/2692 (81%)	1978 (90%)	206 (9%)	4 (0%)	50	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	309	ILE
1	B	309	ILE
1	C	63	GLY
1	E	159	VAL

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	311/320 (97%)	278 (89%)	33 (11%)	6	32
1	B	310/320 (97%)	281 (91%)	29 (9%)	8	38
1	C	312/320 (98%)	286 (92%)	26 (8%)	11	42
1	D	309/320 (97%)	278 (90%)	31 (10%)	7	35
1	E	309/320 (97%)	294 (95%)	15 (5%)	25	59
2	F	107/246 (44%)	99 (92%)	8 (8%)	13	45
2	G	107/246 (44%)	101 (94%)	6 (6%)	21	56
2	H	107/246 (44%)	96 (90%)	11 (10%)	7	34
All	All	1872/2338 (80%)	1713 (92%)	159 (8%)	14	41

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	16	LEU
1	A	28	ARG
1	A	30	VAL
1	A	34	ILE
1	A	44	MET
1	A	54	VAL
1	A	56	ASP
1	A	61	LYS
1	A	62	ARG
1	A	93	GLU
1	A	111	ASN
1	A	134	VAL
1	A	143	TYR
1	A	148	THR
1	A	157	ASP
1	A	162	ASN
1	A	179	ASP
1	A	191	LYS

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Mol	Chain	Res	Type
1	A	193	LEU
1	A	213	LYS
1	A	253	GLU
1	A	254	ARG
1	A	260	THR
1	A	275	HIS
1	A	288	ASP
1	A	292	ASP
1	A	297	ASN
1	A	303	THR
1	A	312	ARG
1	A	324	THR
1	A	344	SER
1	A	372	ARG
1	B	14	SER
1	B	16	LEU
1	B	34	ILE
1	B	56	ASP
1	B	61	LYS
1	B	89	THR
1	B	93	GLU
1	B	118	LYS
1	B	120	THR
1	B	132	MET
1	B	134	VAL
1	B	142	LEU
1	B	148	THR
1	B	154	ASP
1	B	157	ASP
1	B	159	VAL
1	B	167	GLU
1	B	175	ILE
1	B	179	ASP
1	B	201	VAL
1	B	247	VAL
1	B	253	GLU
1	B	275	HIS
1	B	278	THR
1	B	292	ASP
1	B	300	SER
1	B	312	ARG
1	B	335	ARG

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Mol	Chain	Res	Type
1	B	372	ARG
1	C	6	THR
1	C	16	LEU
1	C	30	VAL
1	C	34	ILE
1	C	54	VAL
1	C	56	ASP
1	C	57	GLU
1	C	66	THR
1	C	75	ILE
1	C	107	GLU
1	C	111	ASN
1	C	132	MET
1	C	134	VAL
1	C	162	ASN
1	C	167	GLU
1	C	191	LYS
1	C	198	TYR
1	C	201	VAL
1	C	236	LEU
1	C	253	GLU
1	C	275	HIS
1	C	296	ASN
1	C	323	SER
1	C	324	THR
1	C	353	GLN
1	C	370	VAL
1	D	11	ASP
1	D	45	VAL
1	D	56	ASP
1	D	64	ILE
1	D	75	ILE
1	D	81	ASP
1	D	92	ASN
1	D	107	GLU
1	D	111	ASN
1	D	134	VAL
1	D	148	THR
1	D	159	VAL
1	D	162	ASN
1	D	167	GLU
1	D	180	LEU

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Mol	Chain	Res	Type
1	D	191	LYS
1	D	193	LEU
1	D	201	VAL
1	D	249	THR
1	D	253	GLU
1	D	254	ARG
1	D	286	ASP
1	D	288	ASP
1	D	296	ASN
1	D	297	ASN
1	D	312	ARG
1	D	320	LEU
1	D	324	THR
1	D	334	GLU
1	D	335	ARG
1	D	351	THR
1	E	34	ILE
1	E	66	THR
1	E	111	ASN
1	E	115	ASN
1	E	134	VAL
1	E	154	ASP
1	E	161	HIS
1	E	179	ASP
1	E	261	LEU
1	E	286	ASP
1	E	288	ASP
1	E	320	LEU
1	E	328	LYS
1	E	334	GLU
1	E	372	ARG
2	F	18	PHE
2	F	22	ILE
2	F	45	PHE
2	F	53	ILE
2	F	55	ASP
2	F	107	LEU
2	F	108	VAL
2	F	124	LEU
2	G	18	PHE
2	G	22	ILE
2	G	53	ILE

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Mol	Chain	Res	Type
2	G	100	LEU
2	G	108	VAL
2	G	119	ASN
2	H	22	ILE
2	H	28	GLU
2	H	36	THR
2	H	69	LEU
2	H	70	LEU
2	H	78	LEU
2	H	94	ASN
2	H	107	LEU
2	H	108	VAL
2	H	109	ASN
2	H	124	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	101	HIS
1	A	162	ASN
1	A	353	GLN
1	B	88	HIS
1	B	92	ASN
1	B	162	ASN
1	C	88	HIS
1	C	111	ASN
1	C	161	HIS
1	C	275	HIS
1	D	40	HIS
1	D	88	HIS
1	D	111	ASN
1	D	137	GLN
1	D	275	HIS
1	E	88	HIS
1	E	111	ASN
1	E	137	GLN
1	E	275	HIS
2	F	29	HIS
2	F	30	ASN
2	F	33	GLN
2	F	88	HIS

