



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 07:27 pm GMT

PDB ID : 6QS8
EMDB ID : EMD-4627
Title : ClpB (DWB and K476C mutant) bound to casein in presence of ATPgammaS
- state KC-2B
Authors : Deville, C.; Saibil, H.R.
Deposited on : 2019-02-20
Resolution : 3.90 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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

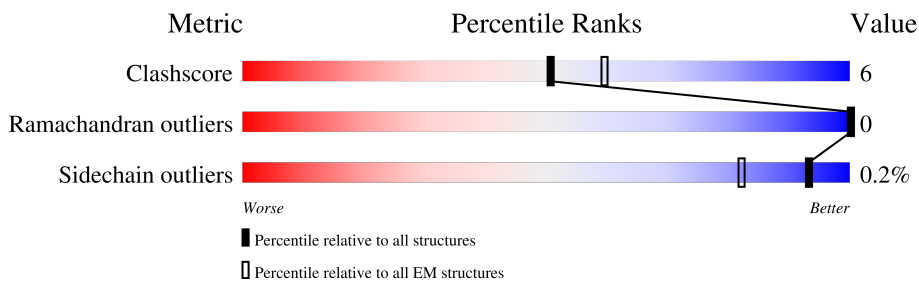
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	858	
1	B	858	
1	C	858	
1	D	858	
1	E	858	
1	F	858	
2	S	24	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 28875 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
			Total	C	N	O	S		
1	A	568	4472	2809	813	836	14	0	0
1	B	582	4562	2864	830	852	16	0	0
1	C	630	4976	3120	900	938	18	0	0
1	D	625	4952	3106	895	933	18	0	0
1	E	625	4952	3106	895	933	18	0	0
1	F	573	4496	2823	818	841	14	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	GLU	engineered mutation	UNP P63284
A	476	CYS	LYS	engineered mutation	UNP P63284
A	678	ALA	GLU	engineered mutation	UNP P63284
A	858	HIS	-	expression tag	UNP P63284
B	279	ALA	GLU	engineered mutation	UNP P63284
B	476	CYS	LYS	engineered mutation	UNP P63284
B	678	ALA	GLU	engineered mutation	UNP P63284
B	858	HIS	-	expression tag	UNP P63284
C	279	ALA	GLU	engineered mutation	UNP P63284
C	476	CYS	LYS	engineered mutation	UNP P63284
C	678	ALA	GLU	engineered mutation	UNP P63284
C	858	HIS	-	expression tag	UNP P63284
D	279	ALA	GLU	engineered mutation	UNP P63284
D	476	CYS	LYS	engineered mutation	UNP P63284
D	678	ALA	GLU	engineered mutation	UNP P63284
D	858	HIS	-	expression tag	UNP P63284
E	279	ALA	GLU	engineered mutation	UNP P63284
E	476	CYS	LYS	engineered mutation	UNP P63284

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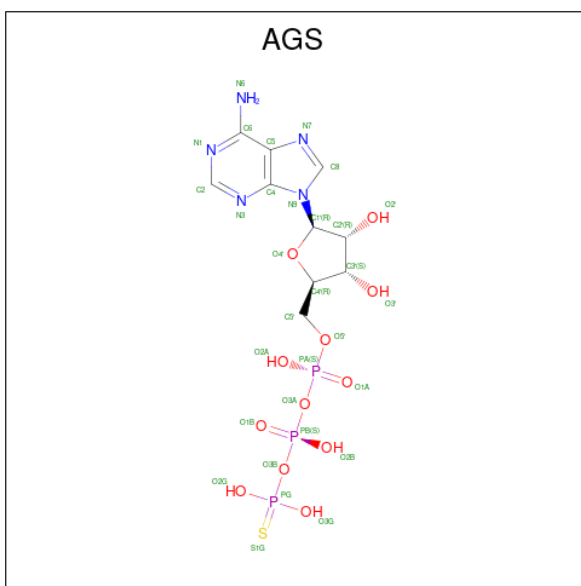
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Chain	Residue	Modelled	Actual	Comment	Reference
E	678	ALA	GLU	engineered mutation	UNP P63284
E	858	HIS	-	expression tag	UNP P63284
F	279	ALA	GLU	engineered mutation	UNP P63284
F	476	CYS	LYS	engineered mutation	UNP P63284
F	678	ALA	GLU	engineered mutation	UNP P63284
F	858	HIS	-	expression tag	UNP P63284

- 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 (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
3	A	1	31	10	5	12	3	1	0
3	B	1	62	20	10	24	6	2	0
3	B	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0
3	C	1	62	20	10	24	6	2	0

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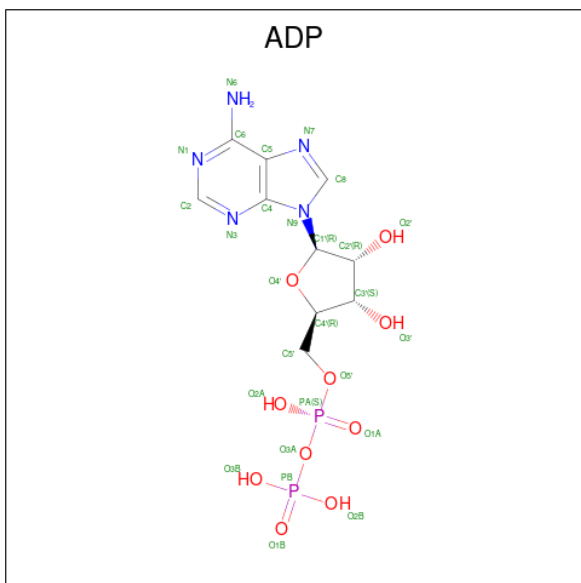
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Mol	Chain	Residues	Atoms						AltConf
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	D	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	E	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
3	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	2	Total	Mg	0
			2	2	
4	C	2	Total	Mg	0
			2	2	
4	D	2	Total	Mg	0
			2	2	
4	E	1	Total	Mg	0
			1	1	

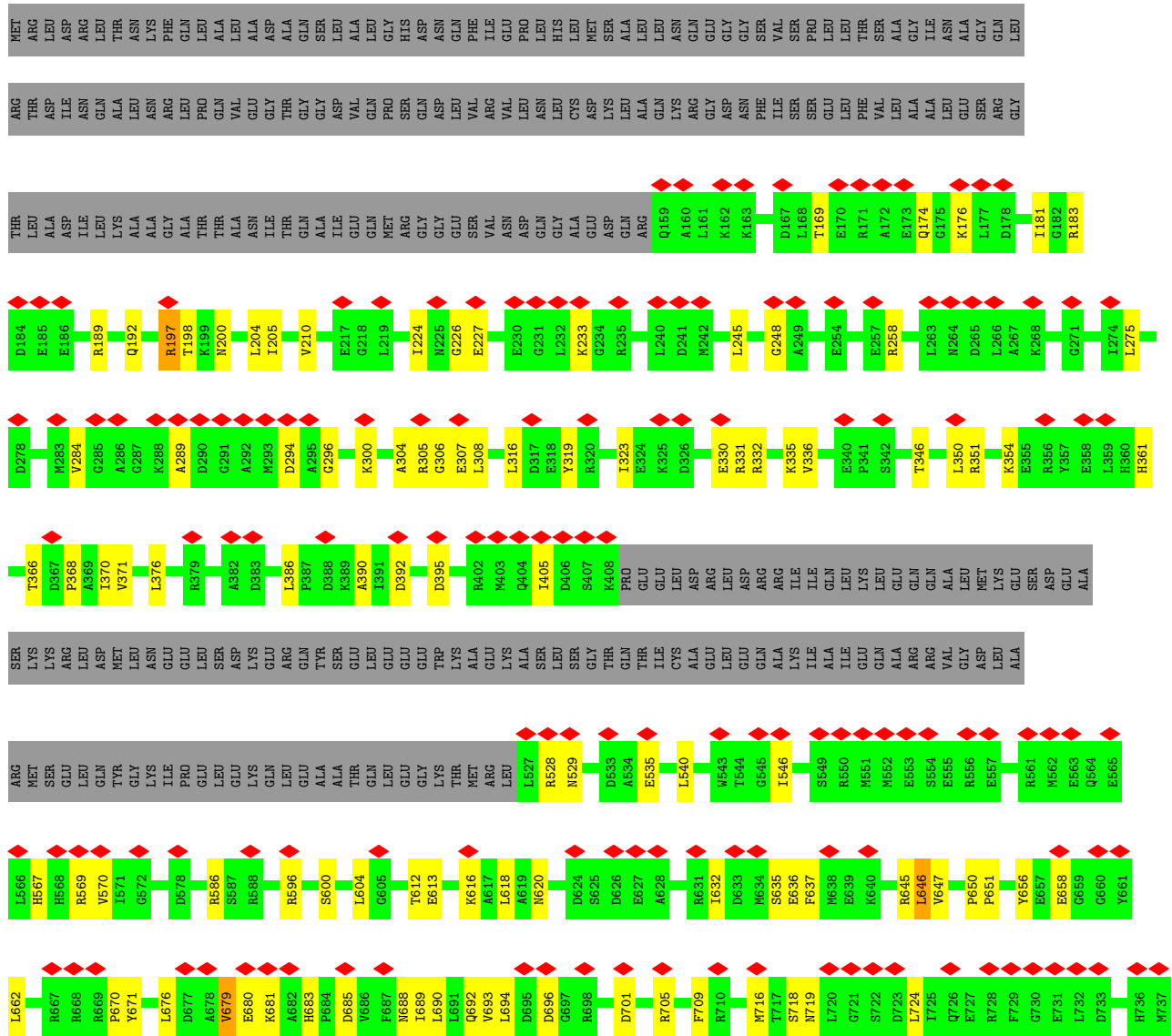
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

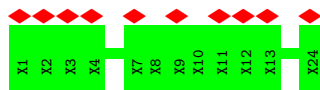


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	F	1	27	10	5	10	2	0



● Molecule 1: Chaperone protein ClpB





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39739	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	0.090	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	302.4, 302.4, 302.4	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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: AGS, MG, ADP

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	0.39	0/4537	0.54	0/6120
1	B	0.57	0/4630	0.65	2/6249 (0.0%)
1	C	0.59	0/5047	0.67	3/6805 (0.0%)
1	D	0.56	0/5022	0.65	1/6769 (0.0%)
1	E	0.46	0/5022	0.61	2/6769 (0.0%)
1	F	0.29	0/4561	0.50	1/6152 (0.0%)
All	All	0.49	0/28819	0.61	9/38864 (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	C	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	646	LEU	CA-CB-CG	6.93	131.25	115.30
1	C	646	LEU	CA-CB-CG	6.89	131.14	115.30
1	B	316	LEU	CA-CB-CG	6.76	130.86	115.30
1	B	646	LEU	CA-CB-CG	6.76	130.84	115.30
1	E	646	LEU	CA-CB-CG	6.19	129.54	115.30
1	C	618	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	F	766	LEU	CA-CB-CG	5.33	127.55	115.30
1	E	559	LEU	CA-CB-CG	5.20	127.25	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ALA	C-N-CA	-5.07	111.66	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	ASP	Peptide
1	C	293	MET	Peptide

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	4472	0	4530	45	0
1	B	4562	0	4622	88	0
1	C	4976	0	5029	83	0
1	D	4952	0	5013	79	0
1	E	4952	0	5011	51	0
1	F	4496	0	4550	42	0
2	S	120	0	29	0	0
3	A	31	0	12	1	0
3	B	62	0	23	6	0
3	C	62	0	24	6	0
3	D	62	0	24	2	0
3	E	62	0	23	4	0
3	F	31	0	12	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
5	F	27	0	12	1	0
All	All	28875	0	28914	341	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 6.

