



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 07:54 PM UTC

PDB ID : 6RN4 / pdb_00006rn4
EMDB ID : EMD-4942
Title : ClpB (DWB mutant) bound to casein in presence of ATPgammaS - state WT-2B
Authors : Deville, C.; Saibil, H.R.
Deposited on : 2019-05-08
Resolution : 4.20 Å(reported)
Based on initial model : 1CIU

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

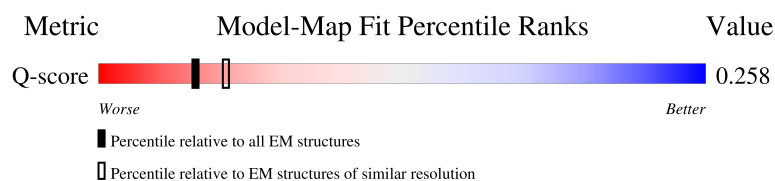
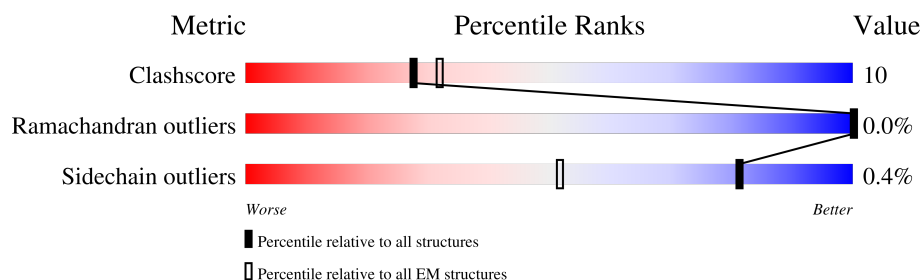
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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	858	23% 60% 18% 21%
1	B	858	17% 60% 20% 20%
1	C	858	15% 63% 17% 20%
1	D	858	15% 59% 21% 20%

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Mol	Chain	Length	Quality of chain
1	E	858	15% 61% 19% 20%
1	F	858	30% 59% 19% • 21%
2	S	24	• 88% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32833 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 Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	675	Total	C	N	O	S	0	0
			5340	3345	964	1013	18		
1	B	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	C	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	D	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	E	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	F	680	Total	C	N	O	S	0	0
			5364	3359	969	1018	18		

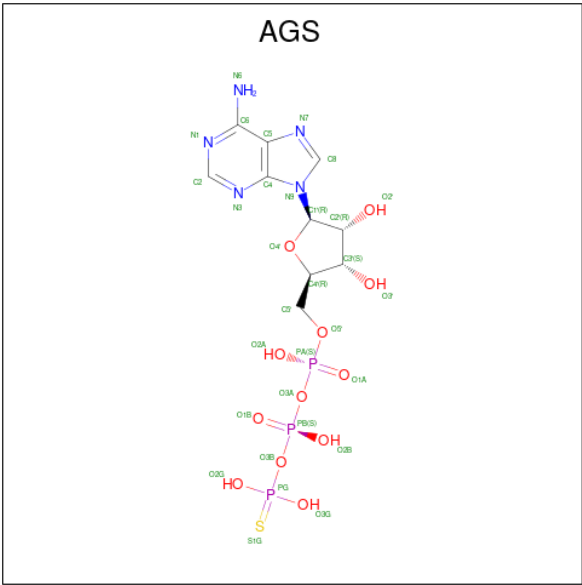
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	GLU	engineered mutation	UNP V2RJ62
A	678	ALA	GLU	engineered mutation	UNP V2RJ62
A	858	HIS	-	expression tag	UNP V2RJ62
B	279	ALA	GLU	engineered mutation	UNP V2RJ62
B	678	ALA	GLU	engineered mutation	UNP V2RJ62
B	858	HIS	-	expression tag	UNP V2RJ62
C	279	ALA	GLU	engineered mutation	UNP V2RJ62
C	678	ALA	GLU	engineered mutation	UNP V2RJ62
C	858	HIS	-	expression tag	UNP V2RJ62
D	279	ALA	GLU	engineered mutation	UNP V2RJ62
D	678	ALA	GLU	engineered mutation	UNP V2RJ62
D	858	HIS	-	expression tag	UNP V2RJ62
E	279	ALA	GLU	engineered mutation	UNP V2RJ62
E	678	ALA	GLU	engineered mutation	UNP V2RJ62
E	858	HIS	-	expression tag	UNP V2RJ62
F	279	ALA	GLU	engineered mutation	UNP V2RJ62
F	678	ALA	GLU	engineered mutation	UNP V2RJ62
F	858	HIS	-	expression tag	UNP V2RJ62

- Molecule 2 is a protein called casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	24	120	72	24	24	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



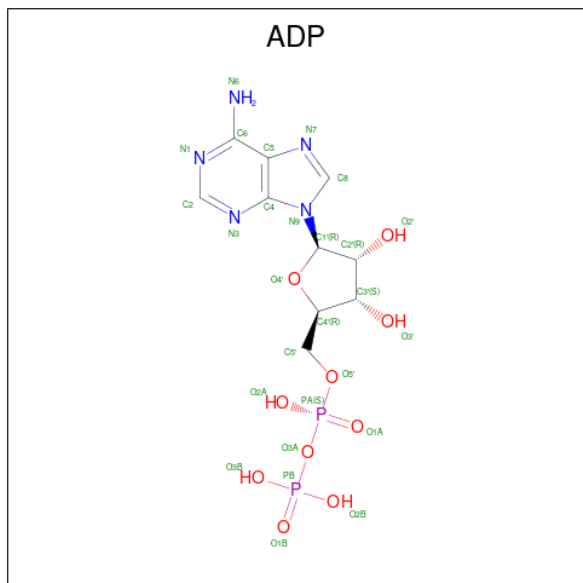
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	A	1	Total 31	10	5	12	3	1	0
3	B	1	Total 31	10	5	12	3	1	0
3	B	1	Total 31	10	5	12	3	1	0
3	C	1	Total 31	10	5	12	3	1	0
3	C	1	Total 31	10	5	12	3	1	0
3	D	1	Total 31	10	5	12	3	1	0
3	D	1	Total 31	10	5	12	3	1	0
3	E	1	Total 31	10	5	12	3	1	0
3	E	1	Total 31	10	5	12	3	1	0

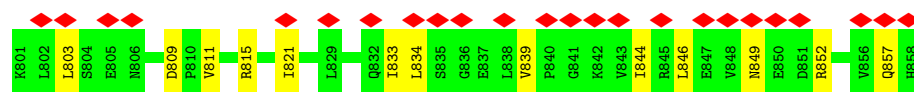
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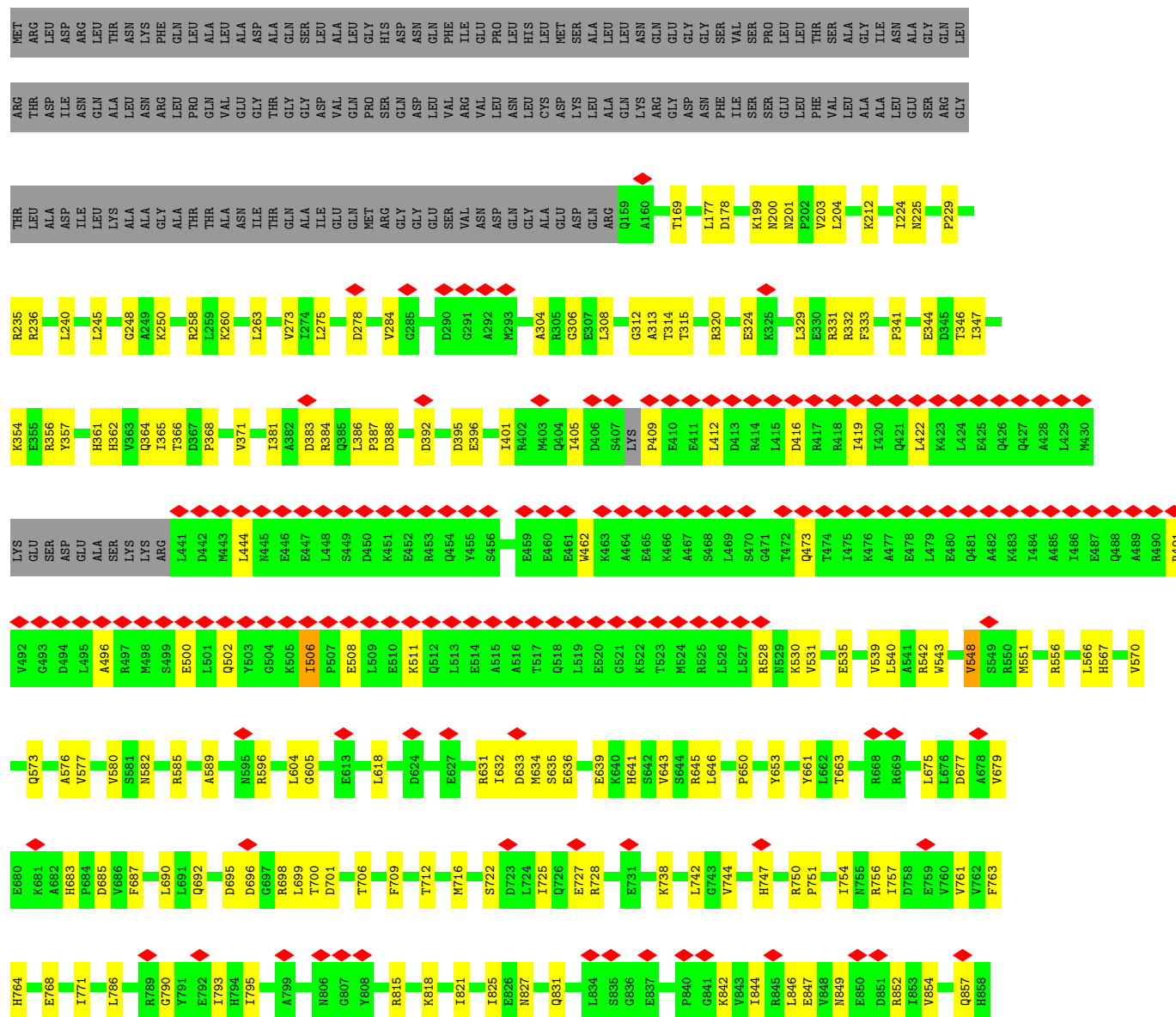
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	F	1	31	10	5	12	3	1	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

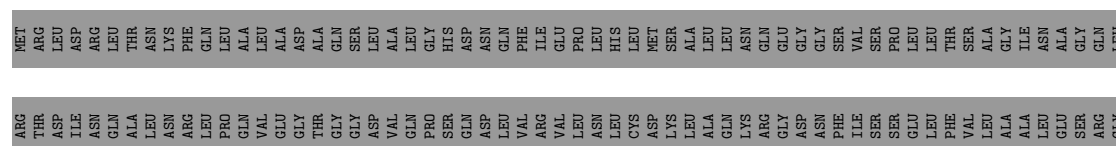


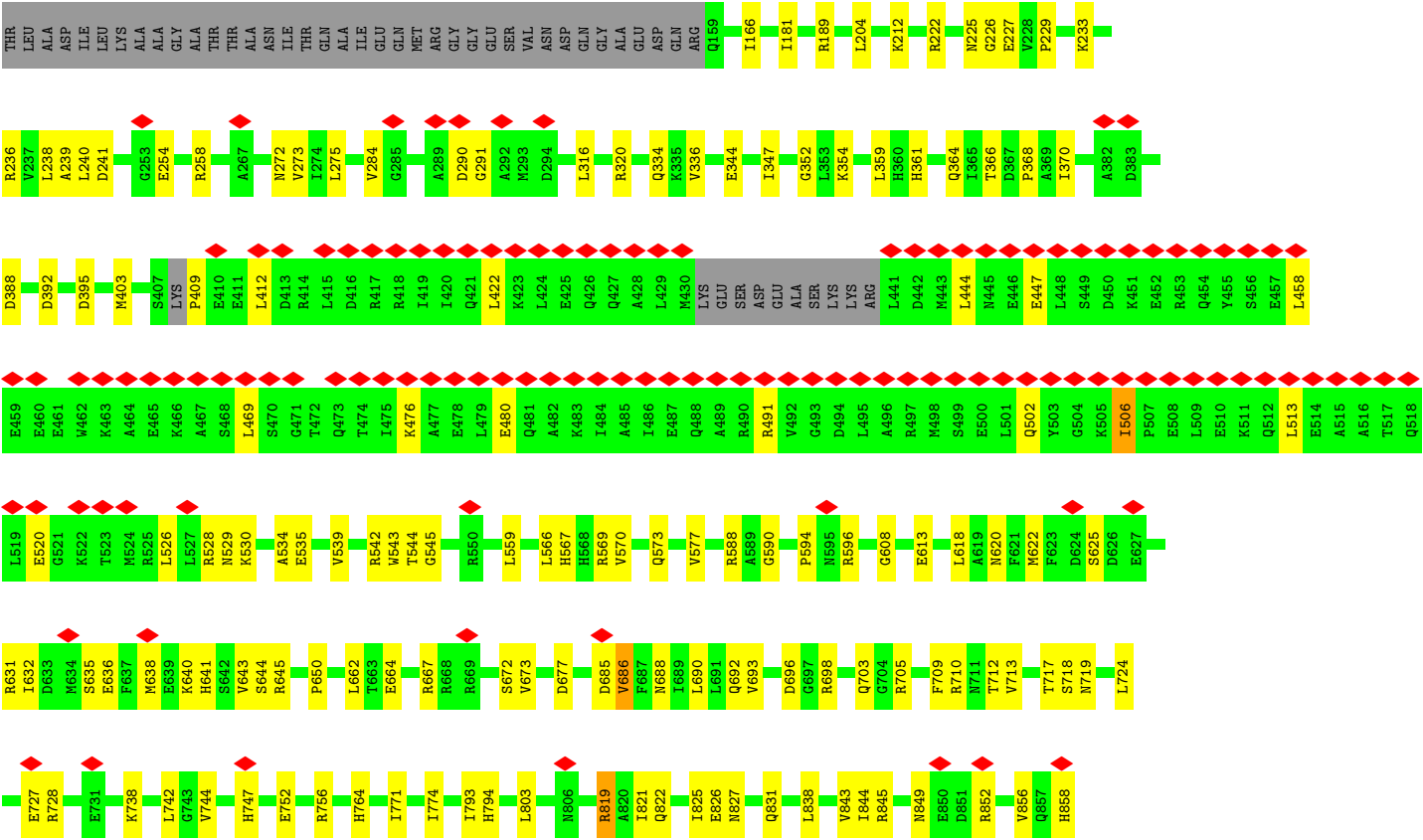


• Molecule 1: Chaperone protein ClpB

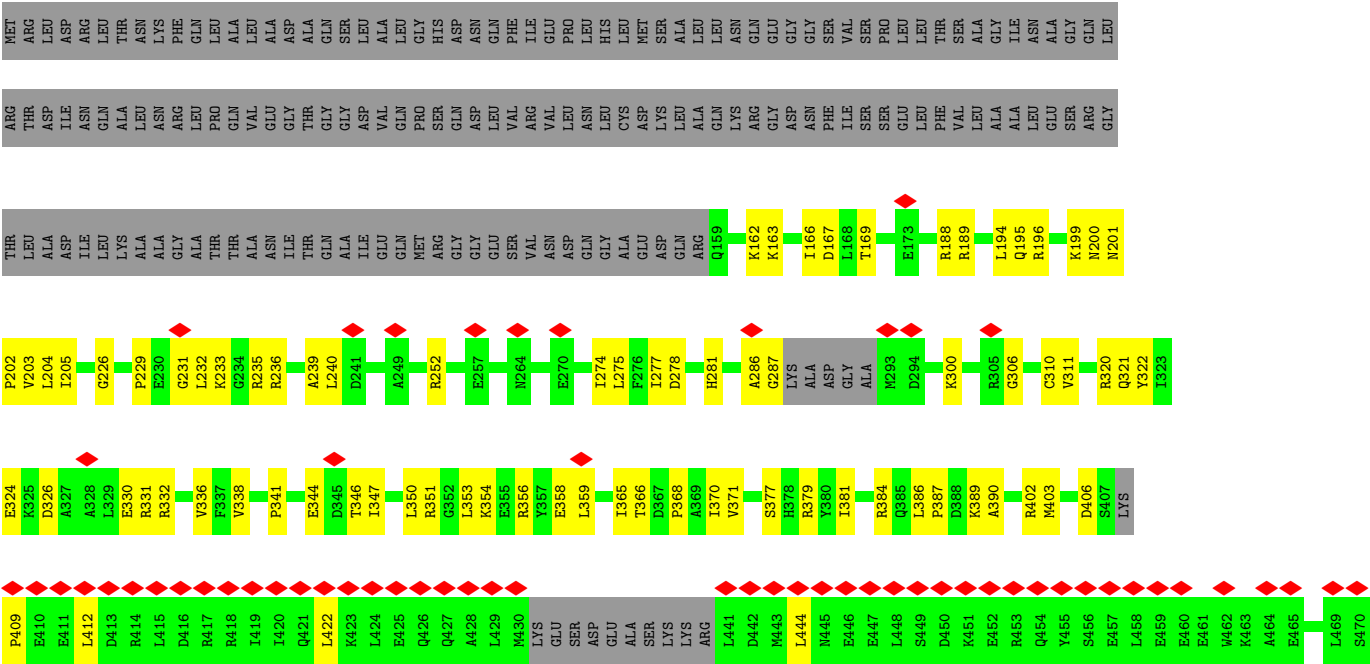


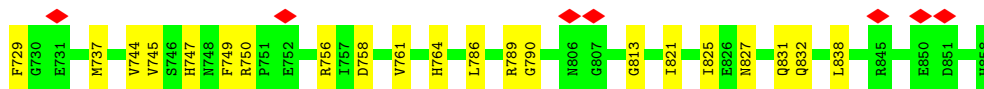
• Molecule 1: Chaperone protein ClpB



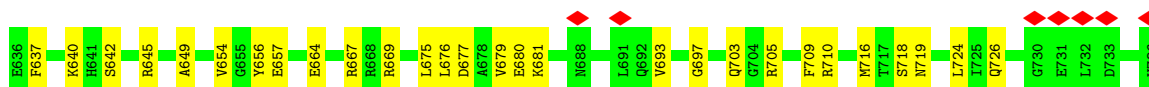


● Molecule 1: Chaperone protein ClpB



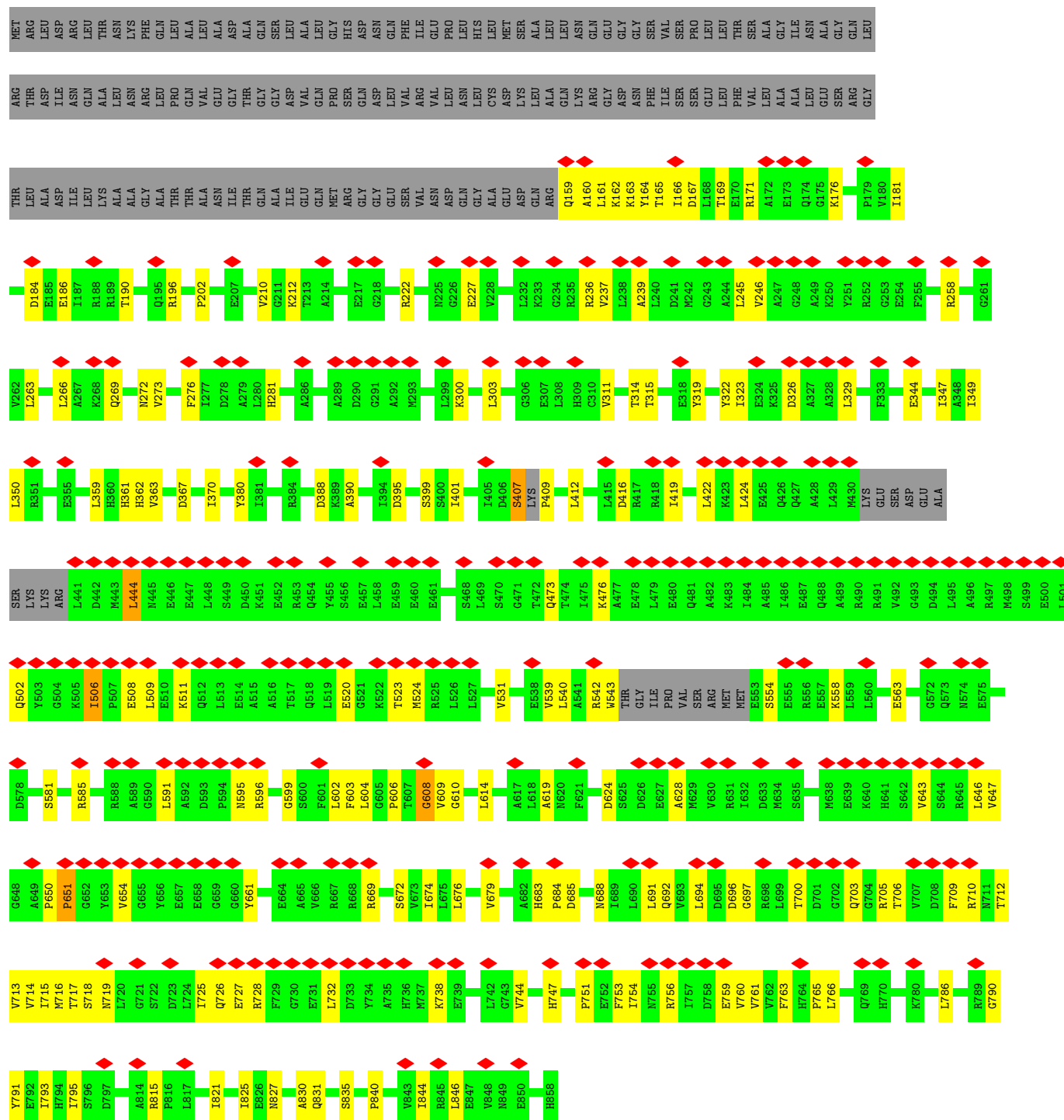


- Molecule 1: Chaperone protein ClpB

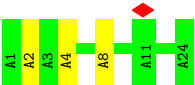
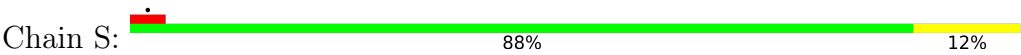




• Molecule 1: Chaperone protein ClpB



• Molecule 2: casein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	29268	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.156	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/5409	0.59	0/7283
1	B	0.53	0/5503	0.70	0/7415
1	C	0.63	0/5503	0.77	1/7416 (0.0%)
1	D	0.63	0/5477	0.76	0/7376
1	E	0.52	0/5479	0.71	1/7383 (0.0%)
1	F	0.33	0/5436	0.64	4/7326 (0.1%)
2	S	0.52	0/119	0.78	0/165
All	All	0.52	0/32926	0.70	6/44364 (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	B	0	1
1	D	0	1
1	F	0	2
All	All	0	5

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	407	SER	CA-C-N	8.80	148.13	127.00
1	F	407	SER	C-N-CA	8.80	148.13	127.00
1	C	686	VAL	N-CA-C	-8.10	103.26	113.22
1	F	407	SER	C-N-CD	-7.98	103.04	120.60
1	F	444	LEU	N-CA-C	-5.98	106.14	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	444	LEU	N-CA-C	-5.38	106.88	113.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	656	TYR	Peptide
1	B	548	VAL	Peptide
1	D	682	ALA	Peptide
1	F	608	GLY	Peptide
1	F	651	PRO	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	5340	0	5413	111	0
1	B	5430	0	5507	123	0
1	C	5430	0	5505	105	0
1	D	5406	0	5486	126	0
1	E	5406	0	5486	106	0
1	F	5364	0	5431	117	0
2	S	120	0	122	3	0
3	A	31	0	11	3	0
3	B	62	0	22	7	0
3	C	62	0	24	10	0
3	D	62	0	24	8	0
3	E	62	0	22	8	0
3	F	31	0	10	8	0
4	F	27	0	9	0	0
All	All	32833	0	33072	641	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 10.