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Mol	Chain	Res	Type
2	F	94	ASN
2	F	98	GLN
2	F	120	HIS
2	G	29	HIS
2	G	33	GLN
2	G	88	HIS
2	G	119	ASN
2	G	120	HIS
2	H	29	HIS
2	H	33	GLN
2	H	88	HIS
2	H	103	ASN
2	H	120	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	E	402	3	24,29,29	0.95	1 (4%)	29,45,45	1.49	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	A	402	3	24,29,29	1.00	1 (4%)	29,45,45	1.57	4 (13%)
4	ADP	D	402	3	24,29,29	0.96	1 (4%)	29,45,45	1.43	4 (13%)
4	ADP	B	402	3	24,29,29	0.98	1 (4%)	29,45,45	1.54	5 (17%)
4	ADP	C	402	3	24,29,29	0.95	0	29,45,45	1.47	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	E	402	3	-	5/12/32/32	0/3/3/3
4	ADP	A	402	3	-	0/12/32/32	0/3/3/3
4	ADP	D	402	3	-	3/12/32/32	0/3/3/3
4	ADP	B	402	3	-	0/12/32/32	0/3/3/3
4	ADP	C	402	3	-	2/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	402	ADP	C2'-C1'	-2.18	1.50	1.53
4	B	402	ADP	C2'-C1'	-2.11	1.50	1.53
4	D	402	ADP	C5-C4	2.08	1.46	1.40
4	E	402	ADP	C5-C4	2.06	1.46	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ADP	PA-O3A-PB	-4.42	117.67	132.83
4	A	402	ADP	PA-O3A-PB	-4.36	117.85	132.83
4	C	402	ADP	PA-O3A-PB	-3.73	120.02	132.83
4	D	402	ADP	C3'-C2'-C1'	3.50	106.25	100.98
4	E	402	ADP	PA-O3A-PB	-3.49	120.85	132.83
4	C	402	ADP	C3'-C2'-C1'	3.37	106.05	100.98
4	A	402	ADP	C3'-C2'-C1'	3.28	105.92	100.98
4	E	402	ADP	N3-C2-N1	-3.21	123.65	128.68
4	B	402	ADP	C3'-C2'-C1'	3.21	105.81	100.98
4	D	402	ADP	PA-O3A-PB	-3.18	121.90	132.83
4	E	402	ADP	C3'-C2'-C1'	3.15	105.72	100.98
4	C	402	ADP	N3-C2-N1	-3.05	123.91	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	ADP	N3-C2-N1	-3.02	123.95	128.68
4	A	402	ADP	N3-C2-N1	-2.83	124.25	128.68
4	D	402	ADP	N3-C2-N1	-2.54	124.70	128.68
4	C	402	ADP	C4-C5-N7	-2.32	106.98	109.40
4	E	402	ADP	C4-C5-N7	-2.30	107.00	109.40
4	A	402	ADP	C4-C5-N7	-2.29	107.01	109.40
4	D	402	ADP	C4-C5-N7	-2.15	107.16	109.40
4	B	402	ADP	C4-C5-N7	-2.14	107.17	109.40
4	B	402	ADP	O3B-PB-O2B	2.03	115.38	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	402	ADP	C5'-O5'-PA-O2A
4	E	402	ADP	PA-O3A-PB-O2B
4	E	402	ADP	PA-O3A-PB-O3B
4	E	402	ADP	C5'-O5'-PA-O1A
4	E	402	ADP	C5'-O5'-PA-O2A
4	D	402	ADP	C5'-O5'-PA-O3A
4	E	402	ADP	C5'-O5'-PA-O3A
4	C	402	ADP	C3'-C4'-C5'-O5'
4	C	402	ADP	O4'-C4'-C5'-O5'
4	D	402	ADP	C5'-O5'-PA-O1A

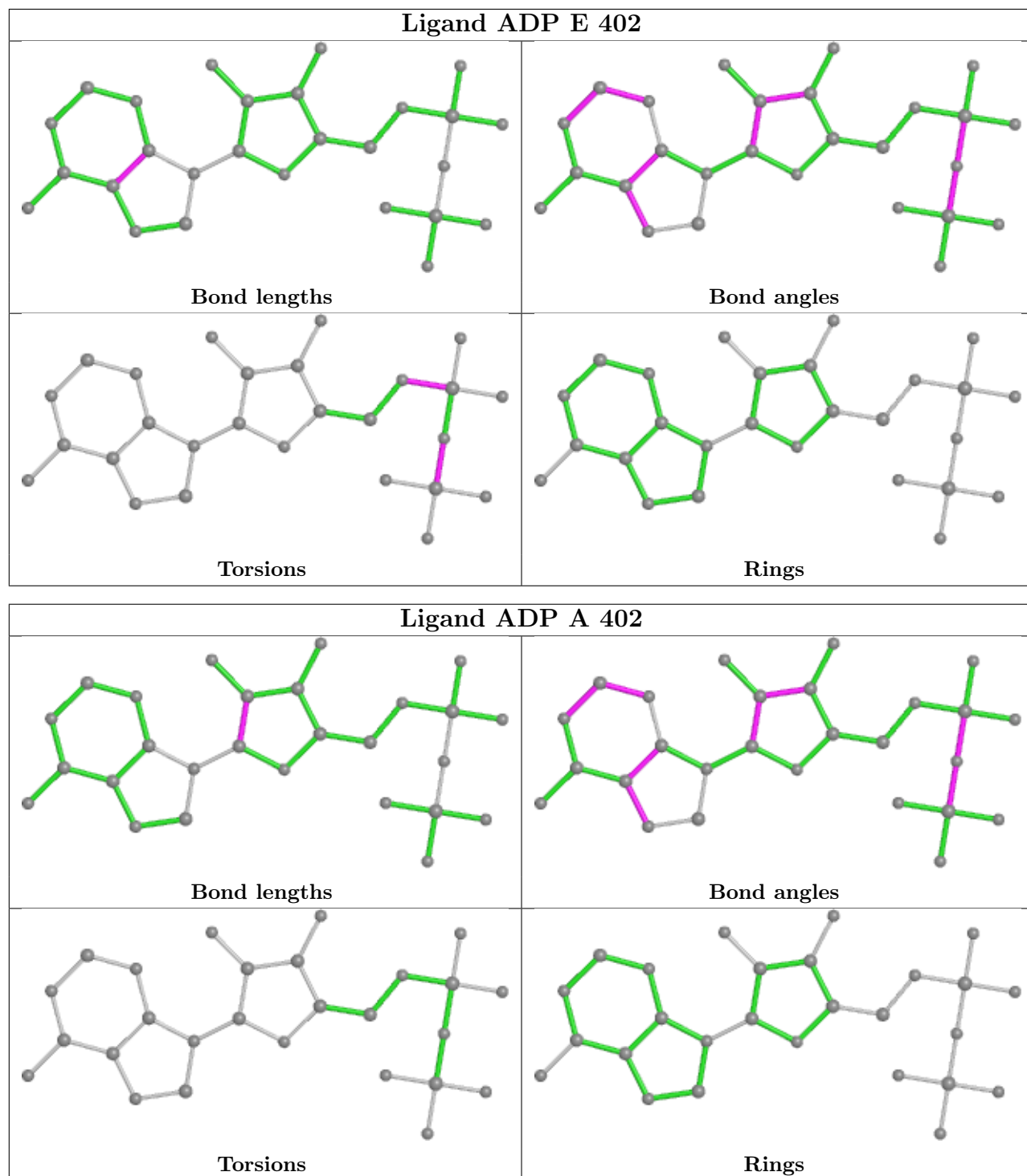
There are no ring outliers.