All (341) 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:E:561:ARG:O	1:E:565:GLU:HB2	1.77	0.84
1:A:296:GLY:O	1:A:300:LYS:HB2	1.84	0.78
1:B:227:GLU:HB3	1:C:417:ARG:HH22	1.47	0.77
1:B:692:GLN:HE22	1:C:636:GLU:HG3	1.50	0.77
1:C:227:GLU:HB3	1:D:417:ARG:HH22	1.51	0.75
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.52	0.73
1:D:692:GLN:HE22	1:E:636:GLU:HG3	1.54	0.72
1:A:366:THR:HG22	1:A:368:PRO:HD2	1.74	0.69
1:F:366:THR:HG22	1:F:368:PRO:HD2	1.75	0.68
1:A:651:PRO:HD2	1:B:645:ARG:HA	1.74	0.68
1:B:331:ARG:NH1	3:C:1001:AGS:S1G	2.67	0.68
1:D:366:THR:HG22	1:D:368:PRO:HD2	1.76	0.67
1:B:546:ILE:HG13	1:B:671:TYR:HB2	1.77	0.67
1:C:366:THR:HG22	1:C:368:PRO:HD2	1.76	0.67
1:C:692:GLN:NE2	1:D:635:SER:OG	2.28	0.67
1:D:227:GLU:HB3	1:E:417:ARG:HH22	1.60	0.66
1:B:332:ARG:NH2	3:C:1001:AGS:S1G	2.69	0.65
1:D:684:PRO:HA	1:D:687:PHE:HD2	1.61	0.65
1:C:702:GLY:HA2	1:D:645:ARG:HE	1.62	0.65
1:D:692:GLN:NE2	1:E:635:SER:OG	2.29	0.64
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.80	0.63
1:B:679:VAL:HG12	1:B:718:SER:HB2	1.79	0.63
1:A:752:GLU:OE2	1:B:719:ASN:ND2	2.32	0.63
1:F:625:SER:HB3	1:F:628:ALA:HB2	1.81	0.62
1:F:793:ILE:HG12	1:F:844:ILE:HB	1.82	0.62
1:A:692:GLN:HE22	1:B:636:GLU:HG3	1.64	0.61
1:A:688:ASN:HB3	1:B:635:SER:HB2	1.82	0.61
1:D:422:LEU:HD22	1:D:444:LEU:HD11	1.81	0.61
1:A:332:ARG:NH2	3:B:1001:AGS:S1G	2.74	0.61
1:F:248:GLY:H	1:F:258:ARG:HH12	1.49	0.61
1:A:692:GLN:NE2	1:B:635:SER:OG	2.32	0.61
1:B:756:ARG:NH2	3:C:1002:AGS:S1G	2.69	0.61
1:C:680:GLU:OE2	1:C:681:LYS:NZ	2.34	0.60
1:D:793:ILE:HG12	1:D:844:ILE:HB	1.82	0.60
1:B:692:GLN:NE2	1:C:635:SER:OG	2.26	0.60
1:C:651:PRO:HD2	1:D:645:ARG:HA	1.84	0.60
1:B:376:LEU:HB3	1:B:540:LEU:HD22	1.84	0.59
1:F:323:ILE:HG23	1:F:329:LEU:HG	1.84	0.59
1:F:727:GLU:HG2	1:F:728:ARG:HG3	1.82	0.59
1:C:832:GLN:HB3	1:C:838:LEU:HD13	1.84	0.59
1:C:404:GLN:NE2	1:C:410:GLU:OE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1001:AGS:H8	3:C:1001:AGS:H5'1	1.84	0.58
1:B:815:ARG:NH1	3:B:1002:AGS:S1G	2.74	0.58
1:B:632:ILE:HD11	1:B:662:LEU:HD13	1.84	0.58
1:F:281:HIS:HB2	1:F:322:TYR:HD2	1.69	0.58
1:B:366:THR:HG22	1:B:368:PRO:HD2	1.86	0.58
1:C:328:ALA:O	1:C:332:ARG:NH2	2.37	0.57
1:F:786:LEU:HD13	1:F:793:ILE:HD12	1.87	0.57
1:D:832:GLN:HB3	1:D:838:LEU:HD13	1.86	0.57
1:B:351:ARG:NH1	1:C:425:GLU:OE2	2.38	0.57
1:B:183:ARG:NH2	1:B:210:VAL:O	2.38	0.57
1:F:631:ARG:HG3	1:F:675:LEU:HD23	1.87	0.56
1:D:376:LEU:HB3	1:D:540:LEU:HD22	1.85	0.56
1:E:565:GLU:OE2	1:E:568:HIS:ND1	2.38	0.56
1:C:679:VAL:HG12	1:C:718:SER:HB2	1.86	0.56
1:C:771:ILE:HG23	1:C:817:LEU:HD22	1.87	0.56
1:B:680:GLU:OE2	1:B:681:LYS:NZ	2.38	0.56
1:D:243:GLY:O	1:D:247:ALA:HB2	2.05	0.56
1:E:832:GLN:HB3	1:E:838:LEU:HD13	1.88	0.56
1:D:197:ARG:HH12	1:E:356:ARG:HG3	1.70	0.56
1:D:354:LYS:HB2	1:D:370:ILE:HD11	1.87	0.56
1:D:637:PHE:HE1	1:D:645:ARG:HD2	1.71	0.56
1:D:317:ASP:OD1	1:E:668:ARG:NH2	2.39	0.56
1:D:200:ASN:ND2	1:D:306:GLY:O	2.39	0.55
1:C:351:ARG:NH1	1:D:425:GLU:OE2	2.39	0.55
1:C:422:LEU:HD22	1:C:444:LEU:HD11	1.88	0.55
1:C:546:ILE:HG13	1:C:671:TYR:HB2	1.88	0.55
1:C:815:ARG:NH1	3:C:1002:AGS:S1G	2.77	0.55
1:E:346:THR:HG21	1:E:386:LEU:HD22	1.87	0.55
1:E:724:LEU:HD21	1:E:740:LEU:HG	1.89	0.55
1:B:688:ASN:HB3	1:C:635:SER:HB2	1.89	0.54
1:D:646:LEU:HD12	1:D:647:VAL:HG23	1.89	0.54
1:C:243:GLY:O	1:C:247:ALA:HB2	2.07	0.54
1:B:637:PHE:HE2	1:B:646:LEU:HD23	1.71	0.54
1:F:849:ASN:HD22	1:F:852:ARG:HB2	1.72	0.54
1:B:192:GLN:OE1	1:C:542:ARG:NH2	2.40	0.54
1:B:656:TYR:OH	1:C:658:GLU:OE1	2.22	0.54
1:B:613:GLU:HG3	3:B:1002:AGS:H2'	1.88	0.54
1:F:766:LEU:HB2	1:F:770:HIS:HB2	1.89	0.54
1:E:361:HIS:NE2	1:E:395:ASP:OD1	2.36	0.54
1:F:361:HIS:NE2	1:F:395:ASP:OD1	2.41	0.54
1:A:305:ARG:NH1	1:A:307:GLU:OE2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:ASP:OD2	1:C:631:ARG:NH2	2.41	0.53
1:C:248:GLY:HA3	1:C:258:ARG:HH22	1.72	0.53
1:F:539:VAL:HG22	1:F:542:ARG:HH22	1.73	0.53
1:D:651:PRO:HD2	1:E:645:ARG:HA	1.89	0.53
1:E:554:SER:O	1:E:558:LYS:HB2	2.09	0.53
1:E:174:GLN:OE1	1:E:176:LYS:NZ	2.41	0.53
1:A:645:ARG:HH11	1:F:640:LYS:HD2	1.73	0.53
1:B:596:ARG:NH2	1:B:756:ARG:O	2.41	0.53
1:B:528:ARG:NH2	1:B:535:GLU:OE2	2.41	0.53
1:C:771:ILE:HD12	1:C:808:TYR:HD1	1.73	0.53
1:F:703:GLN:OE1	1:F:705:ARG:NH2	2.42	0.52
1:C:696:ASP:OD2	1:D:631:ARG:NH2	2.40	0.52
3:D:902:AGS:O2B	3:D:902:AGS:O2A	2.27	0.52
1:B:693:VAL:HG13	1:B:709:PHE:HD2	1.75	0.52
1:C:611:LYS:NZ	1:C:718:SER:O	2.31	0.52
1:C:698:ARG:NH1	1:D:633:ASP:OD2	2.42	0.52
1:D:803:LEU:HD11	1:D:825:ILE:HD11	1.92	0.52
1:D:248:GLY:HA3	1:D:258:ARG:HH22	1.74	0.52
1:E:296:GLY:O	1:E:300:LYS:HB3	2.09	0.52
1:E:193:VAL:HG22	1:E:196:ARG:HH12	1.74	0.52
1:E:613:GLU:HG3	3:E:1002:AGS:H2'	1.92	0.52
1:A:642:SER:HA	1:A:645:ARG:HE	1.74	0.52
1:C:688:ASN:HB3	1:D:635:SER:HB2	1.91	0.52
1:C:690:LEU:HA	1:C:693:VAL:HB	1.91	0.52
1:E:636:GLU:O	1:E:645:ARG:NH1	2.43	0.52
1:F:821:ILE:HG23	1:F:825:ILE:HD12	1.91	0.52
1:B:651:PRO:HD2	1:C:645:ARG:HA	1.91	0.51
1:C:606:PRO:HG2	1:C:609:VAL:HG11	1.92	0.51
1:F:554:SER:O	1:F:558:LYS:HB2	2.09	0.51
1:F:646:LEU:HA	1:F:661:TYR:HB2	1.92	0.51
1:C:738:LYS:O	1:C:742:LEU:HB2	2.11	0.51
1:E:226:GLY:O	1:E:233:LYS:NZ	2.43	0.51
1:F:683:HIS:ND1	1:F:685:ASP:OD1	2.41	0.51
1:B:197:ARG:HD3	1:B:198:THR:HG23	1.92	0.51
1:A:316:LEU:HD11	1:A:320:ARG:HH11	1.74	0.51
1:A:599:GLY:HA3	1:A:713:VAL:HG13	1.92	0.51
1:A:728:ARG:HB3	1:A:732:LEU:HD12	1.92	0.51
1:B:296:GLY:O	1:B:300:LYS:HB2	2.10	0.51
1:B:771:ILE:HG23	1:B:817:LEU:HD22	1.93	0.51
1:C:422:LEU:HB2	1:C:448:LEU:HD13	1.92	0.51
1:B:827:ASN:O	1:B:831:GLN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:648:GLY:HA3	1:F:701:ASP:HB2	1.93	0.51
1:B:701:ASP:O	1:C:645:ARG:NH2	2.43	0.50
1:B:690:LEU:HA	1:B:693:VAL:HB	1.93	0.50
1:A:368:PRO:HA	1:A:371:VAL:HG12	1.94	0.50
1:C:350:LEU:HD11	1:C:390:ALA:HB1	1.93	0.50
1:D:724:LEU:HD21	1:D:740:LEU:HG	1.93	0.50
3:E:1002:AGS:O2A	3:E:1002:AGS:O1B	2.30	0.50
1:D:569:ARG:HH11	1:D:620:ASN:HD22	1.59	0.50
3:F:1002:AGS:O1A	3:F:1002:AGS:O2G	2.30	0.50
1:A:726:GLN:HE22	1:A:811:VAL:HA	1.77	0.50
1:B:226:GLY:O	1:B:233:LYS:NZ	2.44	0.50
1:C:333:PHE:O	1:D:384:ARG:NH2	2.42	0.50
1:E:582:ASN:OD1	1:E:585:ARG:NH2	2.45	0.49
3:B:1002:AGS:O2G	3:B:1002:AGS:O1B	2.30	0.49
1:D:240:LEU:HB2	1:D:275:LEU:HD11	1.93	0.49
1:A:331:ARG:NE	3:B:1001:AGS:S1G	2.78	0.49
1:D:240:LEU:HB3	1:D:277:ILE:HG12	1.94	0.49
1:D:422:LEU:HB2	1:D:448:LEU:HD13	1.95	0.49
1:D:546:ILE:HG13	1:D:671:TYR:HB2	1.93	0.49
1:C:610:GLY:HA2	1:C:613:GLU:HB2	1.95	0.49
1:B:849:ASN:HB2	1:B:852:ARG:H	1.77	0.49
1:B:305:ARG:NH1	1:B:307:GLU:OE1	2.45	0.49
1:B:803:LEU:HD13	1:B:821:ILE:HG12	1.95	0.49
1:C:361:HIS:NE2	1:C:395:ASP:OD1	2.44	0.49
1:A:795:ILE:HG13	1:A:846:LEU:HB2	1.95	0.49
1:D:350:LEU:HD11	1:D:390:ALA:HB1	1.93	0.49
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.94	0.49
1:C:286:ALA:HB3	1:C:295:ALA:HB3	1.94	0.49
1:C:695:ASP:HB2	1:C:756:ARG:HH11	1.78	0.49
1:E:236:ARG:HB2	1:E:273:VAL:HG22	1.94	0.49
1:F:585:ARG:O	1:F:589:ALA:HB2	2.13	0.49
1:A:252:ARG:HD3	1:B:289:ALA:HB2	1.94	0.48
1:D:401:ILE:HD11	1:D:535:GLU:HG3	1.94	0.48
1:E:404:GLN:NE2	1:E:410:GLU:OE2	2.45	0.48
1:E:703:GLN:OE1	1:E:705:ARG:NH1	2.40	0.48
1:B:757:ILE:O	1:C:819:ARG:NH1	2.46	0.48
1:C:533:ASP:OD1	1:C:533:ASP:N	2.46	0.48
1:C:612:THR:HG22	1:C:616:LYS:HE3	1.94	0.48
1:C:703:GLN:OE1	1:C:705:ARG:NH1	2.34	0.48
1:C:809:ASP:OD1	1:C:809:ASP:N	2.43	0.48
1:B:354:LYS:HD3	1:B:370:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:771:ILE:HG23	1:D:817:LEU:HD22	1.96	0.48
1:B:676:LEU:HB2	1:B:716:MET:HG2	1.94	0.48
1:E:169:THR:HB	1:E:224:ILE:HD11	1.95	0.48
1:E:803:LEU:HD11	1:E:825:ILE:HD11	1.95	0.48
1:C:559:LEU:HD11	1:C:588:ARG:HG3	1.96	0.48
1:C:600:SER:HB2	1:C:694:LEU:HD22	1.96	0.48
3:B:1002:AGS:O2A	3:B:1002:AGS:O2B	2.31	0.48
3:C:1001:AGS:O2A	3:C:1001:AGS:O2B	2.32	0.48
1:F:631:ARG:NH2	3:F:1002:AGS:O3G	2.44	0.48
1:A:240:LEU:HD22	1:A:275:LEU:HD21	1.95	0.47
1:D:368:PRO:HA	1:D:371:VAL:HG12	1.96	0.47
1:D:688:ASN:HB3	1:E:635:SER:HB2	1.96	0.47
1:E:683:HIS:ND1	1:E:685:ASP:OD1	2.43	0.47
1:A:646:LEU:HA	1:A:661:TYR:HB3	1.97	0.47
1:C:596:ARG:NH2	1:C:756:ARG:O	2.45	0.47
1:A:344:GLU:HA	1:A:347:ILE:HD12	1.95	0.47
1:A:695:ASP:HB2	1:A:756:ARG:HD2	1.97	0.47
1:C:200:ASN:ND2	1:C:306:GLY:O	2.47	0.47
1:B:586:ARG:NH1	1:C:822:GLN:HE21	2.13	0.47
1:E:631:ARG:HG3	1:E:675:LEU:HD23	1.96	0.47
1:B:275:LEU:HD22	1:B:308:LEU:HD11	1.97	0.46
1:E:300:LYS:HG3	1:E:329:LEU:HD22	1.97	0.46
1:A:786:LEU:HD13	1:A:793:ILE:HD12	1.97	0.46
1:D:462:TRP:HD1	1:D:527:LEU:HD21	1.80	0.46
1:F:174:GLN:OE1	1:F:176:LYS:NZ	2.43	0.46
1:A:573:GLN:NE2	1:A:764:HIS:O	2.47	0.46
1:A:586:ARG:NH1	1:B:822:GLN:HE21	2.13	0.46
1:C:656:TYR:OH	1:D:658:GLU:OE1	2.26	0.46
1:F:368:PRO:HA	1:F:371:VAL:HG12	1.98	0.46
1:D:619:ALA:O	1:D:623:PHE:HB2	2.15	0.46
1:B:181:ILE:HG23	1:C:421:GLN:HE22	1.80	0.46
1:C:586:ARG:CZ	1:D:822:GLN:HE21	2.28	0.46
1:A:560:LEU:HD11	1:B:835:SER:HA	1.97	0.46
1:B:169:THR:HB	1:B:224:ILE:HD11	1.98	0.46
1:D:361:HIS:NE2	1:D:395:ASP:OD1	2.39	0.46
1:E:303:LEU:HD22	1:E:329:LEU:HD21	1.98	0.46
1:E:689:ILE:HG23	1:E:699:LEU:HD11	1.97	0.46
1:A:196:ARG:NH2	1:B:392:ASP:OD1	2.38	0.45
1:B:200:ASN:ND2	1:B:306:GLY:O	2.49	0.45
1:B:604:LEU:O	1:B:763:PHE:N	2.46	0.45
1:F:635:SER:HA	1:F:681:LYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:634:MET:HG3	1:D:679:VAL:HG23	1.97	0.45
1:F:664:GLU:OE1	1:F:667:ARG:NE	2.43	0.45
1:C:405:ILE:HD11	1:C:529:ASN:HA	1.97	0.45
1:D:169:THR:HB	1:D:224:ILE:HD11	1.98	0.45
1:B:724:LEU:HD21	1:B:740:LEU:HG	1.98	0.45
1:D:197:ARG:HD3	1:D:198:THR:HG23	1.97	0.45
1:D:586:ARG:CZ	1:E:822:GLN:HE21	2.30	0.45
1:D:299:LEU:HB3	1:D:303:LEU:HD13	1.98	0.45
1:A:584:ILE:HD11	1:A:618:LEU:HD11	1.98	0.45
1:B:405:ILE:HD11	1:B:529:ASN:HA	1.98	0.45
1:B:618:LEU:HA	1:B:618:LEU:HD23	1.71	0.45
1:C:239:ALA:HA	1:C:276:PHE:HB3	1.98	0.45
1:D:161:LEU:O	1:D:165:THR:OG1	2.31	0.45
1:E:605:GLY:HA3	1:E:763:PHE:HB2	1.99	0.45
1:A:304:ALA:HB2	1:A:332:ARG:HE	1.82	0.45
1:B:600:SER:HB2	1:B:694:LEU:HD22	1.98	0.45
1:B:692:GLN:H	1:B:692:GLN:HG3	1.54	0.45
1:B:809:ASP:OD1	1:B:809:ASP:N	2.49	0.45
1:C:688:ASN:HA	1:C:691:LEU:HG	1.98	0.45
1:F:698:ARG:HA	1:F:708:ASP:HA	1.99	0.45
1:B:646:LEU:HD11	1:B:689:ILE:HG21	1.97	0.45
1:C:188:ARG:HH21	1:D:413:ASP:HB3	1.81	0.45
1:B:174:GLN:OE1	1:B:176:LYS:NZ	2.42	0.44
1:C:663:THR:HB	1:C:707:VAL:HG21	1.99	0.44
1:A:809:ASP:OD1	1:A:809:ASP:N	2.50	0.44
1:B:248:GLY:H	1:B:258:ARG:HH12	1.66	0.44
1:B:683:HIS:ND1	1:B:685:ASP:OD1	2.46	0.44
1:C:462:TRP:HD1	1:C:527:LEU:HD21	1.82	0.44
1:D:533:ASP:OD1	1:D:533:ASP:N	2.50	0.44
1:D:332:ARG:NH2	3:E:1001:AGS:S1G	2.85	0.44
1:C:376:LEU:HB3	1:C:540:LEU:HD22	1.99	0.44
1:D:611:LYS:NZ	1:D:718:SER:O	2.38	0.44
1:F:172:ALA:HB2	1:F:177:LEU:HD12	2.00	0.44
1:C:317:ASP:OD1	1:D:668:ARG:NH2	2.50	0.44
1:D:331:ARG:NH1	3:E:1001:AGS:S1G	2.88	0.44
1:A:786:LEU:O	1:A:790:GLY:N	2.49	0.44
3:A:1001:AGS:O2G	3:A:1001:AGS:O1B	2.36	0.44
1:B:650:PRO:HB3	1:C:645:ARG:HB3	2.00	0.44
1:B:204:LEU:HD23	1:B:336:VAL:HB	1.98	0.43
1:B:361:HIS:NE2	1:B:395:ASP:OD1	2.43	0.43
1:C:248:GLY:H	1:C:258:ARG:HH12	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ASP:OD2	1:D:815:ARG:NH2	2.50	0.43
1:D:612:THR:HG22	1:D:616:LYS:HE3	1.99	0.43
1:F:350:LEU:HD11	1:F:390:ALA:HB1	1.99	0.43
1:C:192:GLN:HE22	1:D:542:ARG:HH12	1.65	0.43
1:D:680:GLU:OE2	1:D:681:LYS:NZ	2.51	0.43
1:D:721:GLY:HA3	1:D:741:VAL:HG23	2.00	0.43
1:E:771:ILE:HG23	1:E:817:LEU:HD22	2.01	0.43
1:F:845:ARG:HH21	1:F:858:HIS:CD2	2.36	0.43
1:B:319:TYR:OH	1:B:330:GLU:OE2	2.36	0.43
1:E:287:GLY:N	1:E:294:ASP:OD2	2.52	0.43
1:B:646:LEU:HD12	1:B:647:VAL:HG13	2.00	0.43
1:D:698:ARG:NH1	1:E:633:ASP:OD2	2.52	0.43
1:F:738:LYS:NZ	1:F:759:GLU:OE2	2.51	0.43
1:B:718:SER:OG	1:B:719:ASN:N	2.51	0.43
1:D:402:ARG:HA	1:D:402:ARG:HD2	1.81	0.43
1:A:693:VAL:HG13	1:A:709:PHE:HD2	1.84	0.43
1:C:401:ILE:HG13	1:C:531:VAL:HG22	1.99	0.43
1:D:771:ILE:HD12	1:D:808:TYR:HD1	1.84	0.43
1:E:197:ARG:HH12	1:F:356:ARG:HG3	1.83	0.43
1:F:674:ILE:HB	1:F:714:VAL:HA	2.01	0.43
1:C:695:ASP:HB2	1:C:756:ARG:HD2	2.01	0.43
1:A:612:THR:OG1	1:A:815:ARG:NH2	2.52	0.42
1:B:685:ASP:HB3	1:B:750:ARG:HH22	1.83	0.42
1:D:181:ILE:HD11	1:D:352:GLY:HA3	2.00	0.42
1:E:612:THR:HG22	1:E:616:LYS:HE3	2.00	0.42
1:E:177:LEU:HD13	1:E:217:GLU:HB3	2.01	0.42
1:E:302:ALA:HA	1:E:305:ARG:HB2	1.99	0.42
1:C:192:GLN:OE1	1:D:542:ARG:NH2	2.52	0.42
1:C:683:HIS:HB3	1:C:686:VAL:HG23	2.02	0.42
1:B:849:ASN:HD22	1:B:852:ARG:HB2	1.83	0.42
1:E:663:THR:HB	1:E:707:VAL:HG21	2.02	0.42
1:B:205:ILE:HD12	1:B:335:LYS:HG2	2.01	0.42
1:B:612:THR:HG22	1:B:616:LYS:HE3	2.00	0.42
1:C:196:ARG:NH2	1:D:392:ASP:OD1	2.45	0.42
1:E:293:MET:N	1:E:297:ASN:OD1	2.52	0.42
1:E:294:ASP:OD1	1:E:294:ASP:N	2.53	0.42
1:A:600:SER:HB2	1:A:694:LEU:HD22	2.01	0.42
1:B:676:LEU:HD22	1:B:690:LEU:HD11	2.01	0.42
1:A:663:THR:HB	1:A:707:VAL:HG21	2.01	0.42
1:C:161:LEU:O	1:C:165:THR:OG1	2.27	0.42
1:D:795:ILE:HG13	1:D:846:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:211:GLY:N	5:F:1001:ADP:O1A	2.42	0.42
1:D:600:SER:HB2	1:D:694:LEU:HD22	2.02	0.42
1:F:326:ASP:HB3	1:F:329:LEU:HB3	2.02	0.42
1:C:683:HIS:ND1	1:C:685:ASP:OD1	2.48	0.42
1:D:317:ASP:OD1	1:D:320:ARG:NH1	2.53	0.42
1:E:286:ALA:N	1:E:294:ASP:OD2	2.53	0.42
1:F:744:VAL:HA	1:F:747:HIS:HD2	1.84	0.42
1:B:569:ARG:HH11	1:B:620:ASN:HD22	1.68	0.41
1:C:169:THR:HB	1:C:224:ILE:HD11	2.02	0.41
1:B:567:HIS:ND1	1:B:570:VAL:O	2.54	0.41
1:D:637:PHE:CD1	1:D:642:SER:HB3	2.55	0.41
1:D:809:ASP:OD1	1:D:809:ASP:N	2.52	0.41
1:B:304:ALA:HB2	1:B:332:ARG:NE	2.35	0.41
1:C:240:LEU:HD11	1:C:245:LEU:HD11	2.02	0.41
1:D:192:GLN:OE1	1:E:542:ARG:NH2	2.54	0.41
1:D:596:ARG:NH2	1:D:756:ARG:O	2.52	0.41
1:D:632:ILE:HD11	1:D:662:LEU:HD13	2.02	0.41
1:D:663:THR:HB	1:D:707:VAL:HG21	2.02	0.41
1:A:628:ALA:HB1	1:A:669:ARG:HH21	1.84	0.41
1:A:778:GLN:HA	1:A:781:ARG:HG2	2.02	0.41
1:F:328:ALA:HA	1:F:331:ARG:HG2	2.01	0.41
1:B:294:ASP:N	1:B:294:ASP:OD1	2.53	0.41
1:B:350:LEU:HD11	1:B:390:ALA:HB1	2.01	0.41
1:E:570:VAL:HG21	1:E:614:LEU:HA	2.02	0.41
1:F:619:ALA:HB1	1:F:628:ALA:HB3	2.03	0.41
1:A:634:MET:HE1	1:A:686:VAL:HG11	2.01	0.41
1:B:245:LEU:O	1:B:258:ARG:NH1	2.47	0.41
1:C:724:LEU:HD21	1:C:740:LEU:HG	2.02	0.41
1:D:212:LYS:HE2	1:D:212:LYS:HB2	1.91	0.41
1:A:299:LEU:HB3	1:A:303:LEU:HD13	2.01	0.41
1:B:189:ARG:NE	1:C:396:GLU:OE2	2.53	0.41
1:B:368:PRO:HA	1:B:371:VAL:HG12	2.01	0.41
1:C:720:LEU:HD23	1:C:720:LEU:HA	1.90	0.41
1:D:204:LEU:HD23	1:D:336:VAL:HB	2.02	0.41
1:E:679:VAL:HG12	1:E:718:SER:HB2	2.03	0.41
1:B:346:THR:HG21	1:B:386:LEU:HD22	2.03	0.41
1:B:546:ILE:HD11	1:B:670:PRO:HB2	2.03	0.41
1:F:226:GLY:O	1:F:233:LYS:NZ	2.54	0.41
1:A:688:ASN:HD21	1:A:750:ARG:HH12	1.69	0.40
1:C:183:ARG:NH2	1:C:210:VAL:O	2.53	0.40
1:E:558:LYS:HG2	1:E:621:PHE:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:LEU:HD23	1:B:786:LEU:HA	1.87	0.40
3:D:901:AGS:O2A	3:D:901:AGS:O2B	2.39	0.40
1:F:806:ASN:HB3	1:F:824:GLN:HE22	1.85	0.40
1:A:294:ASP:OD1	1:A:294:ASP:N	2.55	0.40
1:A:376:LEU:HB3	1:A:540:LEU:HD22	2.02	0.40
1:E:401:ILE:HD13	1:E:401:ILE:HA	1.93	0.40
1:F:791:TYR:HE1	1:F:840:PRO:HG3	1.86	0.40
1:A:632:ILE:HG12	1:A:661:TYR:HE2	1.87	0.40
1:A:656:TYR:OH	1:B:658:GLU:OE1	2.26	0.40
1:B:284:VAL:HG21	1:B:323:ILE:HG12	2.03	0.40
1:E:296:GLY:O	1:E:300:LYS:CB	2.69	0.40
1:B:692:GLN:NE2	1:C:636:GLU:HG3	2.28	0.40
1:C:809:ASP:HA	1:C:810:PRO:HD3	1.82	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	560/858 (65%)	522 (93%)	38 (7%)	0	100	100
1	B	578/858 (67%)	542 (94%)	36 (6%)	0	100	100
1	C	624/858 (73%)	584 (94%)	40 (6%)	0	100	100
1	D	617/858 (72%)	581 (94%)	36 (6%)	0	100	100
1	E	617/858 (72%)	569 (92%)	48 (8%)	0	100	100
1	F	565/858 (66%)	523 (93%)	42 (7%)	0	100	100
All	All	3561/5148 (69%)	3321 (93%)	240 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	473/714 (66%)	473 (100%)	0	100	100
1	B	481/714 (67%)	478 (99%)	3 (1%)	86	91
1	C	527/714 (74%)	524 (99%)	3 (1%)	86	91
1	D	527/714 (74%)	526 (100%)	1 (0%)	93	96
1	E	527/714 (74%)	527 (100%)	0	100	100
1	F	473/714 (66%)	473 (100%)	0	100	100
All	All	3008/4284 (70%)	3001 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	ARG
1	B	679	VAL
1	B	705	ARG
1	C	315	THR
1	C	679	VAL
1	C	819	ARG
1	D	197	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
1	A	692	GLN
1	A	726	GLN
1	A	806	ASN
1	B	281	HIS
1	B	297	ASN
1	B	692	GLN
1	B	849	ASN
1	B	858	HIS
1	C	421	GLN

