Full wwPDB EM Validation Report (i)

May 18, 2024 – 11:54 AM EDT

PDB ID	:	6W6H
EMDB ID	:	EMD-21555
Title	:	The Mycobacterium tuberculosis ClpB disaggregase hexamer structure in conformation II in the presence of DnaK chaperone and a model substrate
Authors	:	Yin, Y.; Li, H.
Deposited on	:	2020-03-16
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

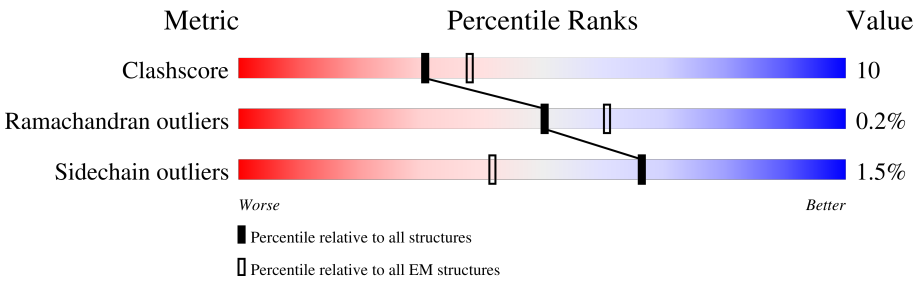
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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 <=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	848	61% 12% 27%
1	B	848	60% 13% 26%
1	C	848	56% 16% • 25%
1	D	848	53% 13% 34%
1	E	848	48% 17% 35%
1	F	848	58% 15% 27%
2	N	31	81% • 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 28427 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.

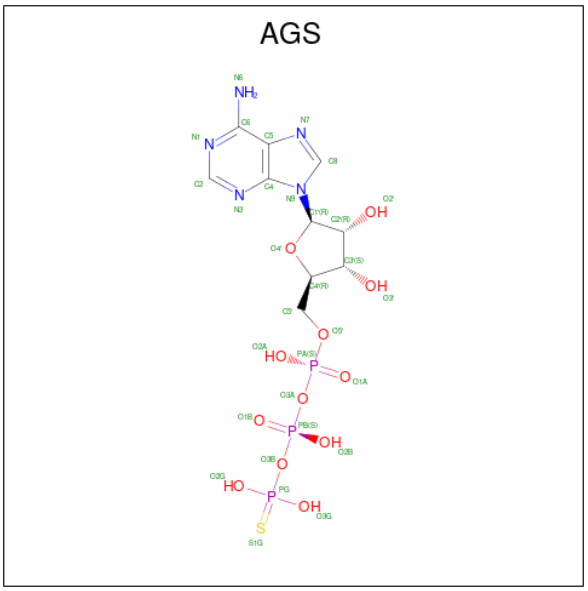
- Molecule 1 is a protein called Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	620	4796	2990	876	920	10	0	0
1	B	629	4872	3038	889	935	10	0	0
1	C	636	4918	3066	896	945	11	0	0
1	D	562	4321	2701	790	821	9	0	0
1	E	548	4230	2647	772	802	9	0	0
1	F	620	4796	2990	876	920	10	0	0

- Molecule 2 is a protein called Substrate.

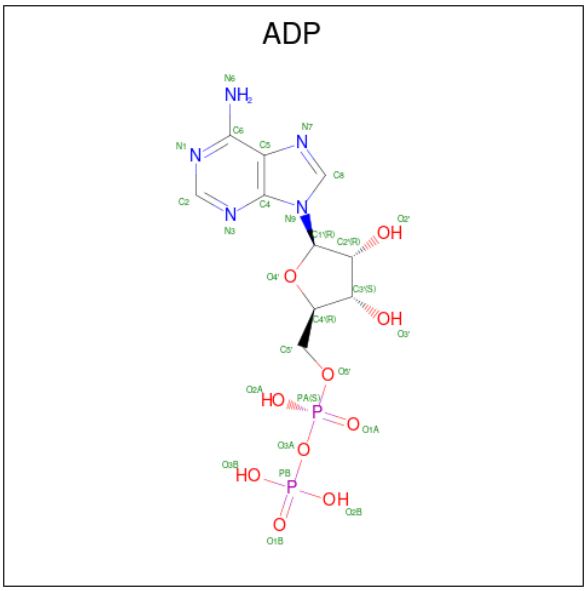
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	N	26	130	78	26	26	0	0

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

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



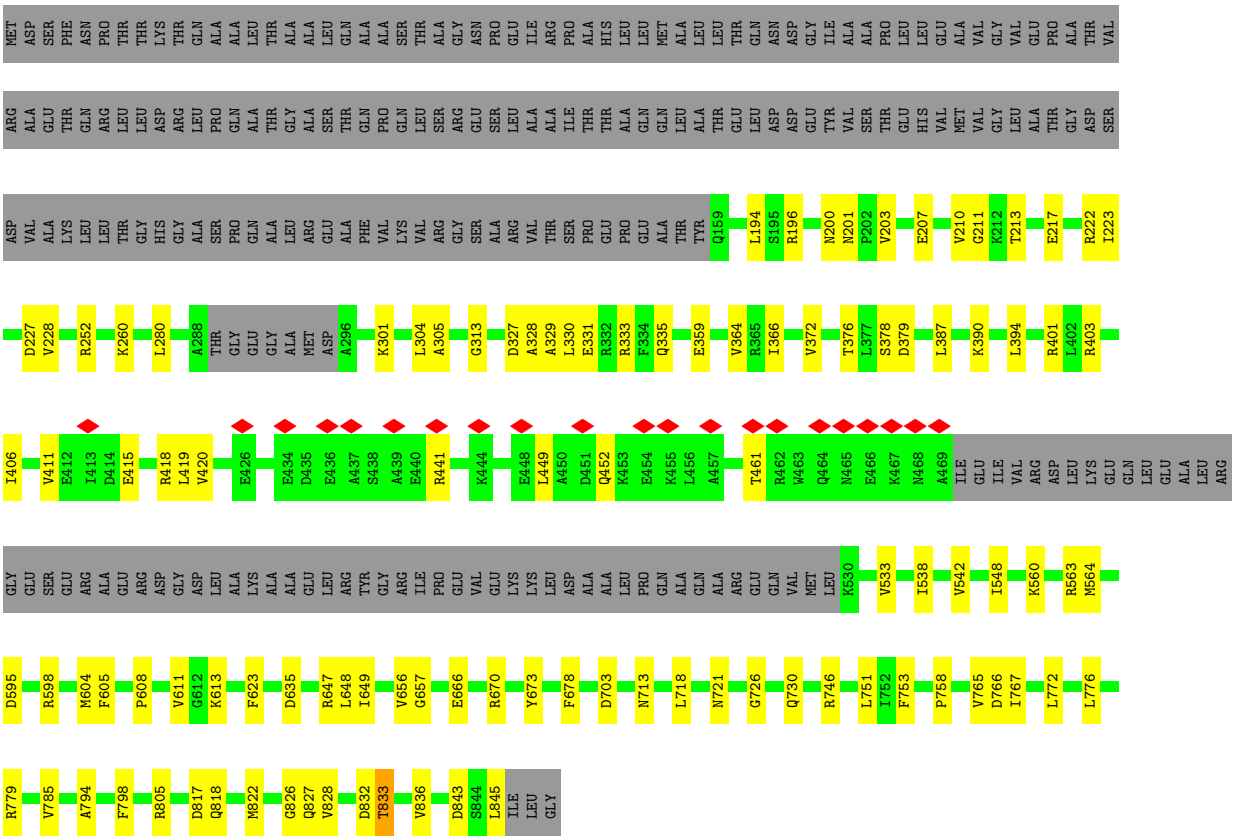
Mol	Chain	Residues	Atoms					AltConf
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