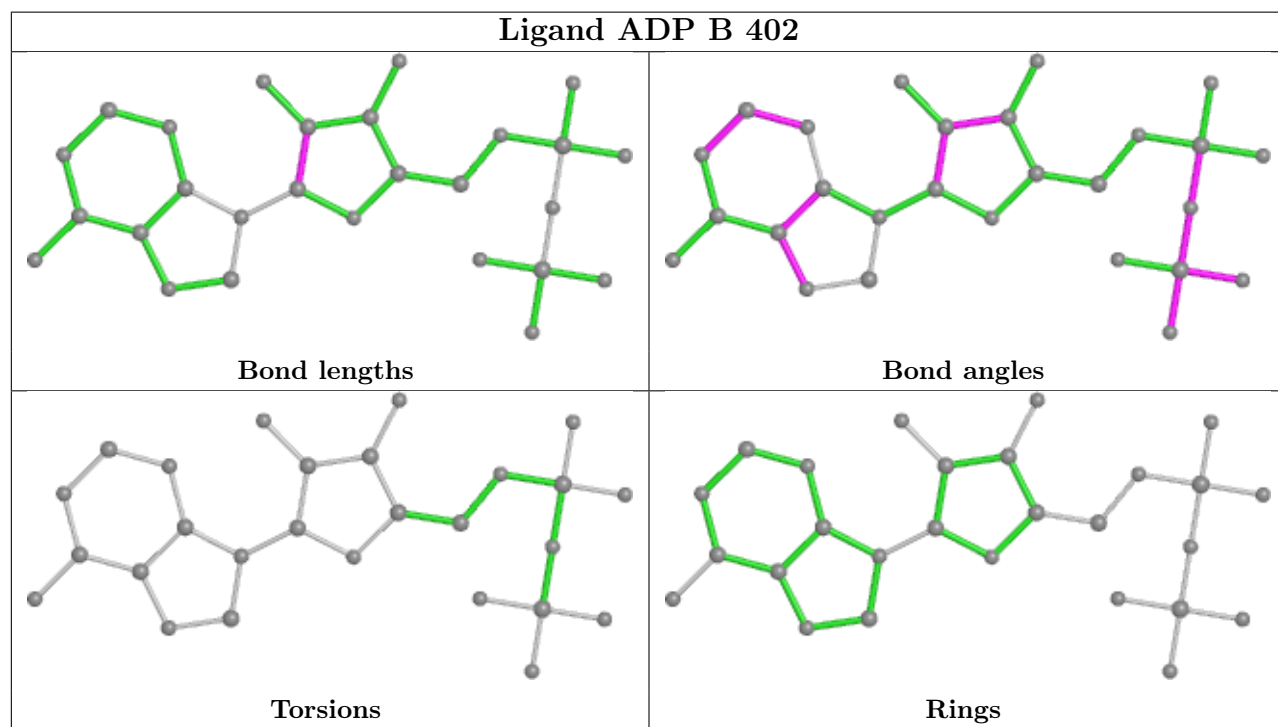
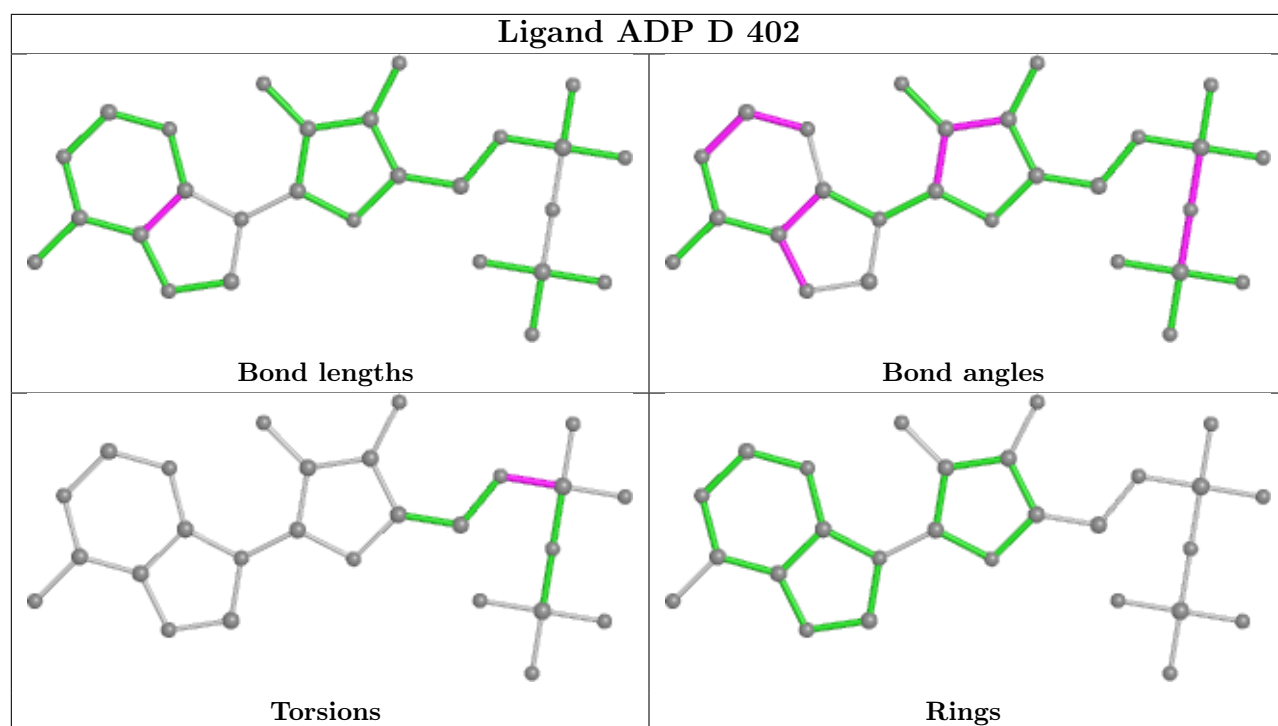
5 monomers are involved in 11 short contacts:

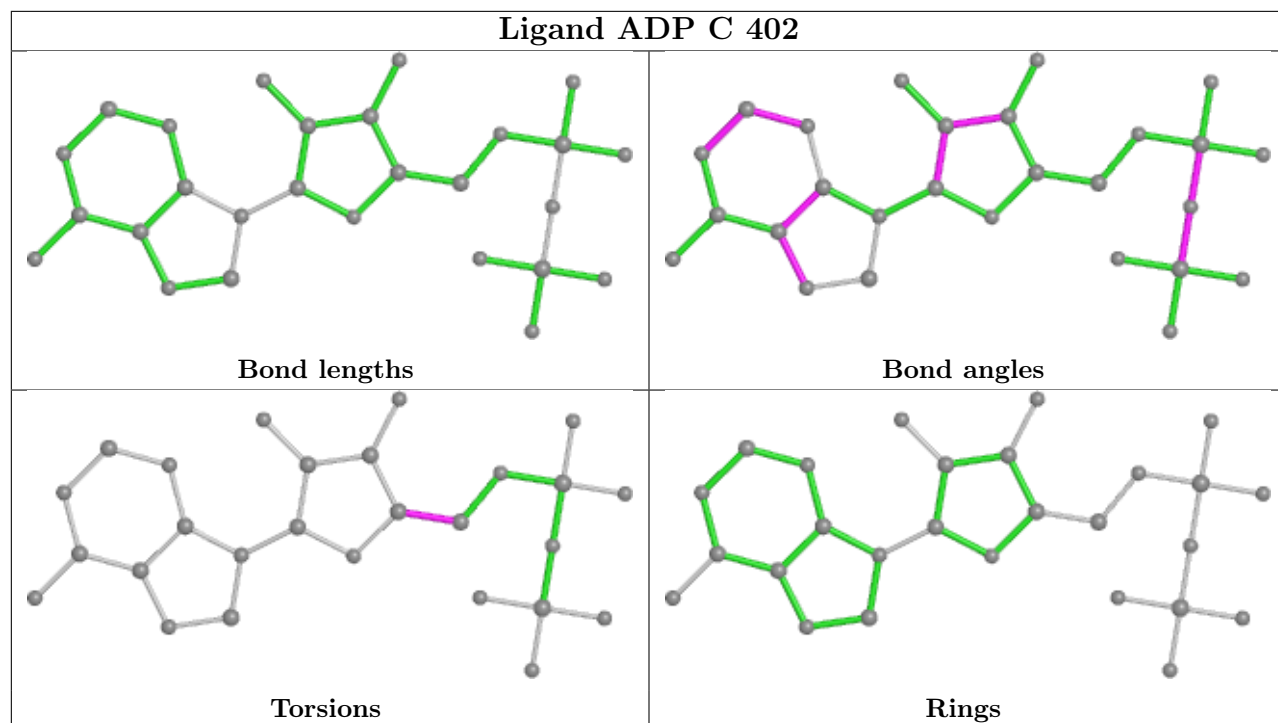
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	402	ADP	1	0
4	A	402	ADP	2	0
4	D	402	ADP	3	0
4	B	402	ADP	3	0
4	C	402	ADP	2	0

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.

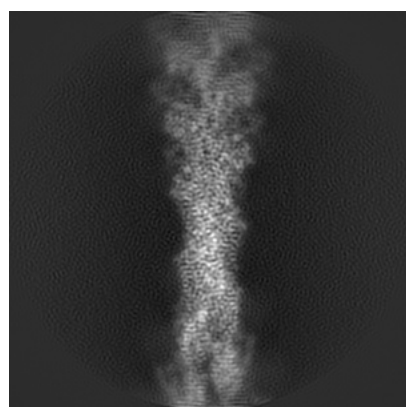
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30085. These allow visual inspection of the internal detail of the map and identification of artifacts.

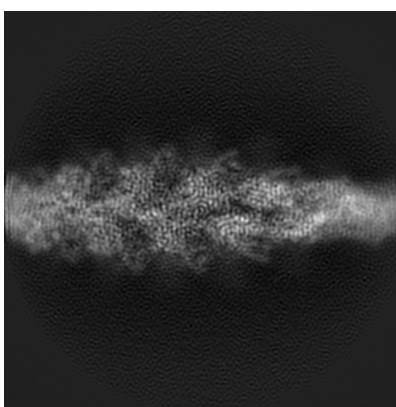
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

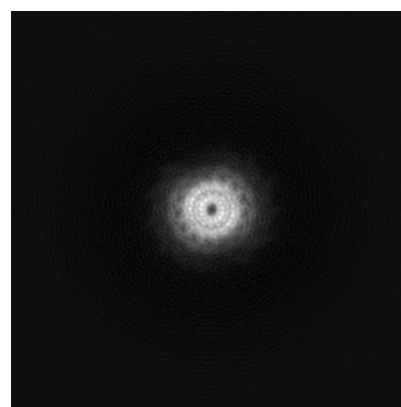
6.1.1 Primary map



X



Y

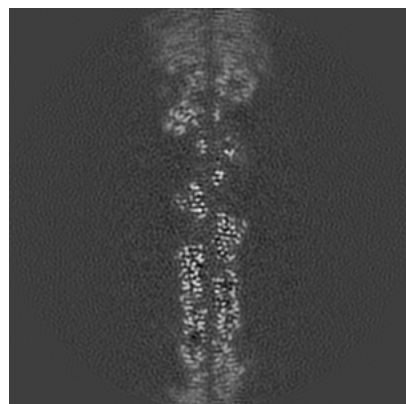


Z

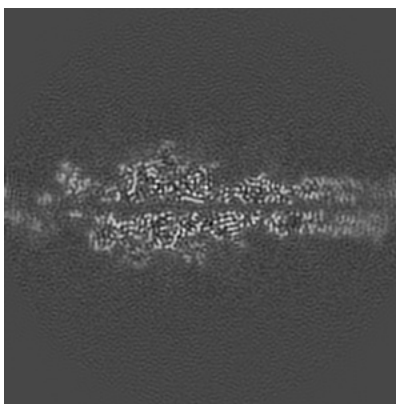
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

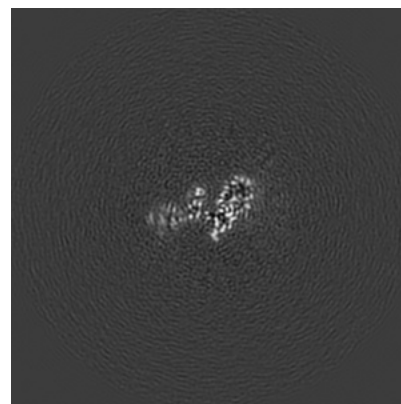
6.2.1 Primary map



X Index: 128



Y Index: 128

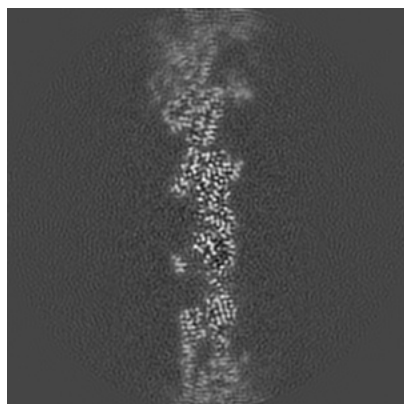


Z Index: 128

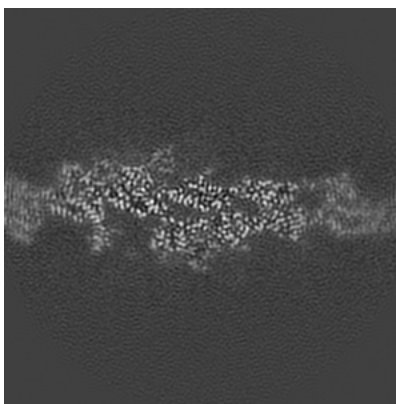
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