All (641) 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:539:VAL:O	1:B:543:TRP:HB2	1.72	0.89
1:C:672:SER:H	1:C:712:THR:HG22	1.50	0.76
1:C:752:GLU:HG2	1:D:719:ASN:HD21	1.54	0.71
1:B:366:THR:HG22	1:B:368:PRO:HD2	1.73	0.71
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.75	0.69
1:A:642:SER:HA	1:A:645:ARG:HE	1.58	0.69
1:E:637:PHE:HD1	1:E:642:SER:HB3	1.58	0.68
1:E:178:ASP:O	1:E:221:GLN:NE2	2.27	0.68
1:A:672:SER:H	1:A:712:THR:HG22	1.58	0.68
1:A:211:GLY:HA3	3:A:1001:AGS:H8	1.74	0.68
1:B:331:ARG:NH1	3:C:1001:AGS:S1G	2.67	0.67
1:D:332:ARG:NH2	3:E:1001:AGS:S1G	2.68	0.66
1:D:679:VAL:HG12	1:D:718:SER:HB2	1.77	0.66
1:E:631:ARG:HG3	1:E:675:LEU:HD23	1.78	0.66
1:A:781:ARG:HG3	1:A:785:ARG:HH22	1.61	0.65
1:E:559:LEU:HD11	1:E:585:ARG:HG2	1.78	0.65
1:A:331:ARG:NH1	3:B:1001:AGS:S1G	2.69	0.65
1:C:573:GLN:HE22	1:C:764:HIS:H	1.45	0.65
1:E:821:ILE:HG23	1:E:825:ILE:HD12	1.79	0.64
1:F:786:LEU:HB3	1:F:791:TYR:HB2	1.78	0.64
1:C:719:ASN:ND2	3:C:1002:AGS:S1G	2.71	0.64
1:F:795:ILE:HA	1:F:846:LEU:HB2	1.80	0.64
1:A:171:ARG:HE	1:A:177:LEU:HD21	1.63	0.63
1:A:328:ALA:O	1:A:332:ARG:HB2	1.97	0.63
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.63	0.63
1:E:573:GLN:NE2	1:E:764:HIS:O	2.31	0.63
1:C:189:ARG:HH12	1:C:336:VAL:HA	1.62	0.63
1:E:183:ARG:NH2	1:E:339:ALA:O	2.32	0.62
1:A:692:GLN:NE2	1:B:635:SER:OG	2.32	0.62
3:E:1001:AGS:O1B	3:E:1001:AGS:O2A	2.17	0.62
1:A:284:VAL:HG21	1:A:322:TYR:HB3	1.81	0.62
1:A:195:GLN:HE21	1:A:232:LEU:HG	1.64	0.62
1:C:528:ARG:HH22	1:C:534:ALA:HB3	1.63	0.62
1:D:166:ILE:HB	1:D:239:ALA:HB3	1.82	0.62
1:A:573:GLN:NE2	1:A:764:HIS:O	2.33	0.61
1:D:366:THR:HG22	1:D:368:PRO:HD2	1.81	0.61
1:F:606:PRO:HB3	1:F:726:GLN:HE21	1.65	0.61
1:F:363:VAL:O	1:F:476:LYS:NZ	2.34	0.61
1:F:815:ARG:NH2	3:F:1001:AGS:O2G	2.34	0.61
1:D:674:ILE:HD12	1:D:714:VAL:HG22	1.81	0.61
1:E:544:THR:O	1:E:669:ARG:NH1	2.33	0.61
1:B:756:ARG:NH2	3:C:1002:AGS:O2G	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LYS:NZ	3:C:1001:AGS:O3B	2.29	0.60
1:F:608:GLY:N	3:F:1001:AGS:O3B	2.34	0.60
1:B:634:MET:HG3	1:B:679:VAL:HG23	1.82	0.60
1:E:703:GLN:OE1	1:E:705:ARG:NH1	2.30	0.60
1:E:310:CYS:SG	1:E:311:VAL:N	2.74	0.60
1:B:757:ILE:O	1:C:819:ARG:NH1	2.35	0.60
1:B:422:LEU:HD22	1:B:444:LEU:HD11	1.84	0.60
1:F:563:GLU:OE2	1:F:585:ARG:NH1	2.35	0.60
1:A:599:GLY:HA3	1:A:713:VAL:HG13	1.84	0.60
1:A:776:GLN:HG2	1:A:800:LEU:HD11	1.83	0.60
1:A:169:THR:O	1:A:173:GLU:HB2	2.01	0.60
1:A:409:PRO:HD2	1:A:412:LEU:HD22	1.83	0.59
1:A:524:MET:HE3	1:A:527:LEU:HB3	1.83	0.59
1:C:334:GLN:HA	1:D:384:ARG:HH22	1.66	0.59
1:C:354:LYS:HD3	1:C:370:ILE:HD11	1.84	0.59
1:D:354:LYS:HD3	1:D:370:ILE:HD11	1.83	0.59
1:E:296:GLY:O	1:E:300:LYS:HB2	2.02	0.59
1:F:300:LYS:HA	1:F:303:LEU:HD13	1.83	0.59
1:E:738:LYS:NZ	1:E:759:GLU:OE2	2.34	0.59
1:F:609:VAL:HG12	1:F:766:LEU:HD22	1.83	0.59
1:D:341:PRO:HG3	1:D:387:PRO:HD3	1.84	0.59
1:B:683:HIS:ND1	1:B:685:ASP:OD1	2.35	0.59
1:E:402:ARG:O	1:E:406:ASP:HB2	2.03	0.59
1:F:181:ILE:HB	1:F:349:ILE:HG12	1.84	0.59
1:A:618:LEU:O	1:A:622:MET:CB	2.51	0.59
1:A:299:LEU:HB3	1:A:303:LEU:HD13	1.85	0.58
1:C:632:ILE:HD11	1:C:662:LEU:HD13	1.85	0.58
1:D:703:GLN:OE1	1:D:705:ARG:NH1	2.36	0.58
1:D:605:GLY:O	1:D:611:LYS:NZ	2.36	0.58
1:A:520:GLU:OE1	1:A:529:ASN:ND2	2.36	0.58
1:A:676:LEU:HB2	1:A:716:MET:HA	1.86	0.58
1:A:618:LEU:O	1:A:622:MET:HB3	2.02	0.58
1:B:650:PRO:HG3	1:C:641:HIS:HB3	1.86	0.58
1:C:366:THR:HG22	1:C:368:PRO:HD2	1.84	0.58
1:F:166:ILE:HB	1:F:239:ALA:HB3	1.85	0.58
1:B:199:LYS:NZ	1:C:388:ASP:OD2	2.35	0.58
1:B:361:HIS:NE2	1:B:395:ASP:OD1	2.32	0.58
1:D:544:THR:OG1	1:D:545:GLY:N	2.35	0.58
1:C:794:HIS:HB2	1:C:845:ARG:HG2	1.84	0.58
1:E:361:HIS:NE2	1:E:395:ASP:OD1	2.35	0.58
1:F:603:PHE:HB2	1:F:717:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:619:ALA:O	1:F:624:ASP:N	2.37	0.58
1:D:613:GLU:HG3	3:D:1002:AGS:H2'	1.85	0.57
1:E:184:ASP:OD1	1:E:222:ARG:NH1	2.36	0.57
1:E:554:SER:O	1:E:558:LYS:HB2	2.04	0.57
1:D:569:ARG:NH1	1:D:626:ASP:OD1	2.37	0.57
1:A:834:LEU:HD13	1:F:585:ARG:HB3	1.86	0.57
1:B:827:ASN:O	1:B:831:GLN:HB2	2.05	0.57
1:F:323:ILE:HG23	1:F:329:LEU:HG	1.85	0.57
1:F:786:LEU:O	1:F:790:GLY:N	2.36	0.57
1:C:166:ILE:HB	1:C:239:ALA:HB3	1.87	0.57
1:D:189:ARG:NH1	1:E:542:ARG:O	2.36	0.57
1:A:181:ILE:O	3:A:1001:AGS:N6	2.33	0.57
3:B:1001:AGS:O1B	3:B:1001:AGS:O2G	2.22	0.57
1:A:602:LEU:HB3	1:A:760:VAL:HG22	1.87	0.57
1:D:744:VAL:HA	1:D:747:HIS:HD2	1.70	0.57
1:E:594:PRO:O	1:E:710:ARG:NH1	2.38	0.57
1:E:615:CYS:HB3	1:E:629:MET:HE1	1.86	0.57
1:A:344:GLU:HA	1:A:347:ILE:HD12	1.85	0.57
1:C:225:ASN:OD1	1:C:491:ARG:NH1	2.38	0.57
1:C:738:LYS:O	1:C:742:LEU:HB2	2.03	0.57
1:D:573:GLN:NE2	1:D:764:HIS:O	2.35	0.57
1:B:409:PRO:HD2	1:B:412:LEU:HD22	1.86	0.56
1:A:363:VAL:O	1:A:476:LYS:NZ	2.38	0.56
1:B:687:PHE:HA	1:B:690:LEU:HD12	1.87	0.56
1:D:538:GLU:HB3	1:D:542:ARG:HH21	1.68	0.56
1:B:260:LYS:NZ	1:C:241:ASP:OD2	2.38	0.56
3:C:1002:AGS:O3G	3:C:1002:AGS:O1B	2.24	0.56
1:D:729:PHE:HA	1:D:737:MET:HE1	1.86	0.56
1:F:643:VAL:O	1:F:647:VAL:HB	2.05	0.56
1:D:745:VAL:O	1:D:749:PHE:N	2.38	0.56
1:B:240:LEU:HB2	1:B:275:LEU:HD11	1.86	0.56
1:C:727:GLU:HG2	1:C:728:ARG:HG3	1.87	0.56
1:A:183:ARG:HH12	1:A:339:ALA:HB3	1.70	0.56
1:D:358:GLU:OE2	1:D:365:ILE:N	2.38	0.56
1:E:401:ILE:HG13	1:E:531:VAL:HG22	1.87	0.56
1:F:684:PRO:O	1:F:688:ASN:ND2	2.38	0.56
3:C:1001:AGS:O2G	3:C:1001:AGS:O1B	2.22	0.56
1:B:502:GLN:HA	1:B:506:ILE:HD13	1.88	0.56
1:B:384:ARG:NH1	1:B:392:ASP:OD2	2.39	0.56
1:D:324:GLU:HG2	1:D:330:GLU:HG3	1.86	0.56
1:F:236:ARG:HB2	1:F:273:VAL:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:HD2	1:B:250:LYS:HB2	1.72	0.55
1:B:698:ARG:NH2	1:B:700:THR:OG1	2.39	0.55
1:C:641:HIS:O	1:C:644:SER:N	2.40	0.55
1:F:672:SER:H	1:F:712:THR:HG22	1.72	0.55
1:A:786:LEU:HD13	1:A:793:ILE:HD12	1.88	0.55
1:B:821:ILE:HG23	1:B:825:ILE:HD12	1.87	0.55
1:D:229:PRO:HG2	1:E:403:MET:HE3	1.87	0.55
1:E:422:LEU:HD22	1:E:444:LEU:HD11	1.87	0.55
1:B:821:ILE:O	1:B:825:ILE:HB	2.07	0.55
3:F:1001:AGS:O2G	3:F:1001:AGS:O2B	2.23	0.55
1:B:324:GLU:OE2	1:C:667:ARG:NH1	2.40	0.55
1:C:821:ILE:HG23	1:C:825:ILE:HD12	1.87	0.55
1:E:180:VAL:H	1:E:221:GLN:HE22	1.54	0.55
1:A:332:ARG:NH2	3:B:1001:AGS:S1G	2.79	0.55
1:D:320:ARG:NH1	1:E:664:GLU:OE1	2.40	0.55
1:E:563:GLU:OE2	1:E:585:ARG:NH1	2.39	0.55
1:B:551:MET:HB3	1:B:556:ARG:HB2	1.89	0.55
1:B:566:LEU:O	1:B:570:VAL:N	2.35	0.55
1:F:554:SER:O	1:F:558:LYS:HB2	2.07	0.55
1:F:595:ASN:HA	1:F:710:ARG:HH11	1.71	0.55
1:D:188:ARG:HG3	1:E:403:MET:HE1	1.87	0.55
1:E:319:TYR:HA	1:E:323:ILE:HD12	1.89	0.55
1:C:539:VAL:HG22	1:C:542:ARG:HH21	1.72	0.55
1:D:199:LYS:NZ	1:E:392:ASP:OD2	2.33	0.55
1:D:600:SER:HB2	1:D:694:LEU:HD22	1.89	0.55
1:D:602:LEU:HD13	1:D:716:MET:HE3	1.87	0.55
1:D:632:ILE:HD11	1:D:662:LEU:HD13	1.89	0.55
1:C:422:LEU:HD22	1:C:444:LEU:HD11	1.89	0.54
3:D:1002:AGS:O2G	3:D:1002:AGS:O1B	2.25	0.54
1:F:502:GLN:HA	1:F:506:ILE:HD13	1.89	0.54
1:E:354:LYS:HD3	1:E:370:ILE:HD11	1.88	0.54
3:B:1001:AGS:O2B	3:B:1001:AGS:O2A	2.23	0.54
1:D:520:GLU:OE1	1:D:529:ASN:ND2	2.40	0.54
1:A:520:GLU:HA	1:A:523:THR:HG22	1.89	0.54
1:D:821:ILE:HG23	1:D:825:ILE:HD12	1.89	0.54
1:F:738:LYS:HE2	1:F:761:VAL:HA	1.88	0.54
1:B:573:GLN:NE2	1:B:764:HIS:O	2.40	0.54
1:B:692:GLN:NE2	1:C:635:SER:OG	2.37	0.54
3:D:1001:AGS:O2B	3:D:1001:AGS:O1A	2.24	0.54
1:F:692:GLN:O	1:F:696:ASP:HB2	2.08	0.54
1:B:567:HIS:ND1	1:B:570:VAL:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:GLU:OE2	1:C:258:ARG:NE	2.40	0.54
1:C:566:LEU:HD12	1:C:577:VAL:HG13	1.88	0.54
1:C:344:GLU:HA	1:C:347:ILE:HD12	1.90	0.54
1:C:520:GLU:HB3	1:C:529:ASN:HD21	1.72	0.54
1:C:240:LEU:HD22	1:C:275:LEU:HD21	1.90	0.54
1:F:181:ILE:HD12	1:F:349:ILE:HA	1.89	0.54
1:F:202:PRO:HG2	1:F:311:VAL:HG13	1.90	0.53
1:F:520:GLU:O	1:F:524:MET:N	2.40	0.53
1:B:332:ARG:NH2	3:C:1001:AGS:S1G	2.68	0.53
1:C:458:LEU:HD22	1:C:526:LEU:HD21	1.90	0.53
1:C:756:ARG:NH2	3:D:1002:AGS:O2G	2.42	0.53
1:F:314:THR:OG1	1:F:315:THR:N	2.41	0.53
1:B:346:THR:HG21	1:B:386:LEU:HD22	1.90	0.53
1:C:718:SER:OG	1:C:719:ASN:N	2.39	0.53
1:F:676:LEU:HB2	1:F:716:MET:HG2	1.91	0.53
1:F:827:ASN:O	1:F:831:GLN:HB2	2.07	0.53
1:C:569:ARG:NH2	1:C:613:GLU:OE1	2.41	0.53
1:A:502:GLN:HA	1:A:506:ILE:HD13	1.90	0.53
1:A:673:VAL:HG22	1:A:713:VAL:HB	1.89	0.53
1:C:620:ASN:HA	1:C:625:SER:H	1.74	0.53
1:E:502:GLN:HA	1:E:506:ILE:HD13	1.91	0.53
1:F:683:HIS:ND1	1:F:685:ASP:OD1	2.41	0.53
1:C:469:LEU:HD11	1:C:529:ASN:HD22	1.73	0.53
1:B:744:VAL:HA	1:B:747:HIS:HD2	1.73	0.53
1:C:544:THR:OG1	1:C:545:GLY:N	2.41	0.53
1:F:610:GLY:O	1:F:614:LEU:N	2.39	0.53
1:D:634:MET:HG3	1:D:679:VAL:HG23	1.91	0.53
1:E:559:LEU:HD21	1:E:585:ARG:HD3	1.90	0.53
1:A:323:ILE:HG23	1:A:329:LEU:HG	1.91	0.52
1:B:585:ARG:O	1:B:589:ALA:HB2	2.08	0.52
1:C:409:PRO:HB2	1:C:412:LEU:HB2	1.91	0.52
1:E:591:LEU:HD22	1:F:830:ALA:HB2	1.90	0.52
1:A:171:ARG:HA	1:A:176:LYS:HZ2	1.75	0.52
1:E:293:MET:N	1:E:297:ASN:OD1	2.42	0.52
3:E:1002:AGS:O2A	3:E:1002:AGS:O1B	2.27	0.52
1:F:361:HIS:NE2	1:F:395:ASP:OD1	2.42	0.52
1:E:300:LYS:HA	1:E:303:LEU:HB2	1.91	0.52
1:C:359:LEU:HD21	1:C:480:GLU:HG2	1.92	0.52
1:F:703:GLN:OE1	1:F:705:ARG:NH2	2.42	0.52
1:B:364:GLN:HB2	1:B:530:LYS:HG2	1.92	0.52
1:D:368:PRO:HA	1:D:371:VAL:HG12	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:610:GLY:N	3:D:1002:AGS:O2A	2.42	0.52
1:E:631:ARG:NH2	1:E:677:ASP:OD2	2.39	0.52
1:F:380:TYR:HD2	1:F:540:LEU:HD21	1.75	0.52
1:D:300:LYS:NZ	1:D:326:ASP:OD2	2.42	0.52
1:C:677:ASP:OD1	1:C:717:THR:OG1	2.27	0.52
1:E:613:GLU:HG3	3:E:1002:AGS:H2'	1.90	0.52
1:F:269:GLN:HB3	1:F:272:ASN:HB3	1.91	0.52
1:C:222:ARG:HG3	1:C:227:GLU:HB2	1.92	0.52
1:F:751:PRO:HA	1:F:754:ILE:HG12	1.92	0.52
1:A:833:ILE:HD13	1:F:591:LEU:HD22	1.91	0.51
3:E:1002:AGS:O3A	3:E:1002:AGS:O2G	2.28	0.51
1:F:608:GLY:N	3:F:1001:AGS:S1G	2.82	0.51
1:B:815:ARG:HA	1:B:818:LYS:HD3	1.92	0.51
1:E:751:PRO:HA	1:E:754:ILE:HG12	1.90	0.51
1:F:596:ARG:NH2	1:F:756:ARG:O	2.43	0.51
1:B:698:ARG:HH21	1:B:706:THR:HG22	1.75	0.51
1:C:590:GLY:HA3	1:D:789:ARG:HH21	1.75	0.51
1:D:321:GLN:NE2	1:E:657:GLU:O	2.42	0.51
1:F:821:ILE:O	1:F:825:ILE:HB	2.09	0.51
1:A:197:ARG:HE	1:B:357:TYR:HE1	1.58	0.51
1:A:314:THR:OG1	1:A:315:THR:N	2.39	0.51
1:F:602:LEU:HB3	1:F:760:VAL:HG22	1.92	0.51
3:C:1002:AGS:O1B	3:C:1002:AGS:O2A	2.25	0.51
1:A:605:GLY:O	1:A:611:LYS:NZ	2.43	0.51
1:C:189:ARG:HH21	1:D:543:TRP:HA	1.76	0.51
1:E:724:LEU:HD21	1:E:740:LEU:HG	1.93	0.51
1:B:169:THR:HB	1:B:224:ILE:HD11	1.93	0.51
1:B:692:GLN:HE22	1:C:636:GLU:HG3	1.76	0.51
1:C:334:GLN:OE1	1:D:384:ARG:NH1	2.33	0.51
3:D:1001:AGS:O2B	3:D:1001:AGS:O2G	2.28	0.51
1:E:160:ALA:HA	1:E:163:LYS:HB2	1.93	0.51
1:A:362:HIS:CD2	1:A:473:GLN:HG2	2.46	0.51
1:D:606:PRO:HG3	1:D:726:GLN:HG3	1.92	0.51
1:F:409:PRO:HD2	1:F:412:LEU:HD22	1.92	0.51
1:A:222:ARG:O	1:A:226:GLY:N	2.44	0.51
1:B:540:LEU:HD23	1:B:548:VAL:HG21	1.93	0.51
1:C:559:LEU:HD11	1:C:588:ARG:HG3	1.91	0.51
1:D:508:GLU:HG3	1:D:509:LEU:HD12	1.93	0.51
1:F:319:TYR:HA	1:F:323:ILE:HD12	1.92	0.51
1:A:189:ARG:NH2	1:B:396:GLU:OE2	2.45	0.50
1:B:365:ILE:HA	1:B:531:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ARG:HG3	1:A:675:LEU:HD23	1.93	0.50
1:A:679:VAL:HG12	1:A:718:SER:HB2	1.93	0.50
1:B:679:VAL:HG11	1:B:716:MET:HB3	1.94	0.50
1:A:422:LEU:HD22	1:A:444:LEU:HD11	1.93	0.50
1:F:786:LEU:O	1:F:791:TYR:N	2.41	0.50
1:C:236:ARG:HB2	1:C:273:VAL:HA	1.93	0.50
1:C:709:PHE:O	1:C:712:THR:OG1	2.27	0.50
1:A:738:LYS:NZ	1:A:759:GLU:OE2	2.42	0.50
1:B:236:ARG:HB2	1:B:273:VAL:HG22	1.94	0.50
1:D:231:GLY:O	1:D:235:ARG:NH2	2.45	0.50
1:E:304:ALA:HA	1:E:332:ARG:HE	1.76	0.50
1:C:502:GLN:HA	1:C:506:ILE:HD13	1.93	0.50
1:D:377:SER:HB2	1:D:389:LYS:HG3	1.92	0.50
1:B:178:ASP:OD2	3:B:1001:AGS:O2'	2.29	0.50
1:B:225:ASN:OD1	1:B:491:ARG:NH1	2.45	0.50
1:D:281:HIS:HB2	1:D:322:TYR:HD2	1.77	0.50
1:E:193:VAL:HG22	1:E:196:ARG:HH12	1.77	0.50
1:A:539:VAL:HG22	1:A:542:ARG:HH22	1.77	0.50
1:A:603:PHE:HB2	1:A:717:THR:HG22	1.93	0.50
1:E:697:GLY:O	1:E:709:PHE:N	2.42	0.50
1:D:786:LEU:O	1:D:790:GLY:N	2.45	0.49
1:F:161:LEU:O	1:F:165:THR:OG1	2.28	0.49
1:C:596:ARG:NH2	1:C:756:ARG:O	2.45	0.49
1:E:169:THR:HB	1:E:224:ILE:HD11	1.95	0.49
1:F:401:ILE:HG13	1:F:531:VAL:HG22	1.92	0.49
1:A:573:GLN:HG2	1:A:766:LEU:HD21	1.94	0.49
1:B:229:PRO:HG2	1:C:403:MET:HE3	1.95	0.49
1:C:640:LYS:NZ	1:D:638:MET:SD	2.81	0.49
1:D:502:GLN:HA	1:D:506:ILE:HD13	1.93	0.49
1:A:603:PHE:O	1:A:718:SER:N	2.45	0.49
1:B:663:THR:HG21	1:B:701:ASP:HB3	1.94	0.49
1:A:380:TYR:HB2	1:A:540:LEU:HD21	1.95	0.49
1:B:631:ARG:NH2	1:B:677:ASP:OD2	2.45	0.49
1:C:827:ASN:O	1:C:831:GLN:HB2	2.12	0.49
1:B:177:LEU:O	1:B:356:ARG:NH2	2.40	0.49
1:D:684:PRO:HA	1:D:687:PHE:HD2	1.77	0.49
1:D:695:ASP:OD2	1:D:756:ARG:NH2	2.45	0.49
1:E:676:LEU:HB2	1:E:716:MET:HG2	1.95	0.49
1:B:639:GLU:HB2	1:B:641:HIS:CE1	2.48	0.49
1:A:172:ALA:HB2	1:A:177:LEU:HD12	1.93	0.49
1:B:695:ASP:OD2	1:C:631:ARG:NH2	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:LYS:NZ	1:F:388:ASP:OD1	2.40	0.49
1:A:612:THR:OG1	1:A:815:ARG:NH2	2.45	0.49
1:F:599:GLY:HA3	1:F:713:VAL:HG13	1.95	0.49
1:F:821:ILE:HG23	1:F:825:ILE:HD12	1.94	0.49
1:D:344:GLU:HA	1:D:347:ILE:HD12	1.94	0.48
1:D:537:ALA:HB1	1:D:549:SER:HA	1.93	0.48
1:D:727:GLU:HG2	1:D:728:ARG:HG3	1.94	0.48
1:D:226:GLY:O	1:D:233:LYS:NZ	2.46	0.48
1:A:294:ASP:OD1	1:A:295:ALA:N	2.45	0.48
1:A:319:TYR:HA	1:A:323:ILE:HD12	1.94	0.48
1:B:320:ARG:NH1	1:C:664:GLU:OE1	2.46	0.48
1:B:596:ARG:NH2	1:B:756:ARG:O	2.46	0.48
1:D:167:ASP:OD1	1:D:169:THR:OG1	2.28	0.48
1:E:259:LEU:HD11	1:E:299:LEU:HD11	1.94	0.48
1:F:326:ASP:HB3	1:F:329:LEU:HB3	1.94	0.48
1:F:359:LEU:HA	1:F:473:GLN:HE22	1.78	0.48
1:A:293:MET:N	1:A:297:ASN:OD1	2.46	0.48
1:F:520:GLU:O	1:F:523:THR:N	2.46	0.48
1:B:636:GLU:OE1	1:B:645:ARG:NH1	2.47	0.48
1:A:168:LEU:HD23	1:A:171:ARG:HD3	1.96	0.48
1:A:401:ILE:HG13	1:A:531:VAL:HG22	1.95	0.48
1:C:567:HIS:ND1	1:C:570:VAL:O	2.44	0.48
1:C:573:GLN:NE2	1:C:764:HIS:O	2.47	0.48
1:D:553:GLU:OE1	1:D:556:ARG:NH2	2.47	0.48
1:F:263:LEU:HD23	1:F:266:LEU:HD12	1.95	0.48
1:B:793:ILE:HA	1:B:844:ILE:HB	1.96	0.48
1:E:612:THR:HG22	1:E:616:LYS:HE3	1.96	0.48
1:F:276:PHE:HD1	1:F:311:VAL:HB	1.78	0.48
1:B:245:LEU:O	1:B:258:ARG:NH1	2.45	0.47
1:F:159:GLN:HB2	1:F:162:LYS:HG2	1.96	0.47
1:F:604:LEU:O	1:F:763:PHE:N	2.39	0.47
1:F:793:ILE:HG12	1:F:844:ILE:HB	1.96	0.47
1:A:585:ARG:O	1:A:589:ALA:HB3	2.14	0.47
1:B:344:GLU:HA	1:B:347:ILE:HD12	1.95	0.47
1:B:722:SER:HA	1:B:725:ILE:HD12	1.96	0.47
1:C:744:VAL:HA	1:C:747:HIS:HD2	1.79	0.47
1:D:667:ARG:HD3	1:D:707:VAL:HG22	1.96	0.47