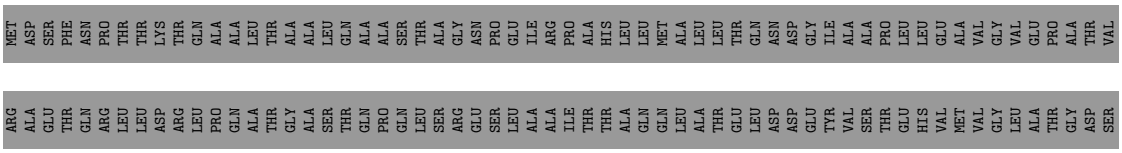
• Molecule 1: Chaperone protein ClpB

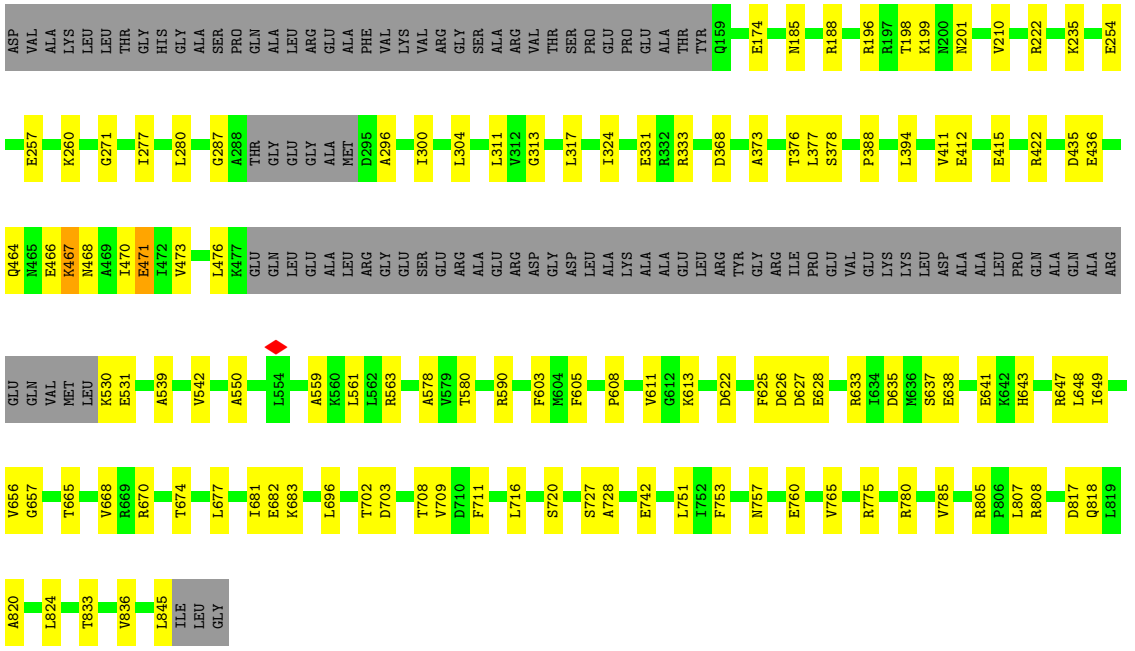
Chain A: 61% 12% 27%



• Molecule 1: Chaperone protein ClpB

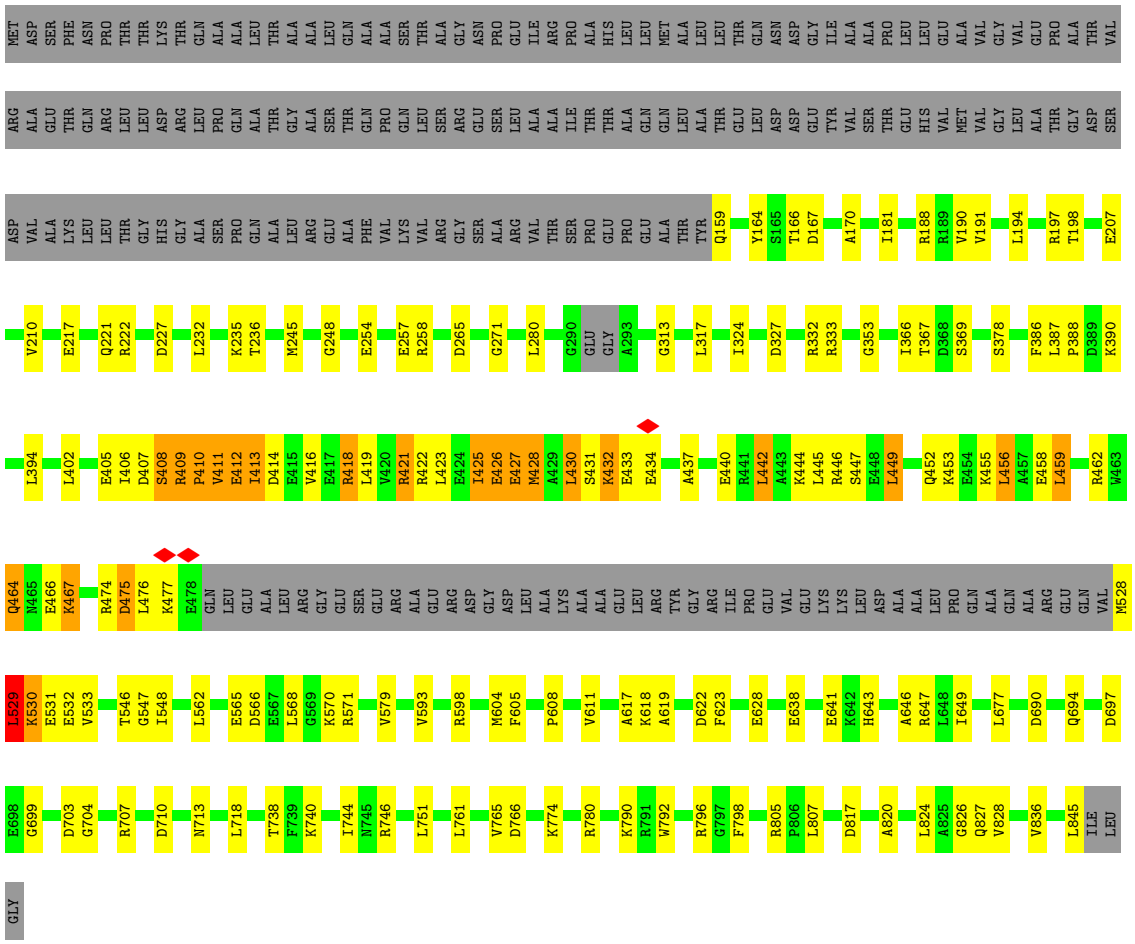
Chain B: 60% 13% 26%





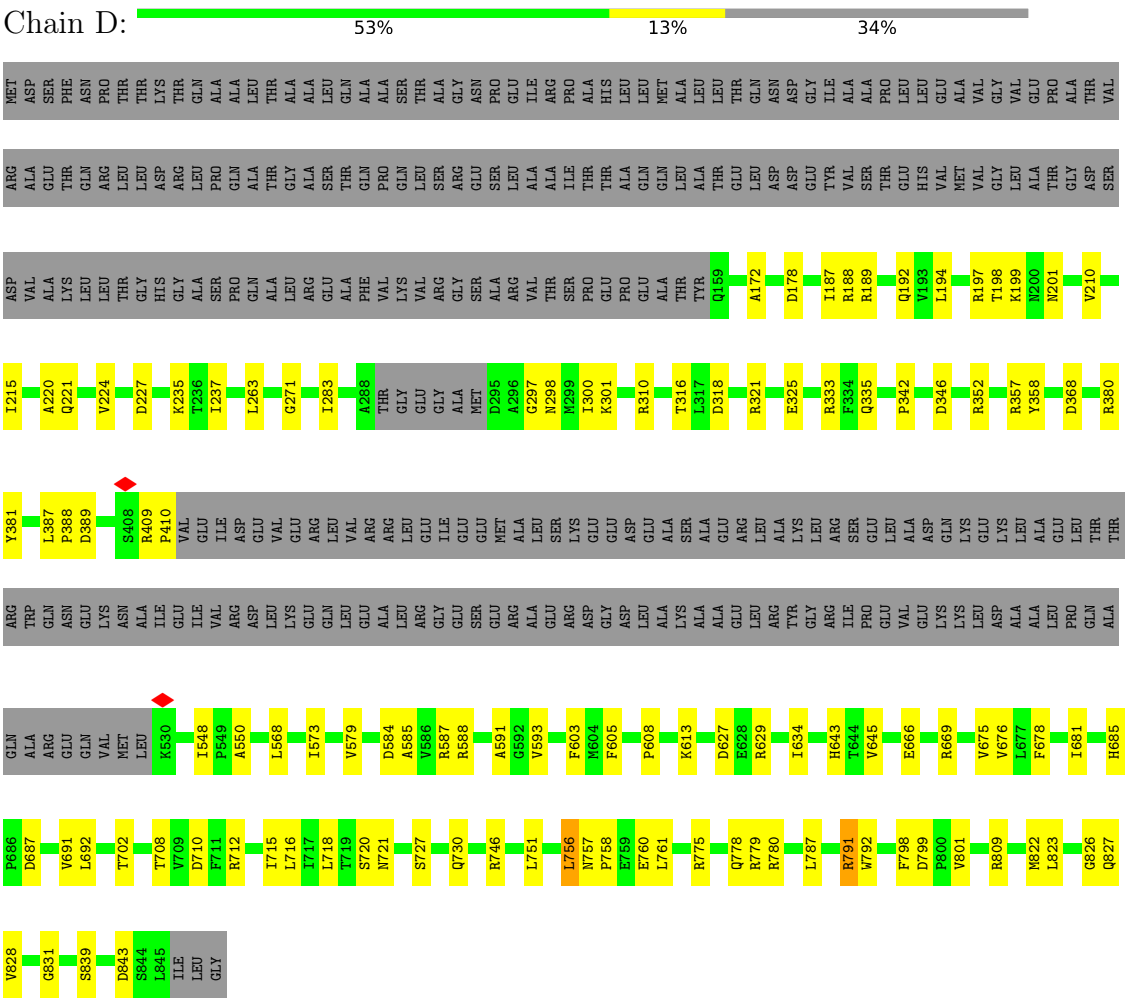
- Molecule 1: Chaperone protein ClpB