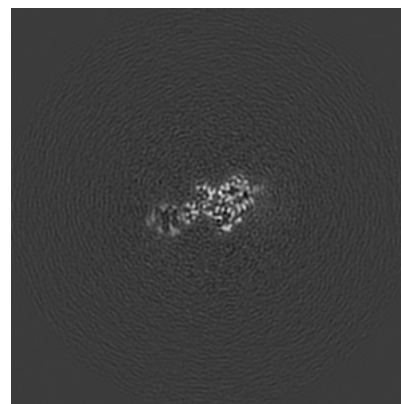
6.3.1 Primary map



X Index: 121



Y Index: 122



Z Index: 123

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

6.4 Orthogonal surface views [i](#)

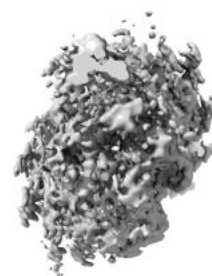
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0464. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

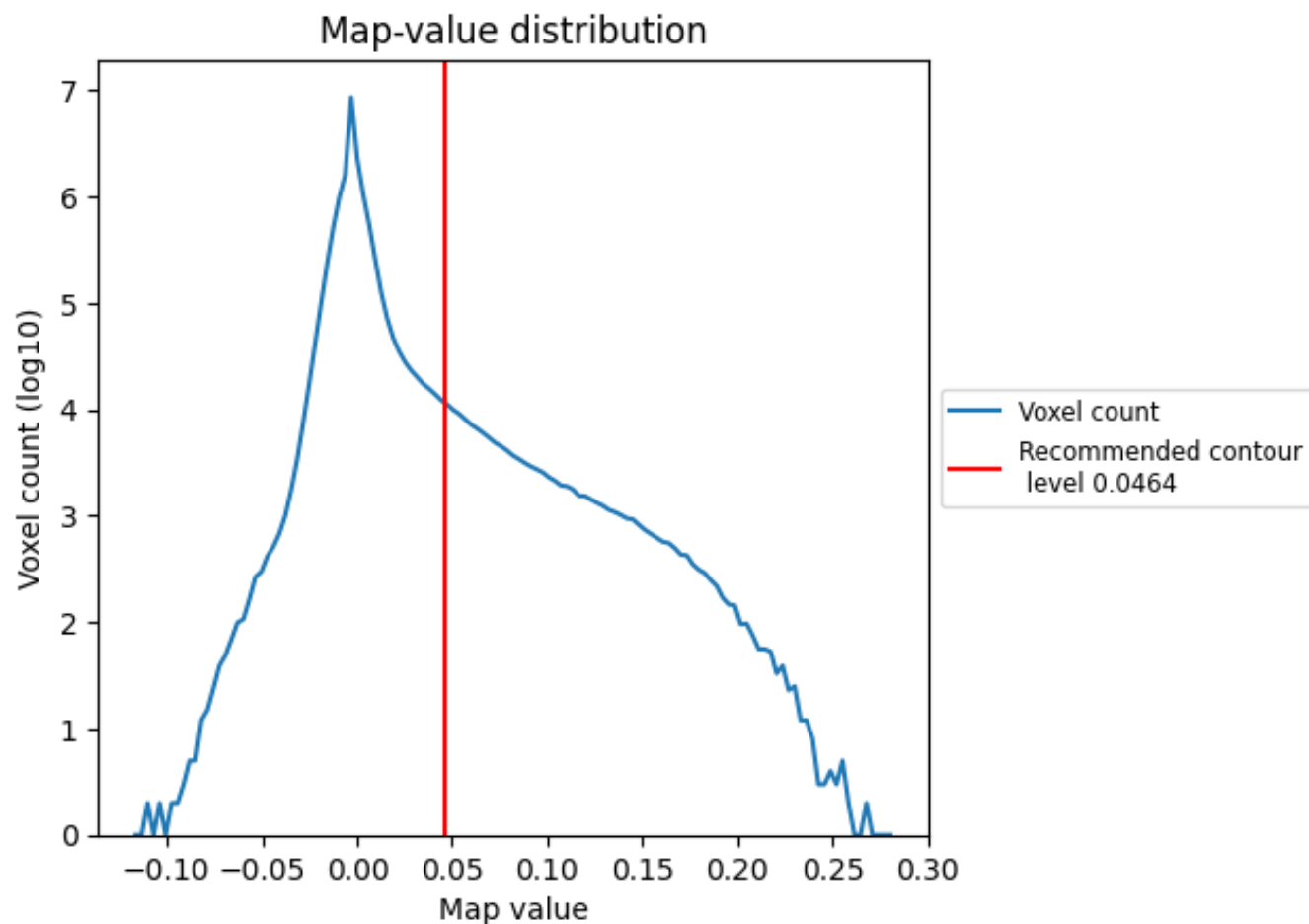
6.5 Mask visualisation