1:A:695:ASP:HB2	1:A:756:ARG:HH12	1.79	0.47
1:C:803:LEU:HD11	1:C:825:ILE:HD11	1.96	0.47
1:D:827:ASN:O	1:D:831:GLN:HB2	2.14	0.47
1:E:680:GLU:OE2	1:E:681:LYS:NZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:691:LEU:HD22	1:F:756:ARG:HH11	1.79	0.47
1:A:619:ALA:HA	1:A:622:MET:HE2	1.95	0.47
1:C:673:VAL:HG13	1:C:713:VAL:HB	1.96	0.47
1:D:196:ARG:NH1	1:D:199:LYS:O	2.47	0.47
1:B:528:ARG:NH2	1:B:535:GLU:OE2	2.41	0.47
1:B:815:ARG:NH1	3:B:1002:AGS:S1G	2.87	0.47
1:D:240:LEU:HD23	1:D:277:ILE:HG12	1.97	0.47
1:F:539:VAL:HG22	1:F:542:ARG:HH22	1.78	0.47
1:F:744:VAL:HA	1:F:747:HIS:HD2	1.80	0.47
1:E:540:LEU:HD23	1:E:548:VAL:HG11	1.97	0.47
1:E:693:VAL:HG13	1:E:709:PHE:HD2	1.80	0.47
1:B:631:ARG:NE	1:B:633:ASP:OD1	2.42	0.47
1:E:362:HIS:CD2	1:E:473:GLN:HG2	2.50	0.47
1:F:691:LEU:HD21	1:F:753:PHE:HA	1.96	0.47
1:B:248:GLY:H	1:B:258:ARG:HH22	1.61	0.47
1:C:696:ASP:OD2	1:D:631:ARG:NH2	2.36	0.47
1:C:822:GLN:O	1:C:826:GLU:HB2	2.15	0.47
1:F:184:ASP:OD1	1:F:222:ARG:NH1	2.45	0.47
1:A:684:PRO:O	1:A:750:ARG:NH2	2.48	0.47
1:B:203:VAL:HG23	1:B:312:GLY:HA3	1.96	0.47
1:D:202:PRO:HG2	1:D:311:VAL:HG22	1.97	0.47
1:E:367:ASP:HA	1:E:370:ILE:HD12	1.97	0.47
1:E:782:LEU:HD13	1:E:785:ARG:HH21	1.78	0.47
1:E:793:ILE:HG12	1:E:844:ILE:HB	1.97	0.47
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.96	0.47
1:F:520:GLU:HA	1:F:523:THR:HG22	1.97	0.47
1:A:839:VAL:H	1:A:857:GLN:HE22	1.62	0.46
1:D:580:VAL:HG11	1:D:618:LEU:HD11	1.96	0.46
1:B:842:LYS:HD3	1:B:857:GLN:HB3	1.98	0.46
1:D:204:LEU:HD23	1:D:336:VAL:HB	1.98	0.46
1:A:199:LYS:NZ	1:B:392:ASP:OD2	2.33	0.46
1:B:768:GLU:HA	1:B:771:ILE:HD12	1.96	0.46
1:B:650:PRO:HG2	1:B:653:TYR:HD2	1.81	0.46
1:D:652:GLY:H	1:E:654:VAL:HB	1.79	0.46
1:A:341:PRO:HG2	1:A:386:LEU:HB2	1.98	0.46
1:C:849:ASN:HD22	1:C:852:ARG:HB2	1.80	0.46
1:F:554:SER:O	1:F:558:LYS:CB	2.64	0.46
1:A:286:ALA:N	1:A:294:ASP:OD2	2.35	0.46
1:C:690:LEU:HA	1:C:693:VAL:HB	1.97	0.46
1:D:688:ASN:OD1	1:D:750:ARG:NH1	2.49	0.46
1:B:585:ARG:O	1:B:589:ALA:CB	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:LEU:HB2	1:D:716:MET:HG2	1.97	0.46
1:A:239:ALA:HA	1:A:276:PHE:HB3	1.97	0.46
1:B:786:LEU:O	1:B:790:GLY:N	2.47	0.46
1:D:200:ASN:HD22	1:D:306:GLY:HA2	1.81	0.46
1:D:600:SER:H	1:D:758:ASP:HB2	1.80	0.46
1:D:622:MET:HE3	1:D:622:MET:HB2	1.82	0.46
1:E:296:GLY:O	1:E:300:LYS:CB	2.64	0.46
1:C:226:GLY:O	1:C:233:LYS:NZ	2.49	0.46
1:F:646:LEU:HA	1:F:661:TYR:HB2	1.97	0.46
1:A:303:LEU:HD23	1:A:332:ARG:HB3	1.97	0.46
1:B:212:LYS:N	3:B:1001:AGS:O2B	2.48	0.46
1:D:356:ARG:HA	1:D:359:LEU:HD13	1.98	0.46
1:D:545:GLY:HA3	1:D:669:ARG:HH22	1.80	0.46
1:B:566:LEU:HD12	1:B:577:VAL:HG13	1.98	0.45
1:D:571:ILE:HD12	1:D:571:ILE:HA	1.84	0.45
1:D:582:ASN:OD1	1:D:585:ARG:NH2	2.42	0.45
3:D:1002:AGS:O1A	3:D:1002:AGS:O2B	2.29	0.45
1:A:326:ASP:OD2	1:A:329:LEU:N	2.46	0.45
1:A:803:LEU:HD22	1:A:821:ILE:HG23	1.99	0.45
1:C:838:LEU:HD23	1:C:844:ILE:HD13	1.98	0.45
1:E:556:ARG:NH1	1:F:835:SER:O	2.47	0.45
1:F:676:LEU:N	1:F:715:ILE:O	2.48	0.45
1:F:679:VAL:HG12	1:F:718:SER:HB2	1.98	0.45
1:F:827:ASN:O	1:F:831:GLN:CB	2.64	0.45
1:C:622:MET:HE3	1:C:622:MET:HB2	1.79	0.45
1:B:368:PRO:HA	1:B:371:VAL:HG12	1.98	0.45
1:B:580:VAL:HG11	1:B:618:LEU:HD13	1.99	0.45
1:D:195:GLN:O	1:E:399:SER:OG	2.26	0.45
1:E:487:GLU:OE2	1:E:490:ARG:NH1	2.50	0.45
1:E:501:LEU:O	1:E:505:LYS:HB2	2.17	0.45
1:F:422:LEU:HD22	1:F:444:LEU:HD11	1.99	0.45
1:F:791:TYR:HE1	1:F:840:PRO:HG3	1.81	0.45
1:A:585:ARG:O	1:A:589:ALA:CB	2.65	0.45
3:F:1001:AGS:O2B	3:F:1001:AGS:O2A	2.33	0.45
1:C:291:GLY:HA2	1:D:286:ALA:HA	1.98	0.45
1:C:539:VAL:O	1:C:543:TRP:HB2	2.17	0.45
1:C:640:LYS:NZ	1:C:685:ASP:O	2.50	0.45
1:E:211:GLY:H	3:E:1001:AGS:H5'1	1.82	0.45
1:D:664:GLU:O	1:D:668:ARG:HG2	2.16	0.45
1:D:609:VAL:N	3:D:1002:AGS:O2A	2.50	0.45
1:F:697:GLY:HA2	1:F:709:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ILE:HD11	1:C:352:GLY:HA3	1.98	0.45
1:C:238:LEU:HD13	1:C:273:VAL:HG13	1.99	0.45
1:C:771:ILE:HA	1:C:774:ILE:HD12	1.97	0.45
1:D:252:ARG:HH12	2:S:2:ALA:HB3	1.82	0.45
1:D:351:ARG:HG2	1:D:370:ILE:HD13	1.99	0.45
1:B:416:ASP:HA	1:B:419:ILE:HG12	1.99	0.44
1:C:212:LYS:HZ1	3:C:1001:AGS:PG	2.37	0.44
1:E:498:MET:HB3	1:F:424:LEU:HD21	1.99	0.44
1:A:656:TYR:CZ	1:A:703:GLN:HG2	2.53	0.44
1:C:608:GLY:H	3:C:1002:AGS:PB	2.40	0.44
1:E:235:ARG:NH1	1:E:271:GLY:O	2.51	0.44
1:F:539:VAL:O	1:F:543:TRP:N	2.48	0.44
1:F:694:LEU:HD13	1:F:756:ARG:HB2	1.99	0.44
1:A:657:GLU:HB2	1:F:651:PRO:HB2	1.98	0.44
1:B:566:LEU:HD23	1:B:566:LEU:HA	1.84	0.44
1:E:281:HIS:CD2	1:E:318:GLU:HG2	2.51	0.44
1:F:628:ALA:HA	1:F:669:ARG:HH21	1.82	0.44
1:F:738:LYS:NZ	1:F:759:GLU:OE2	2.50	0.44
1:A:183:ARG:NH2	1:A:339:ALA:O	2.51	0.44
1:A:650:PRO:HG2	1:A:653:TYR:CD2	2.52	0.44
1:C:724:LEU:HD12	1:C:724:LEU:HA	1.87	0.44
1:E:236:ARG:HB2	1:E:273:VAL:HA	1.98	0.44
1:E:634:MET:HA	1:E:637:PHE:HD2	1.83	0.44
1:C:688:ASN:HB3	1:D:635:SER:HB2	1.99	0.44
1:D:275:LEU:HD23	1:D:310:CYS:HB2	1.98	0.44
1:E:212:LYS:N	3:E:1001:AGS:O1B	2.42	0.44
1:E:508:GLU:HA	1:E:511:LYS:HE3	1.99	0.44
1:F:222:ARG:O	1:F:227:GLU:N	2.45	0.44
1:A:184:ASP:OD1	1:A:222:ARG:NH1	2.41	0.44
1:C:856:VAL:HB	1:C:858:HIS:HD2	1.82	0.44
1:F:725:ILE:HG22	1:F:765:PRO:HD3	2.00	0.44
1:B:496:ALA:O	1:B:500:GLU:HB2	2.18	0.44
1:B:751:PRO:HA	1:B:754:ILE:HG12	2.00	0.44
1:C:236:ARG:N	1:C:272:ASN:O	2.51	0.44
1:F:350:LEU:HD11	1:F:390:ALA:HB1	2.00	0.44
3:F:1001:AGS:O2A	3:F:1001:AGS:O1B	2.35	0.44
1:A:203:VAL:HG23	1:A:312:GLY:HA3	2.00	0.44
1:A:786:LEU:O	1:A:790:GLY:N	2.43	0.44
1:C:476:LYS:HE2	1:C:513:LEU:HD21	2.00	0.44
1:C:594:PRO:O	1:C:710:ARG:NH1	2.49	0.44
1:D:162:LYS:HB2	1:D:163:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:PRO:HB2	1:D:750:ARG:NH2	2.33	0.44
1:E:634:MET:HG3	1:E:679:VAL:HG23	2.00	0.44
1:A:169:THR:O	1:A:173:GLU:CB	2.66	0.43
1:A:650:PRO:HG3	1:B:641:HIS:CD2	2.53	0.43
1:A:754:ILE:HA	1:A:757:ILE:HG12	2.00	0.43
1:D:252:ARG:HG2	2:S:4:ALA:HB2	1.98	0.43
1:D:618:LEU:HA	1:D:618:LEU:HD23	1.78	0.43
1:E:208:PRO:HD3	1:E:315:THR:HG23	2.00	0.43
1:D:350:LEU:HD11	1:D:390:ALA:HB1	2.00	0.43
1:D:422:LEU:HD22	1:D:444:LEU:HD11	1.99	0.43
1:E:368:PRO:HA	1:E:371:VAL:HG12	2.00	0.43
1:F:167:ASP:OD1	1:F:169:THR:OG1	2.34	0.43
1:F:319:TYR:O	1:F:323:ILE:HB	2.17	0.43
1:A:643:VAL:HG22	1:A:686:VAL:HG22	1.98	0.43
1:B:304:ALA:HB2	1:B:332:ARG:CZ	2.48	0.43
1:D:508:GLU:HA	1:D:511:LYS:HE3	2.00	0.43
1:F:508:GLU:HA	1:F:511:LYS:HE3	1.99	0.43
1:B:201:ASN:HB3	1:B:333:PHE:CD1	2.53	0.43
1:B:225:ASN:HA	1:B:491:ARG:HD2	2.00	0.43
1:C:843:VAL:HG12	1:C:845:ARG:HG3	1.99	0.43
1:D:533:ASP:N	1:D:533:ASP:OD1	2.51	0.43
1:F:171:ARG:O	1:F:176:LYS:N	2.48	0.43
1:A:251:TYR:HB3	2:S:8:ALA:HB3	2.00	0.43
1:B:709:PHE:O	1:B:712:THR:OG1	2.28	0.43
1:D:236:ARG:O	1:D:274:ILE:N	2.50	0.43
1:A:303:LEU:HD12	1:A:308:LEU:HD23	2.00	0.43
1:A:751:PRO:HA	1:A:754:ILE:HG12	2.01	0.43
1:B:278:ASP:OD1	1:B:278:ASP:N	2.46	0.43
1:D:201:ASN:OD1	1:D:310:CYS:N	2.51	0.43
1:A:201:ASN:OD1	1:A:310:CYS:N	2.52	0.43
1:B:235:ARG:HD3	1:B:235:ARG:HA	1.82	0.43
1:B:354:LYS:HD2	1:B:365:ILE:HB	2.01	0.43
1:B:381:ILE:HG22	1:B:383:ASP:H	1.84	0.43
1:F:160:ALA:HA	1:F:163:LYS:HG2	2.00	0.43
1:F:728:ARG:HB3	1:F:732:LEU:HD13	2.01	0.43
1:A:171:ARG:HG2	1:A:176:LYS:HD2	2.01	0.43
1:A:212:LYS:HA	1:A:215:ILE:HD12	2.01	0.43
1:A:783:TYR:HD1	1:A:786:LEU:HD12	1.83	0.43
1:E:576:ALA:HB2	1:E:761:VAL:HG21	2.00	0.43
1:F:610:GLY:N	3:F:1001:AGS:O1B	2.29	0.43
1:F:674:ILE:HD12	1:F:714:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ILE:HA	1:A:844:ILE:HB	2.01	0.43
1:B:278:ASP:HA	1:B:313:ALA:HB3	2.01	0.43
1:C:229:PRO:HG2	1:D:403:MET:HE3	2.01	0.43
1:E:809:ASP:HB2	1:E:811:VAL:HG22	2.01	0.43
1:B:199:LYS:HZ1	1:C:388:ASP:CG	2.26	0.43
1:B:582:ASN:OD1	1:B:585:ARG:NH2	2.45	0.43
1:B:727:GLU:HG2	1:B:728:ARG:HG3	2.00	0.43
1:C:703:GLN:OE1	1:C:705:ARG:NH1	2.49	0.43
1:D:709:PHE:O	1:D:712:THR:OG1	2.36	0.43
1:D:744:VAL:HA	1:D:747:HIS:CD2	2.52	0.43
1:E:236:ARG:HB2	1:E:273:VAL:HG22	2.01	0.43
1:E:412:LEU:O	1:E:416:ASP:HB2	2.19	0.43
1:F:245:LEU:O	1:F:258:ARG:NH1	2.52	0.43
1:D:832:GLN:HB3	1:D:838:LEU:HD13	2.00	0.42
1:A:368:PRO:HA	1:A:371:VAL:HG12	2.01	0.42
1:A:658:GLU:HB2	1:F:650:PRO:HA	2.01	0.42
1:A:361:HIS:HE1	1:F:196:ARG:HA	1.84	0.42
1:B:699:LEU:HD12	1:B:699:LEU:HA	1.87	0.42
1:D:737:MET:HE2	1:D:737:MET:HB2	1.75	0.42
1:A:849:ASN:HD22	1:A:852:ARG:HB2	1.84	0.42
1:D:685:ASP:OD1	1:D:686:VAL:N	2.53	0.42
1:A:732:LEU:HD23	1:A:732:LEU:HA	1.90	0.42
1:E:409:PRO:HG2	1:E:412:LEU:HD22	2.01	0.42
1:E:561:ARG:O	1:E:565:GLU:HB2	2.19	0.42
1:F:608:GLY:HA2	3:F:1001:AGS:H5'1	2.02	0.42
1:A:559:LEU:HA	1:A:562:MET:HB2	2.01	0.42
1:D:195:GLN:HE21	1:D:232:LEU:HG	1.83	0.42
1:E:248:GLY:HA3	1:E:258:ARG:HH22	1.85	0.42
1:F:416:ASP:HA	1:F:419:ILE:HG12	2.01	0.42
1:B:200:ASN:ND2	1:B:306:GLY:O	2.50	0.42
1:B:508:GLU:HA	1:B:511:LYS:HE3	2.00	0.42
1:B:738:LYS:O	1:B:742:LEU:HB2	2.20	0.42
1:D:409:PRO:HD2	1:D:412:LEU:HD22	2.02	0.42
1:E:204:LEU:HB2	1:E:313:ALA:HA	2.02	0.42
1:A:606:PRO:HG3	1:A:726:GLN:HE21	1.84	0.42
1:B:341:PRO:HG3	1:B:387:PRO:HD3	2.01	0.42
1:B:847:GLU:N	1:B:854:VAL:O	2.52	0.42
1:C:793:ILE:HG12	1:C:844:ILE:HB	2.02	0.42
1:F:186:GLU:O	1:F:190:THR:OG1	2.32	0.42
1:A:676:LEU:HD22	1:A:716:MET:HG2	2.01	0.42
1:A:795:ILE:HG13	1:A:846:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:ASP:HB2	1:A:811:VAL:HG22	2.02	0.42
1:B:260:LYS:HA	1:B:263:LEU:HD12	2.02	0.42
1:D:689:ILE:HD13	1:D:689:ILE:HA	1.93	0.42
1:E:165:THR:HA	1:E:240:LEU:HA	2.02	0.42
1:E:195:GLN:NE2	1:F:399:SER:O	2.53	0.42
1:E:216:VAL:HG21	1:E:276:PHE:CE1	2.54	0.42
1:F:727:GLU:HG2	1:F:728:ARG:HG3	2.02	0.42
1:B:284:VAL:HG22	1:B:329:LEU:HD23	2.01	0.42
1:F:691:LEU:HD23	1:F:694:LEU:HD12	2.01	0.42
1:F:718:SER:OG	1:F:719:ASN:N	2.53	0.42
1:A:180:VAL:HG13	3:A:1001:AGS:C6	2.50	0.41
1:D:479:LEU:HG	1:D:483:LYS:HE3	2.02	0.41
1:D:701:ASP:OD1	1:D:705:ARG:N	2.53	0.41
1:B:199:LYS:NZ	1:C:392:ASP:OD2	2.32	0.41
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.76	0.41
1:F:164:TYR:HD2	1:F:245:LEU:HD23	1.85	0.41
1:A:684:PRO:HA	1:A:687:PHE:HD2	1.86	0.41
1:B:700:THR:O	1:C:645:ARG:NH2	2.53	0.41
1:C:361:HIS:NE2	1:C:395:ASP:OD1	2.53	0.41
1:C:643:VAL:HG22	1:C:686:VAL:HG13	2.02	0.41
1:D:278:ASP:N	1:D:278:ASP:OD1	2.43	0.41
1:D:608:GLY:HA3	1:D:813:GLY:HA3	2.02	0.41
1:E:169:THR:HG23	1:E:237:VAL:HB	2.02	0.41
1:E:596:ARG:NH2	1:E:600:SER:OG	2.53	0.41
1:E:726:GLN:NE2	1:E:810:PRO:O	2.53	0.41
1:A:724:LEU:HD21	1:A:740:LEU:HG	2.02	0.41
1:B:275:LEU:HD22	1:B:308:LEU:HD11	2.03	0.41
1:C:650:PRO:HG3	1:D:641:HIS:HD2	1.85	0.41
1:D:346:THR:HG21	1:D:386:LEU:HD22	2.02	0.41
1:E:649:ALA:HB3	1:E:656:TYR:HA	2.02	0.41
1:B:405:ILE:O	1:B:462:TRP:NE1	2.48	0.41
1:B:604:LEU:HD23	1:B:604:LEU:HA	1.94	0.41
1:D:324:GLU:OE1	1:E:667:ARG:NH1	2.49	0.41
1:D:688:ASN:HB3	1:E:635:SER:HB2	2.03	0.41
1:E:350:LEU:HD23	1:E:350:LEU:HA	1.93	0.41
1:F:210:VAL:HG23	1:F:212:LYS:HG3	2.03	0.41
1:F:362:HIS:CD2	1:F:473:GLN:HG2	2.54	0.41
1:B:849:ASN:N	1:B:852:ARG:O	2.44	0.41
1:E:771:ILE:HG23	1:E:817:LEU:HD22	2.03	0.41
1:F:359:LEU:HA	1:F:473:GLN:NE2	2.36	0.41
1:A:508:GLU:HA	1:A:511:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:ARG:HG2	1:F:591:LEU:HD21	2.02	0.41
1:B:632:ILE:HG12	1:B:661:TYR:HE2	1.84	0.41
1:D:205:ILE:O	1:D:338:VAL:N	2.41	0.41
1:D:559:LEU:HD11	1:D:588:ARG:HG3	2.03	0.41
1:D:693:VAL:HG13	1:D:709:PHE:CD2	2.55	0.41
1:E:637:PHE:HE1	1:E:645:ARG:HD2	1.86	0.41
1:F:581:SER:HB3	1:F:585:ARG:HH12	1.86	0.41
1:B:750:ARG:HA	1:B:751:PRO:HD3	1.93	0.41
1:D:331:ARG:HD3	3:E:1001:AGS:S1G	2.61	0.41
1:A:359:LEU:HD12	1:A:476:LYS:HG2	2.03	0.41
1:B:314:THR:OG1	1:B:315:THR:N	2.54	0.41
1:B:362:HIS:CD2	1:B:473:GLN:HG2	2.55	0.41
1:B:401:ILE:HD13	1:B:401:ILE:HA	1.85	0.41
1:B:576:ALA:HB2	1:B:761:VAL:HG21	2.02	0.41
1:B:605:GLY:HA3	1:B:763:PHE:HB2	2.03	0.41
1:B:643:VAL:HG21	1:C:638:MET:HE1	2.02	0.41
1:B:795:ILE:HA	1:B:846:LEU:HB2	2.02	0.41
1:C:316:LEU:HD11	1:D:668:ARG:HD2	2.03	0.41
1:C:618:LEU:HA	1:C:618:LEU:HD23	1.77	0.41
1:C:640:LYS:HB3	1:C:640:LYS:HE3	1.82	0.41
1:C:685:ASP:OD1	1:C:685:ASP:N	2.38	0.41
1:D:199:LYS:NZ	1:E:388:ASP:OD2	2.49	0.41
1:D:331:ARG:HA	1:E:384:ARG:HH22	1.86	0.41
1:D:789:ARG:HD3	1:D:789:ARG:HA	1.89	0.41
1:E:403:MET:HB3	1:E:403:MET:HE2	1.86	0.41
1:E:718:SER:OG	1:E:719:ASN:N	2.54	0.41
1:E:786:LEU:HA	1:E:786:LEU:HD23	1.85	0.41
1:E:809:ASP:N	1:E:809:ASP:OD1	2.54	0.41
1:A:189:ARG:HE	1:B:542:ARG:HE	1.68	0.41
1:A:328:ALA:HA	1:A:332:ARG:HH21	1.86	0.41
1:A:331:ARG:NH2	1:B:388:ASP:OD1	2.51	0.41
1:B:618:LEU:HD23	1:B:618:LEU:HA	1.88	0.41
1:B:631:ARG:HG3	1:B:675:LEU:HD23	2.02	0.41
1:C:204:LEU:HD23	1:C:204:LEU:HA	1.80	0.41
1:C:364:GLN:HB2	1:C:530:LYS:HG2	2.03	0.41
1:D:600:SER:OG	1:D:758:ASP:N	2.54	0.41
1:D:695:ASP:OD1	1:E:815:ARG:NH1	2.53	0.41
1:E:640:LYS:HD3	1:F:654:VAL:HG22	2.03	0.41
1:F:409:PRO:HB2	1:F:412:LEU:HD13	2.02	0.41
1:B:849:ASN:HD22	1:B:852:ARG:HB2	1.86	0.40
1:C:290:ASP:O	1:D:287:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ARG:HH11	1:C:320:ARG:HD3	1.72	0.40
1:C:444:LEU:HD12	1:C:447:GLU:HB3	2.03	0.40
1:D:566:LEU:HA	1:D:566:LEU:HD23	1.90	0.40
1:E:541:ALA:HB2	1:E:548:VAL:HB	2.02	0.40
1:F:314:THR:HG21	1:F:319:TYR:HB2	2.03	0.40
1:C:528:ARG:NH2	1:C:535:GLU:OE2	2.54	0.40
1:D:194:LEU:HD23	1:D:194:LEU:HA	1.84	0.40
1:D:353:LEU:HD23	1:D:353:LEU:HA	1.90	0.40
1:F:281:HIS:HB2	1:F:322:TYR:HB2	2.03	0.40
1:A:718:SER:OG	1:A:719:ASN:N	2.54	0.40
1:E:416:ASP:HA	1:E:419:ILE:HG12	2.04	0.40
1:A:241:ASP:OD1	1:A:242:MET:N	2.54	0.40
1:B:386:LEU:HD23	1:B:386:LEU:HA	1.94	0.40
1:B:696:ASP:HB2	1:B:698:ARG:HG2	2.02	0.40
1:D:379:ARG:NH2	1:D:594:PRO:HB3	2.36	0.40
1:D:402:ARG:O	1:D:406:ASP:HB2	2.21	0.40
1:F:169:THR:HG23	1:F:237:VAL:HB	2.03	0.40
1:B:496:ALA:O	1:B:500:GLU:CB	2.69	0.40
1:C:698:ARG:NH1	1:D:633:ASP:OD2	2.55	0.40
1:E:194:LEU:HD21	1:E:274:ILE:HD13	2.03	0.40
1:E:597:PRO:HA	1:E:710:ARG:HA	2.04	0.40
1:E:834:LEU:HD23	1:E:834:LEU:HA	1.89	0.40
1:F:367:ASP:HA	1:F:370:ILE:HD12	2.04	0.40
1:F:508:GLU:HG3	1:F:509:LEU:HD12	2.04	0.40
1:F:700:THR:HA	1:F:706:THR:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	663/858 (77%)	606 (91%)	57 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	683/858 (80%)	627 (92%)	56 (8%)	0	100	100
1	C	683/858 (80%)	613 (90%)	70 (10%)	0	100	100
1	D	674/858 (79%)	611 (91%)	63 (9%)	0	100	100
1	E	678/858 (79%)	612 (90%)	66 (10%)	0	100	100
1	F	674/858 (79%)	610 (90%)	63 (9%)	1 (0%)	48	82
2	S	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	4077/5172 (79%)	3699 (91%)	377 (9%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	407	SER