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Mol	Chain	Res	Type
1	C	692	GLN
1	C	778	GLN
1	C	858	HIS
1	D	692	GLN
1	D	822	GLN
1	E	297	ASN
1	E	309	HIS
1	E	822	GLN
1	E	857	GLN
1	F	281	HIS
1	F	309	HIS
1	F	360	HIS
1	F	573	GLN
1	F	747	HIS
1	F	824	GLN
1	F	831	GLN
1	F	849	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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
5	ADP	F	1001	-	24,29,29	0.93	1 (4%)	29,45,45	1.49	4 (13%)
3	AGS	C	1002	4	26,33,33	0.75	0	26,52,52	1.25	3 (11%)
3	AGS	D	901	4	26,33,33	0.83	1 (3%)	26,52,52	1.16	2 (7%)
3	AGS	F	1002	-	26,33,33	0.74	1 (3%)	26,52,52	1.15	2 (7%)
3	AGS	A	1001	4	26,33,33	0.77	1 (3%)	26,52,52	1.24	3 (11%)
3	AGS	E	1001	-	26,33,33	0.70	0	26,52,52	1.20	2 (7%)
3	AGS	E	1002	4	26,33,33	0.77	0	26,52,52	1.16	3 (11%)
3	AGS	C	1001	4	26,33,33	0.72	1 (3%)	26,52,52	1.32	3 (11%)
3	AGS	D	902	4	26,33,33	0.86	1 (3%)	26,52,52	1.29	3 (11%)
3	AGS	B	1001	4	26,33,33	0.80	0	26,52,52	1.26	2 (7%)
3	AGS	B	1002	4	26,33,33	0.71	0	26,52,52	1.31	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	F	1001	-	-	2/12/32/32	0/3/3/3
3	AGS	C	1002	4	-	0/17/38/38	0/3/3/3
3	AGS	D	901	4	-	5/17/38/38	0/3/3/3
3	AGS	F	1002	-	-	3/17/38/38	0/3/3/3
3	AGS	A	1001	4	-	6/17/38/38	0/3/3/3
3	AGS	E	1001	-	-	4/17/38/38	0/3/3/3
3	AGS	E	1002	4	-	3/17/38/38	0/3/3/3
3	AGS	C	1001	4	-	4/17/38/38	0/3/3/3
3	AGS	D	902	4	-	0/17/38/38	0/3/3/3
3	AGS	B	1001	4	-	2/17/38/38	0/3/3/3
3	AGS	B	1002	4	-	5/17/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1001	ADP	C5-C4	2.38	1.47	1.40
3	D	902	AGS	PG-S1G	2.25	1.95	1.90
3	D	901	AGS	PG-S1G	2.18	1.95	1.90
3	F	1002	AGS	PG-S1G	2.17	1.95	1.90
3	A	1001	AGS	PG-S1G	2.04	1.95	1.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1001	AGS	C8-N7	-2.01	1.31	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1001	AGS	PA-O3A-PB	-5.16	115.14	132.83
3	B	1001	AGS	PA-O3A-PB	-4.92	115.94	132.83
3	A	1001	AGS	PA-O3A-PB	-4.90	116.02	132.83
3	B	1002	AGS	PA-O3A-PB	-4.62	116.97	132.83
3	F	1002	AGS	PA-O3A-PB	-4.46	117.53	132.83
3	E	1001	AGS	PA-O3A-PB	-4.44	117.61	132.83
3	C	1002	AGS	PA-O3A-PB	-4.42	117.65	132.83
3	D	901	AGS	PA-O3A-PB	-4.30	118.06	132.83
3	D	902	AGS	PA-O3A-PB	-4.10	118.76	132.83
5	F	1001	ADP	PA-O3A-PB	-3.78	119.85	132.83
5	F	1001	ADP	C3'-C2'-C1'	3.64	106.45	100.98
5	F	1001	ADP	N3-C2-N1	-3.33	123.47	128.68
3	E	1002	AGS	PA-O3A-PB	-2.73	123.47	132.83
3	E	1002	AGS	C5-C6-N6	2.59	124.29	120.35
3	B	1002	AGS	C5-C6-N6	2.57	124.25	120.35
3	C	1001	AGS	O3G-PG-O3B	2.56	113.18	104.64
3	E	1002	AGS	C3'-C2'-C1'	2.45	104.67	100.98
5	F	1001	ADP	C4-C5-N7	-2.41	106.88	109.40
3	D	901	AGS	C5-C6-N6	2.31	123.86	120.35
3	E	1001	AGS	C5-C6-N6	2.31	123.86	120.35
3	F	1002	AGS	C5-C6-N6	2.30	123.85	120.35
3	C	1001	AGS	C5-C6-N6	2.28	123.82	120.35
3	B	1002	AGS	C3'-C2'-C1'	2.26	104.38	100.98
3	B	1001	AGS	C5-C6-N6	2.22	123.73	120.35
3	A	1001	AGS	C5-C6-N6	2.21	123.72	120.35
3	C	1002	AGS	C5-C6-N6	2.13	123.59	120.35
3	A	1001	AGS	O3G-PG-O3B	2.13	111.73	104.64
3	D	902	AGS	C5-C6-N6	2.11	123.56	120.35
3	D	902	AGS	C3'-C2'-C1'	2.08	104.10	100.98
3	C	1002	AGS	O3G-PG-O3B	2.05	111.48	104.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	AGS	C5'-O5'-PA-O3A
3	B	1001	AGS	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
3	B	1001	AGS	PB-O3B-PG-O3G
3	B	1002	AGS	PB-O3B-PG-O2G
3	B	1002	AGS	PB-O3B-PG-O3G
3	C	1001	AGS	C5'-O5'-PA-O2A
3	C	1001	AGS	O4'-C4'-C5'-O5'
3	E	1001	AGS	C5'-O5'-PA-O3A
5	F	1001	ADP	O4'-C4'-C5'-O5'
3	A	1001	AGS	O4'-C4'-C5'-O5'
5	F	1001	ADP	C3'-C4'-C5'-O5'
3	B	1002	AGS	O4'-C4'-C5'-O5'
3	A	1001	AGS	C3'-C4'-C5'-O5'
3	D	901	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	O4'-C4'-C5'-O5'
3	C	1001	AGS	C5'-O5'-PA-O3A
3	A	1001	AGS	PA-O3A-PB-O1B
3	A	1001	AGS	C5'-O5'-PA-O1A
3	A	1001	AGS	C5'-O5'-PA-O2A
3	C	1001	AGS	C5'-O5'-PA-O1A
3	E	1001	AGS	C5'-O5'-PA-O1A
3	E	1001	AGS	C5'-O5'-PA-O2A
3	B	1002	AGS	PB-O3A-PA-O2A
3	E	1002	AGS	PB-O3A-PA-O2A
3	B	1002	AGS	C3'-C4'-C5'-O5'
3	F	1002	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	PB-O3B-PG-O3G
3	E	1002	AGS	PB-O3A-PA-O1A
3	E	1002	AGS	O4'-C4'-C5'-O5'
3	D	901	AGS	PG-O3B-PB-O2B
3	F	1002	AGS	PA-O3A-PB-O2B
3	D	901	AGS	C5'-O5'-PA-O1A
3	F	1002	AGS	C4'-C5'-O5'-PA

There are no ring outliers.