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

7 Map analysis [i](#)

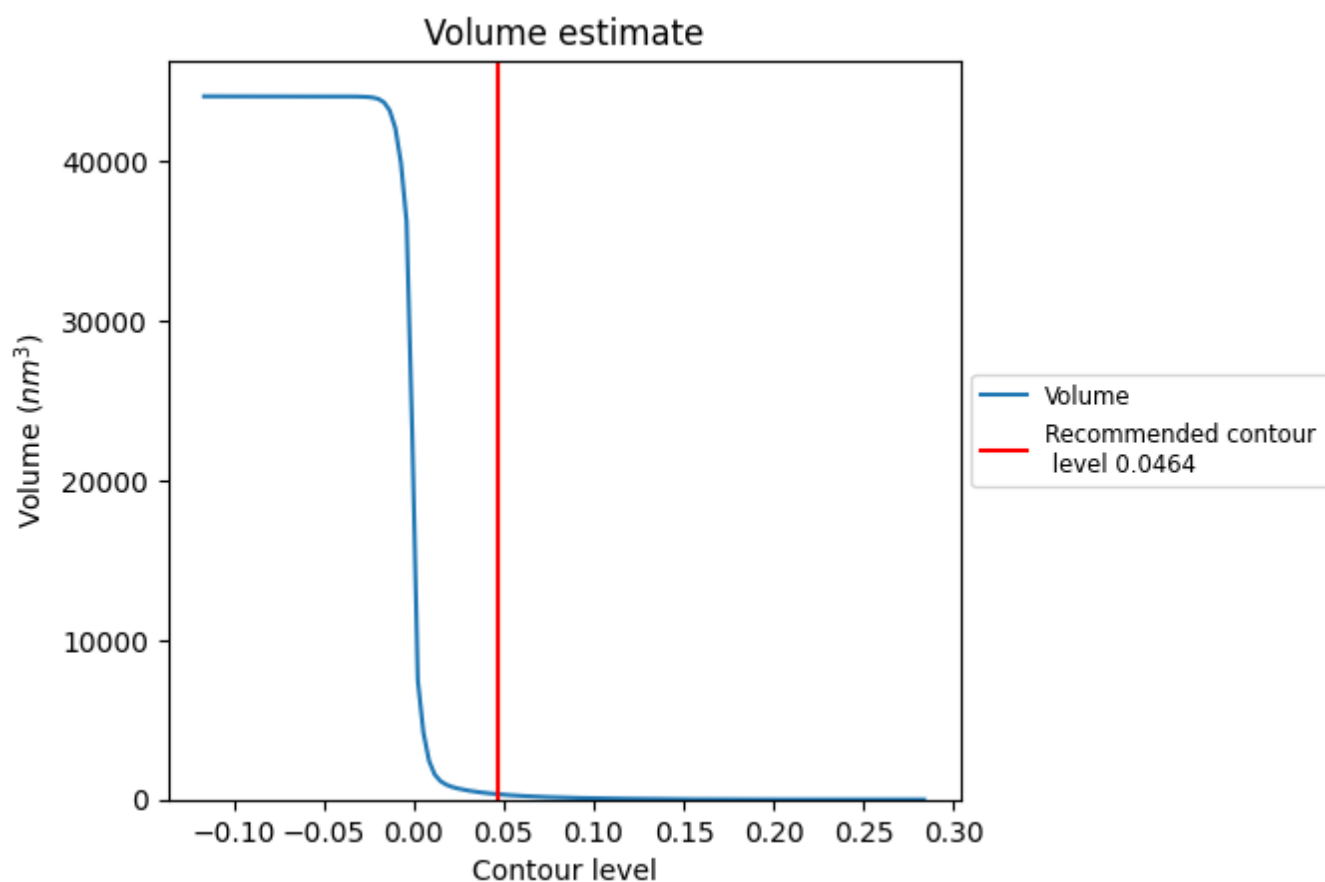
This section contains the results of statistical analysis of the map.

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.

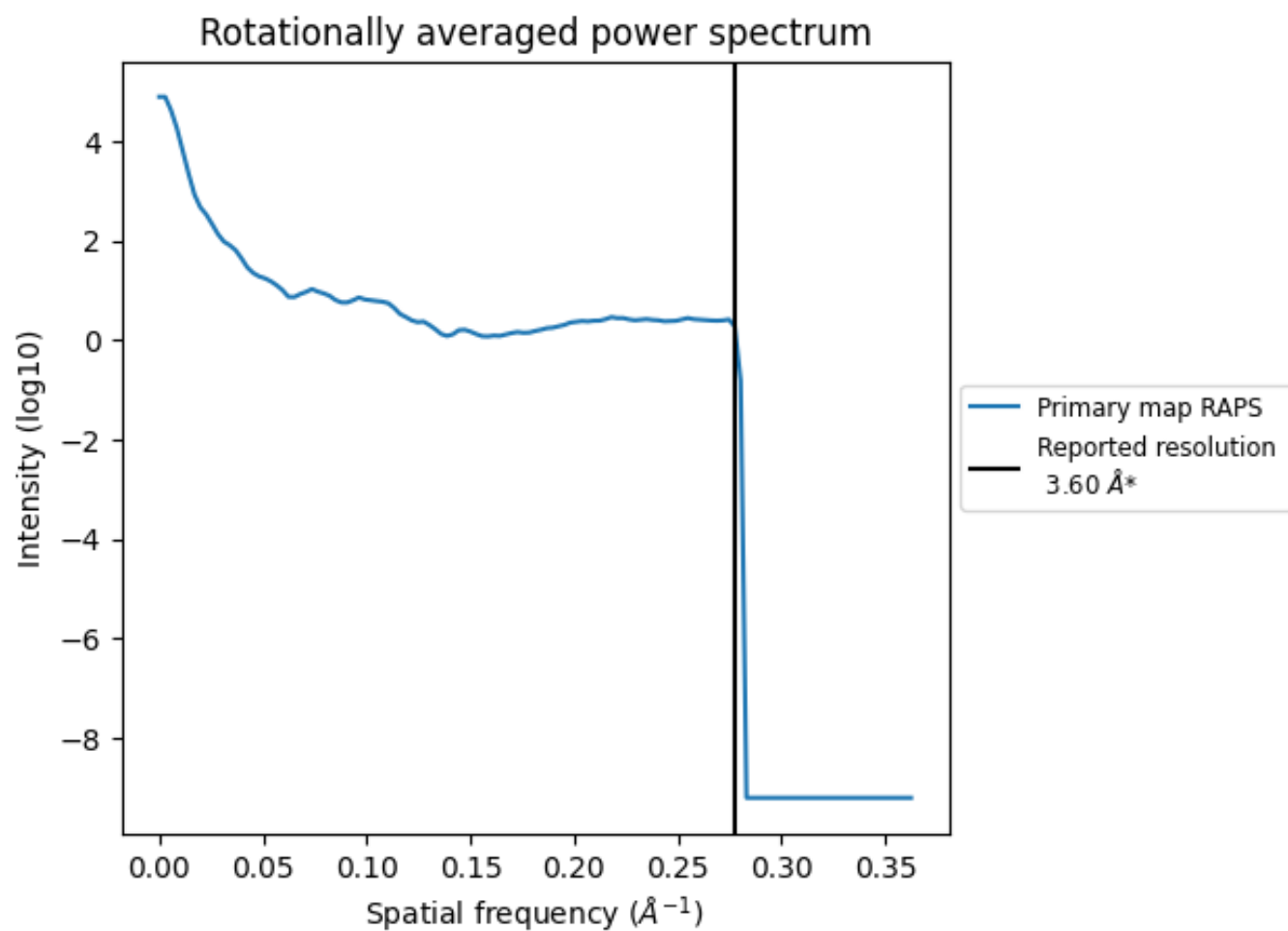
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 340 nm³; this corresponds to an approximate mass of 307 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 ⓘ