Chain C: 56% 16% • 25%



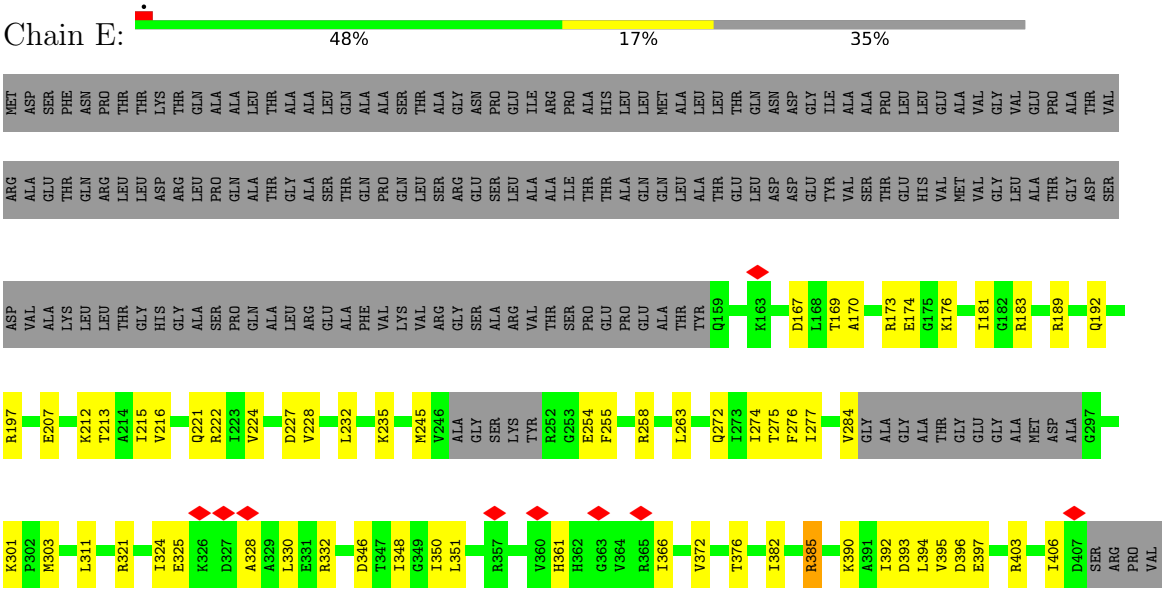
• Molecule 1: Chaperone protein ClpB

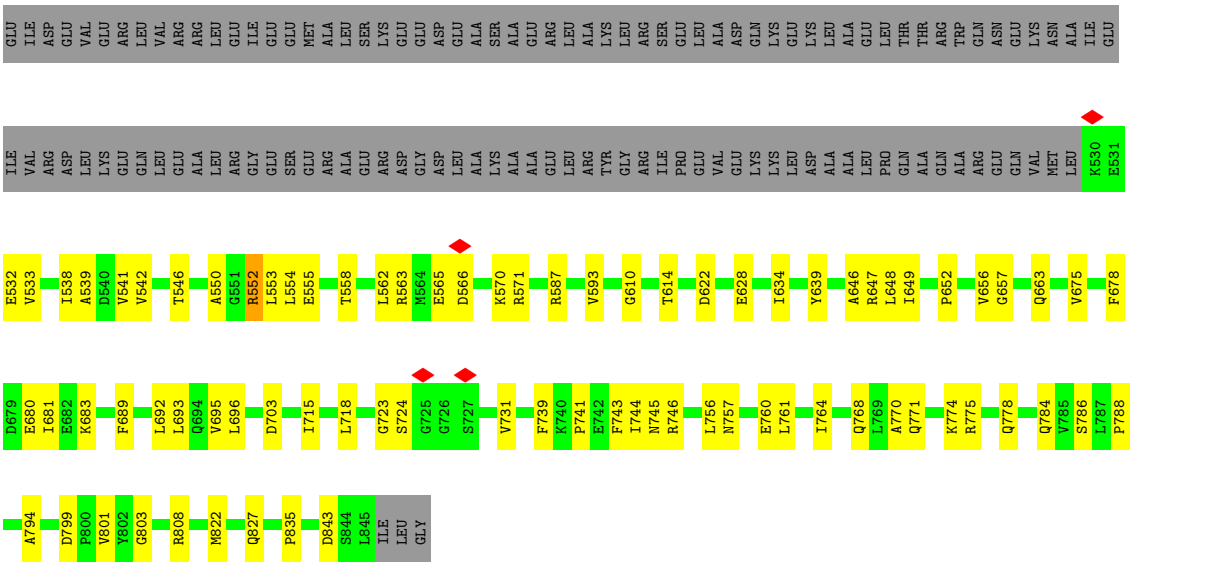
Chain D:



• Molecule 1: Chaperone protein ClpB

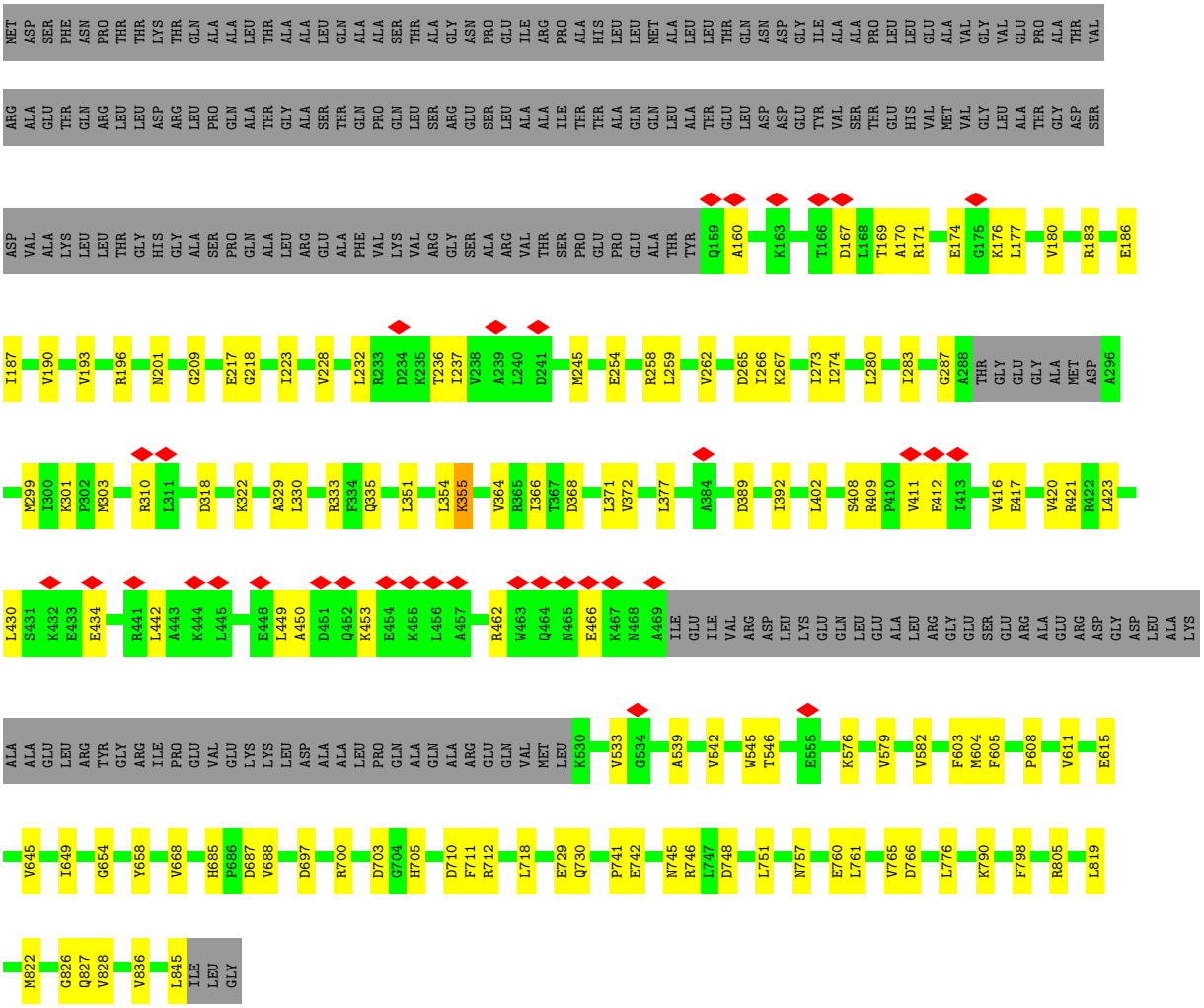
Chain E:





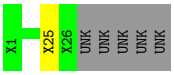
- Molecule 1: Chaperone protein ClpB

Chain F:



• Molecule 2: Substrate

Chain N: 81% • 16%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.106	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0131	Depositor
Map size (Å)	386.64, 386.64, 386.64	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.074, 1.074, 1.074	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.25	0/4857	0.44	0/6551
1	B	0.26	0/4933	0.45	0/6653
1	C	0.32	0/4979	0.47	0/6715
1	D	0.24	0/4380	0.46	1/5914 (0.0%)
1	E	0.24	0/4286	0.46	0/5786
1	F	0.24	0/4857	0.44	0/6551
All	All	0.26	0/28292	0.45	1/38170 (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	C	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	756	LEU	C-N-CA	5.10	134.46	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	387	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	387	LEU	Peptide
1	D	839	SER	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	4796	0	4853	69	0
1	B	4872	0	4935	83	0
1	C	4918	0	4978	168	0
1	D	4321	0	4377	79	0
1	E	4230	0	4292	94	0
1	F	4796	0	4851	90	0
2	N	130	0	35	1	0
3	A	62	0	24	5	0
3	B	62	0	24	6	0
3	C	62	0	24	5	0
3	D	62	0	24	4	0
3	F	62	0	23	9	0
4	E	54	0	24	3	0
All	All	28427	0	28464	557	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 (557) 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:C:530:LYS:NZ	1:C:531:GLU:H	1.37	1.20
1:B:467:LYS:HG2	1:B:471:GLU:OE2	1.43	1.15
1:C:528:MET:O	1:C:529:LEU:HB2	1.45	1.12
1:C:407:ASP:O	1:C:408:SER:O	1.72	1.08
1:C:530:LYS:HZ1	1:C:531:GLU:N	1.54	1.05
1:C:414:ASP:OD2	1:D:188:ARG:NH1	1.89	1.04
1:C:530:LYS:NZ	1:C:531:GLU:N	2.07	1.01
1:B:467:LYS:CG	1:B:471:GLU:OE2	2.08	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:GLU:OE2	1:C:528:MET:N	1.94	0.99
1:C:530:LYS:HE3	1:C:532:GLU:OE1	1.64	0.98
1:C:406:ILE:HD11	1:C:531:GLU:OE1	1.65	0.95
1:C:426:GLU:OE1	1:D:352:ARG:HD2	1.66	0.94
1:C:422:ARG:O	1:C:425:ILE:HG13	1.69	0.92
1:C:530:LYS:HA	1:C:530:LYS:HZ2	1.35	0.90
1:C:416:VAL:CG1	1:C:456:LEU:HB2	2.04	0.87
1:C:474:ARG:O	1:C:477:LYS:N	2.06	0.87
1:C:530:LYS:CE	1:C:532:GLU:OE1	2.22	0.86
1:C:406:ILE:CD1	1:C:531:GLU:OE1	2.24	0.85
1:C:530:LYS:HZ1	1:C:531:GLU:H	1.05	0.85
1:C:405:GLU:OE2	1:C:411:VAL:CG2	2.25	0.85
1:C:456:LEU:HD22	1:C:456:LEU:O	1.78	0.83
1:B:467:LYS:O	1:B:471:GLU:OE2	1.97	0.81
1:E:571:ARG:NH1	1:E:622:ASP:OD2	2.13	0.81
1:C:421:ARG:CB	1:C:421:ARG:HH11	1.94	0.80
1:C:442:LEU:HD12	1:C:442:LEU:O	1.82	0.80
1:B:467:LYS:C	1:B:471:GLU:OE2	2.20	0.79
1:C:416:VAL:HG11	1:C:456:LEU:HB2	1.63	0.79
1:C:422:ARG:O	1:C:425:ILE:CG1	2.32	0.77
1:C:530:LYS:HZ2	1:C:531:GLU:H	1.32	0.77
1:C:437:ALA:HA	1:C:780:ARG:HH22	1.49	0.77
1:A:822:MET:HB3	1:A:828:VAL:HG21	1.67	0.77
1:C:414:ASP:CG	1:D:188:ARG:HH12	1.88	0.76
1:C:437:ALA:HA	1:C:780:ARG:NH2	2.00	0.75
1:C:464:GLN:OE1	1:C:464:GLN:HA	1.87	0.75
1:C:466:GLU:OE2	1:C:528:MET:CA	2.34	0.75
1:C:411:VAL:C	1:C:413:ILE:H	1.91	0.74
1:C:422:ARG:HA	1:C:425:ILE:HD11	1.68	0.73
1:C:426:GLU:OE1	1:D:352:ARG:CD	2.30	0.73
1:C:409:ARG:HB2	1:C:410:PRO:HD2	1.70	0.73
1:F:209:GLY:N	3:F:901:AGS:O3G	2.22	0.72
1:E:385:ARG:NH2	1:E:393:ASP:OD2	2.23	0.71
1:F:177:LEU:HD13	1:F:217:GLU:HG2	1.71	0.71
1:C:428:MET:SD	1:C:428:MET:N	2.64	0.70
1:D:605:PHE:HB3	1:D:751:LEU:HB2	1.73	0.70
1:E:361:HIS:O	1:E:403:ARG:NH1	2.25	0.70
1:C:416:VAL:HG12	1:C:456:LEU:HB2	1.73	0.70
1:C:466:GLU:OE2	1:C:528:MET:C	2.30	0.70
1:C:421:ARG:HH11	1:C:421:ARG:HB2	1.55	0.70
3:C:902:AGS:S1G	1:D:333:ARG:NH1	2.66	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:GLU:OE2	1:C:411:VAL:HG23	1.92	0.69
1:C:449:LEU:C	1:C:449:LEU:HD12	2.14	0.68
1:B:702:THR:HG22	1:B:708:THR:HG22	1.76	0.68
1:C:474:ARG:O	1:C:476:LEU:N	2.26	0.68
1:C:430:LEU:HD22	1:C:430:LEU:O	1.94	0.68
1:F:836:VAL:HG12	1:F:845:LEU:HG	1.75	0.67
1:C:456:LEU:HD22	1:C:456:LEU:C	2.13	0.67
1:C:530:LYS:HZ2	1:C:530:LYS:CA	2.07	0.67
1:F:805:ARG:NH1	3:F:902:AGS:S1G	2.67	0.67
1:D:778:GLN:HG2	1:D:779:ARG:HD2	1.77	0.67
1:C:805:ARG:NH1	3:C:901:AGS:S1G	2.67	0.66
1:E:656:VAL:HG13	2:N:25:UNK:HA	1.77	0.66
3:F:901:AGS:N3	3:F:901:AGS:H2'	2.08	0.66
1:C:462:ARG:NH1	1:C:528:MET:CE	2.58	0.66
1:C:605:PHE:HB3	1:C:751:LEU:HB2	1.79	0.65
1:C:824:LEU:HD21	1:D:587:ARG:HG2	1.79	0.65
1:B:808:ARG:HH22	1:C:598:ARG:HH11	1.43	0.65
1:E:169:THR:HG22	1:E:173:ARG:HH22	1.62	0.65
1:C:604:MET:HB2	1:C:718:LEU:HB2	1.80	0.64
1:C:530:LYS:NZ	1:C:530:LYS:HA	2.11	0.64
1:A:785:VAL:HA	1:A:836:VAL:HG22	1.80	0.64
1:F:615:GLU:OE1	3:F:902:AGS:H2'	1.98	0.64
1:B:235:LYS:NZ	1:B:271:GLY:O	2.30	0.64
1:F:822:MET:HB3	1:F:828:VAL:HG21	1.80	0.64
1:F:603:PHE:HB3	1:F:748:ASP:HB2	1.78	0.64
1:F:710:ASP:HB2	1:F:712:ARG:HD2	1.80	0.64
1:F:654:GLY:H	1:F:658:TYR:HB2	1.61	0.64
1:E:550:ALA:HB1	1:E:553:LEU:HD11	1.80	0.63
3:D:902:AGS:S1G	1:E:332:ARG:NH1	2.71	0.63
1:C:367:THR:HG22	1:C:369:SER:H	1.63	0.63
1:F:377:LEU:HD21	1:F:542:VAL:HG11	1.81	0.63
1:A:805:ARG:NH1	3:A:901:AGS:S1G	2.70	0.63
1:D:357:ARG:HB3	1:E:197:ARG:HH12	1.64	0.63
1:D:702:THR:HG22	1:D:708:THR:HG22	1.79	0.62
1:C:407:ASP:O	1:C:408:SER:C	2.38	0.62
1:D:358:TYR:HE1	1:E:197:ARG:HG2	1.64	0.62
1:D:197:ARG:HG2	1:D:198:THR:HG23	1.81	0.62
1:C:617:ALA:HB1	1:C:677:LEU:HD21	1.81	0.62
3:C:902:AGS:O2G	3:C:902:AGS:O1B	2.17	0.62
1:E:245:MET:HB3	1:E:255:PHE:HD1	1.65	0.62
1:A:280:LEU:HD23	1:A:313:GLY:HA3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ASP:OD2	1:A:598:ARG:NH1	2.33	0.62
1:A:648:LEU:HD12	1:A:649:ILE:HG13	1.81	0.62
1:F:267:LYS:NZ	1:F:303:MET:O	2.34	0.61
1:C:528:MET:O	1:C:529:LEU:CB	2.35	0.61
1:C:449:LEU:HD12	1:C:449:LEU:O	1.99	0.61
1:A:329:ALA:O	1:A:333:ARG:NH1	2.33	0.61
1:E:539:ALA:HB1	1:E:553:LEU:HD22	1.82	0.61
1:E:799:ASP:O	1:E:801:VAL:N	2.29	0.61
1:E:822:MET:SD	1:E:827:GLN:NE2	2.66	0.61
1:B:648:LEU:HD12	1:B:649:ILE:HG13	1.82	0.61
3:B:901:AGS:O2G	3:B:901:AGS:O1B	2.18	0.61
1:C:159:GLN:N	1:C:265:ASP:OD2	2.34	0.61
1:C:411:VAL:O	1:C:413:ILE:N	2.34	0.60
1:F:608:PRO:HG2	1:F:611:VAL:HG11	1.82	0.60
1:F:757:ASN:ND2	1:F:760:GLU:OE1	2.32	0.60
3:B:901:AGS:S1G	1:C:746:ARG:NH2	2.74	0.60
1:E:610:GLY:HA3	1:E:803:GLY:HA3	1.84	0.59
1:F:423:LEU:HD22	1:F:449:LEU:HD13	1.83	0.59
1:F:776:LEU:HD21	1:F:819:LEU:HD21	1.84	0.59
1:C:431:SER:HA	1:C:442:LEU:HD21	1.84	0.59
1:E:692:LEU:HA	1:E:695:VAL:HB	1.84	0.59
1:D:389:ASP:OD2	1:E:332:ARG:NH2	2.35	0.59
1:B:641:GLU:HG3	1:B:643:HIS:CE1	2.37	0.59
1:A:604:MET:HB2	1:A:718:LEU:HB2	1.83	0.59
1:C:571:ARG:NH2	1:C:622:ASP:OD2	2.34	0.59
1:B:185:ASN:OD1	1:B:188:ARG:NH2	2.36	0.59
1:B:817:ASP:OD1	1:B:818:GLN:N	2.36	0.59
1:C:248:GLY:O	1:C:258:ARG:NH2	2.34	0.59
1:E:675:VAL:HG12	1:E:715:ILE:HB	1.85	0.59