11 monomers are involved in 22 short contacts:

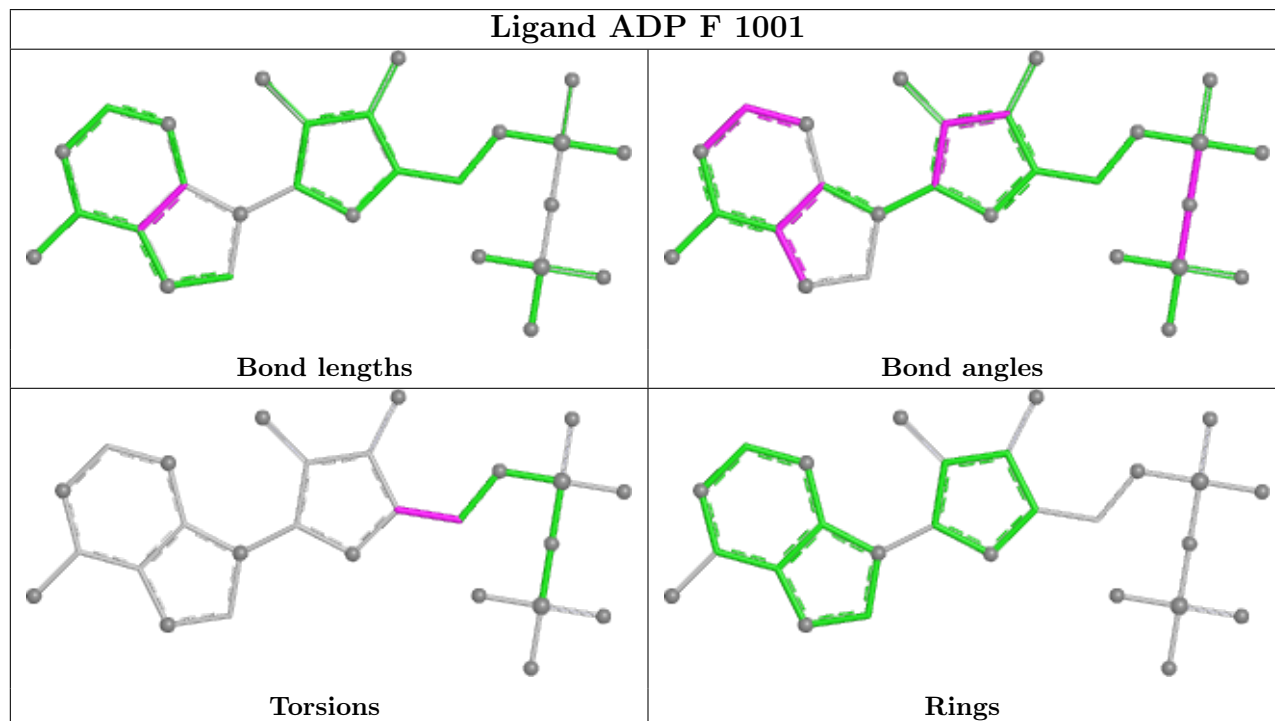
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1001	ADP	1	0
3	C	1002	AGS	2	0
3	D	901	AGS	1	0
3	F	1002	AGS	2	0
3	A	1001	AGS	1	0

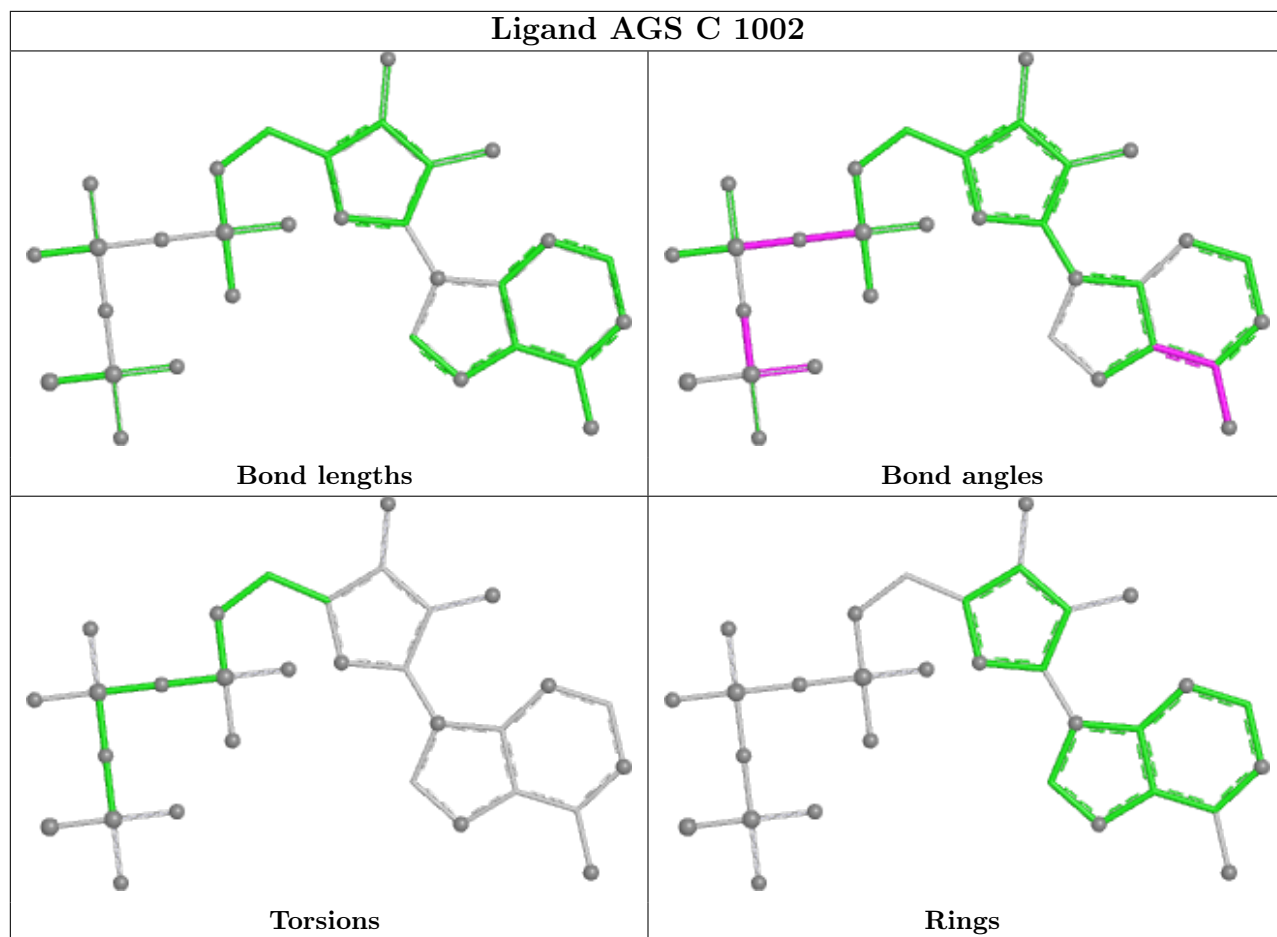
Continued on next page...

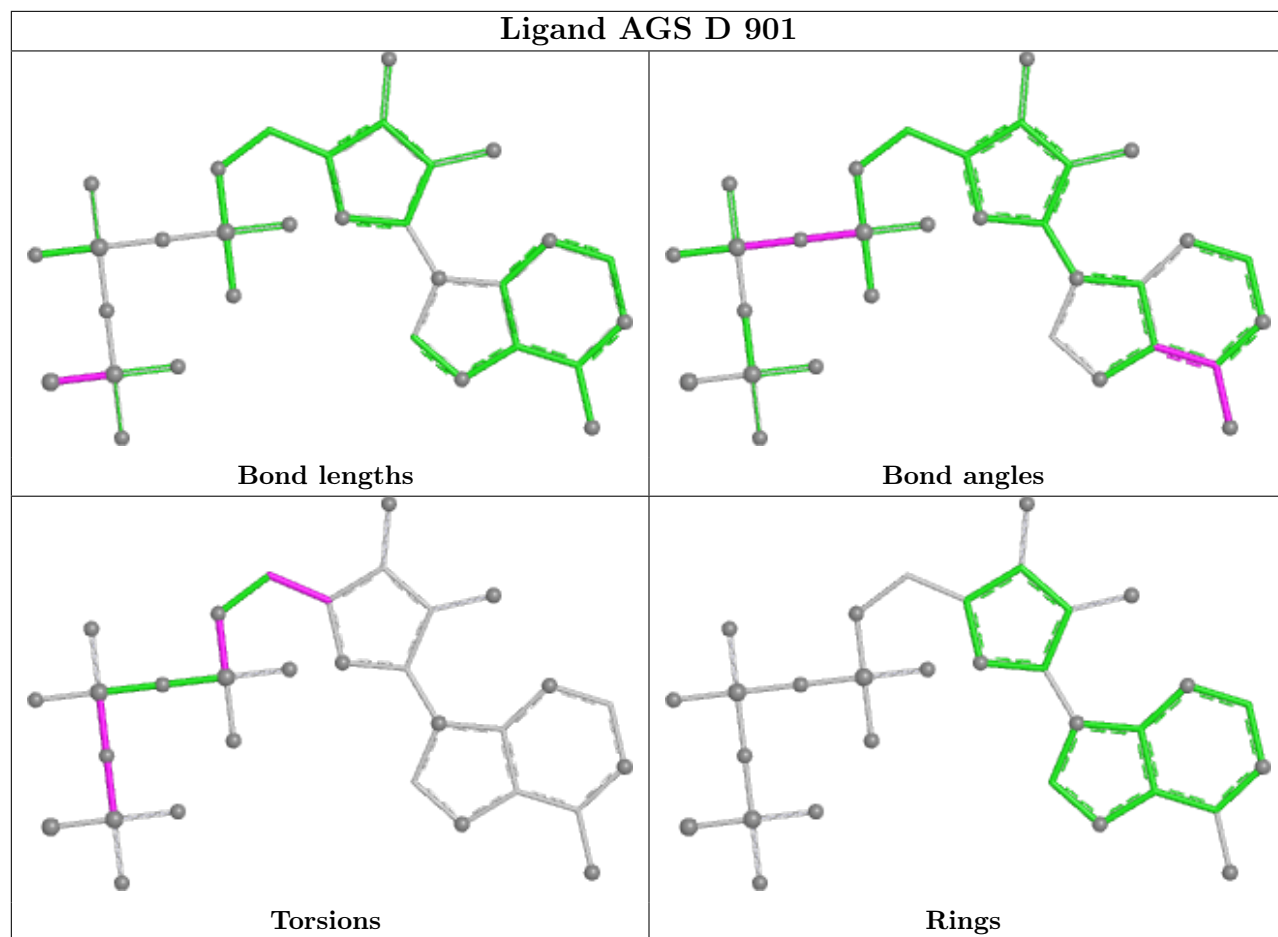
Continued from previous page...

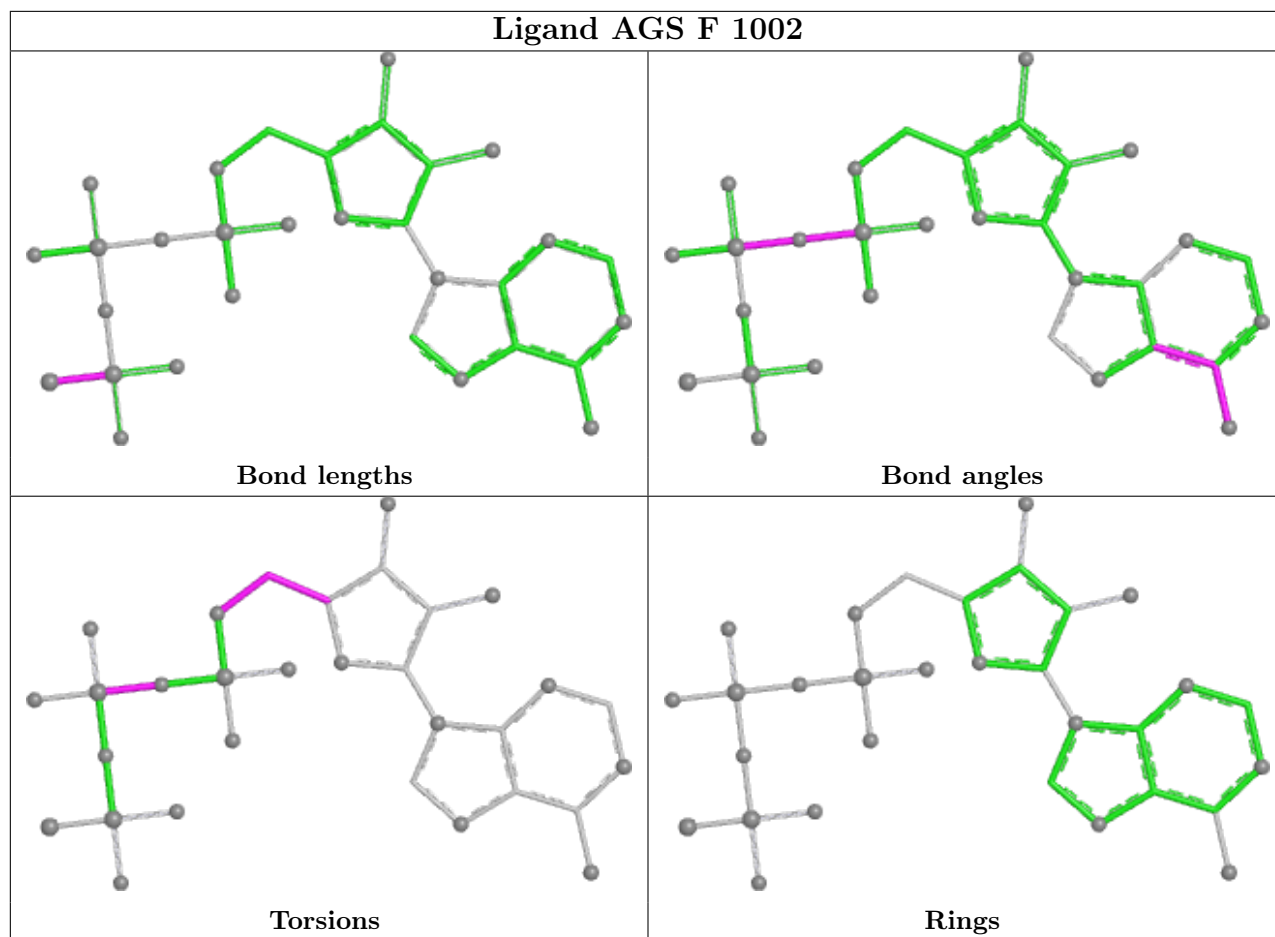
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1001	AGS	2	0
3	E	1002	AGS	2	0
3	C	1001	AGS	4	0
3	D	902	AGS	1	0
3	B	1001	AGS	2	0
3	B	1002	AGS	4	0