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	566/714 (79%)	565 (100%)	1 (0%)	87	85
1	B	574/714 (80%)	572 (100%)	2 (0%)	86	84
1	C	574/714 (80%)	571 (100%)	3 (0%)	81	81
1	D	574/714 (80%)	569 (99%)	5 (1%)	70	75
1	E	574/714 (80%)	573 (100%)	1 (0%)	87	85
1	F	566/714 (79%)	564 (100%)	2 (0%)	84	82
All	All	3428/4284 (80%)	3414 (100%)	14 (0%)	81	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	506	ILE
1	B	506	ILE
1	B	646	LEU

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Mol	Chain	Res	Type
1	C	284	VAL
1	C	506	ILE
1	C	819	ARG
1	D	203	VAL
1	D	381	ILE
1	D	506	ILE
1	D	548	VAL
1	D	761	VAL
1	E	506	ILE
1	F	246	VAL
1	F	506	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	264	ASN
1	A	426	GLN
1	A	573	GLN
1	A	748	ASN
1	A	764	HIS
1	A	806	ASN
1	A	832	GLN
1	A	857	GLN
1	A	858	HIS
1	B	264	ASN
1	B	334	GLN
1	B	620	ASN
1	B	692	GLN
1	B	747	HIS
1	B	806	ASN
1	B	858	HIS
1	C	192	GLN
1	C	264	ASN
1	C	297	ASN
1	C	573	GLN
1	C	692	GLN
1	C	747	HIS
1	C	748	ASN
1	C	778	GLN
1	C	822	GLN
1	C	849	ASN

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Mol	Chain	Res	Type
1	C	858	HIS
1	D	195	GLN
1	D	281	HIS
1	D	309	HIS
1	D	334	GLN
1	D	361	HIS
1	D	378	HIS
1	D	426	GLN
1	D	512	GLN
1	D	564	GLN
1	D	641	HIS
1	D	711	ASN
1	D	719	ASN
1	D	747	HIS
1	D	748	ASN
1	D	806	ASN
1	D	822	GLN
1	E	159	GLN
1	E	195	GLN
1	E	200	ASN
1	E	221	GLN
1	E	297	ASN
1	E	473	GLN
1	E	512	GLN
1	E	567	HIS
1	E	573	GLN
1	E	683	HIS
1	E	688	ASN
1	E	726	GLN
1	E	748	ASN
1	E	764	HIS
1	E	769	GLN
1	E	794	HIS
1	E	806	ASN
1	E	824	GLN
1	F	264	ASN
1	F	297	ASN
1	F	362	HIS
1	F	421	GLN
1	F	688	ASN
1	F	726	GLN
1	F	747	HIS

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Mol	Chain	Res	Type
1	F	748	ASN
1	F	778	GLN
1	F	858	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	AGS	D	1002	-	32,33,33	1.46	3 (9%)	45,52,52	1.05	1 (2%)
3	AGS	D	1001	-	32,33,33	1.81	3 (9%)	45,52,52	0.90	1 (2%)
3	AGS	E	1001	-	32,33,33	1.21	2 (6%)	45,52,52	0.88	2 (4%)
3	AGS	C	1002	-	32,33,33	1.18	3 (9%)	45,52,52	1.01	1 (2%)
3	AGS	E	1002	-	32,33,33	1.14	2 (6%)	45,52,52	1.04	2 (4%)
3	AGS	C	1001	-	32,33,33	1.82	4 (12%)	45,52,52	1.11	1 (2%)
3	AGS	F	1001	-	32,33,33	0.62	1 (3%)	45,52,52	2.10	6 (13%)
4	ADP	F	1002	-	28,29,29	1.41	4 (14%)	43,45,45	2.32	13 (30%)
3	AGS	B	1002	-	32,33,33	1.40	3 (9%)	45,52,52	0.95	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	B	1001	-	32,33,33	1.78	3 (9%)	45,52,52	0.99	2 (4%)
3	AGS	A	1001	-	32,33,33	0.90	3 (9%)	45,52,52	1.01	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	D	1002	-	-	5/21/38/38	0/3/3/3
3	AGS	D	1001	-	-	3/21/38/38	0/3/3/3
3	AGS	E	1001	-	-	6/21/38/38	0/3/3/3
3	AGS	C	1002	-	-	4/21/38/38	0/3/3/3
3	AGS	E	1002	-	-	6/21/38/38	0/3/3/3
3	AGS	C	1001	-	-	3/21/38/38	0/3/3/3
3	AGS	F	1001	-	-	11/21/38/38	0/3/3/3
4	ADP	F	1002	-	-	4/16/32/32	0/3/3/3
3	AGS	B	1002	-	-	4/21/38/38	0/3/3/3
3	AGS	B	1001	-	-	1/21/38/38	0/3/3/3
3	AGS	A	1001	-	-	7/21/38/38	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	AGS	PB-O3A	-6.75	1.52	1.59
3	C	1001	AGS	PB-O3A	-6.24	1.52	1.59
3	C	1001	AGS	PA-O3A	-6.13	1.52	1.59
3	D	1001	AGS	PB-O3B	-5.91	1.53	1.59
3	D	1001	AGS	PA-O3A	-5.53	1.53	1.59
3	D	1002	AGS	PB-O3B	-5.39	1.53	1.59
3	D	1001	AGS	PB-O3A	-5.39	1.53	1.59
3	E	1002	AGS	PA-O3A	-5.38	1.53	1.59
3	B	1001	AGS	PA-O3A	-4.98	1.54	1.59
4	F	1002	ADP	C5-C4	4.87	1.47	1.39
3	B	1001	AGS	PB-O3B	-4.87	1.54	1.59
3	B	1002	AGS	PB-O3A	-4.76	1.54	1.59
3	E	1001	AGS	PB-O3A	-4.76	1.54	1.59
3	B	1002	AGS	PA-O3A	-4.46	1.54	1.59
3	E	1001	AGS	PA-O3A	-4.15	1.55	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	AGS	PB-O3B	-4.05	1.55	1.59
3	D	1002	AGS	PB-O3A	-4.03	1.55	1.59
3	C	1002	AGS	PB-O3B	-3.90	1.55	1.59
3	D	1002	AGS	PA-O3A	-3.61	1.55	1.59
3	B	1002	AGS	PB-O3B	-3.39	1.55	1.59
3	C	1002	AGS	PB-O3A	-3.34	1.55	1.59
3	C	1002	AGS	PA-O3A	-3.19	1.56	1.59
3	A	1001	AGS	PB-O3A	-2.97	1.56	1.59
4	F	1002	ADP	C5-C6	2.82	1.48	1.41
3	F	1001	AGS	PG-S1G	2.66	1.96	1.90
4	F	1002	ADP	C8-N7	2.52	1.36	1.31
3	E	1002	AGS	PB-O3A	-2.48	1.56	1.59
3	A	1001	AGS	PB-O3B	-2.20	1.57	1.59
4	F	1002	ADP	C5-N7	-2.19	1.35	1.39
3	A	1001	AGS	PA-O3A	-2.19	1.57	1.59
3	C	1001	AGS	PA-O1A	-2.18	1.43	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1001	AGS	O2B-PB-O1B	-8.24	74.10	112.44
4	F	1002	ADP	C5-C4-N3	-7.99	115.72	126.72
3	F	1001	AGS	O2B-PB-O3B	-6.74	89.05	107.27
3	F	1001	AGS	O2B-PB-O3A	-6.67	89.25	107.27
3	C	1001	AGS	PB-O3B-PG	-6.63	108.92	133.17
4	F	1002	ADP	N3-C4-N9	6.07	137.49	127.17
3	C	1002	AGS	PB-O3B-PG	-5.54	112.90	133.17
3	D	1002	AGS	PB-O3B-PG	-5.46	113.20	133.17
3	B	1001	AGS	PB-O3B-PG	-5.43	113.31	133.17
3	A	1001	AGS	PB-O3B-PG	-5.11	114.47	133.17
3	D	1001	AGS	PB-O3B-PG	-5.01	114.82	133.17
3	B	1002	AGS	PB-O3B-PG	-5.01	114.82	133.17
4	F	1002	ADP	C2-N3-C4	4.85	123.69	111.83
4	F	1002	ADP	C4-C5-N7	-4.19	105.79	110.58
4	F	1002	ADP	C5-N7-C8	3.82	109.45	103.45
4	F	1002	ADP	N3-C2-N1	-3.62	123.11	128.58
4	F	1002	ADP	C3'-C2'-C1'	3.52	108.12	101.46
3	E	1001	AGS	PB-O3B-PG	-3.35	120.91	133.17
3	F	1001	AGS	PB-O3B-PG	-3.32	121.04	133.17
3	E	1002	AGS	PB-O3B-PG	-2.90	122.56	133.17
4	F	1002	ADP	N9-C8-N7	-2.89	109.83	113.94
3	F	1001	AGS	O3B-PB-O1B	2.86	119.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1001	AGS	O2G-PG-O3B	2.74	113.79	104.64
3	E	1002	AGS	O2B-PB-O3A	-2.37	100.87	107.27
4	F	1002	ADP	O4'-C1'-N9	2.29	112.49	108.09
4	F	1002	ADP	C4-N9-C8	2.24	108.09	105.74
3	F	1001	AGS	O3A-PB-O1B	2.23	117.40	110.70
4	F	1002	ADP	O2A-PA-O1A	2.21	122.74	112.44
4	F	1002	ADP	C6-C5-N7	2.20	136.34	132.09
3	B	1001	AGS	O2B-PB-O3A	-2.20	101.34	107.27
4	F	1002	ADP	O3B-PB-O2B	2.04	115.44	107.80