1:F:237:ILE:HG12	1:F:274:ILE:HB	1.83	0.59
1:D:263:LEU:HD21	1:D:300:ILE:HG22	1.83	0.59
1:A:678:PHE:HB2	1:A:718:LEU:HD23	1.84	0.59
1:B:467:LYS:HG3	1:B:471:GLU:OE2	2.00	0.58
1:D:548:ILE:HG22	1:D:550:ALA:H	1.68	0.58
1:F:228:VAL:HB	1:F:232:LEU:HD23	1.85	0.58
1:A:305:ALA:HB2	1:A:333:ARG:HE	1.67	0.58
1:E:784:GLN:HB3	1:E:835:PRO:HA	1.84	0.58
1:A:666:GLU:OE1	1:A:670:ARG:NH2	2.36	0.58
1:C:530:LYS:HZ2	1:C:531:GLU:N	1.91	0.58
1:C:618:LYS:NZ	1:C:628:GLU:OE1	2.34	0.58
1:E:235:LYS:HD2	1:E:274:ILE:HD11	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:LEU:O	1:E:396:ASP:N	2.37	0.58
1:A:605:PHE:HB3	1:A:751:LEU:HB2	1.84	0.58
3:B:902:AGS:O1B	3:B:902:AGS:O2G	2.22	0.58
1:C:703:ASP:OD2	1:C:707:ARG:NH1	2.37	0.57
1:F:545:TRP:O	1:F:546:THR:OG1	2.22	0.57
1:C:245:MET:O	1:C:258:ARG:NH1	2.36	0.57
1:E:222:ARG:HG3	1:E:227:ASP:HB2	1.86	0.57
1:A:608:PRO:HG2	1:A:611:VAL:HG21	1.86	0.57
1:E:566:ASP:O	1:E:570:LYS:N	2.37	0.57
1:D:380:ARG:NH2	1:D:381:TYR:OH	2.37	0.57
3:A:901:AGS:O2G	3:A:901:AGS:O1B	2.22	0.57
1:B:464:GLN:O	1:B:468:ASN:HB2	2.04	0.57
1:F:411:VAL:O	1:F:412:GLU:HG3	2.04	0.57
1:F:697:ASP:OD2	1:F:746:ARG:NE	2.38	0.57
3:C:901:AGS:O1B	3:C:901:AGS:O2G	2.22	0.57
1:E:346:ASP:N	1:E:346:ASP:OD1	2.38	0.57
1:D:643:HIS:HD2	1:E:652:PRO:HG2	1.70	0.56
1:A:560:LYS:HE2	1:A:563:ARG:HH22	1.70	0.56
1:B:466:GLU:OE2	1:B:530:LYS:NZ	2.38	0.56
1:E:301:LYS:HD2	1:E:330:LEU:HB3	1.87	0.56
1:E:681:ILE:HG12	1:E:718:LEU:HD12	1.88	0.56
1:B:196:ARG:NH1	1:B:198:THR:O	2.38	0.56
1:B:805:ARG:NH2	3:B:901:AGS:S1G	2.77	0.56
1:E:181:ILE:O	4:E:901:ADP:N6	2.36	0.56
1:A:415:GLU:OE1	1:B:188:ARG:NH1	2.29	0.56
1:E:771:GLN:OE1	1:E:808:ARG:NH2	2.38	0.56
1:F:254:GLU:OE2	1:F:258:ARG:NH2	2.39	0.56
1:C:235:LYS:NZ	1:C:271:GLY:O	2.32	0.56
3:D:902:AGS:O2B	3:D:902:AGS:O2A	2.24	0.56
1:E:610:GLY:N	4:E:902:ADP:O3B	2.35	0.56
3:A:902:AGS:O1B	3:A:902:AGS:O2G	2.24	0.55
1:E:207:GLU:O	1:E:212:LYS:NZ	2.38	0.55
1:F:462:ARG:NH1	1:F:466:GLU:OE1	2.39	0.55
1:C:181:ILE:HD11	1:C:353:GLY:HA3	1.88	0.55
1:F:605:PHE:HB3	1:F:751:LEU:HB2	1.87	0.55
1:D:681:ILE:HG21	1:D:718:LEU:HD12	1.88	0.55
1:E:232:LEU:HA	1:E:235:LYS:HE3	1.88	0.55
1:C:414:ASP:HB3	1:D:188:ARG:NH1	2.21	0.55
1:A:378:SER:HB2	1:A:394:LEU:HD11	1.89	0.55
1:B:300:ILE:HG22	1:B:304:LEU:HG	1.89	0.55
1:C:434:GLU:O	1:C:434:GLU:HG2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:ILE:HB	1:E:390:LYS:HD2	1.88	0.55
1:F:169:THR:HG21	1:F:236:THR:HA	1.89	0.55
1:D:675:VAL:HG12	1:D:715:ILE:HB	1.89	0.55
1:E:189:ARG:HD2	1:E:192:GLN:HE21	1.72	0.55
1:F:262:VAL:O	1:F:266:ILE:HG12	2.07	0.55
1:C:422:ARG:HA	1:C:425:ILE:CD1	2.36	0.55
1:C:431:SER:HA	1:C:442:LEU:CD2	2.37	0.55
1:C:409:ARG:HB2	1:C:410:PRO:CD	2.35	0.54
1:C:826:GLY:O	1:C:827:GLN:HG2	2.07	0.54
1:D:826:GLY:O	1:D:827:GLN:HG2	2.07	0.54
1:C:466:GLU:OE2	1:C:528:MET:O	2.25	0.54
1:F:196:ARG:NH2	1:F:335:GLN:OE1	2.39	0.54
1:C:530:LYS:HE3	1:C:532:GLU:CD	2.26	0.54
1:D:199:LYS:HD2	1:D:333:ARG:HA	1.90	0.54
1:F:171:ARG:HG2	1:F:176:LYS:HD2	1.89	0.54
1:F:364:VAL:HG11	1:F:402:LEU:HD22	1.90	0.54
1:F:604:MET:HB2	1:F:718:LEU:HB2	1.88	0.54
1:B:436:GLU:OE1	1:B:780:ARG:NH2	2.41	0.54
1:C:411:VAL:C	1:C:413:ILE:N	2.59	0.54
1:D:584:ASP:OD2	1:D:587:ARG:NH1	2.35	0.54
1:D:761:LEU:HD22	1:D:798:PHE:CZ	2.42	0.54
1:B:174:GLU:OE1	1:B:174:GLU:N	2.41	0.54
1:D:220:ALA:HB2	1:D:237:ILE:HD11	1.89	0.54
1:F:761:LEU:O	1:F:765:VAL:HG23	2.07	0.54
1:B:415:GLU:OE1	1:C:188:ARG:NH2	2.41	0.54
1:B:665:THR:HG23	1:B:709:VAL:HG21	1.90	0.54
1:E:366:ILE:HA	1:E:533:VAL:HG22	1.90	0.54
1:D:757:ASN:HD21	1:D:760:GLU:HB2	1.71	0.54
1:C:197:ARG:HG2	1:C:198:THR:HG23	1.88	0.53
1:D:178:ASP:O	1:D:221:GLN:NE2	2.41	0.53
1:A:252:ARG:NH2	1:F:287:GLY:O	2.41	0.53
1:C:641:GLU:HG3	1:C:643:HIS:CE1	2.44	0.53
1:E:346:ASP:O	1:E:350:ILE:HG13	2.08	0.53
1:D:194:LEU:HD11	1:D:310:ARG:HB3	1.89	0.53
1:F:805:ARG:NE	3:F:902:AGS:H5'1	2.23	0.53
3:B:902:AGS:S1G	1:C:333:ARG:NH1	2.82	0.53
1:C:418:ARG:NH2	1:D:227:ASP:OD1	2.41	0.53
1:C:608:PRO:HG2	1:C:611:VAL:HG21	1.90	0.53
1:E:696:LEU:HD21	1:E:743:PHE:HE1	1.74	0.53
1:C:462:ARG:NH1	1:C:528:MET:HE1	2.24	0.53
1:C:565:GLU:HG2	1:C:579:VAL:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ARG:NH1	1:C:475:ASP:OD1	2.42	0.52
1:E:770:ALA:O	1:E:774:LYS:HG2	2.10	0.52
1:B:324:ILE:HG22	1:B:331:GLU:HB3	1.92	0.52
1:C:280:LEU:HD23	1:C:313:GLY:HA3	1.90	0.52
1:D:775:ARG:NH1	1:E:593:VAL:O	2.42	0.52
1:A:387:LEU:HB2	1:A:390:LYS:HE2	1.90	0.52
1:A:826:GLY:O	1:A:827:GLN:HG2	2.10	0.52
1:D:189:ARG:HA	1:D:192:GLN:HG2	1.92	0.52
1:E:656:VAL:HG23	1:E:657:GLY:H	1.74	0.52
1:C:426:GLU:HG2	1:D:352:ARG:HD2	1.92	0.52
1:C:418:ARG:HA	1:C:421:ARG:HH12	1.74	0.52
1:C:568:LEU:HD23	1:C:579:VAL:HG13	1.92	0.52
1:D:187:ILE:HD13	1:D:215:ILE:HG23	1.90	0.52
1:C:222:ARG:HG2	1:C:227:ASP:HB2	1.92	0.52
1:E:843:ASP:OD1	1:E:843:ASP:N	2.43	0.52
1:C:421:ARG:HB2	1:C:421:ARG:NH1	2.22	0.51
1:B:682:GLU:OE2	1:B:683:LYS:NZ	2.43	0.51
1:C:432:LYS:NZ	1:C:432:LYS:CB	2.73	0.51
1:A:213:THR:O	1:A:217:GLU:HG2	2.10	0.51
1:F:274:ILE:HG12	1:F:310:ARG:HG3	1.92	0.51
1:A:301:LYS:HE2	1:A:330:LEU:HG	1.92	0.51
1:D:568:LEU:HD23	1:D:579:VAL:HG13	1.92	0.51
1:E:394:LEU:O	1:E:397:GLU:N	2.37	0.51
1:C:462:ARG:NH1	1:C:528:MET:HE3	2.25	0.51
1:D:342:PRO:HB2	1:D:346:ASP:HB2	1.93	0.51
1:F:180:VAL:HG11	1:F:218:GLY:HA3	1.91	0.51
1:A:649:ILE:HG23	1:A:703:ASP:HA	1.93	0.51
1:C:467:LYS:CB	1:C:467:LYS:NZ	2.73	0.51
1:C:467:LYS:HZ2	1:C:467:LYS:HB2	1.76	0.51
1:E:284:VAL:HG11	1:E:324:ILE:HG13	1.93	0.51
1:F:301:LYS:HD2	1:F:330:LEU:HD22	1.93	0.51
1:F:826:GLY:O	1:F:827:GLN:HG2	2.11	0.51
1:C:426:GLU:CD	1:D:352:ARG:HD2	2.31	0.51
1:C:546:THR:O	1:C:548:ILE:N	2.44	0.51
1:D:666:GLU:OE2	1:D:669:ARG:NH2	2.43	0.51
1:C:761:LEU:HD12	1:C:798:PHE:HD1	1.76	0.50
1:E:235:LYS:HD3	1:E:272:GLN:HB3	1.92	0.50
1:E:764:ILE:O	1:E:768:GLN:HG2	2.11	0.50
1:A:635:ASP:OD1	1:A:635:ASP:N	2.44	0.50
1:C:166:THR:OG1	1:C:167:ASP:N	2.45	0.50
1:F:430:LEU:HD22	1:F:442:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:HA	1:C:388:PRO:HG2	1.93	0.50
1:E:639:TYR:OH	1:E:647:ARG:NH2	2.45	0.50
1:F:389:ASP:O	1:F:392:ILE:N	2.44	0.50
1:B:608:PRO:HG2	1:B:611:VAL:HG21	1.92	0.50
1:E:538:ILE:O	1:E:542:VAL:HG23	2.11	0.50
1:F:645:VAL:HG22	1:F:688:VAL:HG12	1.94	0.50
1:A:196:ARG:HB2	1:A:200:ASN:HB3	1.92	0.50
1:A:832:ASP:OD1	1:A:833:THR:N	2.44	0.50
1:E:648:LEU:HA	1:E:663:GLN:H	1.77	0.50
1:F:576:LYS:HA	1:F:579:VAL:HG12	1.92	0.50
1:B:199:LYS:HD2	1:B:333:ARG:HA	1.93	0.50
1:D:210:VAL:HA	1:D:388:PRO:HG2	1.93	0.50
1:D:316:THR:HG22	1:D:318:ASP:H	1.76	0.50
1:C:419:LEU:C	1:C:419:LEU:HD23	2.32	0.50