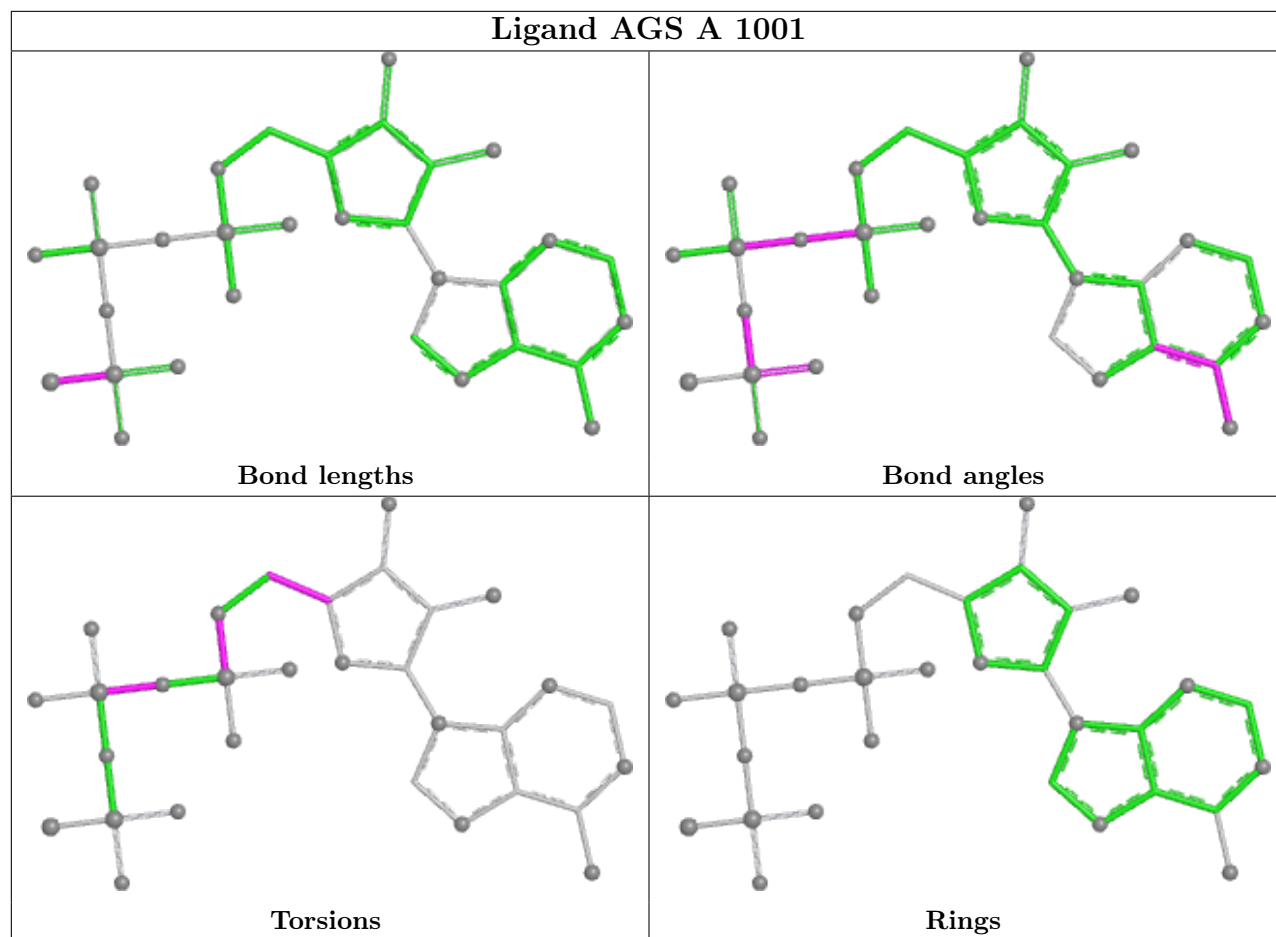
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