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	C5'-O5'-PA-O2A
3	B	1002	AGS	PB-O3B-PG-O2G
3	B	1002	AGS	PB-O3B-PG-O3G
3	C	1001	AGS	PB-O3B-PG-O2G
3	D	1001	AGS	O4'-C4'-C5'-O5'
3	D	1001	AGS	C3'-C4'-C5'-O5'
3	D	1002	AGS	PB-O3B-PG-O2G
3	D	1002	AGS	PB-O3B-PG-O3G
3	D	1002	AGS	C5'-O5'-PA-O1A
3	D	1002	AGS	C5'-O5'-PA-O2A
3	D	1002	AGS	C5'-O5'-PA-O3A
3	E	1001	AGS	C5'-O5'-PA-O1A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	E	1002	AGS	PB-O3B-PG-O2G
3	F	1001	AGS	PB-O3B-PG-O2G
3	F	1001	AGS	PB-O3B-PG-O3G
3	F	1001	AGS	C5'-O5'-PA-O2A
3	F	1001	AGS	C3'-C4'-C5'-O5'
3	A	1001	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	C3'-C4'-C5'-O5'
3	F	1001	AGS	O4'-C4'-C5'-O5'
3	C	1002	AGS	C3'-C4'-C5'-O5'
3	A	1001	AGS	C3'-C4'-C5'-O5'
3	C	1002	AGS	O4'-C4'-C5'-O5'
4	F	1002	ADP	O4'-C4'-C5'-O5'
3	B	1002	AGS	PB-O3A-PA-O1A
3	E	1001	AGS	O4'-C4'-C5'-O5'

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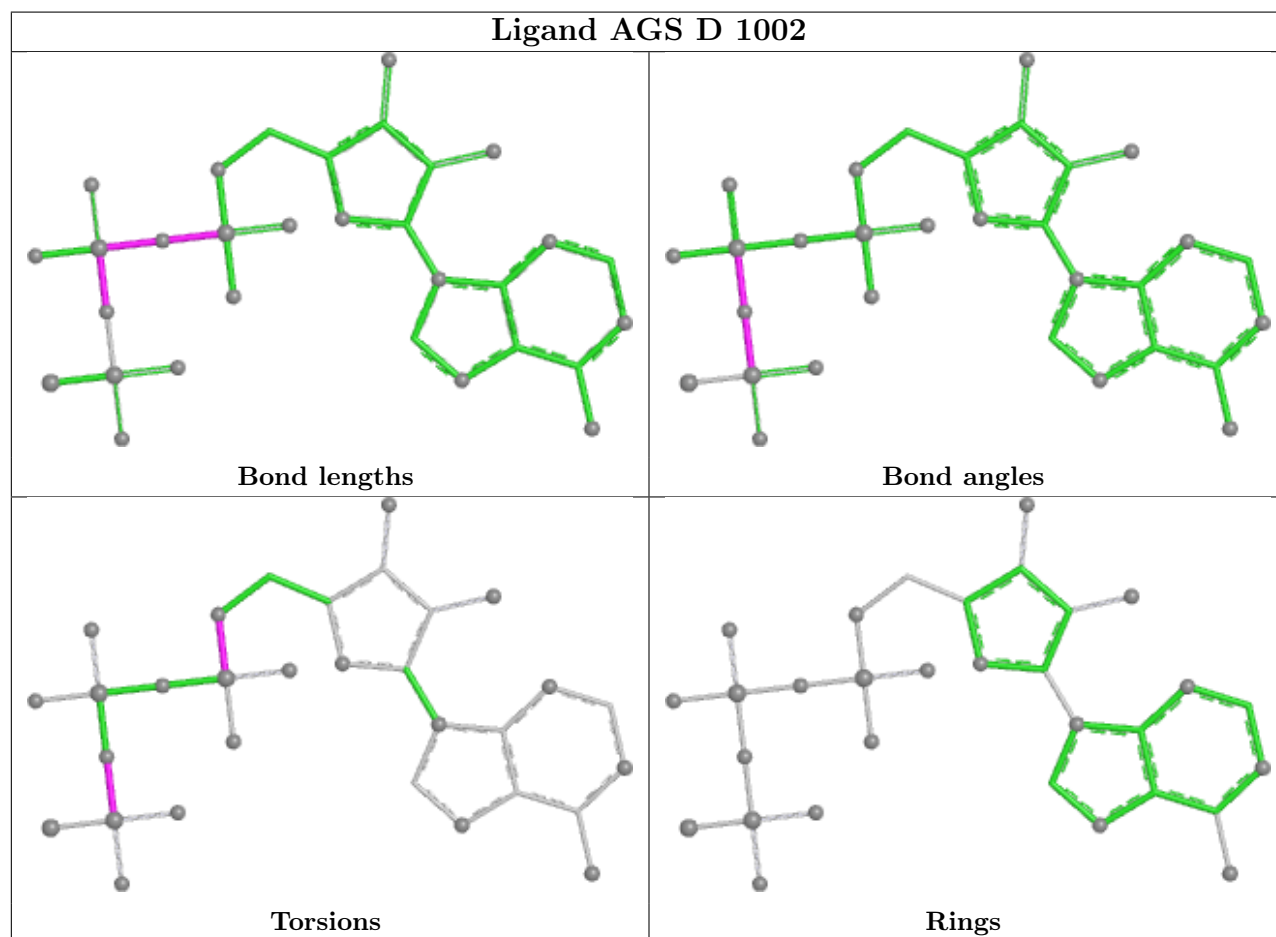
Mol	Chain	Res	Type	Atoms
4	F	1002	ADP	C3'-C4'-C5'-O5'
3	A	1001	AGS	C5'-O5'-PA-O1A
3	A	1001	AGS	C5'-O5'-PA-O3A
3	E	1001	AGS	C5'-O5'-PA-O3A
3	F	1001	AGS	C5'-O5'-PA-O1A
3	F	1001	AGS	C5'-O5'-PA-O3A
4	F	1002	ADP	C5'-O5'-PA-O1A
3	E	1002	AGS	PG-O3B-PB-O1B
3	E	1002	AGS	PG-O3B-PB-O3A
3	F	1001	AGS	PB-O3A-PA-O2A
3	A	1001	AGS	PA-O3A-PB-O1B
3	E	1002	AGS	PB-O3A-PA-O2A
3	F	1001	AGS	PB-O3A-PA-O1A
3	E	1002	AGS	PB-O3B-PG-O3G
3	B	1001	AGS	C4'-C5'-O5'-PA
3	F	1001	AGS	PG-O3B-PB-O1B
3	B	1002	AGS	PB-O3A-PA-O2A
3	C	1002	AGS	PB-O3A-PA-O1A
3	C	1002	AGS	PB-O3A-PA-O2A
3	D	1001	AGS	PB-O3A-PA-O2A
3	E	1002	AGS	PB-O3A-PA-O1A
3	F	1001	AGS	C4'-C5'-O5'-PA
4	F	1002	ADP	C2'-C1'-N9-C8
3	A	1001	AGS	PA-O3A-PB-O2B
3	E	1001	AGS	PA-O3A-PB-O2B
3	E	1001	AGS	PB-O3A-PA-O2A

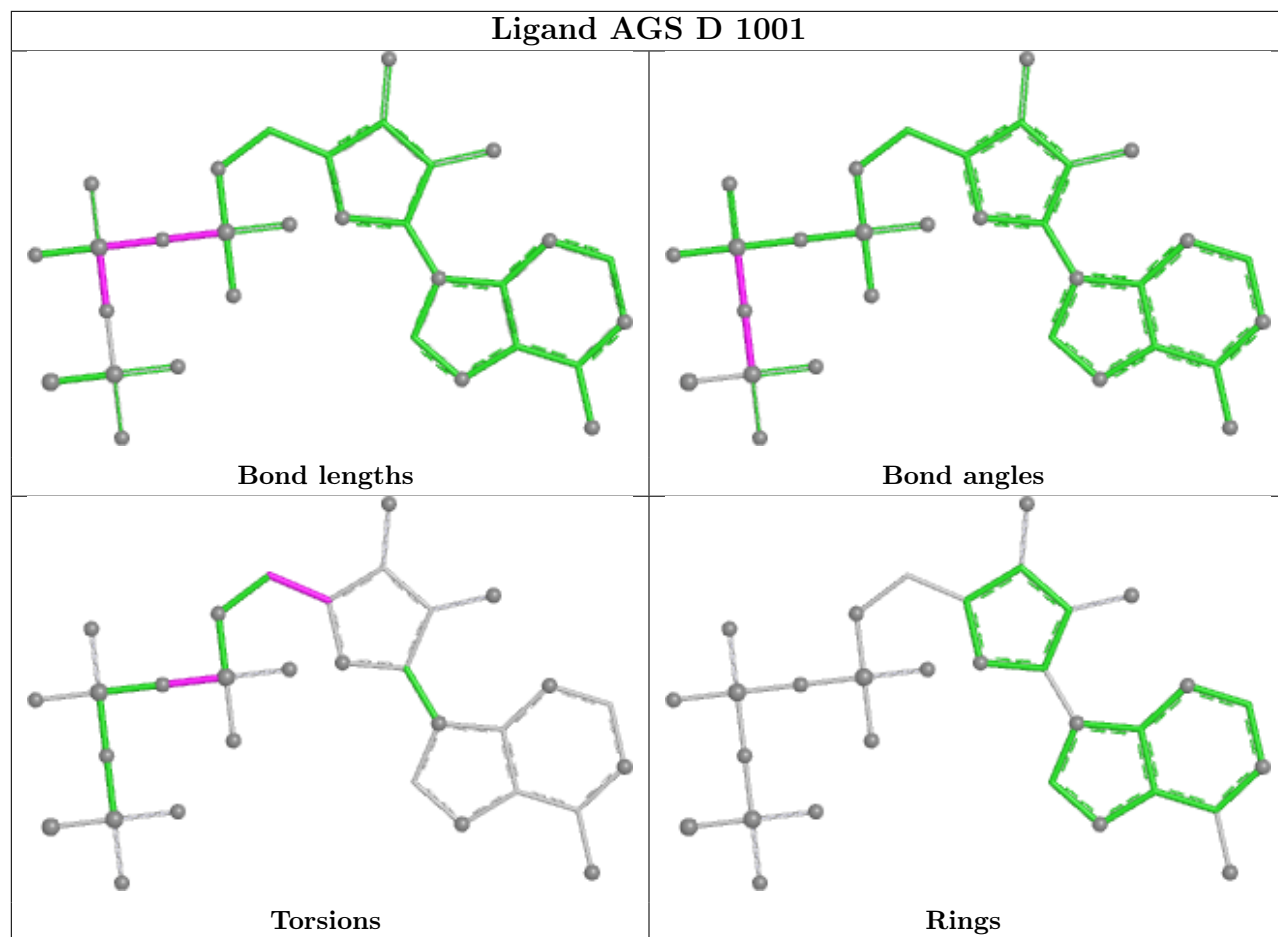
There are no ring outliers.

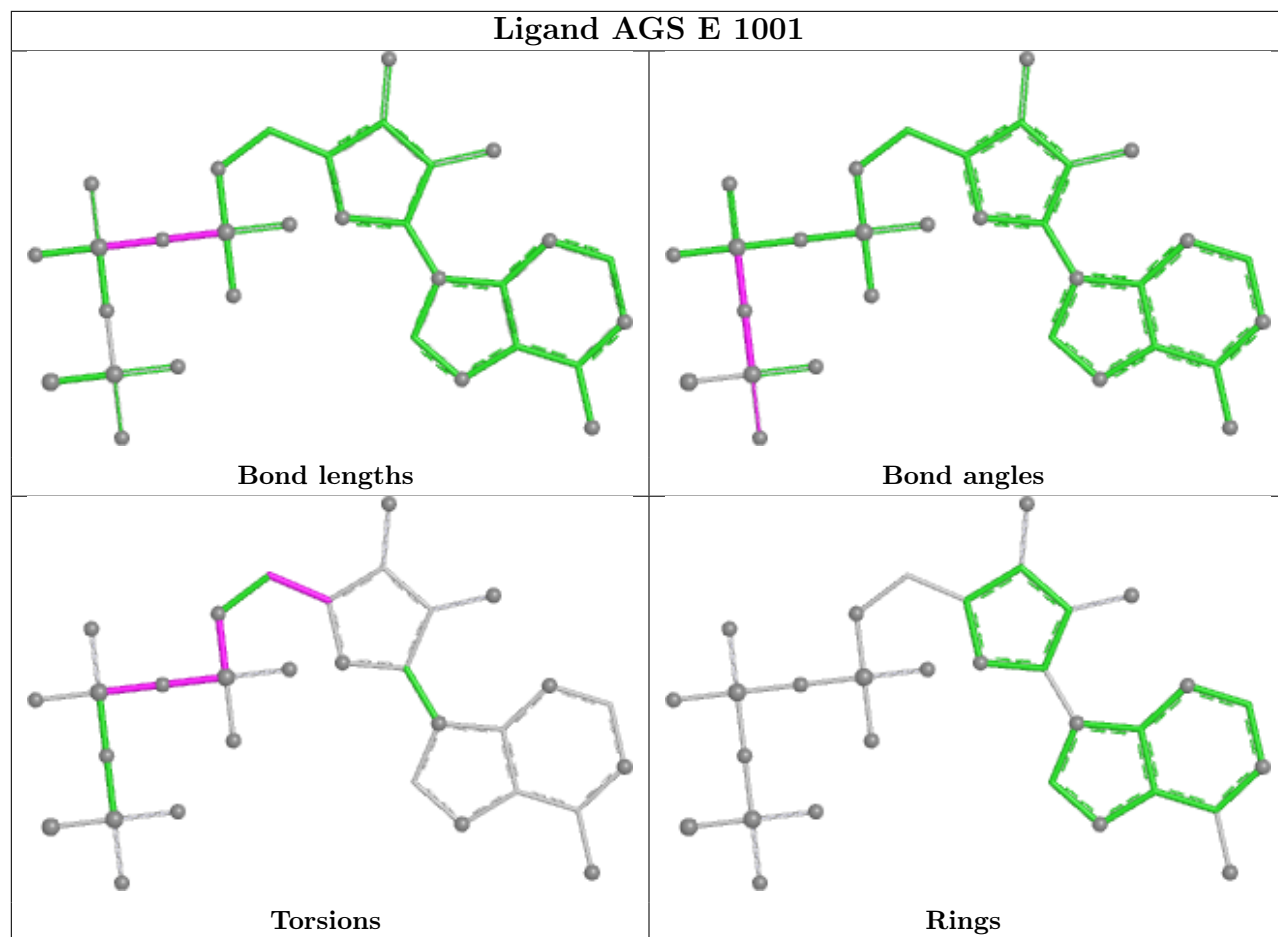
10 monomers are involved in 44 short contacts:

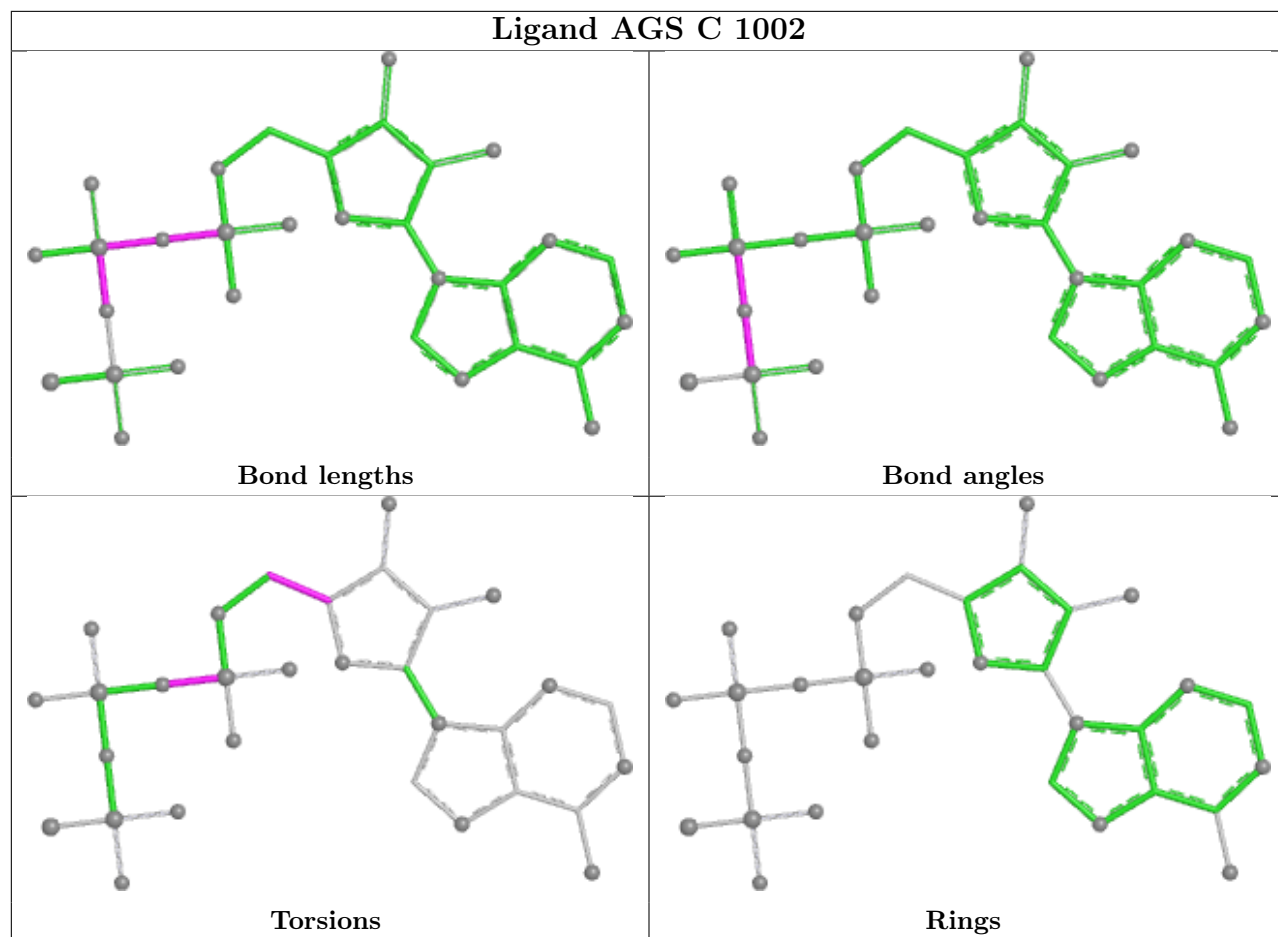
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	AGS	6	0
3	D	1001	AGS	2	0
3	E	1001	AGS	5	0
3	C	1002	AGS	5	0
3	E	1002	AGS	3	0
3	C	1001	AGS	5	0
3	F	1001	AGS	8	0
3	B	1002	AGS	1	0
3	B	1001	AGS	6	0
3	A	1001	AGS	3	0