1:F:805:ARG:NH2	3:F:902:AGS:S1G	2.84	0.50
1:B:196:ARG:HH12	1:B:199:LYS:HB3	1.77	0.49
1:B:681:ILE:HG22	1:B:720:SER:HB3	1.93	0.49
1:E:757:ASN:HB3	1:E:760:GLU:HG3	1.93	0.49
1:C:690:ASP:OD1	1:C:740:LYS:NZ	2.38	0.49
1:E:174:GLU:HB3	1:E:176:LYS:HZ2	1.77	0.49
1:E:213:THR:HA	1:E:216:VAL:HG12	1.93	0.49
1:F:201:ASN:ND2	1:F:333:ARG:O	2.39	0.49
1:A:201:ASN:HD22	1:A:304:LEU:HD22	1.76	0.49
1:C:419:LEU:HD23	1:C:419:LEU:O	2.12	0.49
1:D:645:VAL:HG11	1:D:691:VAL:HG21	1.94	0.49
1:E:775:ARG:O	1:E:778:GLN:NE2	2.46	0.49
1:C:638:GLU:OE1	1:C:647:ARG:NH2	2.46	0.49
1:F:266:ILE:HA	1:F:273:ILE:HD11	1.95	0.49
1:C:407:ASP:C	1:C:408:SER:O	2.49	0.48
1:C:474:ARG:O	1:C:475:ASP:C	2.50	0.48
1:F:416:VAL:O	1:F:420:VAL:HG23	2.13	0.48
1:B:201:ASN:HB3	1:B:311:LEU:H	1.78	0.48
1:D:235:LYS:HE3	1:D:271:GLY:O	2.14	0.48
3:A:902:AGS:S1G	1:B:333:ARG:NH2	2.81	0.48
1:C:568:LEU:HD13	1:C:623:PHE:CE1	2.48	0.48
1:E:348:ILE:HA	1:E:351:LEU:HD12	1.94	0.48
1:C:378:SER:HB3	1:C:394:LEU:HD11	1.95	0.48
1:E:614:THR:OG1	4:E:902:ADP:O2A	2.31	0.48
1:B:277:ILE:HG13	1:B:311:LEU:HD11	1.94	0.48
1:C:530:LYS:NZ	1:C:530:LYS:CA	2.73	0.48
1:C:836:VAL:HG12	1:C:845:LEU:HG	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563:ARG:O	1:E:565:GLU:HG3	2.13	0.48
1:F:366:ILE:HA	1:F:533:VAL:HG22	1.94	0.48
1:A:647:ARG:NH2	1:B:702:THR:OG1	2.47	0.48
1:A:836:VAL:HG12	1:A:845:LEU:HD13	1.95	0.48
1:C:217:GLU:O	1:C:221:GLN:HG3	2.14	0.48
1:C:378:SER:O	1:C:390:LYS:HD2	2.13	0.48
3:C:901:AGS:S1G	1:D:746:ARG:NH2	2.87	0.48
1:D:585:ALA:HB2	1:D:603:PHE:HZ	1.78	0.48
1:E:321:ARG:HA	1:E:325:GLU:HG3	1.95	0.48
1:E:221:GLN:O	1:E:224:VAL:HG12	2.14	0.48
1:F:274:ILE:HG23	1:F:310:ARG:HB2	1.96	0.48
1:B:757:ASN:HB2	1:B:760:GLU:HG2	1.96	0.47
1:F:301:LYS:O	1:F:333:ARG:NH1	2.47	0.47
1:E:757:ASN:N	1:E:760:GLU:OE2	2.46	0.47
1:B:605:PHE:HB3	1:B:751:LEU:HB2	1.96	0.47
1:C:366:ILE:HA	1:C:533:VAL:HG22	1.96	0.47
1:D:199:LYS:HE3	1:D:335:GLN:HE21	1.79	0.47
1:F:259:LEU:HA	1:F:262:VAL:HG22	1.96	0.47
1:D:201:ASN:ND2	1:D:310:ARG:O	2.39	0.47
1:D:780:ARG:HG3	1:D:831:GLY:N	2.30	0.47
1:B:637:SER:OG	1:C:694:GLN:OE1	2.31	0.47
1:C:167:ASP:OD1	1:C:170:ALA:N	2.47	0.47
1:C:191:VAL:HG13	1:C:232:LEU:HD12	1.95	0.47
1:C:467:LYS:NZ	1:C:467:LYS:HB2	2.29	0.47
1:E:552:ARG:H	1:E:552:ARG:HD3	1.79	0.47
1:F:351:LEU:HB3	1:F:371:LEU:HD11	1.96	0.47
1:F:453:LYS:HE3	1:F:453:LYS:HB2	1.74	0.47
1:A:420:VAL:HG13	1:A:449:LEU:HD11	1.96	0.47
3:B:902:AGS:S1G	1:C:332:ARG:HD3	2.55	0.47
1:E:228:VAL:HB	1:E:232:LEU:HD21	1.97	0.47
1:F:354:LEU:HD11	3:F:901:AGS:H2	1.95	0.47
1:C:207:GLU:HG3	1:C:386:PHE:CE1	2.49	0.46
1:C:254:GLU:O	1:C:257:GLU:HG3	2.15	0.46
1:C:824:LEU:HD23	1:D:591:ALA:HB2	1.97	0.46
1:E:634:ILE:HD11	1:E:678:PHE:CE1	2.50	0.46
1:B:765:VAL:HG22	1:B:807:LEU:HD11	1.98	0.46
1:F:223:ILE:HD11	1:F:232:LEU:HD11	1.97	0.46
1:B:638:GLU:OE1	1:B:647:ARG:NH2	2.48	0.46
1:B:703:ASP:OD1	1:B:703:ASP:N	2.49	0.46
1:D:189:ARG:HG3	1:D:192:GLN:HE21	1.80	0.46
1:B:210:VAL:HA	1:B:388:PRO:HG2	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ILE:O	1:C:327:ASP:N	2.48	0.46
1:C:402:LEU:HD11	1:C:530:LYS:O	2.16	0.46
1:F:170:ALA:O	1:F:174:GLU:HG2	2.16	0.46
1:B:578:ALA:HA	1:B:751:LEU:HD13	1.97	0.46
1:D:792:TRP:CZ3	1:D:843:ASP:HB2	2.50	0.46
1:F:167:ASP:OD1	1:F:170:ALA:HB3	2.15	0.46
1:B:373:ALA:O	1:B:377:LEU:HB2	2.16	0.46
1:B:422:ARG:HD2	1:C:181:ILE:HG23	1.97	0.46
1:B:808:ARG:HH22	1:C:598:ARG:NH1	2.12	0.46
1:F:280:LEU:O	1:F:283:ILE:HG12	2.16	0.46
1:B:785:VAL:HA	1:B:836:VAL:HG22	1.96	0.46
1:E:692:LEU:O	1:E:696:LEU:HG	2.16	0.46
1:E:741:PRO:O	1:E:745:ASN:ND2	2.49	0.46
1:E:703:ASP:OD1	1:E:703:ASP:N	2.47	0.46
1:D:822:MET:O	1:D:828:VAL:HB	2.16	0.46
1:E:263:LEU:HD12	1:E:303:MET:SD	2.56	0.45
1:A:223:ILE:HG12	1:A:228:VAL:HG11	1.97	0.45
1:B:670:ARG:HD3	1:C:317:LEU:HD21	1.98	0.45
1:C:792:TRP:HE1	1:C:796:ARG:NH2	2.13	0.45
1:E:372:VAL:O	1:E:376:THR:HG22	2.16	0.45
1:F:539:ALA:HA	1:F:542:VAL:HG12	1.97	0.45
1:A:328:ALA:HA	1:A:331:GLU:HG3	1.98	0.45
1:A:401:ARG:HH22	1:A:411:VAL:HG21	1.82	0.45
1:F:160:ALA:N	1:F:265:ASP:OD2	2.39	0.45
1:F:301:LYS:NZ	1:F:329:ALA:O	2.48	0.45
3:D:901:AGS:O2G	3:D:901:AGS:O1B	2.32	0.45
1:F:368:ASP:O	1:F:372:VAL:HG23	2.16	0.45
1:B:531:GLU:N	1:B:531:GLU:OE1	2.49	0.45
1:B:656:VAL:HG23	1:B:657:GLY:H	1.81	0.45
1:E:183:ARG:HD3	1:E:215:ILE:HD11	1.99	0.45
1:E:254:GLU:HG3	1:E:258:ARG:HG3	1.99	0.45
1:E:555:GLU:OE2	1:E:558:THR:OG1	2.25	0.45
1:D:298:ASN:OD1	1:D:301:LYS:HD3	2.17	0.45
1:B:611:VAL:HG11	1:B:753:PHE:HB3	1.98	0.45
1:E:181:ILE:HD11	1:E:350:ILE:HA	1.99	0.45
1:E:786:SER:OG	1:E:788:PRO:HD2	2.16	0.45
1:A:548:ILE:HD13	1:A:713:ASN:HD21	1.82	0.45
1:C:426:GLU:CG	1:D:352:ARG:HD2	2.46	0.45
1:A:656:VAL:HG23	1:A:657:GLY:H	1.82	0.45
1:A:766:ASP:OD1	1:A:767:ILE:N	2.50	0.45
1:C:422:ARG:O	1:C:425:ILE:HG12	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:566:ASP:O	1:C:570:LYS:NZ	2.47	0.45
1:C:548:ILE:HD13	1:C:713:ASN:HD21	1.82	0.45
1:D:352:ARG:NE	1:D:368:ASP:OD1	2.44	0.45
1:B:201:ASN:OD1	1:B:201:ASN:N	2.50	0.44
1:C:474:ARG:HG2	1:C:475:ASP:N	2.31	0.44
1:C:766:ASP:OD1	1:C:790:LYS:HD3	2.17	0.44
1:C:427:GLU:HA	1:C:445:LEU:HD23	1.99	0.44
1:D:685:HIS:O	1:D:687:ASP:N	2.41	0.44
1:D:822:MET:SD	1:D:827:GLN:NE2	2.90	0.44
1:F:582:VAL:HG22	1:F:603:PHE:CZ	2.52	0.44
1:C:419:LEU:C	1:C:419:LEU:CD2	2.85	0.44
1:A:333:ARG:NH2	3:F:901:AGS:O2G	2.50	0.44
1:A:765:VAL:HG21	1:A:794:ALA:HB2	1.99	0.44
1:B:820:ALA:O	1:B:824:LEU:HG	2.17	0.44
1:C:432:LYS:NZ	1:C:432:LYS:HB3	2.33	0.44
1:C:820:ALA:O	1:C:824:LEU:HG	2.17	0.44
1:B:627:ASP:OD1	1:B:628:GLU:N	2.38	0.44
1:D:321:ARG:HA	1:D:325:GLU:HB2	1.98	0.44
1:A:441:ARG:NH2	1:B:368:ASP:OD2	2.35	0.44
1:B:435:ASP:OD1	1:B:436:GLU:N	2.40	0.44
1:B:561:LEU:HD21	1:B:590:ARG:HG3	1.99	0.44
1:D:634:ILE:HD11	1:D:678:PHE:CE1	2.52	0.44
1:D:685:HIS:CE1	1:D:687:ASP:HB2	2.53	0.44
1:E:403:ARG:O	1:E:406:ILE:HG12	2.18	0.44
1:F:685:HIS:HD2	1:F:687:ASP:HB2	1.83	0.44
1:B:287:GLY:HA3	1:B:296:ALA:H	1.82	0.44
1:C:761:LEU:O	1:C:765:VAL:HG23	2.17	0.44
1:D:409:ARG:HA	1:D:410:PRO:HD3	1.85	0.44
1:A:843:ASP:OD1	1:A:843:ASP:N	2.51	0.44
1:B:647:ARG:HD2	1:C:704:GLY:HA2	2.00	0.44
1:B:775:ARG:NH1	1:C:593:VAL:O	2.50	0.44
1:B:836:VAL:HG12	1:B:845:LEU:HD23	1.98	0.44
1:E:532:GLU:OE1	1:E:532:GLU:N	2.51	0.44
1:B:633:ARG:HG3	1:B:677:LEU:HD23	2.00	0.44
1:E:392:ILE:O	1:E:396:ASP:HB3	2.18	0.44
1:A:538:ILE:O	1:A:542:VAL:HG23	2.18	0.43
1:C:164:TYR:CZ	1:C:258:ARG:HD3	2.53	0.43
1:F:355:LYS:HD2	1:F:355:LYS:O	2.18	0.43
1:A:560:LYS:HE2	1:A:563:ARG:NH2	2.33	0.43
1:A:564:MET:HG3	1:A:623:PHE:CZ	2.54	0.43