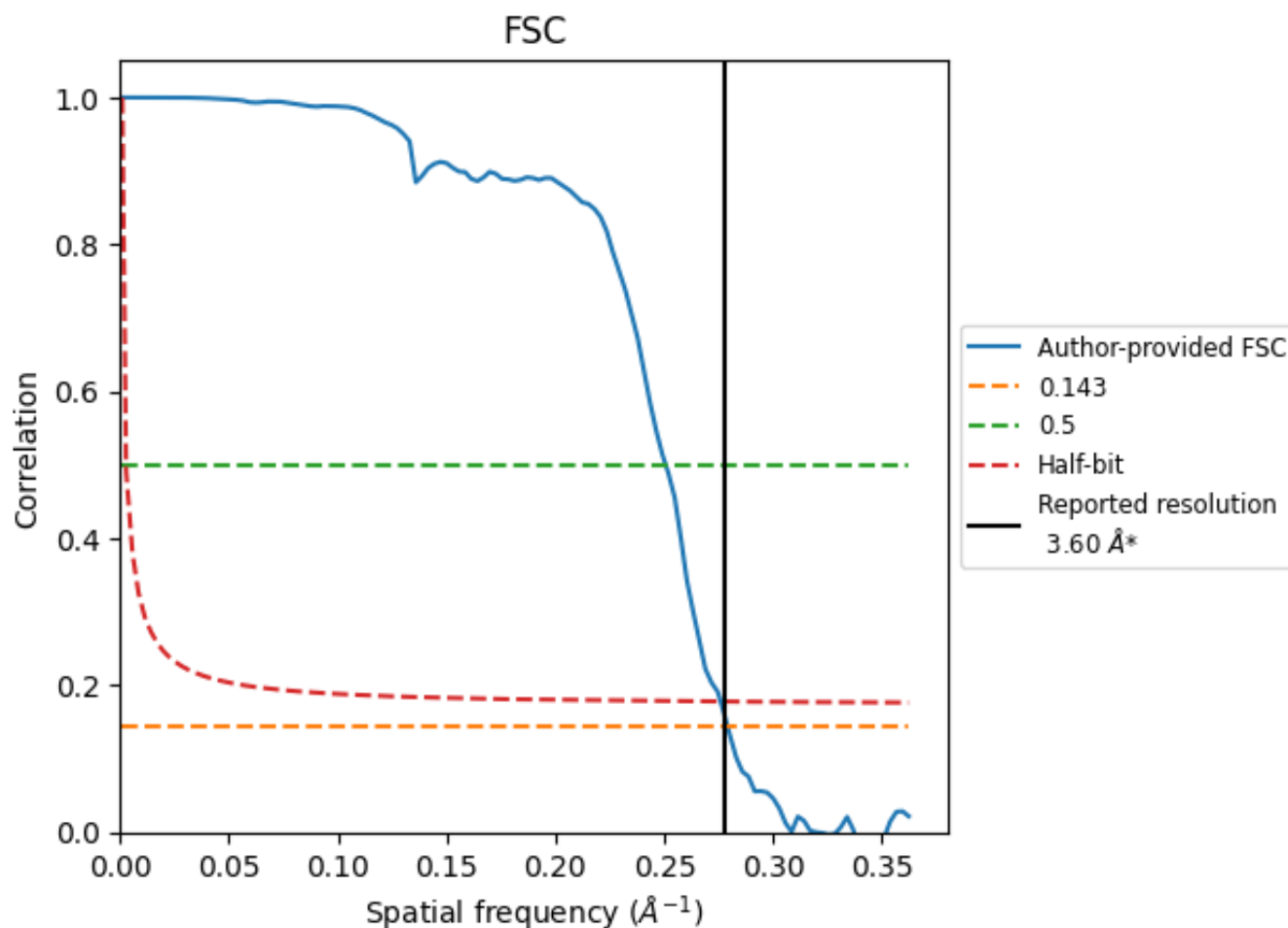


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

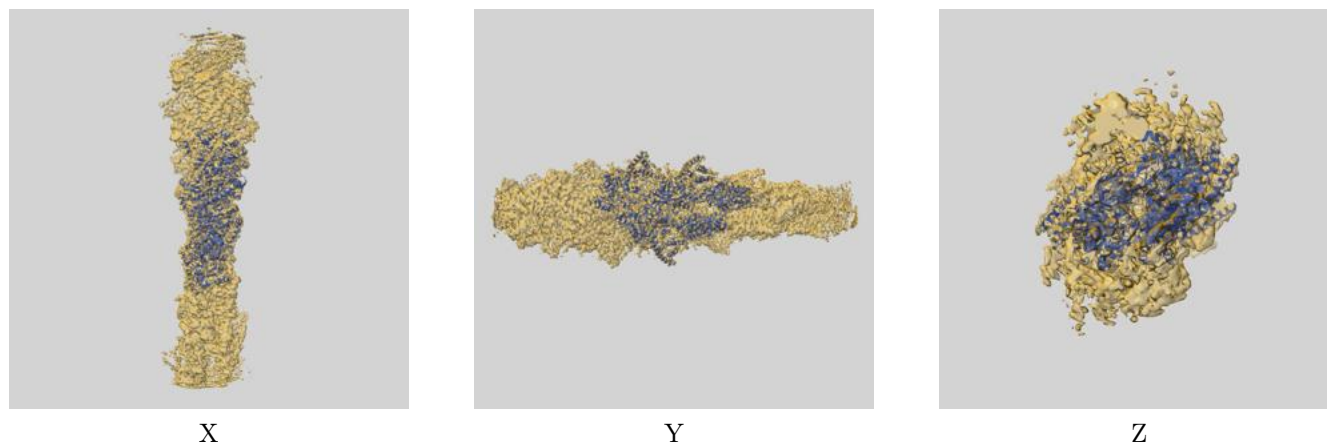
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.99	3.62
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

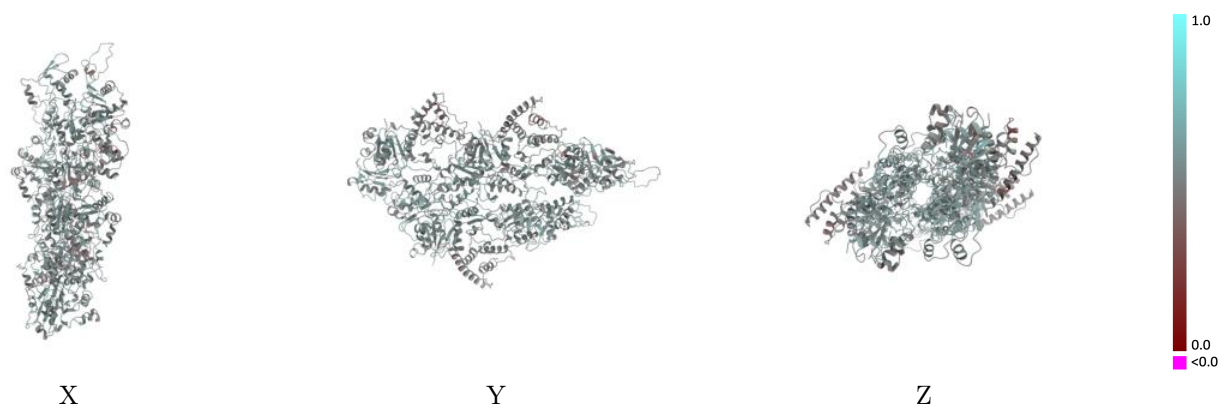
This section contains information regarding the fit between EMDB map EMD-30085 and PDB model 6M5G. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