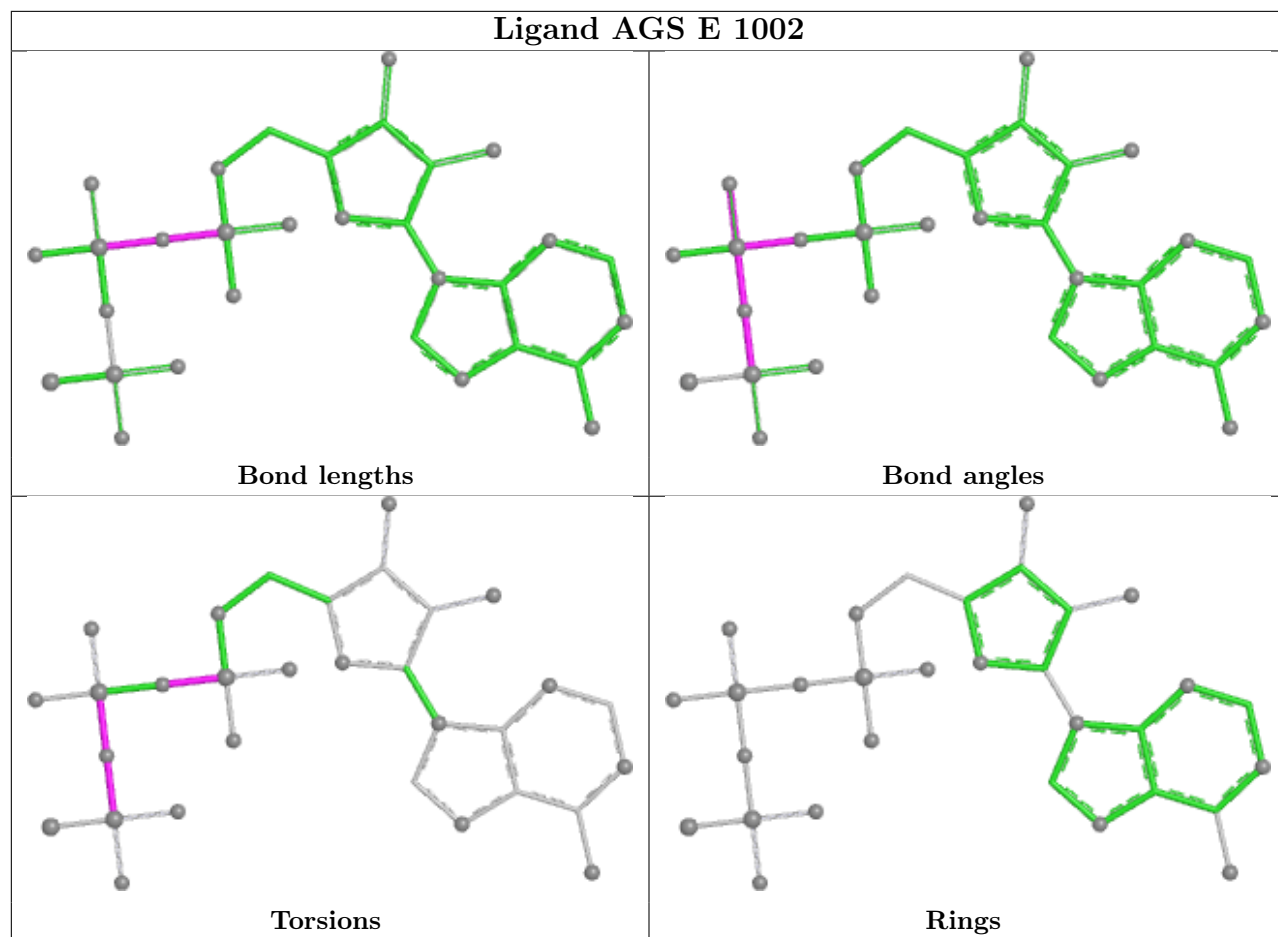
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

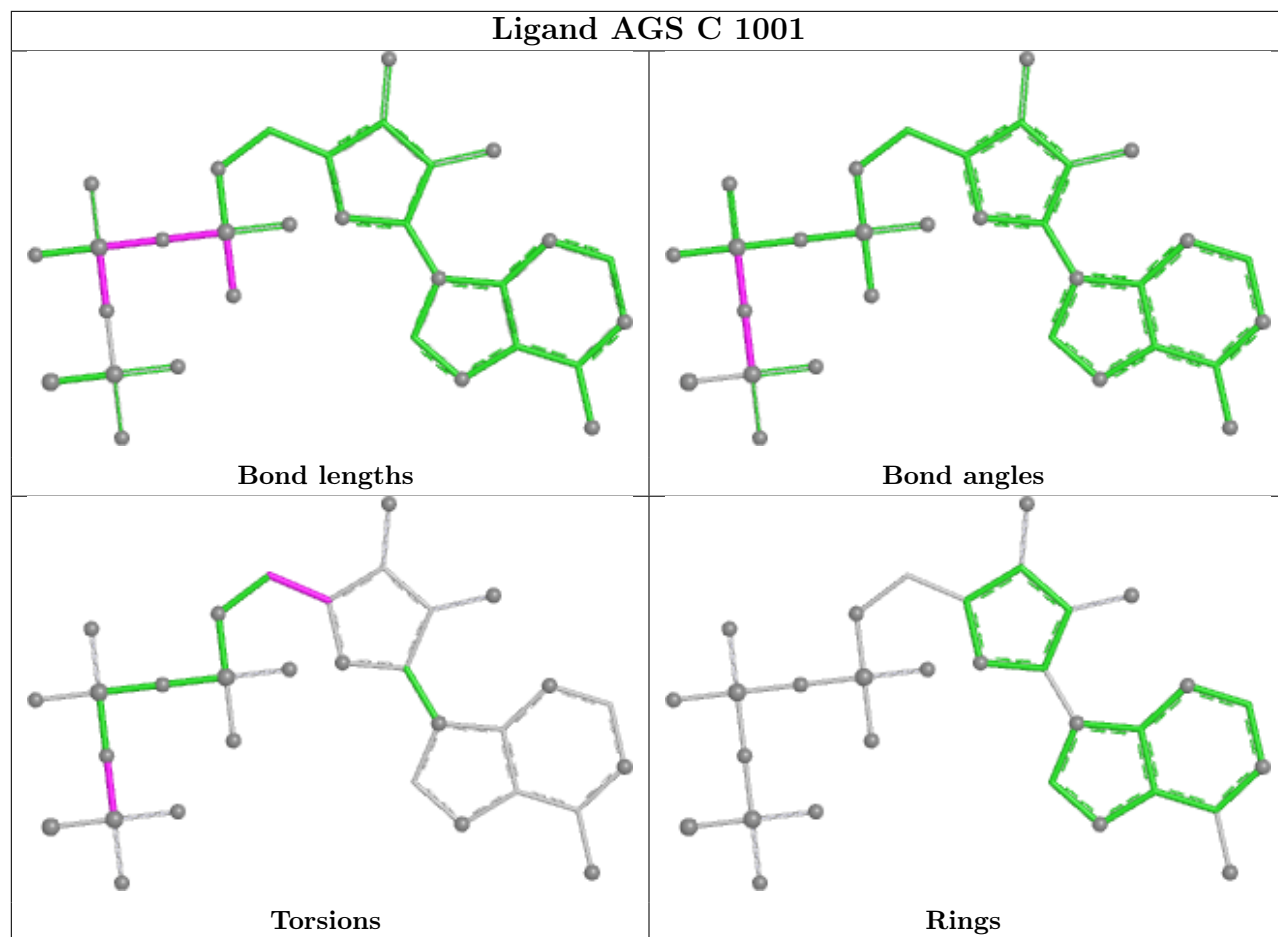


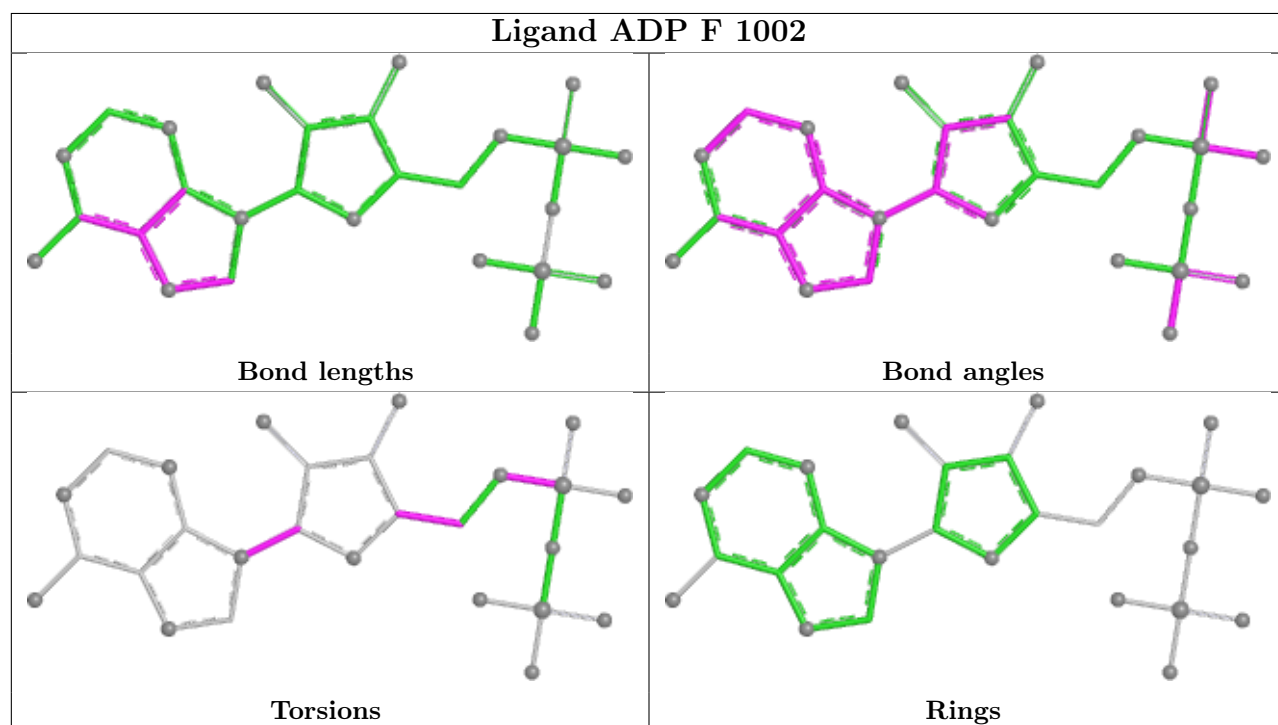
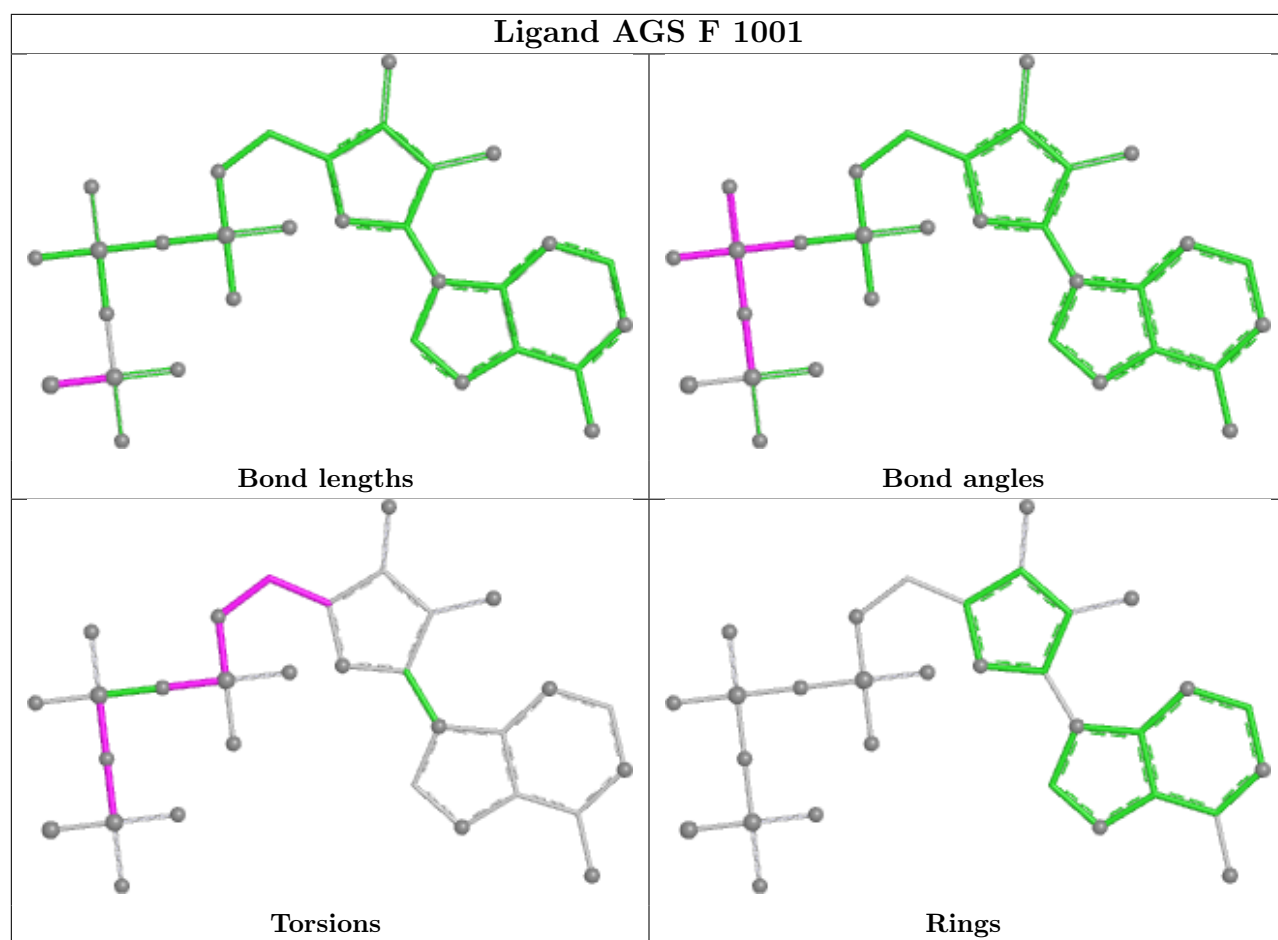


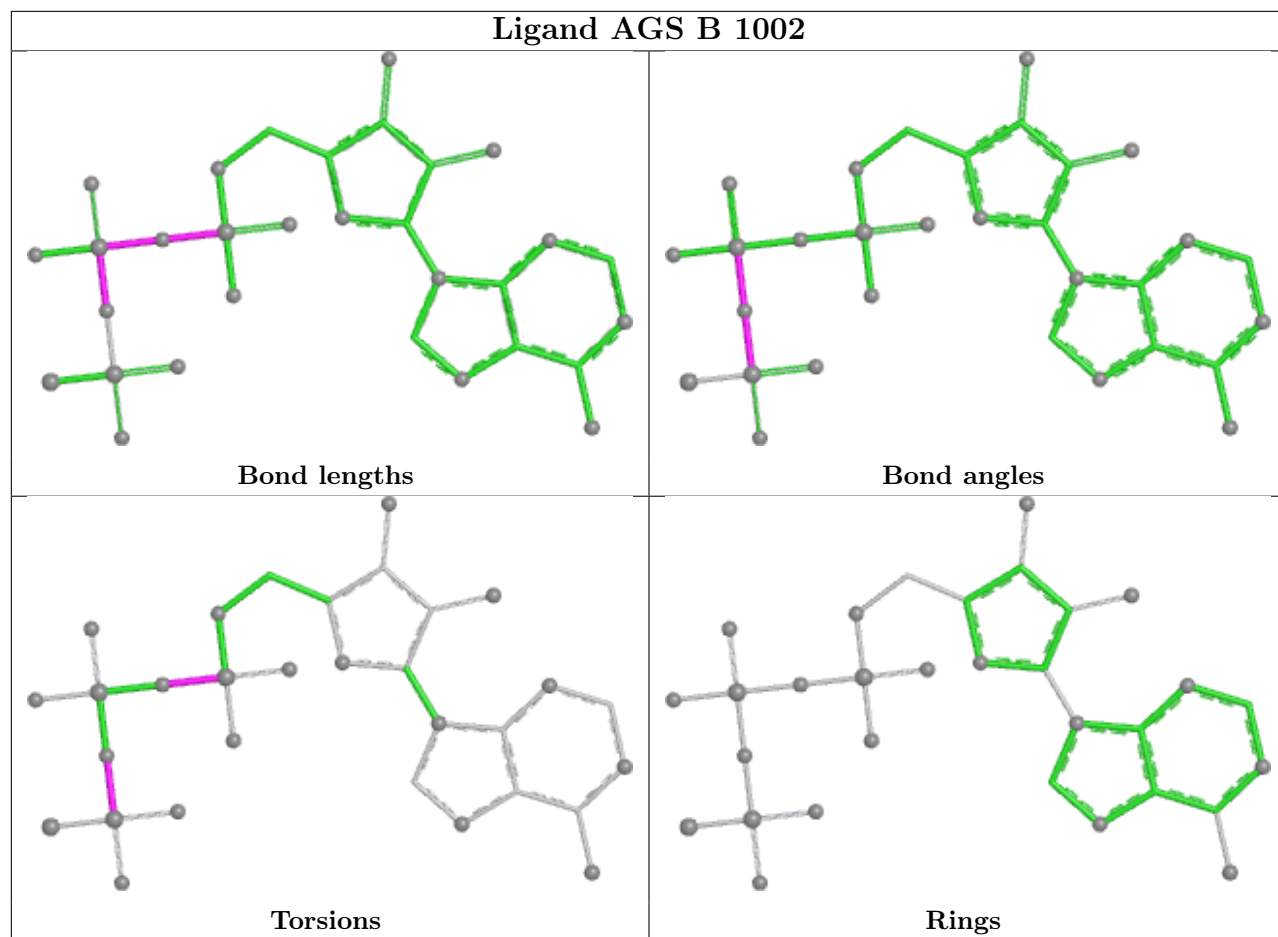


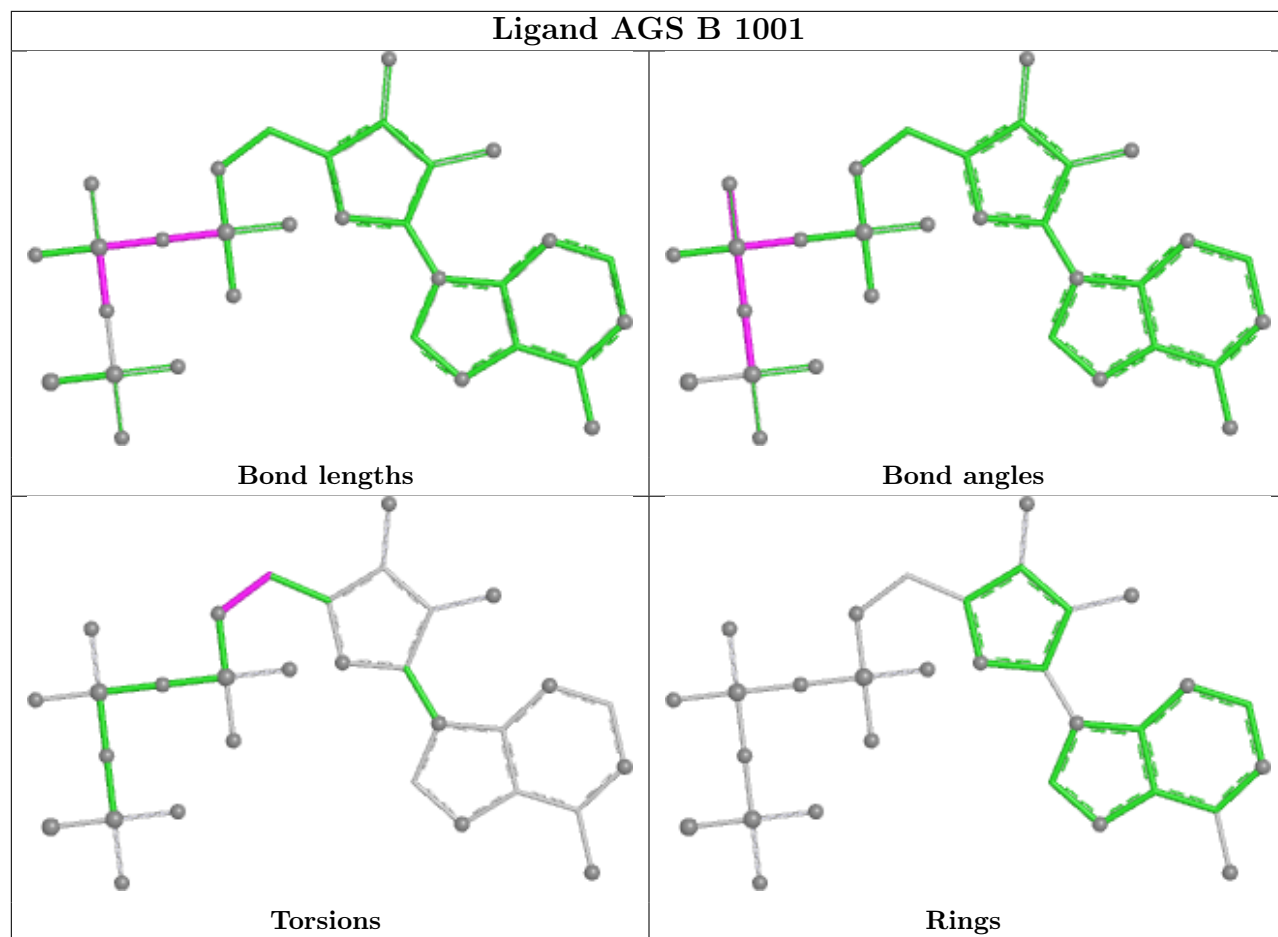


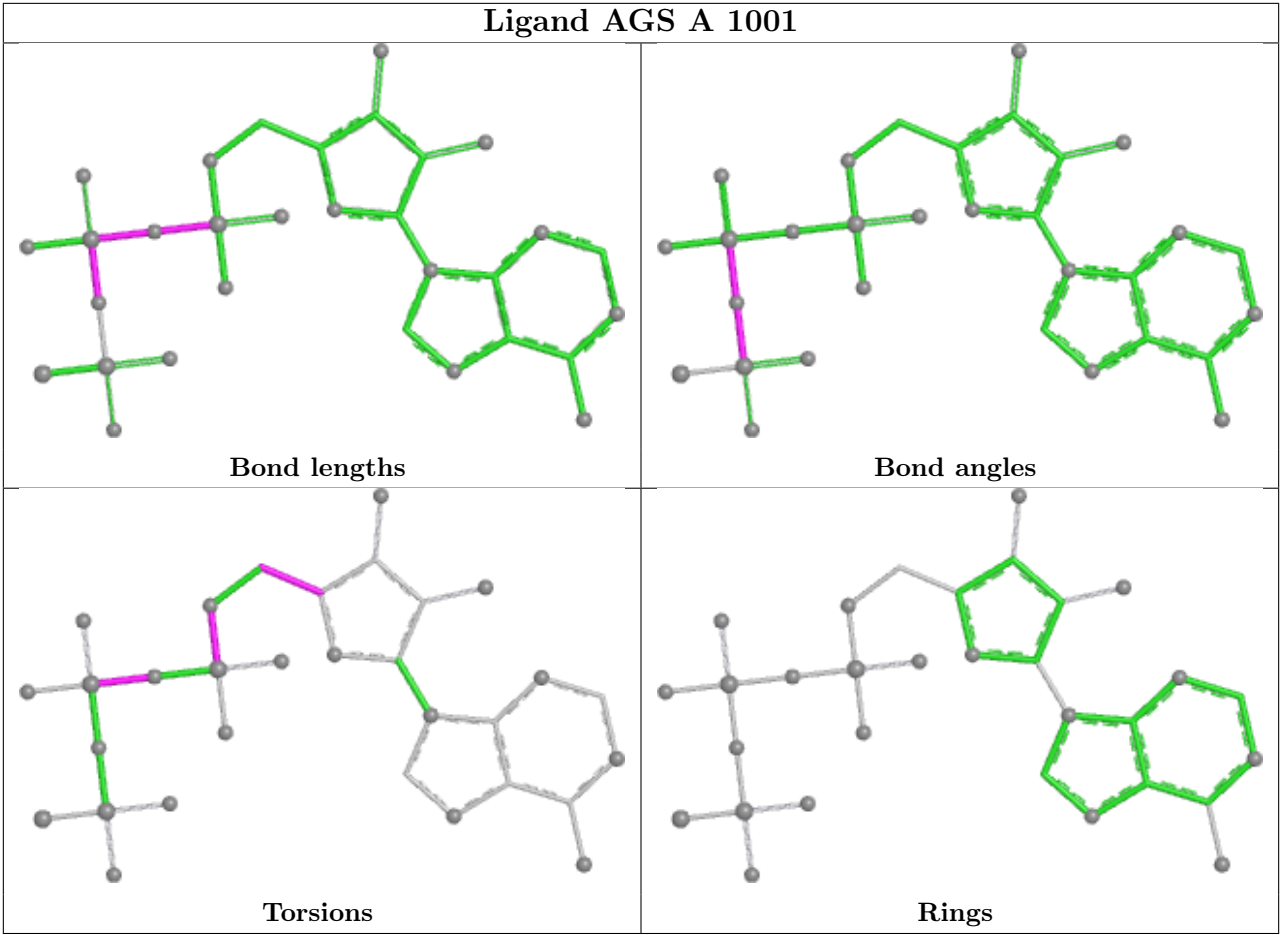












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2
1	D	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	526:LEU	C	527:LEU	N	4.96
1	A	526:LEU	C	527:LEU	N	3.34
1	D	526:LEU	C	527:LEU	N	3.28