1:A:670:ARG:HD3	1:B:317:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ALA:HB1	1:B:550:ALA:O	2.18	0.43
1:C:254:GLU:O	1:C:258:ARG:HG3	2.18	0.43
1:A:418:ARG:HH12	1:B:222:ARG:CZ	2.32	0.43
1:C:456:LEU:C	1:C:456:LEU:CD2	2.86	0.43
1:C:459:LEU:HD12	1:C:459:LEU:O	2.19	0.43
1:E:554:LEU:HD12	1:E:555:GLU:H	1.84	0.43
1:F:760:GLU:OE2	1:F:760:GLU:N	2.51	0.43
1:D:676:VAL:HB	1:D:716:LEU:HD23	1.99	0.43
1:E:542:VAL:O	1:E:546:THR:HG22	2.19	0.43
1:A:419:LEU:HD22	1:A:452:GLN:HG2	2.00	0.43
1:D:692:LEU:HD23	1:D:692:LEU:H	1.84	0.43
1:F:267:LYS:HE3	1:F:303:MET:HB3	2.00	0.43
1:F:417:GLU:OE1	1:F:421:ARG:NH2	2.48	0.43
1:A:372:VAL:O	1:A:376:THR:HG23	2.18	0.43
1:A:613:LYS:HA	1:A:753:PHE:HE2	1.83	0.43
1:C:462:ARG:HH11	1:C:528:MET:HE3	1.82	0.43
1:F:420:VAL:HG13	1:F:449:LEU:HD11	2.01	0.43
1:F:649:ILE:O	1:F:703:ASP:HB2	2.19	0.43
1:C:467:LYS:CB	1:C:467:LYS:HZ2	2.29	0.42
1:F:245:MET:O	1:F:258:ARG:NH1	2.47	0.42
1:F:301:LYS:HE3	1:F:301:LYS:HB3	1.65	0.42
1:F:700:ARG:HH12	1:F:712:ARG:HH21	1.67	0.42
1:A:201:ASN:ND2	1:A:304:LEU:HD22	2.33	0.42
1:A:366:ILE:HA	1:A:533:VAL:HG22	2.00	0.42
1:A:379:ASP:HB2	1:A:387:LEU:HD21	2.01	0.42
1:A:548:ILE:H	1:A:548:ILE:HG13	1.65	0.42
1:A:721:ASN:ND2	1:B:742:GLU:OE1	2.52	0.42
1:B:668:VAL:HG21	1:B:711:PHE:CE1	2.54	0.42
1:C:765:VAL:HG22	1:C:807:LEU:HD11	2.00	0.42
1:D:756:LEU:HD23	1:D:756:LEU:HA	1.80	0.42
1:D:787:LEU:O	1:D:791:ARG:HD3	2.19	0.42
1:E:552:ARG:NH1	1:E:553:LEU:HD23	2.35	0.42
1:F:186:GLU:OE1	1:F:186:GLU:N	2.50	0.42
1:F:668:VAL:HG21	1:F:711:PHE:CZ	2.53	0.42
1:A:260:LYS:HB3	1:A:260:LYS:HE3	1.85	0.42
1:B:373:ALA:HA	1:B:376:THR:HG22	2.02	0.42
1:C:740:LYS:HE3	1:C:740:LYS:HB2	1.84	0.42
1:E:723:GLY:O	1:E:724:SER:OG	2.35	0.42
1:E:739:PHE:HB2	1:E:744:ILE:HD11	2.02	0.42
1:B:280:LEU:HD23	1:B:313:GLY:HA3	2.02	0.42
1:C:817:ASP:N	1:C:817:ASP:OD1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:573:ILE:O	3:D:901:AGS:N6	2.48	0.42
1:E:689:PHE:HA	1:E:692:LEU:HG	2.01	0.42
1:F:434:GLU:O	1:F:434:GLU:HG2	2.20	0.42
1:B:539:ALA:HA	1:B:542:VAL:HG12	2.00	0.42
1:B:590:ARG:HD2	1:B:590:ARG:HA	1.78	0.42
1:B:765:VAL:CG2	1:B:807:LEU:HD11	2.49	0.42
1:E:538:ILE:O	1:E:541:VAL:HG12	2.20	0.42
1:C:422:ARG:HA	1:C:425:ILE:CG1	2.50	0.42
1:C:548:ILE:H	1:C:548:ILE:HG13	1.65	0.42
1:D:588:ARG:HG2	1:D:593:VAL:O	2.20	0.42
1:D:710:ASP:HB2	1:D:712:ARG:HG3	2.01	0.42
1:F:700:ARG:HA	1:F:710:ASP:HA	2.01	0.42
1:F:741:PRO:O	1:F:745:ASN:ND2	2.52	0.42
1:A:327:ASP:O	1:A:330:LEU:N	2.46	0.42
1:B:833:THR:O	1:B:833:THR:OG1	2.37	0.42
1:D:710:ASP:OD1	1:D:710:ASP:N	2.50	0.42
1:D:720:SER:OG	1:D:721:ASN:N	2.52	0.42
1:A:222:ARG:HG3	1:A:227:ASP:HB2	2.02	0.42
1:A:673:TYR:CG	1:A:673:TYR:O	2.73	0.42
1:B:605:PHE:HE2	1:B:613:LYS:O	2.03	0.42
1:F:742:GLU:HA	1:F:745:ASN:HD21	1.84	0.42
1:B:411:VAL:HG12	1:B:412:GLU:N	2.35	0.41
1:C:423:LEU:HD23	1:C:423:LEU:HA	1.84	0.41
1:D:283:ILE:O	1:D:297:GLY:HA3	2.20	0.41
1:D:172:ALA:HB3	1:D:224:VAL:HG21	2.01	0.41
1:E:275:THR:OG1	1:E:276:PHE:N	2.53	0.41
1:E:646:ALA:HA	1:E:649:ILE:HG22	2.02	0.41
1:E:723:GLY:HA3	1:E:731:VAL:HG12	2.01	0.41
1:B:254:GLU:O	1:B:257:GLU:HG3	2.20	0.41
1:B:696:LEU:HD23	1:B:716:LEU:HD22	2.01	0.41
1:E:680:GLU:HG2	1:E:683:LYS:HG2	2.01	0.41
1:F:766:ASP:OD1	1:F:790:LYS:HD3	2.20	0.41
1:B:635:ASP:OD1	1:B:635:ASP:N	2.43	0.41
1:B:638:GLU:OE2	1:C:694:GLN:NE2	2.53	0.41
1:C:761:LEU:HD23	1:C:761:LEU:HA	1.91	0.41
1:F:408:SER:OG	1:F:409:ARG:N	2.54	0.41
1:A:203:VAL:N	1:A:335:GLN:O	2.53	0.41
1:A:207:GLU:O	1:A:210:VAL:HG22	2.20	0.41
1:B:625:PHE:CZ	1:B:674:THR:HA	2.55	0.41
1:C:409:ARG:HG2	1:C:409:ARG:HH11	1.83	0.41
1:E:167:ASP:OD1	1:E:170:ALA:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:729:GLU:HG2	1:F:730:GLN:H	1.85	0.41
1:A:359:GLU:HG2	1:A:364:VAL:O	2.21	0.41
1:A:403:ARG:O	1:A:406:ILE:HG22	2.20	0.41
1:B:622:ASP:O	1:B:626:ASP:N	2.53	0.41
1:C:646:ALA:HA	1:C:649:ILE:HG22	2.02	0.41
1:C:699:GLY:O	1:C:710:ASP:HA	2.21	0.41
1:D:608:PRO:O	1:D:613:LYS:NZ	2.52	0.41
1:D:757:ASN:ND2	1:D:760:GLU:H	2.19	0.41
1:E:756:LEU:HD23	1:E:756:LEU:HA	1.89	0.41
1:F:658:TYR:HH	1:F:705:HIS:CD2	2.34	0.41
1:D:809:ARG:HG3	1:E:746:ARG:HH12	1.85	0.41
1:E:562:LEU:HA	1:E:587:ARG:NH2	2.36	0.41
1:E:678:PHE:HB2	1:E:718:LEU:HD13	2.03	0.41
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.94	0.41
1:A:758:PRO:HG3	1:A:798:PHE:CZ	2.55	0.41
1:B:559:ALA:O	1:B:563:ARG:HG2	2.21	0.41
1:B:727:SER:OG	1:B:728:ALA:N	2.54	0.41
1:C:571:ARG:HD2	1:C:619:ALA:HB2	2.03	0.41
1:C:697:ASP:OD1	1:C:697:ASP:N	2.48	0.41
1:C:828:VAL:HG12	1:C:828:VAL:O	2.21	0.41
1:D:779:ARG:HH12	1:D:823:LEU:HD21	1.85	0.41
1:F:183:ARG:NH2	1:F:186:GLU:OE2	2.53	0.41
1:F:450:ALA:HA	1:F:453:LYS:HE2	2.02	0.41
1:A:726:GLY:HA3	1:A:730:GLN:HB2	2.02	0.41
1:C:562:LEU:HD23	1:C:562:LEU:HA	1.88	0.41
1:D:727:SER:N	1:D:730:GLN:OE1	2.42	0.41
1:E:622:ASP:HB3	1:E:628:GLU:HA	2.02	0.41
1:A:211:GLY:HA2	3:A:902:AGS:O2A	2.20	0.40
1:A:817:ASP:OD1	1:A:818:GLN:N	2.54	0.40
1:F:259:LEU:HD23	1:F:299:MET:SD	2.61	0.40
1:A:548:ILE:HD13	1:A:713:ASN:ND2	2.35	0.40
1:B:260:LYS:HB3	1:B:260:LYS:HE2	1.71	0.40
1:C:414:ASP:CB	1:D:188:ARG:NH1	2.83	0.40
1:C:774:LYS:HB3	1:C:774:LYS:HE2	1.90	0.40
1:D:799:ASP:OD1	1:D:801:VAL:HG12	2.21	0.40
1:F:805:ARG:CZ	3:F:902:AGS:S1G	3.09	0.40
1:C:740:LYS:O	1:C:744:ILE:HG13	2.21	0.40
1:F:236:THR:O	1:F:273:ILE:HA	2.22	0.40
1:F:798:PHE:O	1:F:798:PHE:CG	2.74	0.40
1:A:746:ARG:H	1:A:746:ARG:HG2	1.76	0.40
1:B:808:ARG:HH12	1:C:598:ARG:NH1	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:VAL:O	1:C:194:LEU:HB2	2.21	0.40
1:C:236:THR:O	1:C:236:THR:OG1	2.33	0.40
1:E:277:ILE:HD12	1:E:311:LEU:HD11	2.03	0.40
1:F:190:VAL:HA	1:F:193:VAL:HG22	2.03	0.40
1:F:729:GLU:HG2	1:F:730:GLN:N	2.36	0.40
1:A:403:ARG:HA	1:A:403:ARG:HD2	1.90	0.40
1:A:772:LEU:O	1:A:776:LEU:HG	2.21	0.40
1:B:378:SER:HB3	1:B:394:LEU:HD11	2.03	0.40
1:C:530:LYS:NZ	1:C:530:LYS:C	2.73	0.40
1:D:627:ASP:OD2	1:D:629:ARG:HG2	2.22	0.40
1:D:757:ASN:HA	1:D:758:PRO:HD3	1.96	0.40
1:E:324:ILE:HA	1:E:328:ALA:HB2	2.04	0.40
1:E:693:LEU:HD23	1:E:693:LEU:HA	1.93	0.40
1:E:761:LEU:HD23	1:E:794:ALA:HB1	2.04	0.40
1:F:187:ILE:HA	1:F:190:VAL:HG12	2.04	0.40
1:F:318:ASP:O	1:F:322:LYS:HG2	2.21	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	614/848 (72%)	552 (90%)	62 (10%)	0	100	100
1	B	623/848 (74%)	572 (92%)	51 (8%)	0	100	100
1	C	630/848 (74%)	559 (89%)	65 (10%)	6 (1%)	15	46
1	D	556/848 (66%)	496 (89%)	60 (11%)	0	100	100
1	E	540/848 (64%)	489 (91%)	50 (9%)	1 (0%)	47	77
1	F	614/848 (72%)	549 (89%)	65 (11%)	0	100	100
All	All	3577/5088 (70%)	3217 (90%)	353 (10%)	7 (0%)	50	77