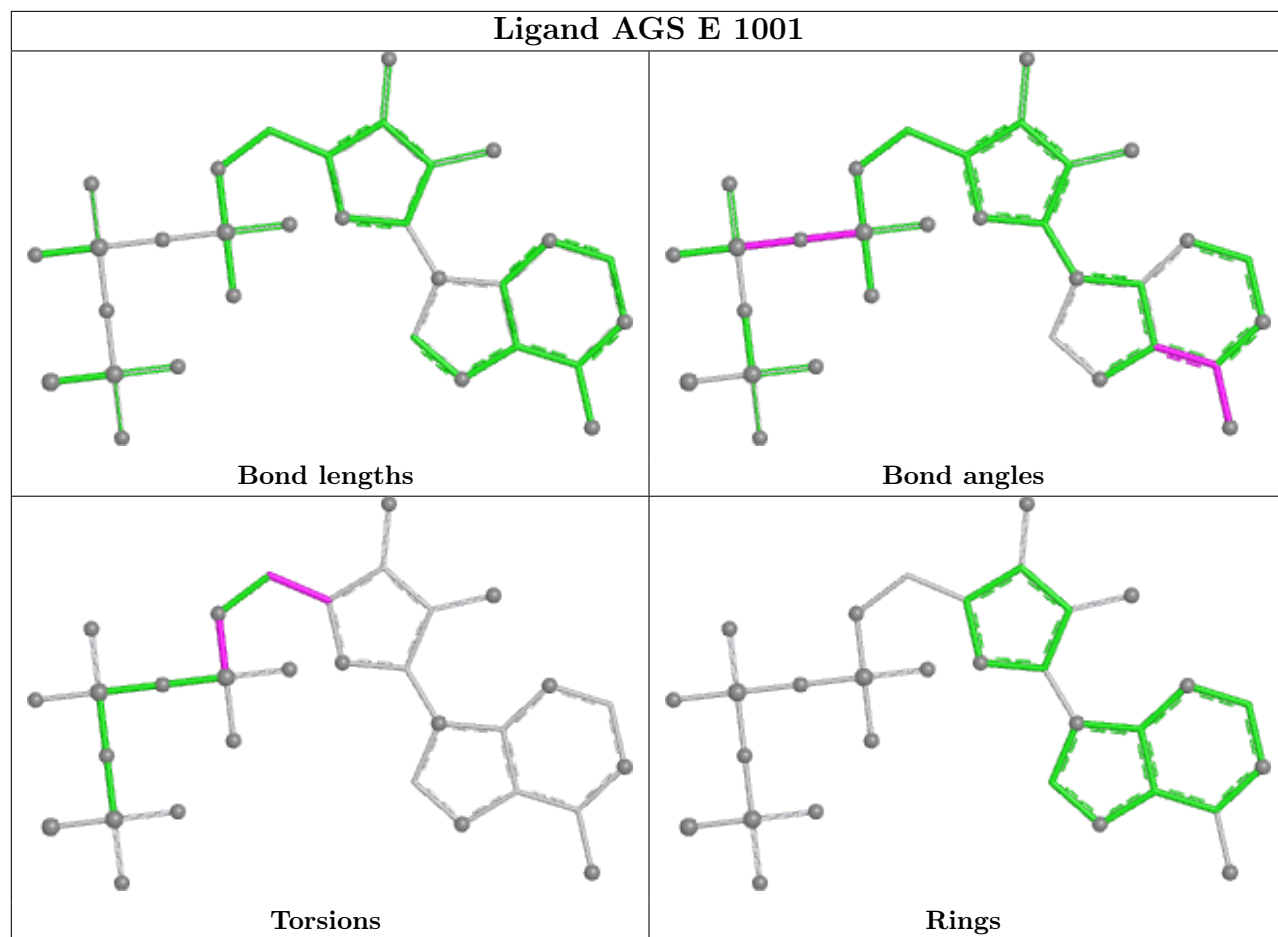


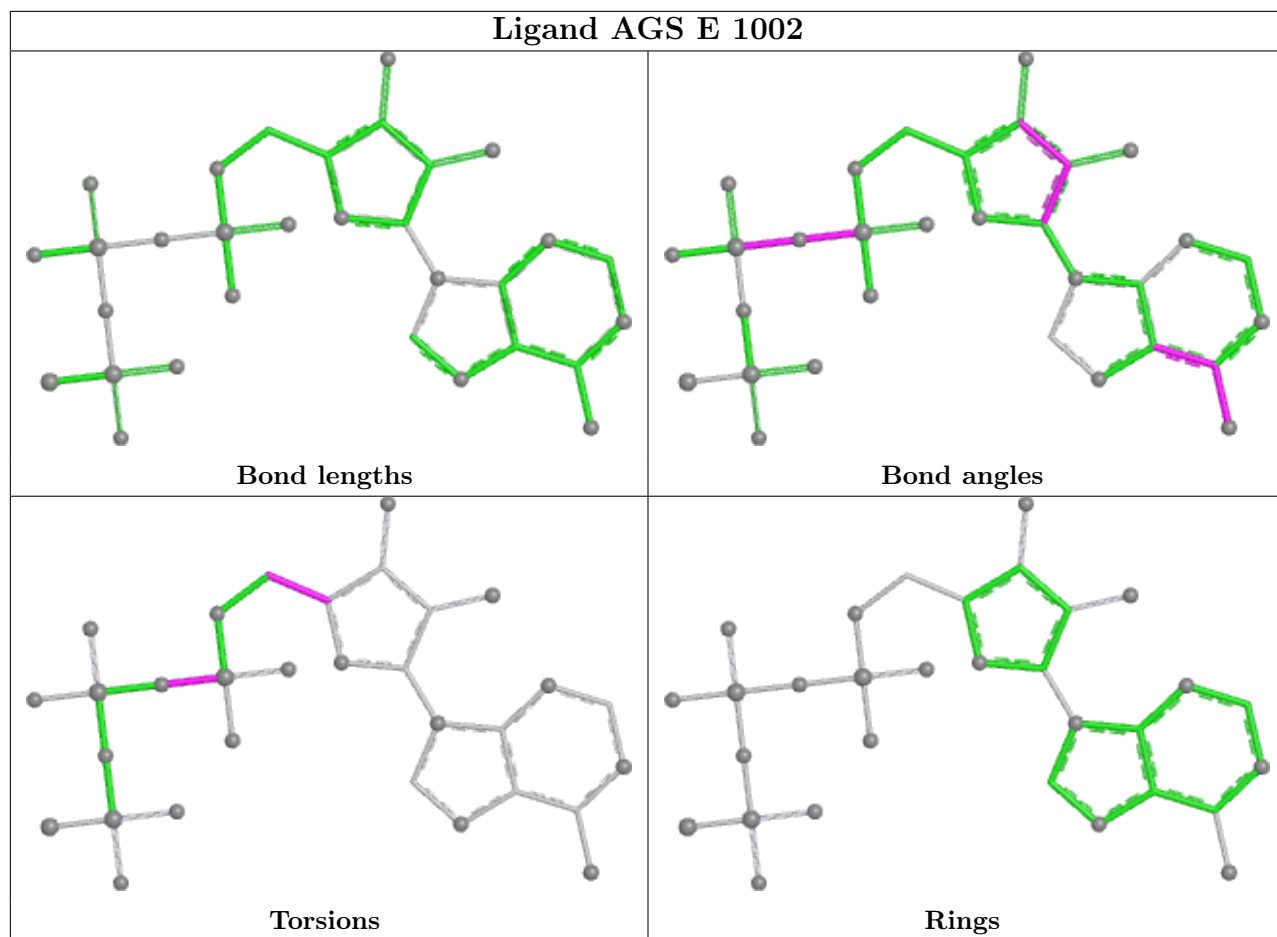


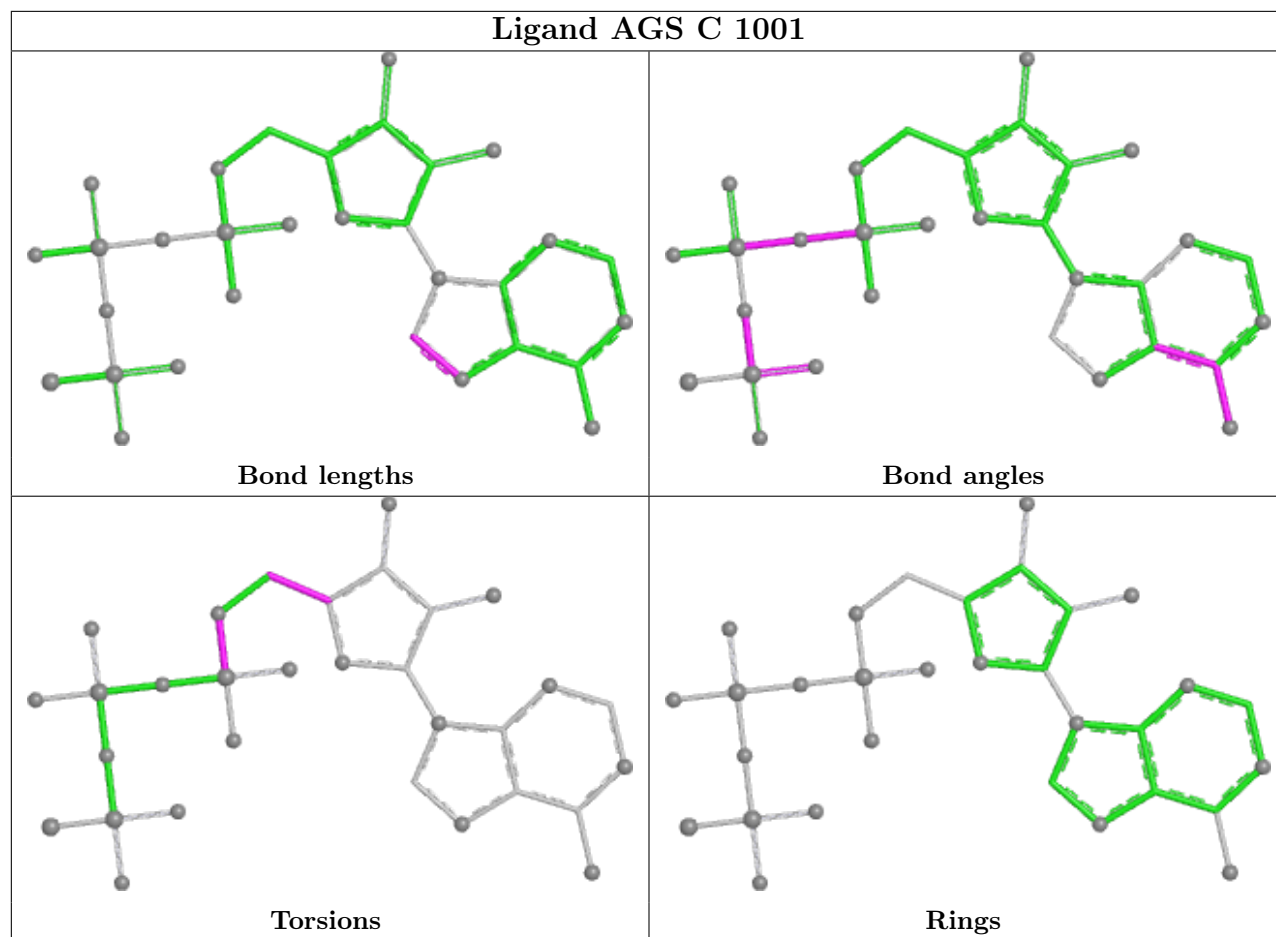


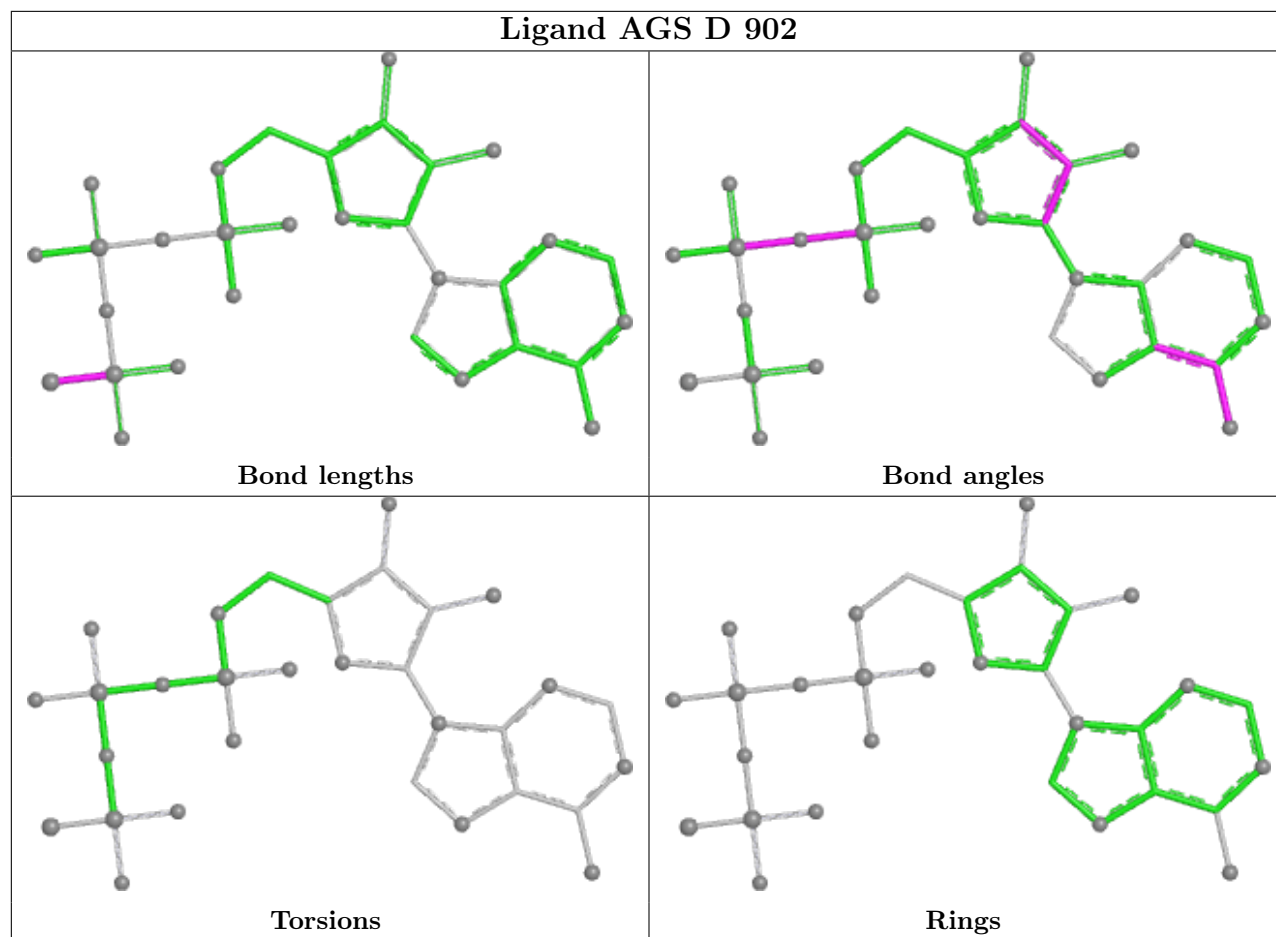


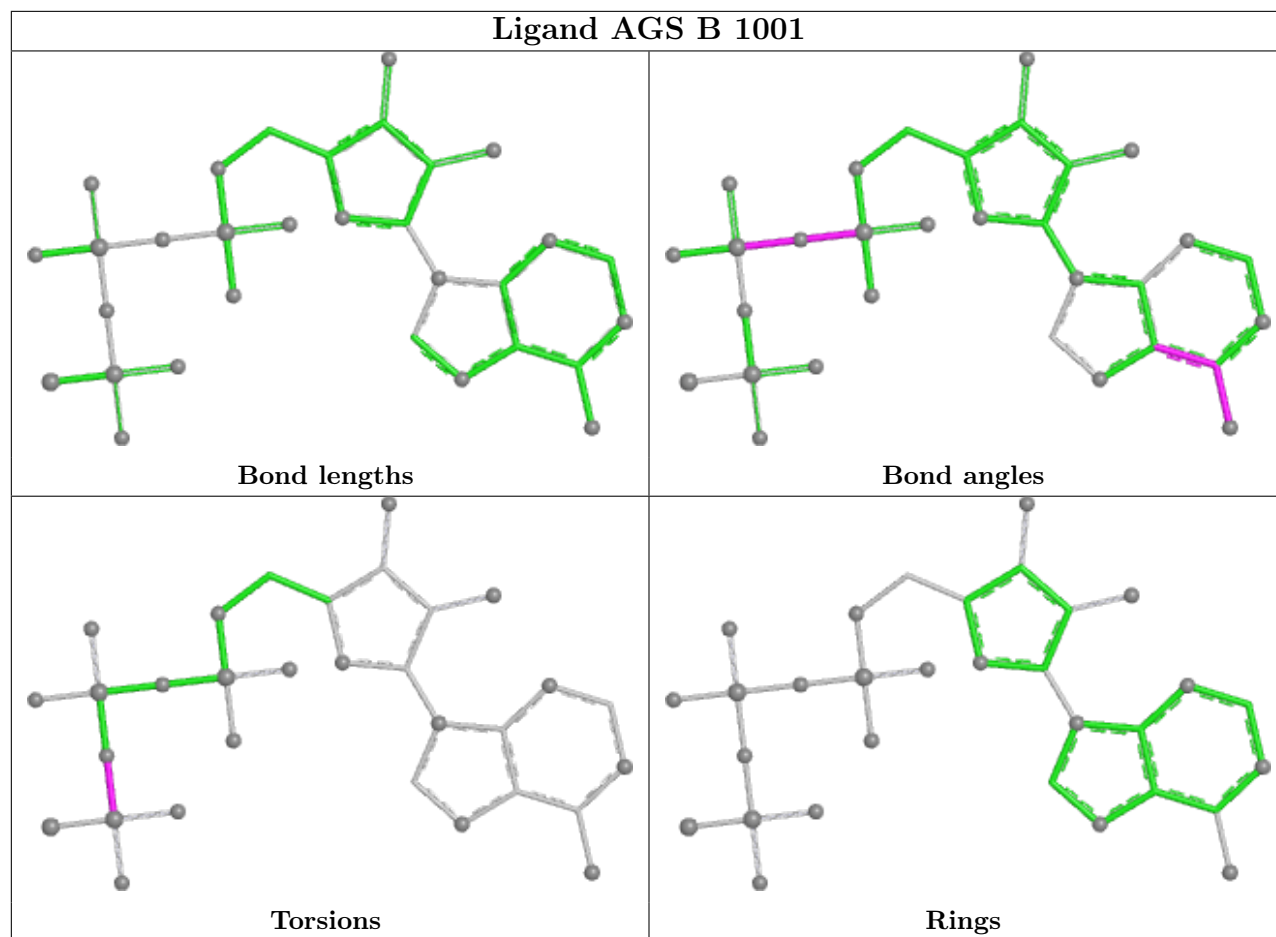


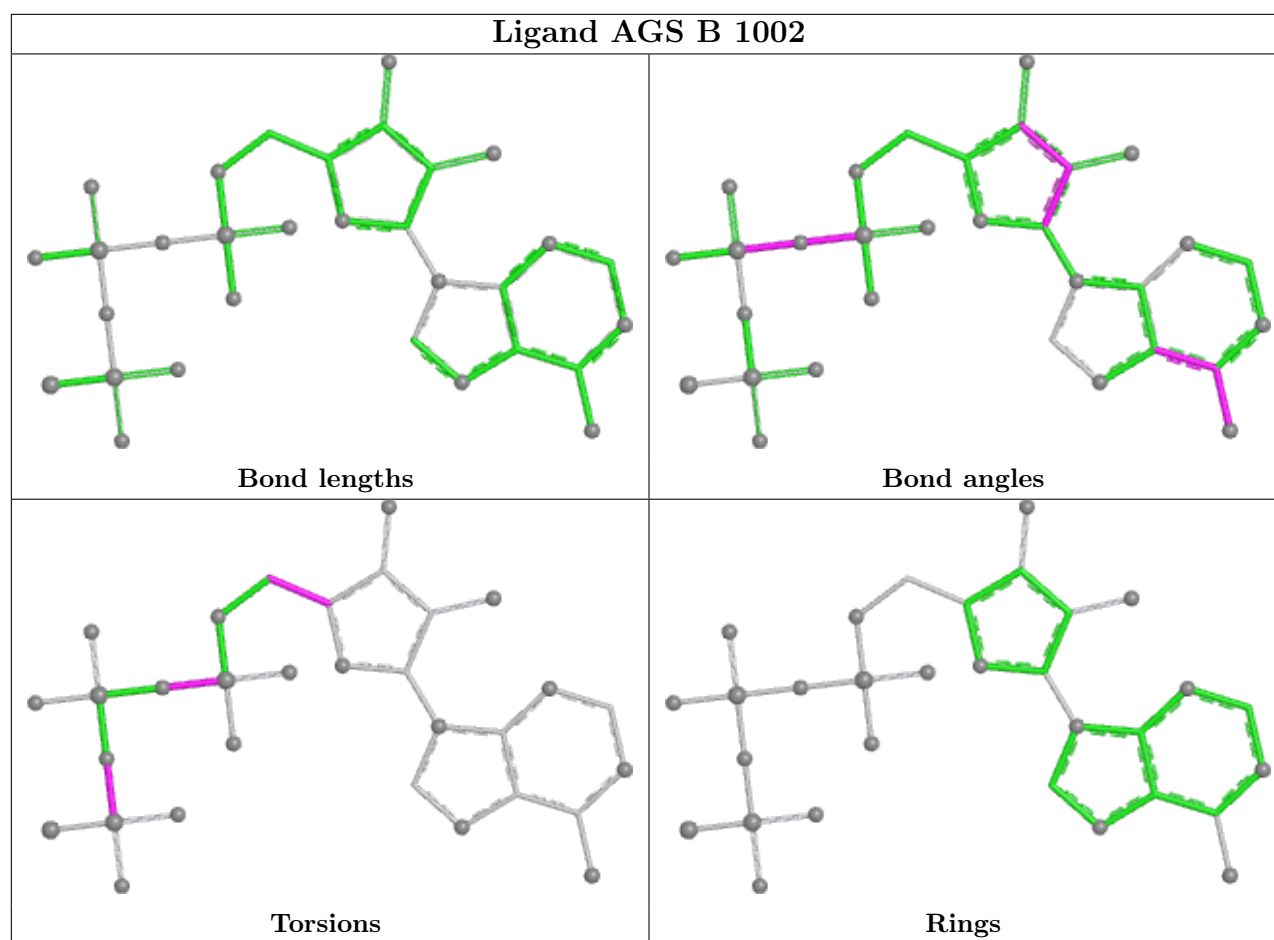












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	764:HIS	C	765:PRO	N	6.27

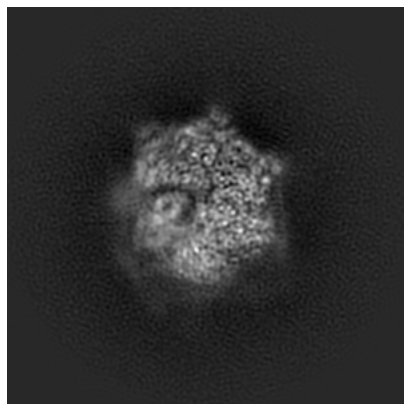
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4627. These allow visual inspection of the internal detail of the map and identification of artifacts.

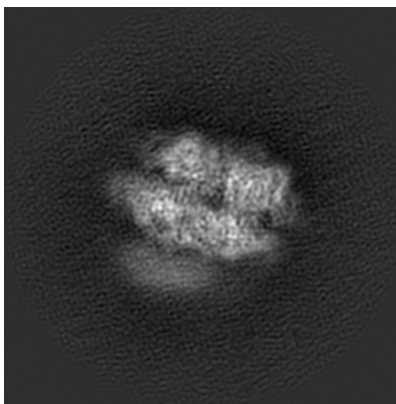
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

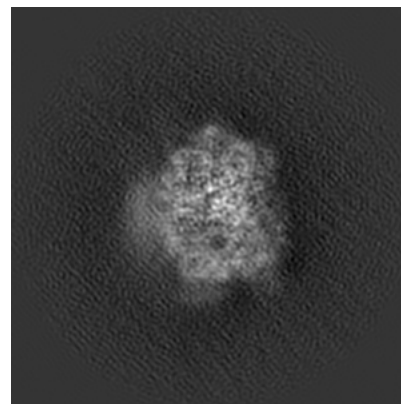
6.1.1 Primary map



X

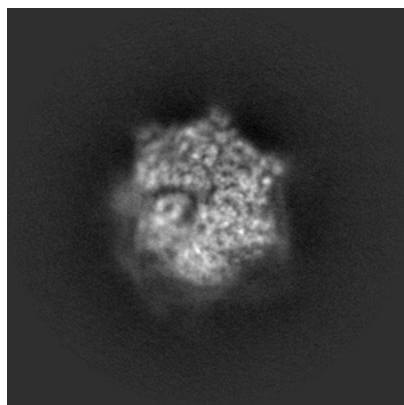


Y

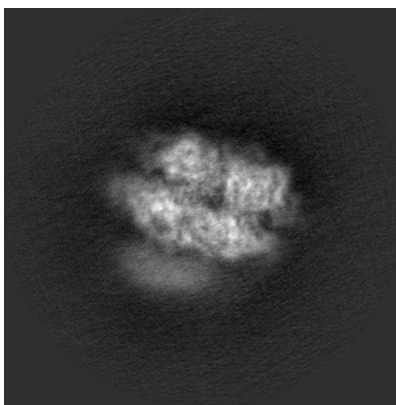


Z

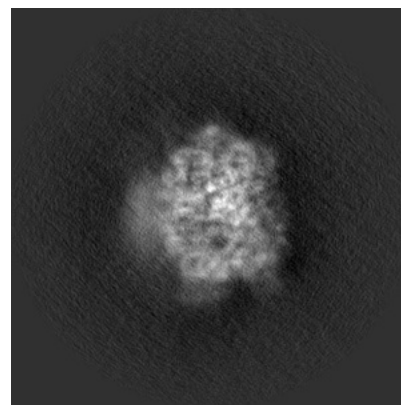
6.1.2 Raw map



X



Y

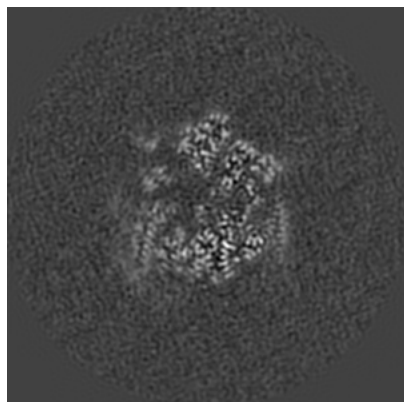


Z

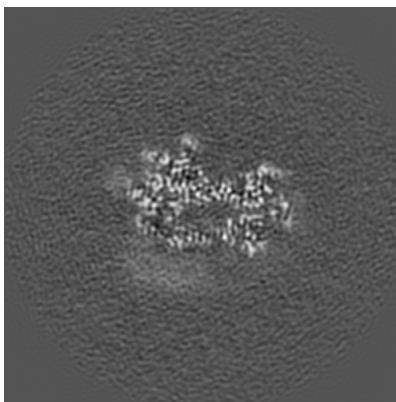
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

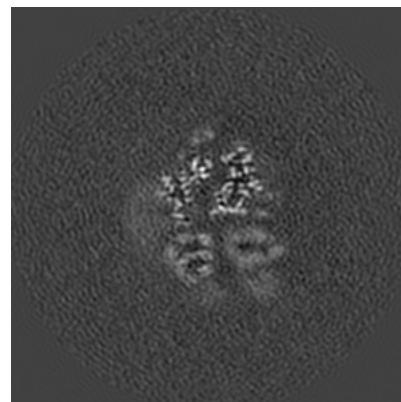
6.2.1 Primary map



X Index: 144

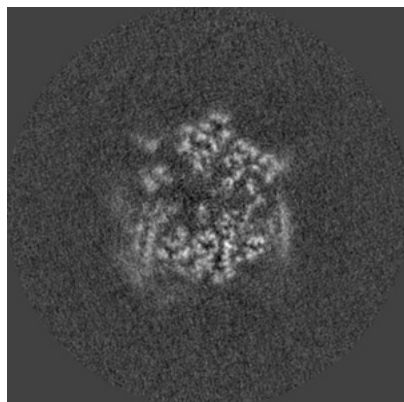


Y Index: 144

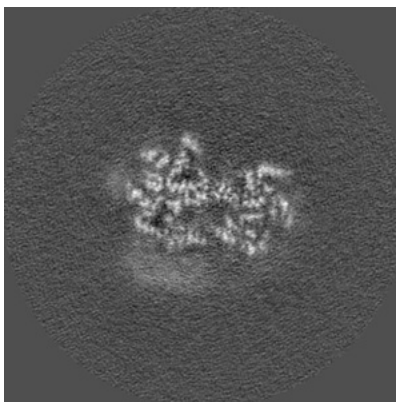


Z Index: 144

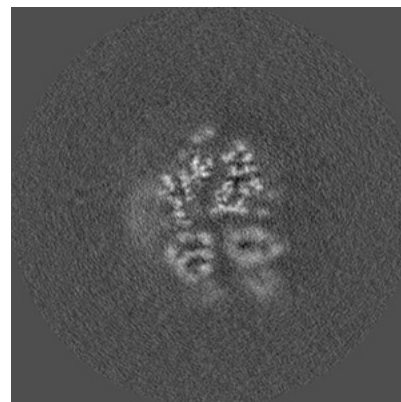
6.2.2 Raw map



X Index: 144



Y Index: 144

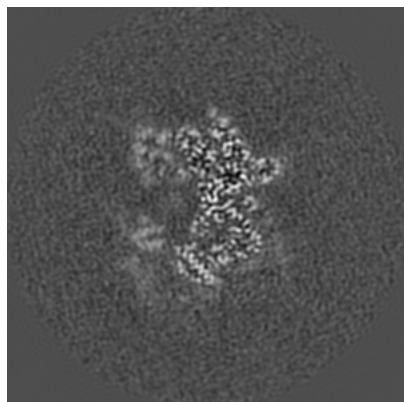


Z Index: 144

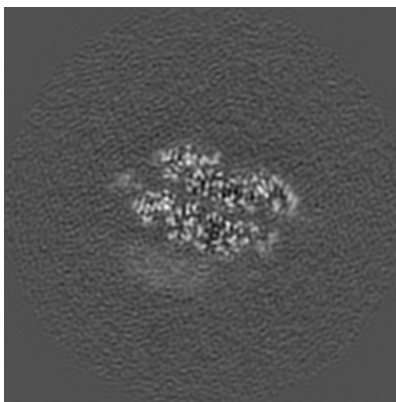
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