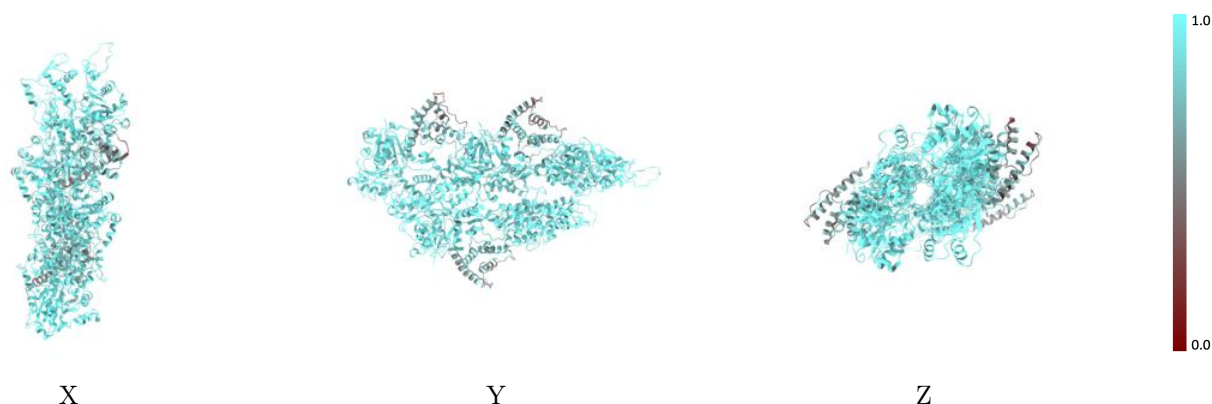
The images above show the 3D surface view of the map at the recommended contour level 0.0464 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



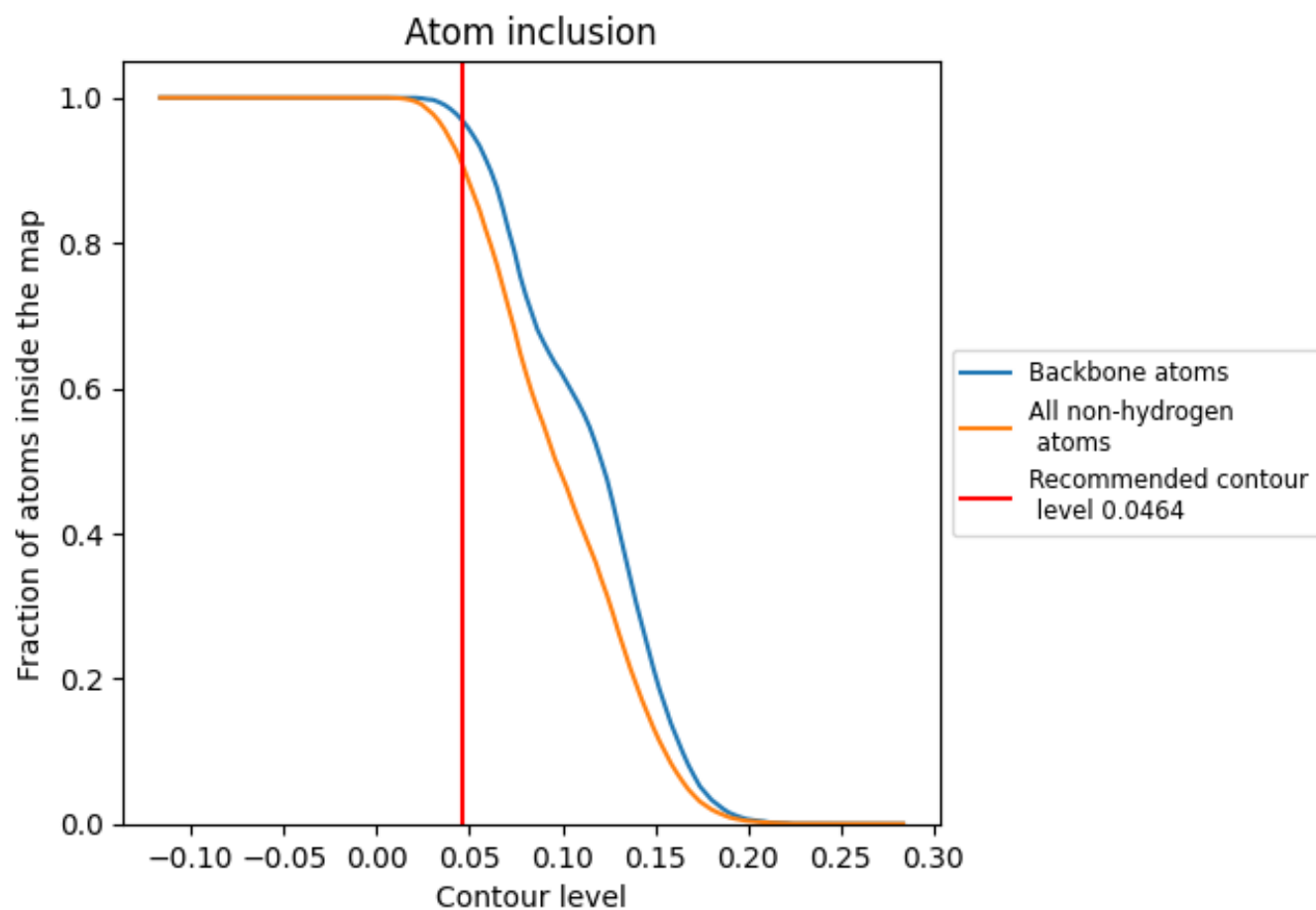
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0464).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.0464) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9065	<div><div></div></div> 0.5300
A	<div><div></div></div> 0.9604	<div><div></div></div> 0.5430
B	<div><div></div></div> 0.9660	<div><div></div></div> 0.5460
C	<div><div></div></div> 0.9576	<div><div></div></div> 0.5450
D	<div><div></div></div> 0.9578	<div><div></div></div> 0.5400
E	<div><div></div></div> 0.9403	<div><div></div></div> 0.5280
F	<div><div></div></div> 0.6638	<div><div></div></div> 0.4770
G	<div><div></div></div> 0.6498	<div><div></div></div> 0.4830
H	<div><div></div></div> 0.6390	<div><div></div></div> 0.4680

1.0

0.0

<0.0