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	749:PHE	C	750:ARG	N	1.20
1	D	749:PHE	C	750:ARG	N	1.16

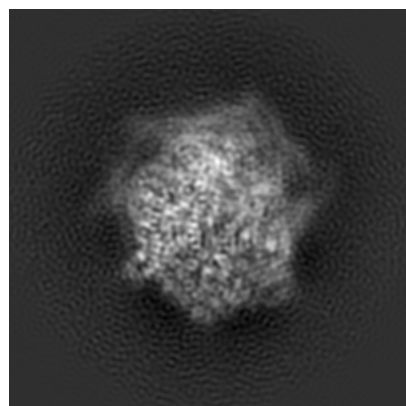
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4942. These allow visual inspection of the internal detail of the map and identification of artifacts.

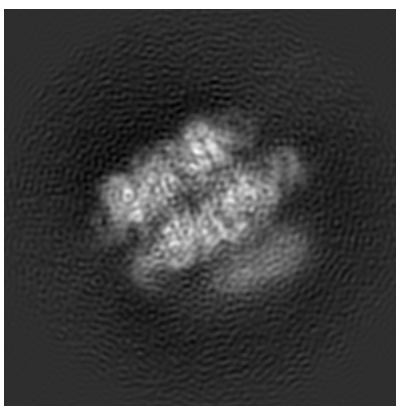
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

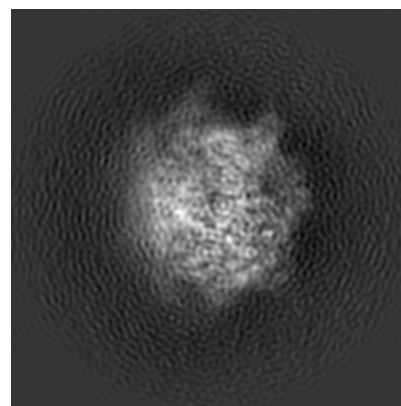
6.1.1 Primary map



X

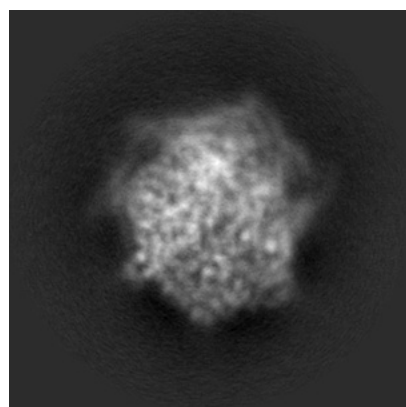


Y

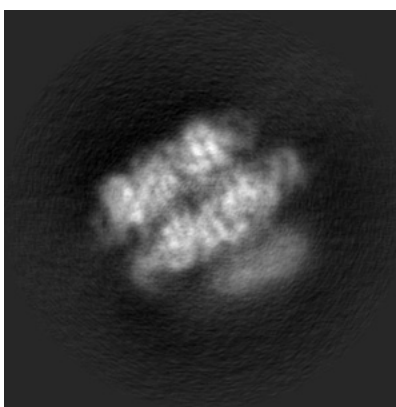


Z

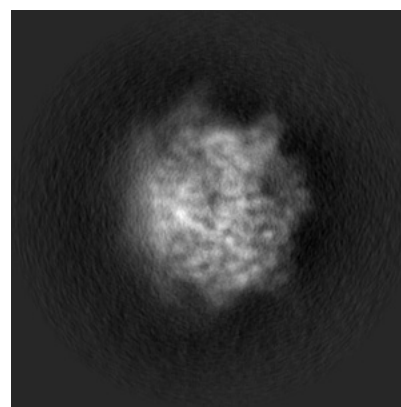
6.1.2 Raw map



X



Y

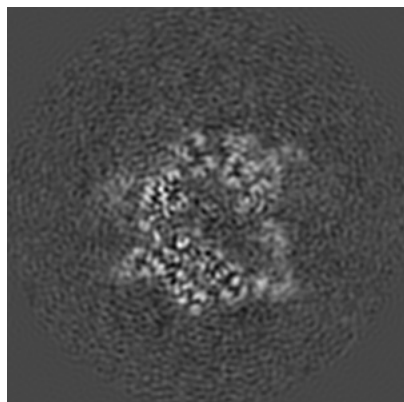


Z

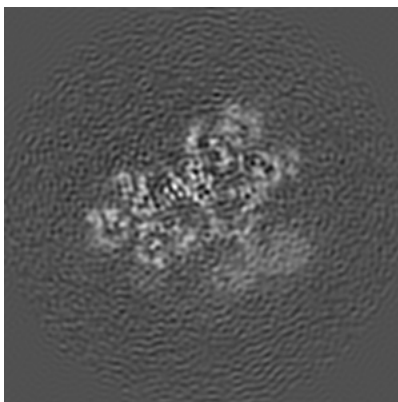
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

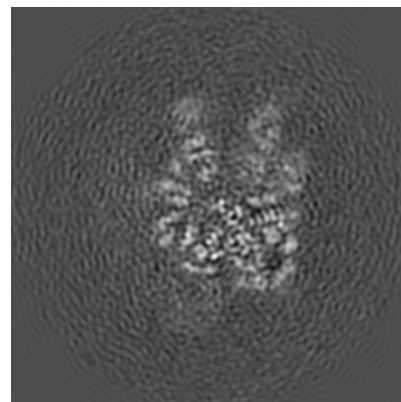
6.2.1 Primary map



X Index: 128

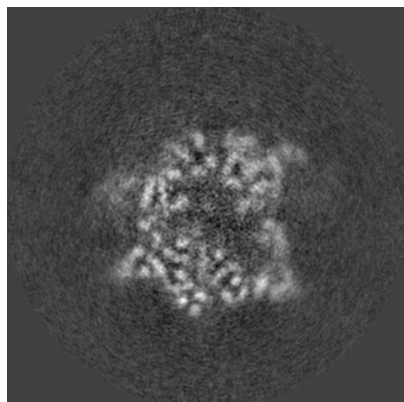


Y Index: 128

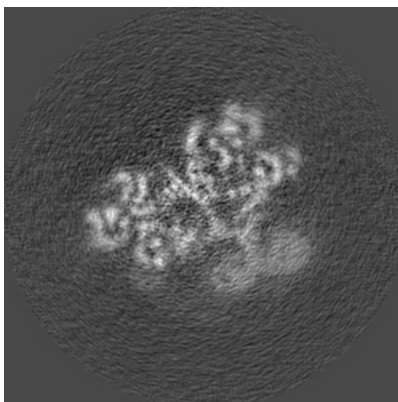


Z Index: 128

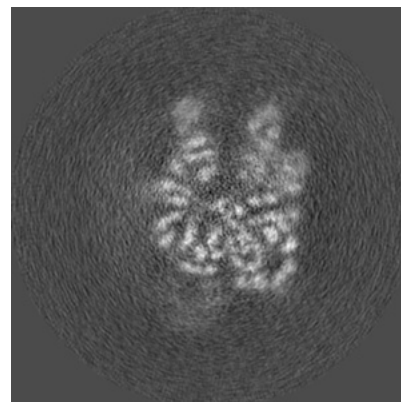
6.2.2 Raw map



X Index: 128



Y Index: 128

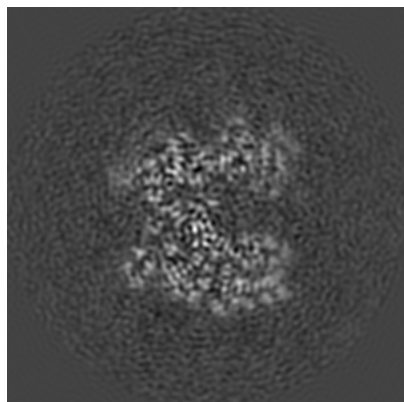


Z Index: 128

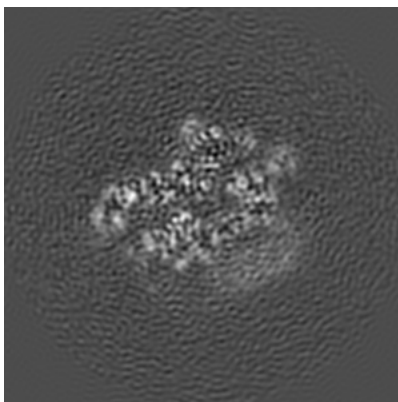
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

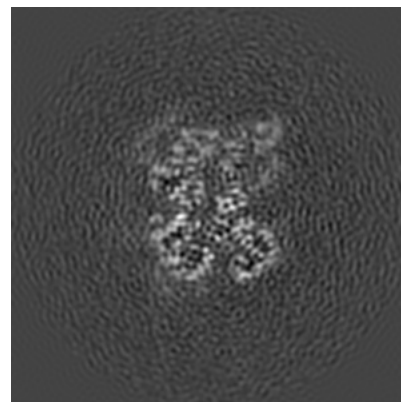
6.3.1 Primary map



X Index: 139

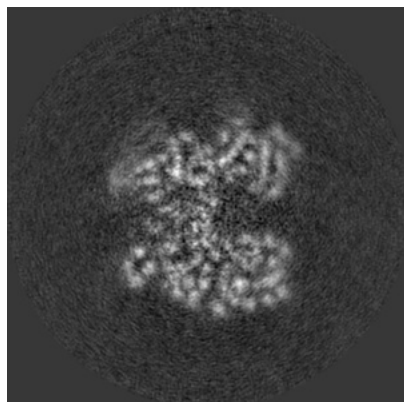


Y Index: 117

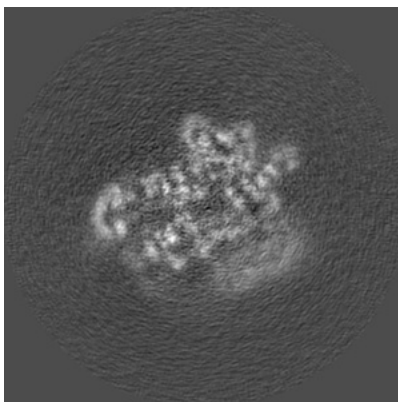


Z Index: 108

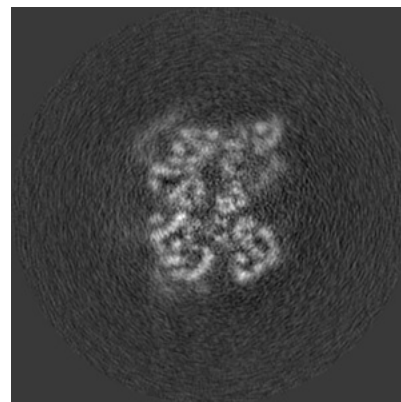
6.3.2 Raw map



X Index: 138



Y Index: 120

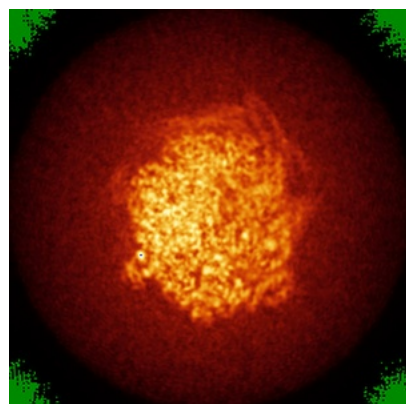


Z Index: 108

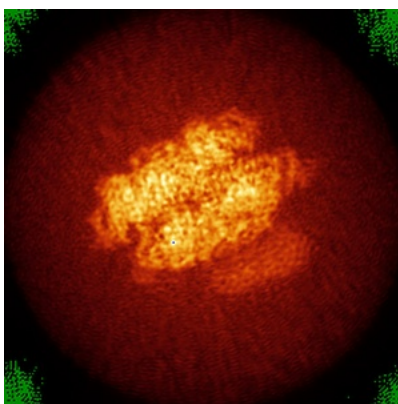
The images above show the largest variance slices of the map in three orthogonal directions.

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

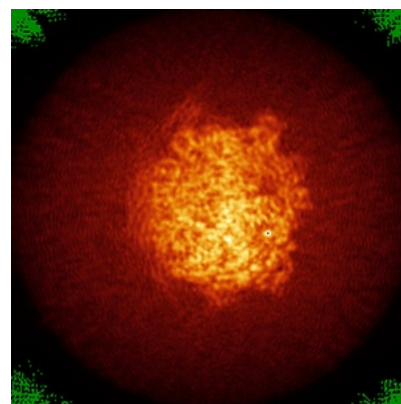
6.4.1 Primary map



X

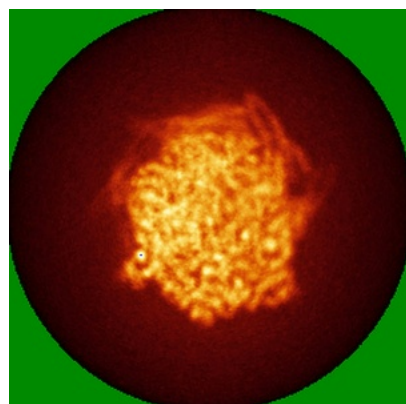


Y

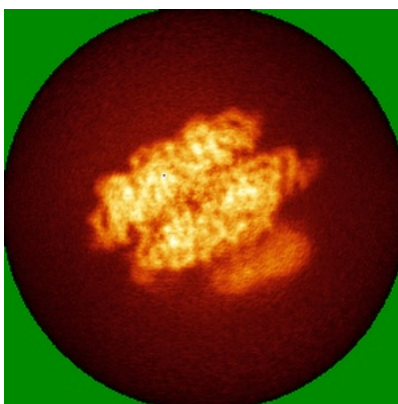


Z

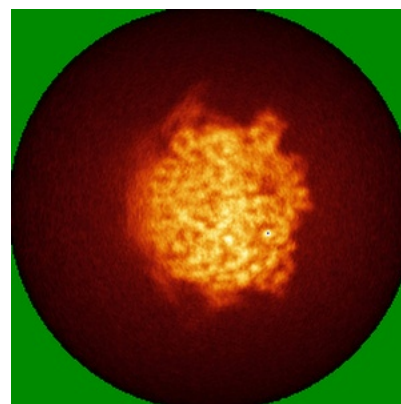
6.4.2 Raw map



X



Y



Z

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

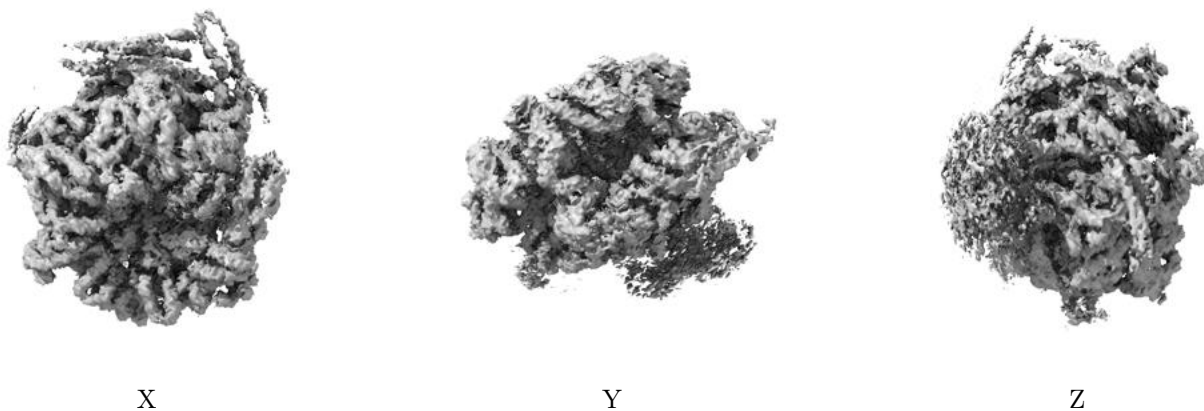
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

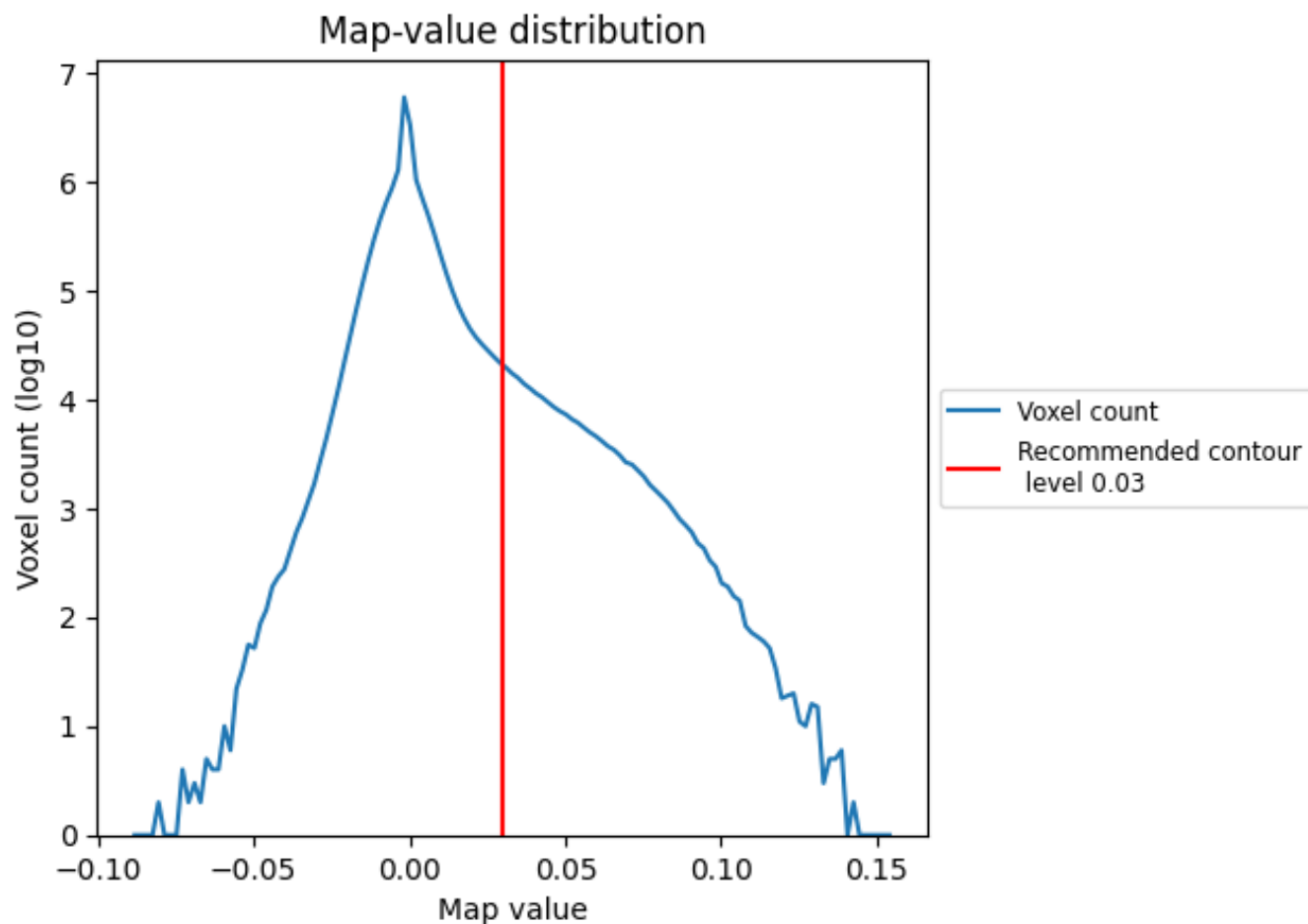
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