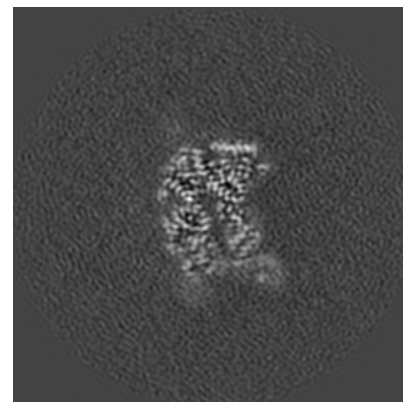
6.3.1 Primary map



X Index: 153

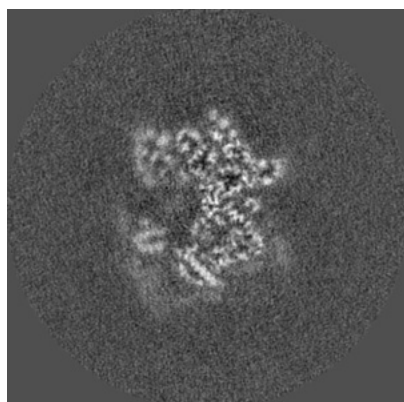


Y Index: 157

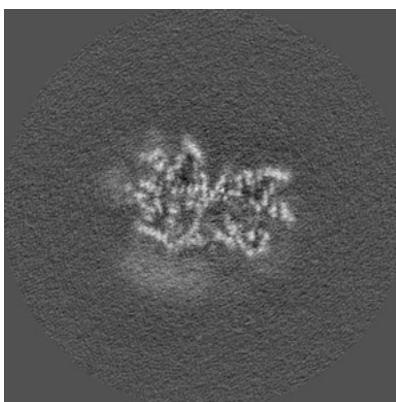


Z Index: 163

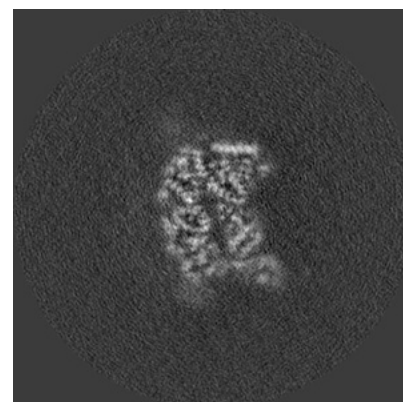
6.3.2 Raw map



X Index: 153



Y Index: 142

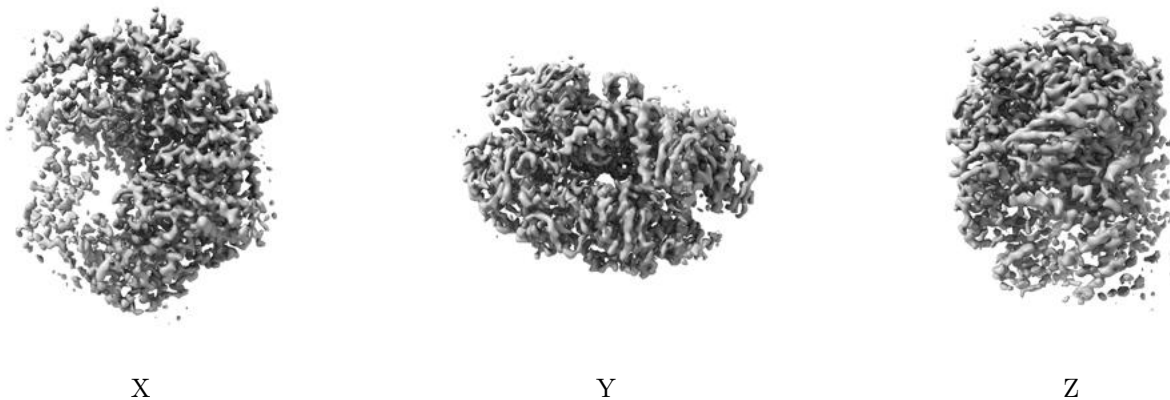


Z Index: 163

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

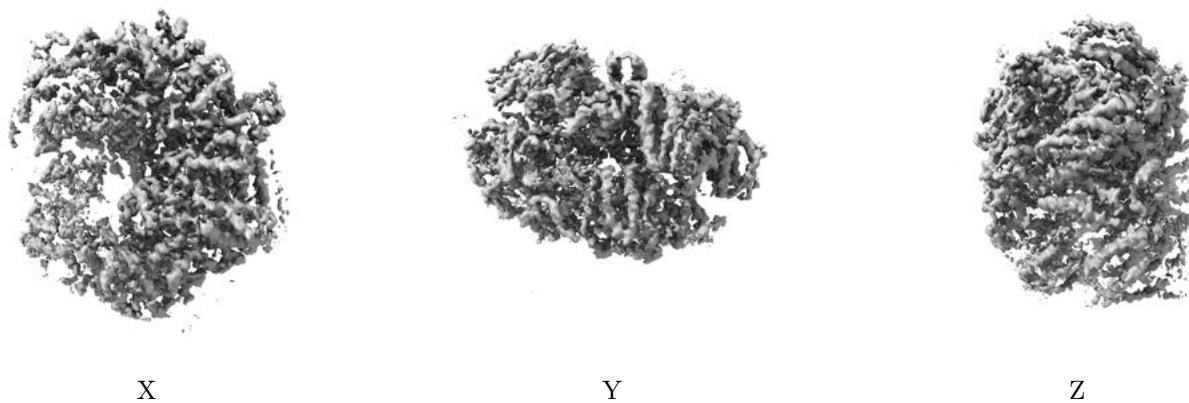
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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.

6.4.2 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.

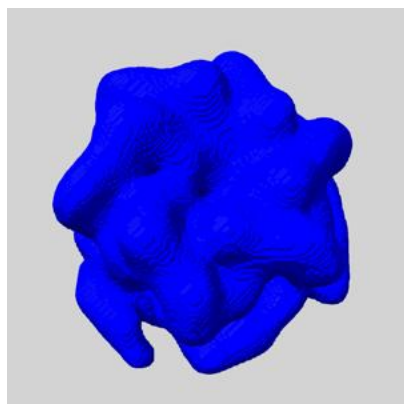
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

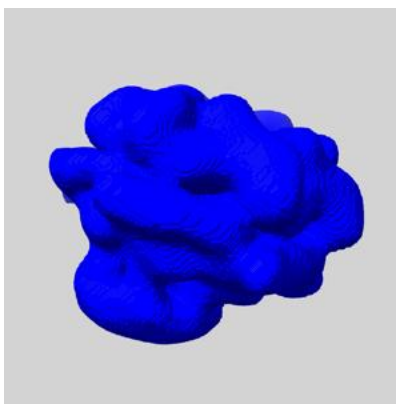
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

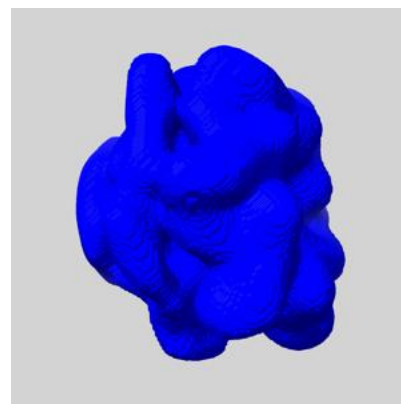
6.5.1 emd_4627_msk_1.map [i](#)



X



Y

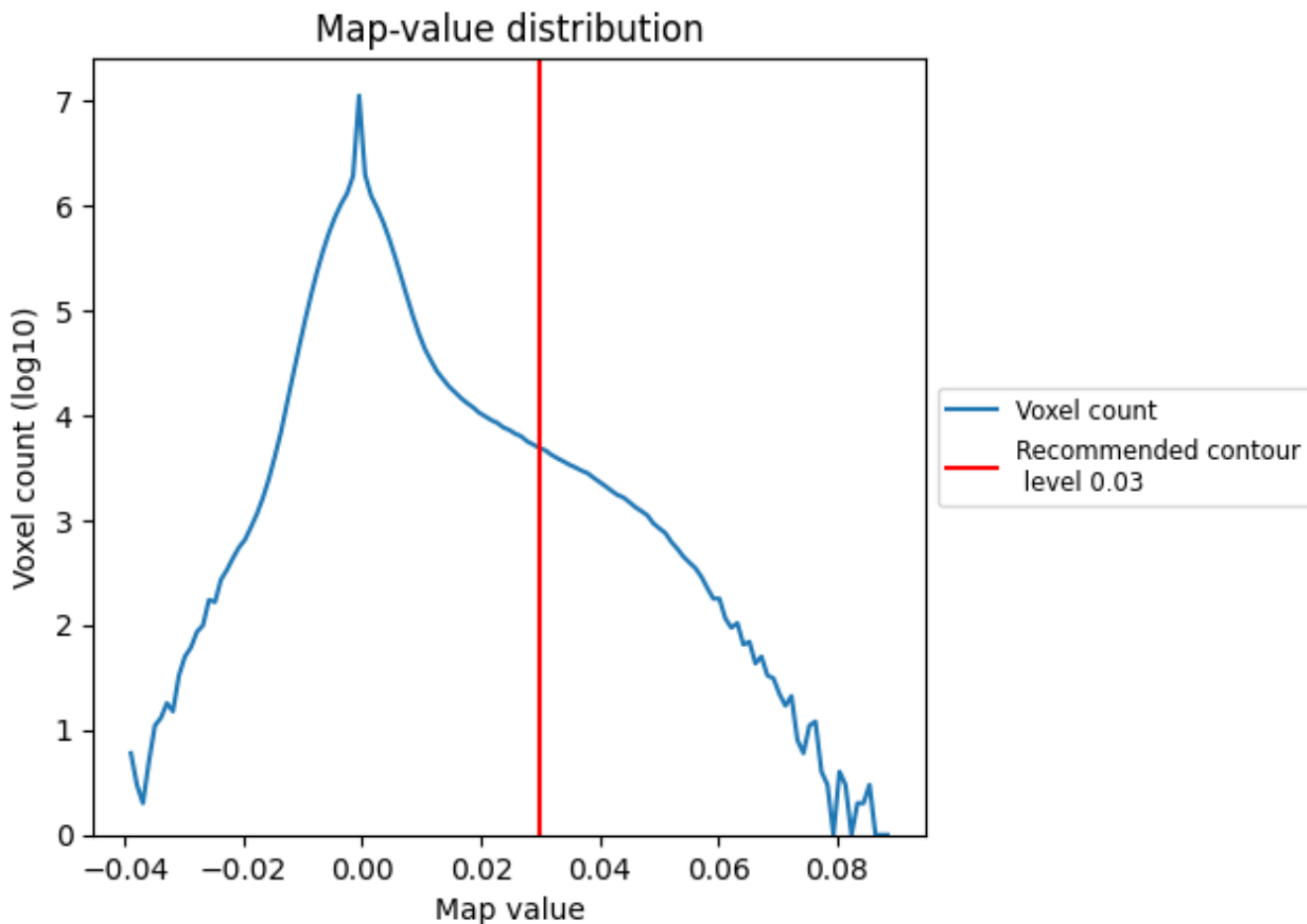


Z

7 Map analysis [i](#)

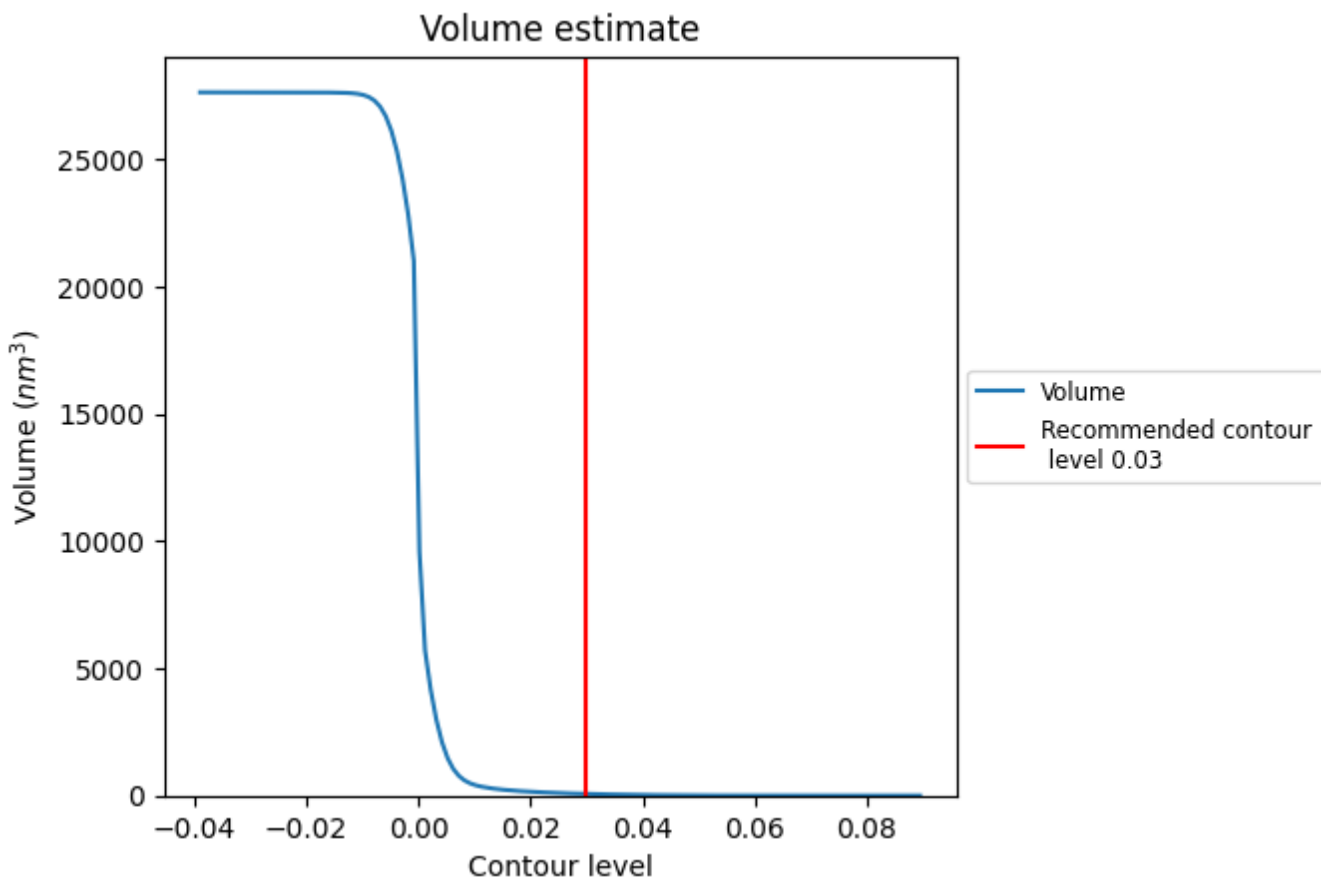
This section contains the results of statistical analysis of the map.

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.

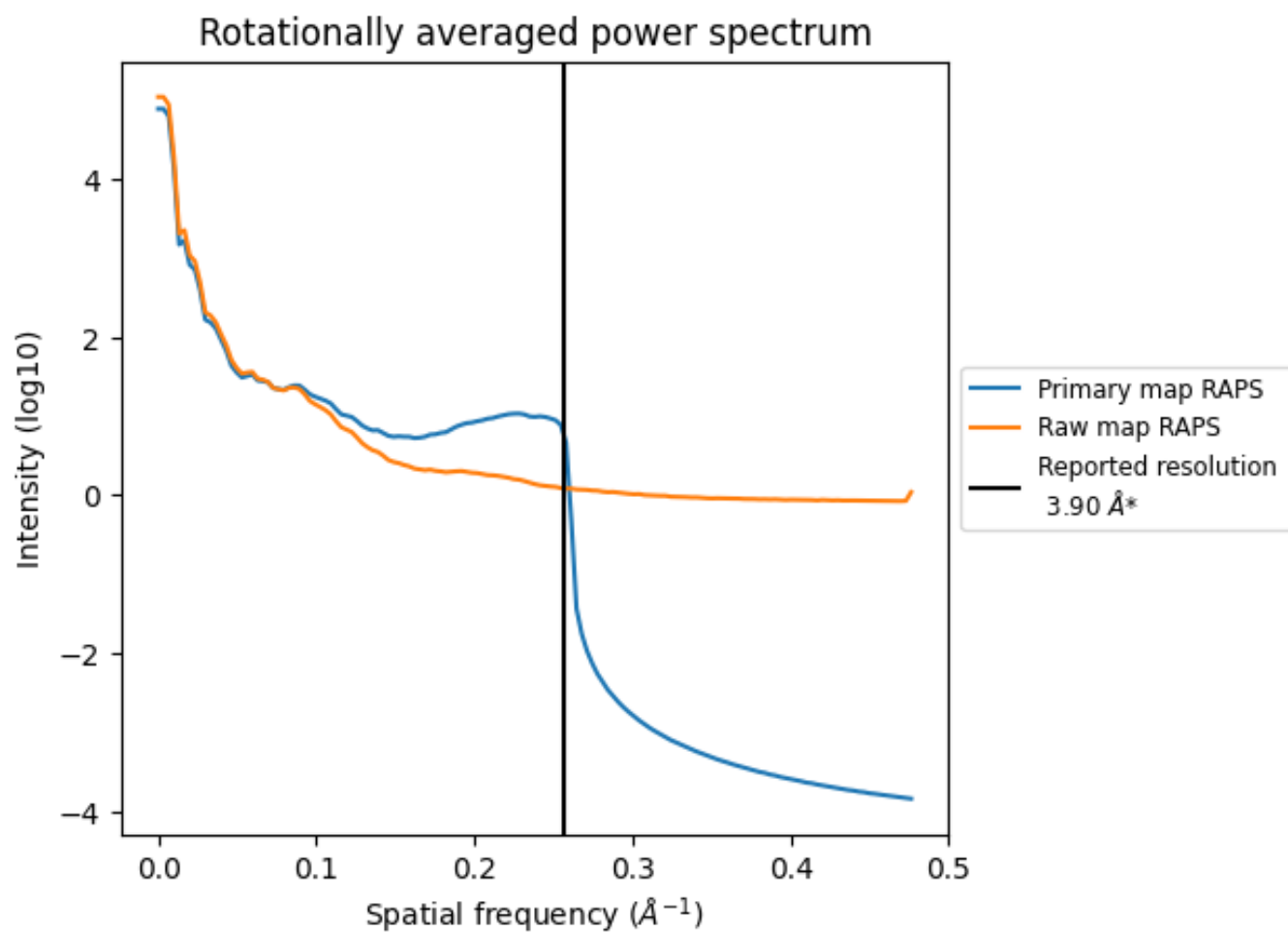
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 65 nm^3 ; this corresponds to an approximate mass of 59 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 i

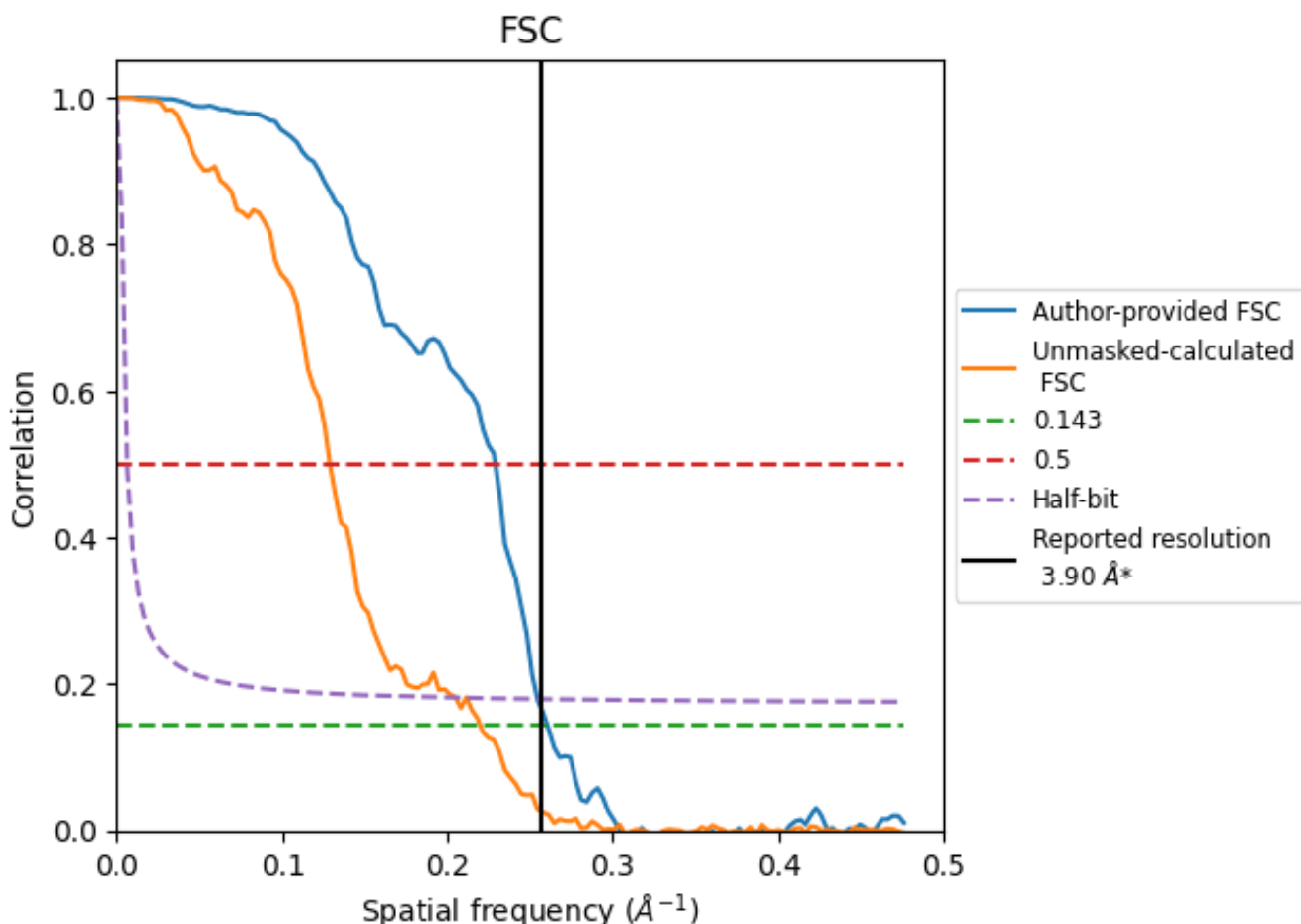


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256\AA^{-1}

8.2 Resolution estimates [i](#)

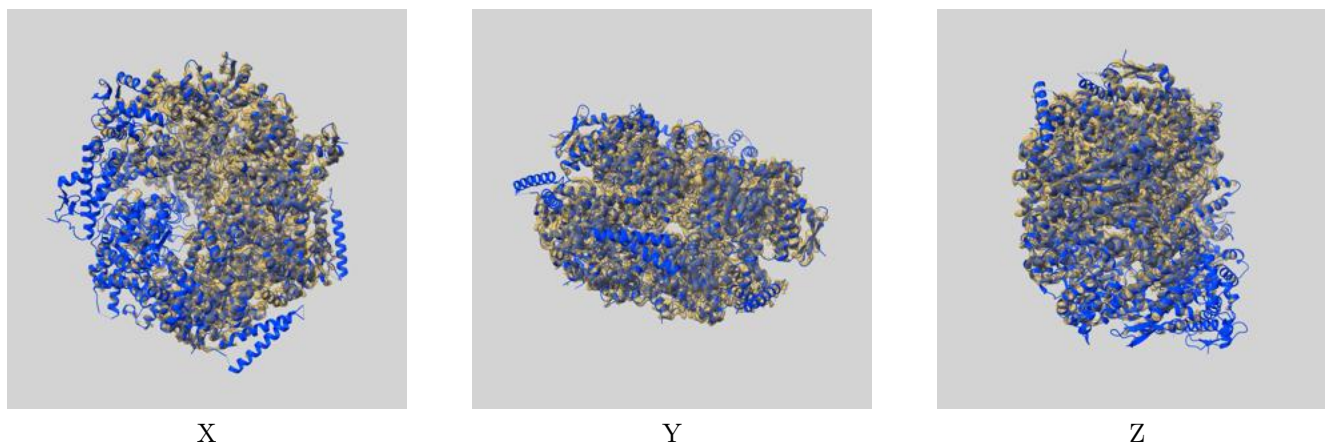
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.84	4.36	3.93
Unmasked-calculated*	4.55	7.76	4.87

*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 4.55 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

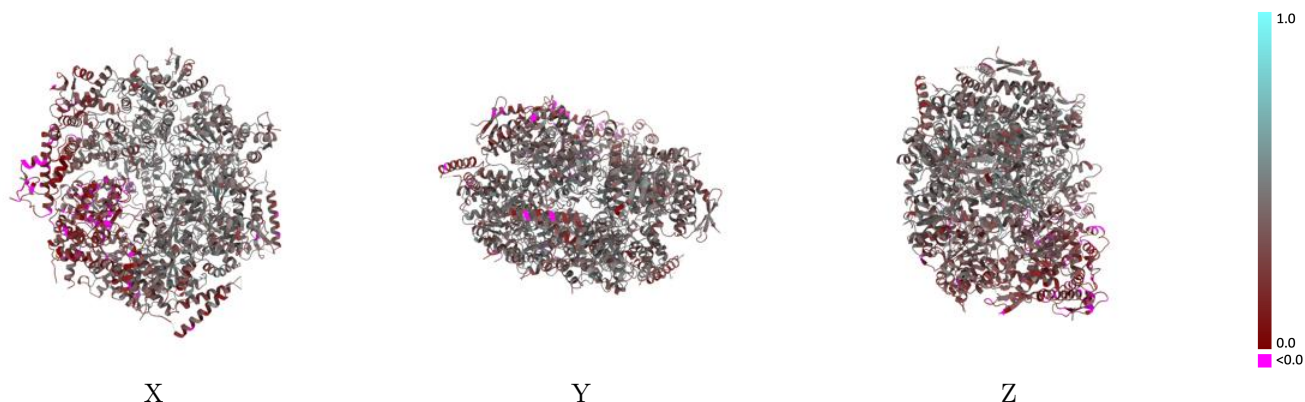
This section contains information regarding the fit between EMDB map EMD-4627 and PDB model 6QS8. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



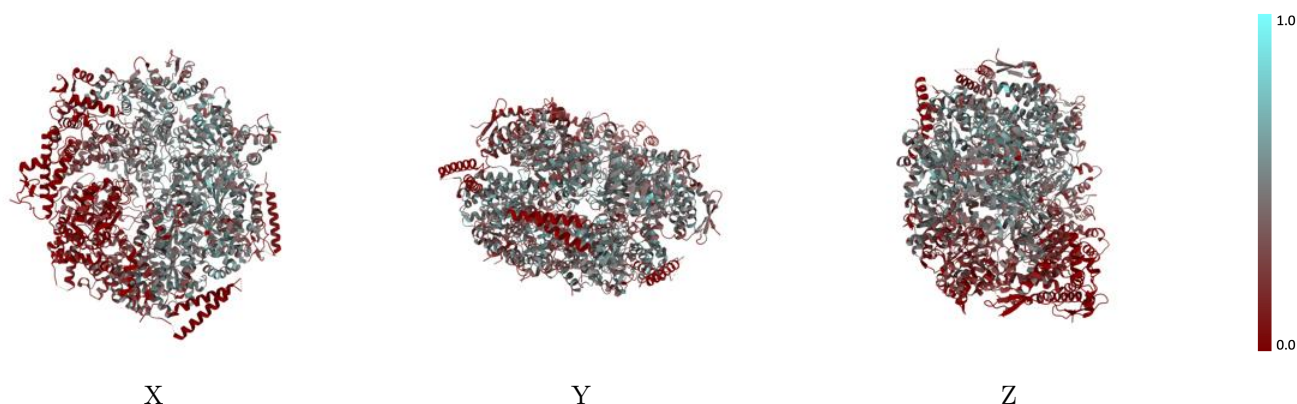
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



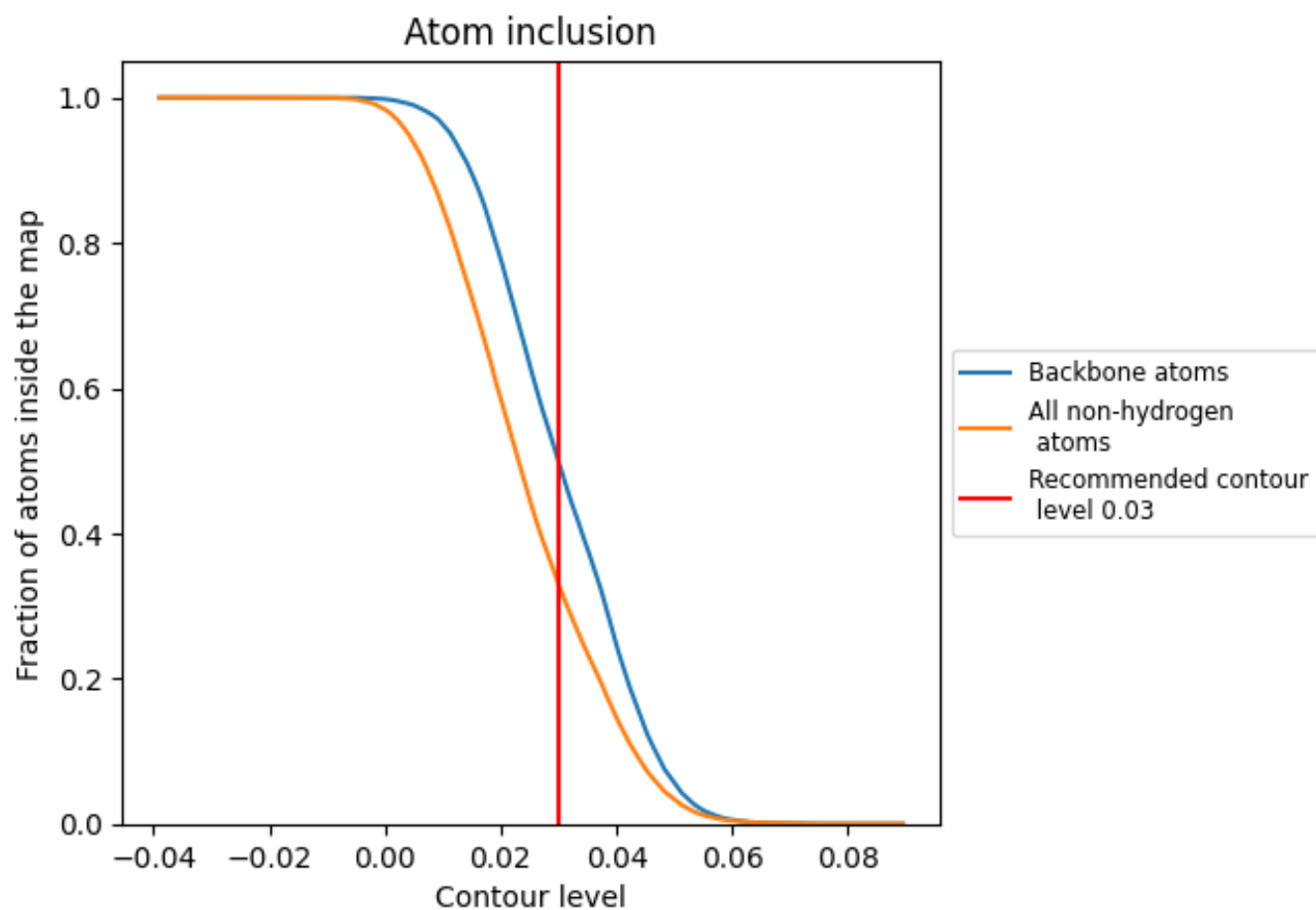
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 50% of all backbone atoms, 33% 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	 0.3304	 0.3600
A	 0.2399	 0.3230
B	 0.4342	 0.4090
C	 0.4622	 0.4240
D	 0.4332	 0.4210
E	 0.3029	 0.3650
F	 0.0821	 0.2030
S	 0.4667	 0.4700