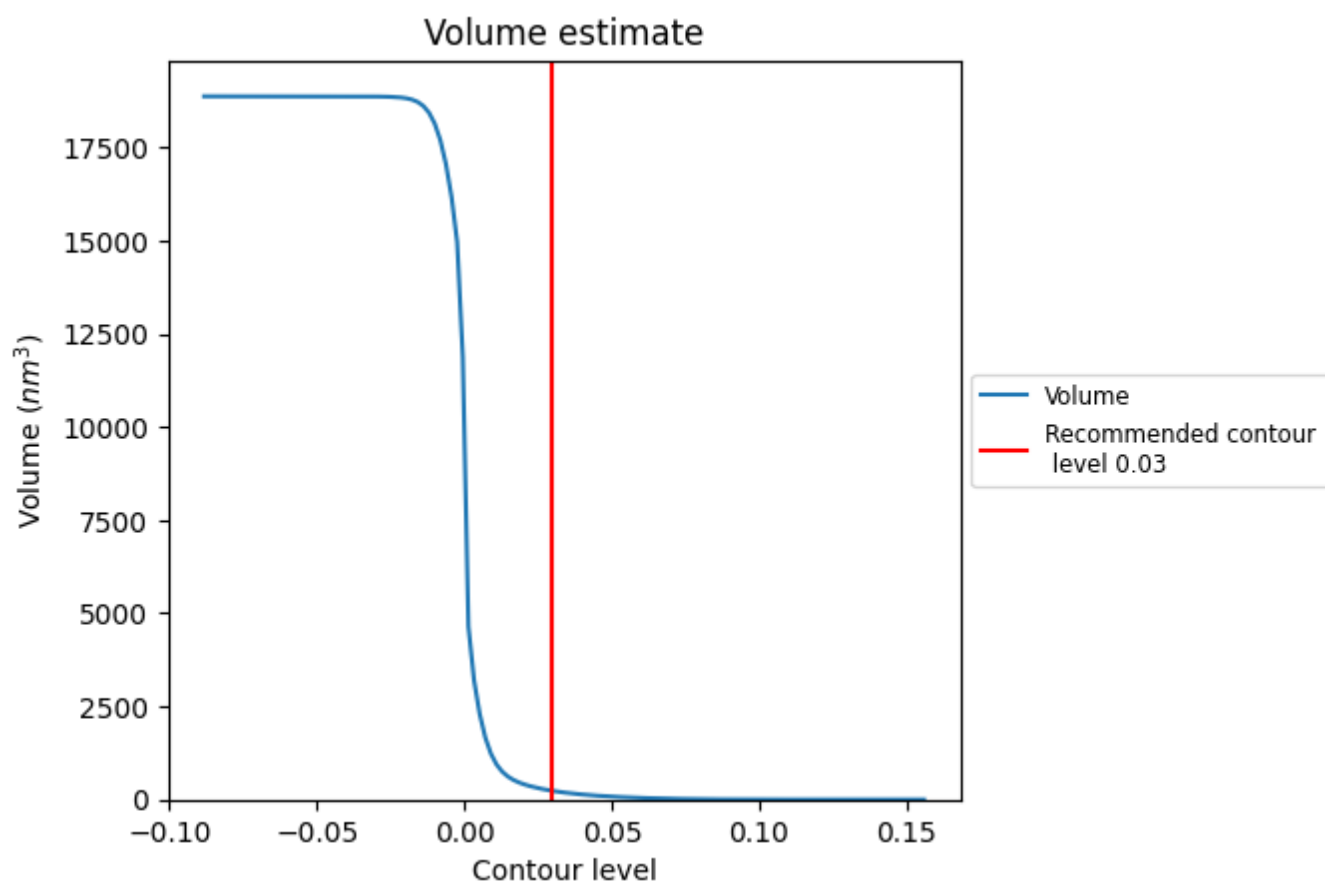
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

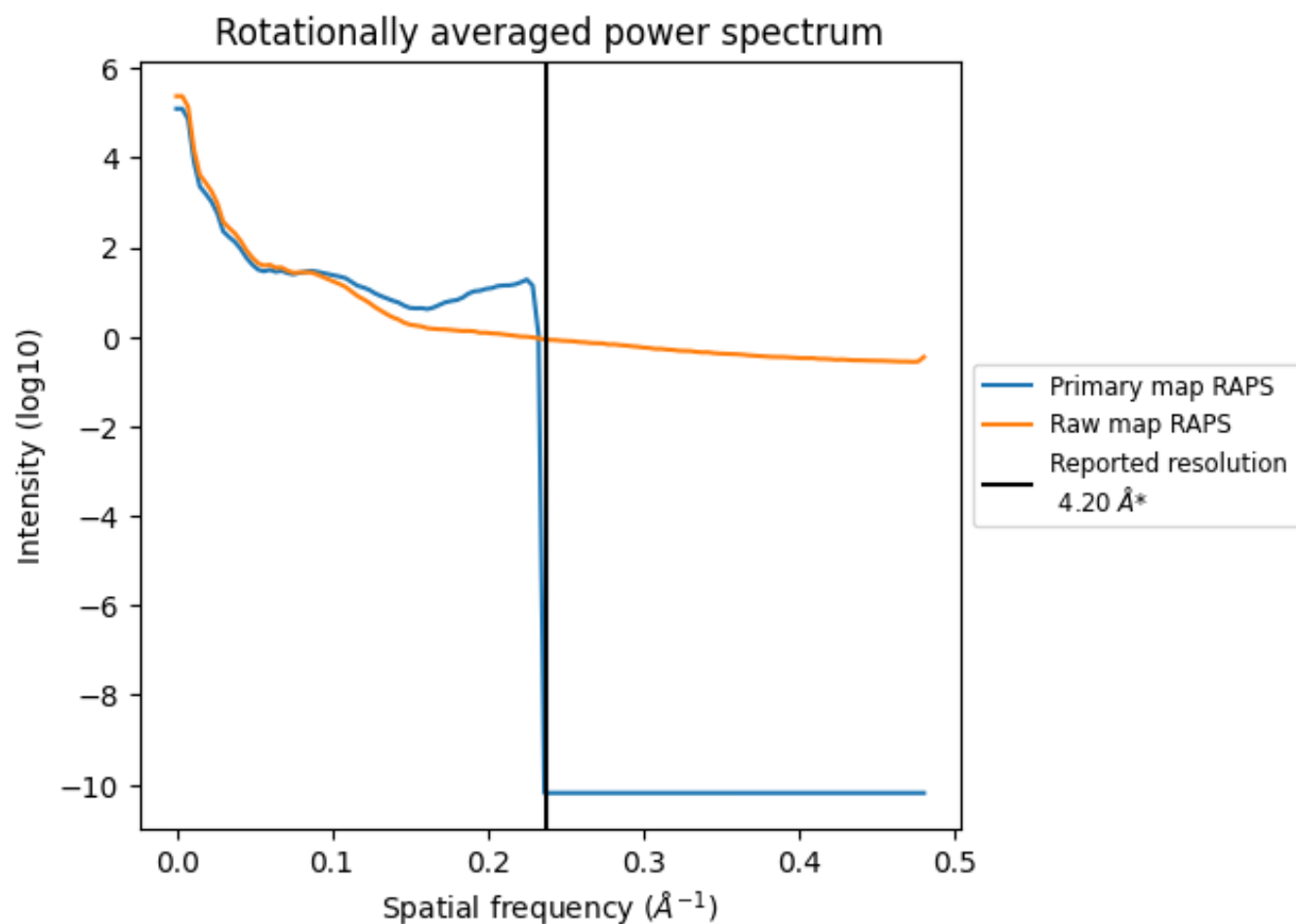
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 233 nm³; this corresponds to an approximate mass of 211 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 ⓘ

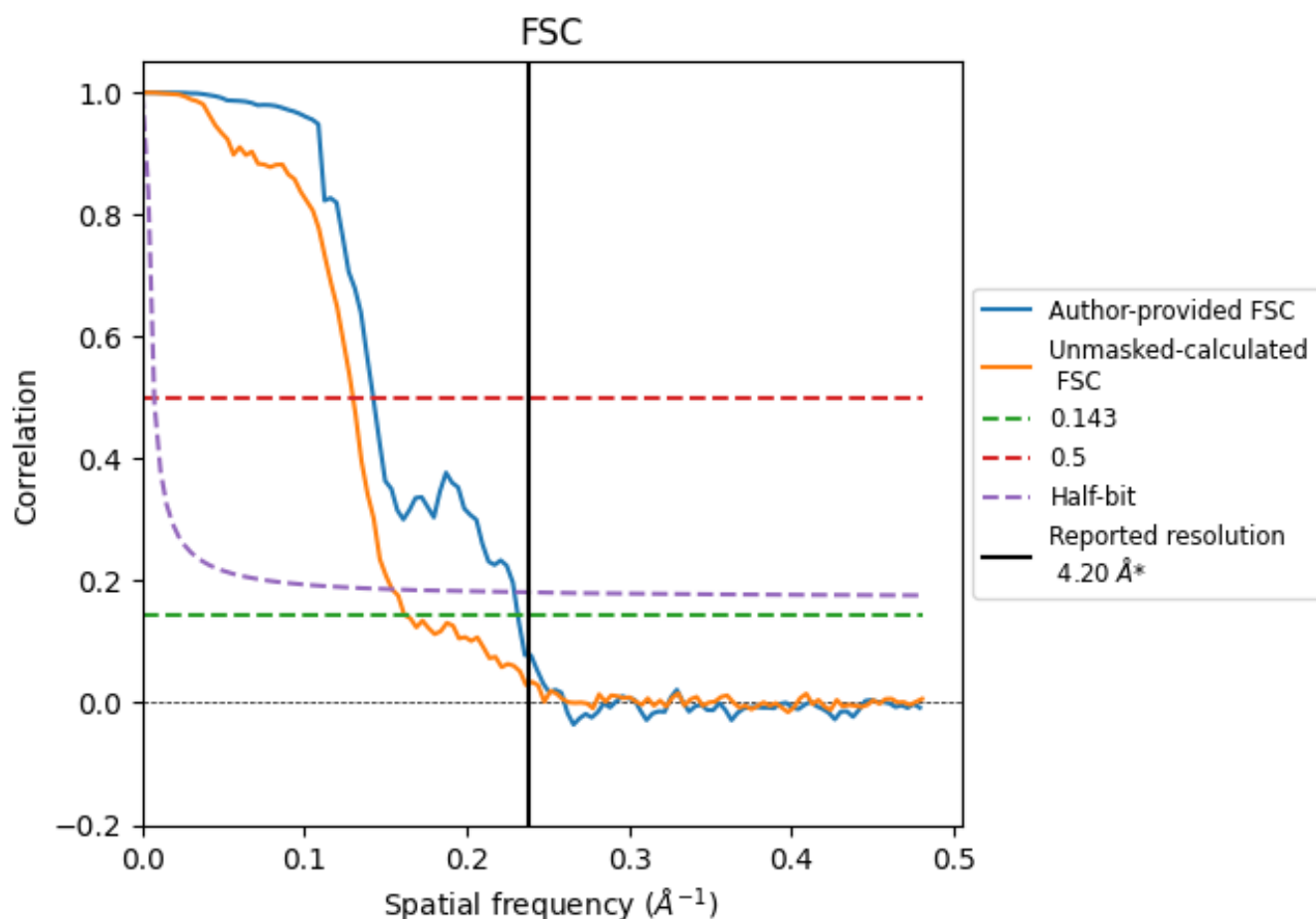


*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

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 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

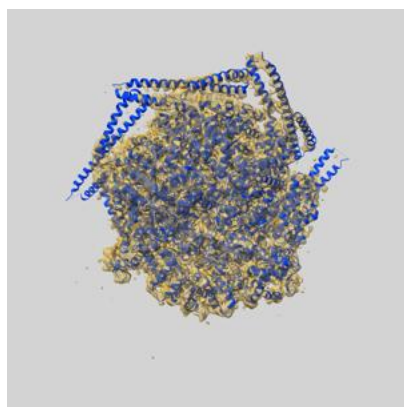
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.32	7.02	4.36
Unmasked-calculated*	6.16	7.70	6.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.16 differs from the reported value 4.2 by more than 10 %

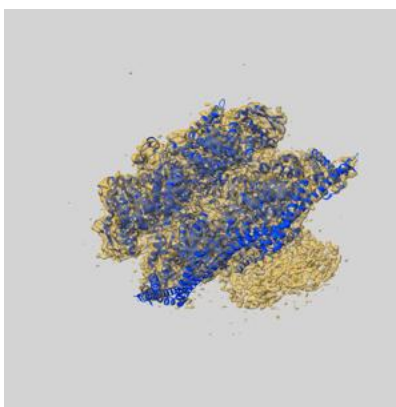
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4942 and PDB model 6RN4. Per-residue inclusion information can be found in section [3](#) on page [7](#).

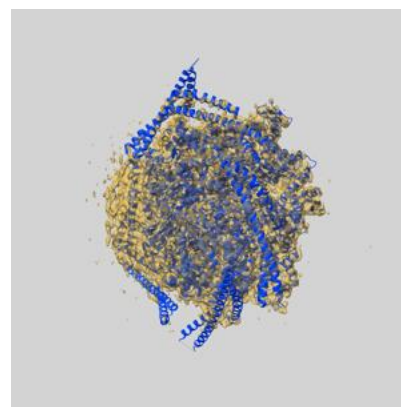
9.1 Map-model overlay [i](#)



X



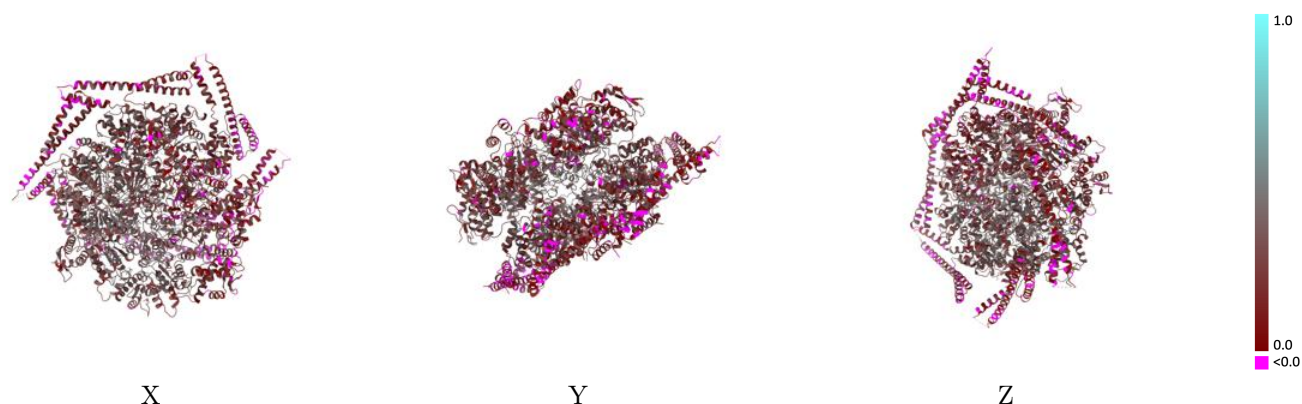
Y



Z

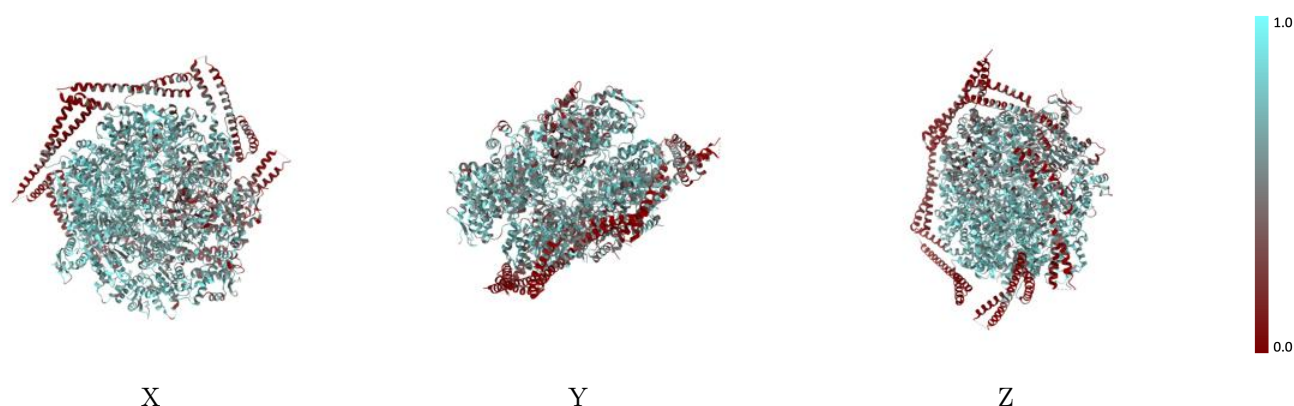
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



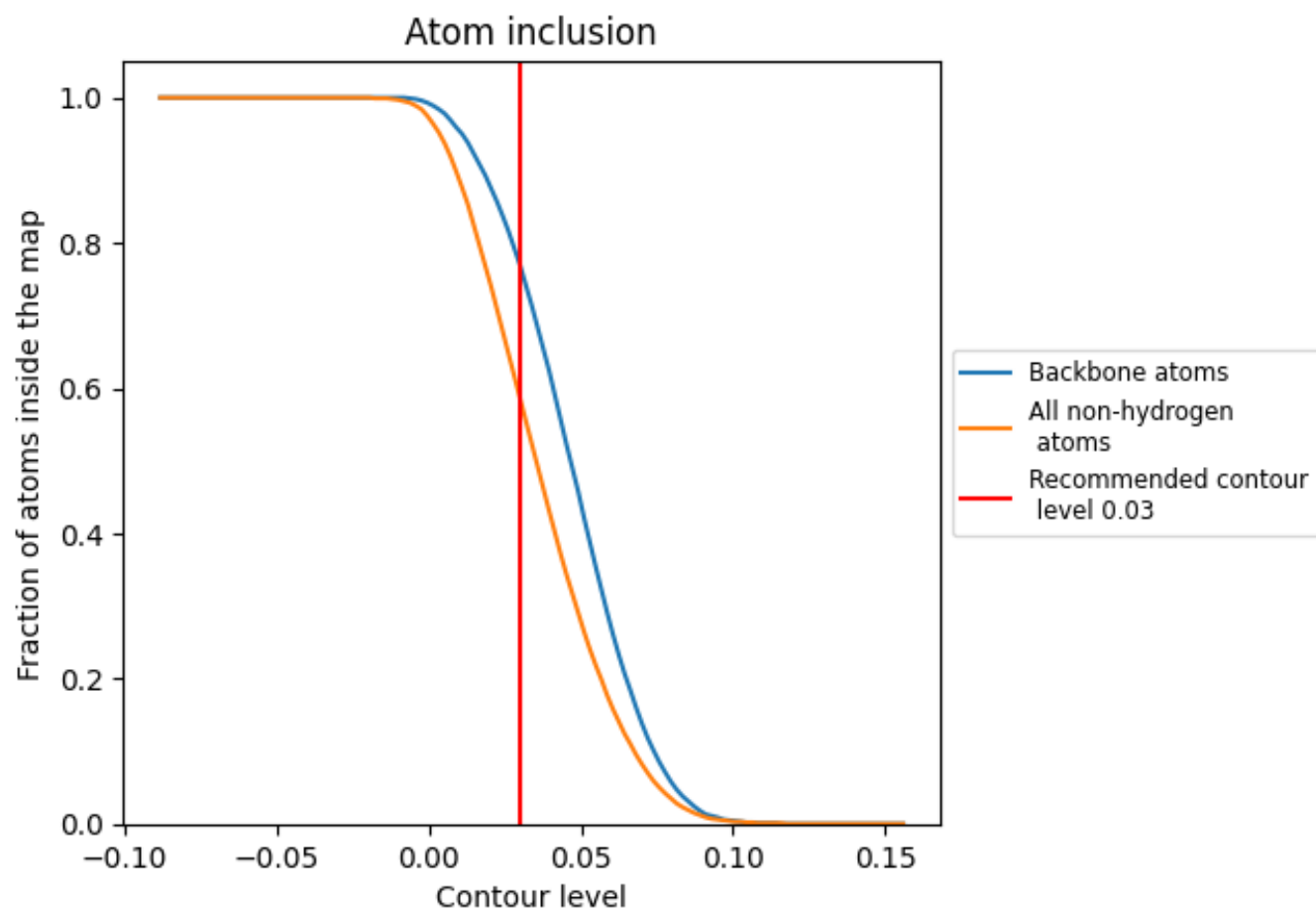
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 59% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5860	0.2580
A	0.5310	0.2120
B	0.6030	0.2750
C	0.6290	0.3010
D	0.6300	0.2970
E	0.6270	0.2710
F	0.4890	0.1850
S	0.8250	0.3790

1.0

0.0

<0.0