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	408	SER
1	C	475	ASP
1	C	529	LEU
1	E	395	VAL
1	C	412	GLU
1	C	410	PRO
1	C	547	GLY

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	506/682 (74%)	503 (99%)	3 (1%)	86	91
1	B	515/682 (76%)	508 (99%)	7 (1%)	67	82
1	C	519/682 (76%)	489 (94%)	30 (6%)	20	50
1	D	455/682 (67%)	454 (100%)	1 (0%)	93	97
1	E	448/682 (66%)	446 (100%)	2 (0%)	91	95
1	F	506/682 (74%)	505 (100%)	1 (0%)	93	97
All	All	2949/4092 (72%)	2905 (98%)	44 (2%)	66	81

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	461	THR
1	A	779	ARG
1	A	833	THR
1	B	467	LYS
1	B	470	ILE
1	B	471	GLU
1	B	473	VAL
1	B	476	LEU
1	B	580	THR
1	B	603	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	409	ARG
1	C	411	VAL
1	C	412	GLU
1	C	413	ILE
1	C	418	ARG
1	C	421	ARG
1	C	425	ILE
1	C	426	GLU
1	C	427	GLU
1	C	428	MET
1	C	430	LEU
1	C	432	LYS
1	C	433	GLU
1	C	440	GLU
1	C	442	LEU
1	C	444	LYS
1	C	446	ARG
1	C	447	SER
1	C	449	LEU
1	C	452	GLN
1	C	453	LYS
1	C	455	LYS
1	C	456	LEU
1	C	458	GLU
1	C	459	LEU
1	C	464	GLN
1	C	467	LYS
1	C	529	LEU
1	C	530	LYS
1	C	738	THR
1	D	791	ARG
1	E	385	ARG
1	E	552	ARG
1	F	355	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	272	GLN
1	B	281	HIS
1	B	361	HIS
1	B	643	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	GLN
1	C	643	HIS
1	C	663	GLN
1	C	685	HIS
1	D	335	GLN
1	D	643	HIS
1	D	757	ASN
1	E	192	GLN
1	E	268	ASN
1	E	323	HIS
1	E	745	ASN
1	F	281	HIS
1	F	361	HIS
1	F	464	GLN
1	F	643	HIS
1	F	685	HIS
1	F	745	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)

12 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	A	901	-	26,33,33	0.72	1 (3%)	26,52,52	1.16	2 (7%)
3	AGS	F	901	-	26,33,33	1.88	3 (11%)	26,52,52	1.58	4 (15%)
4	ADP	E	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
3	AGS	D	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.11	2 (7%)
4	ADP	E	902	-	24,29,29	0.94	1 (4%)	29,45,45	1.50	4 (13%)
3	AGS	C	902	-	26,33,33	0.71	1 (3%)	26,52,52	1.11	2 (7%)
3	AGS	B	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.14	2 (7%)
3	AGS	C	901	-	26,33,33	0.71	1 (3%)	26,52,52	1.16	2 (7%)
3	AGS	A	902	-	26,33,33	0.70	1 (3%)	26,52,52	1.15	2 (7%)
3	AGS	D	902	-	26,33,33	0.71	1 (3%)	26,52,52	1.14	2 (7%)
3	AGS	B	902	-	26,33,33	0.70	0	26,52,52	1.15	2 (7%)
3	AGS	F	902	-	26,33,33	1.86	3 (11%)	26,52,52	1.62	4 (15%)

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	A	901	-	-	3/17/38/38	0/3/3/3
3	AGS	F	901	-	-	3/17/38/38	0/3/3/3
4	ADP	E	901	-	-	2/12/32/32	0/3/3/3
3	AGS	D	901	-	-	0/17/38/38	0/3/3/3
4	ADP	E	902	-	-	1/12/32/32	0/3/3/3
3	AGS	C	902	-	-	5/17/38/38	0/3/3/3
3	AGS	B	901	-	-	5/17/38/38	0/3/3/3
3	AGS	C	901	-	-	2/17/38/38	0/3/3/3
3	AGS	A	902	-	-	4/17/38/38	0/3/3/3
3	AGS	D	902	-	-	5/17/38/38	0/3/3/3
3	AGS	B	902	-	-	6/17/38/38	0/3/3/3
3	AGS	F	902	-	-	1/17/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	AGS	PG-S1G	7.92	2.07	1.90
3	F	902	AGS	PG-S1G	7.88	2.07	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	AGS	C5-C4	2.51	1.47	1.40
4	E	901	ADP	C5-C4	2.48	1.47	1.40
4	E	902	ADP	C5-C4	2.46	1.47	1.40
3	F	902	AGS	C5-C4	2.39	1.47	1.40
3	D	901	AGS	PG-S1G	2.12	1.95	1.90
3	D	902	AGS	PG-S1G	2.08	1.95	1.90
3	A	901	AGS	PG-S1G	2.08	1.95	1.90
3	F	902	AGS	PG-O3G	-2.07	1.48	1.54
3	B	901	AGS	PG-S1G	2.05	1.95	1.90
3	A	902	AGS	PG-S1G	2.04	1.95	1.90
3	C	901	AGS	PG-S1G	2.02	1.95	1.90
3	F	901	AGS	PG-O2G	2.02	1.61	1.54
3	C	902	AGS	PG-S1G	2.02	1.95	1.90

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	AGS	PA-O3A-PB	-4.58	117.11	132.83
3	B	902	AGS	PA-O3A-PB	-4.55	117.21	132.83
3	D	902	AGS	PA-O3A-PB	-4.46	117.53	132.83
3	C	901	AGS	PA-O3A-PB	-4.43	117.62	132.83
3	A	901	AGS	PA-O3A-PB	-4.40	117.73	132.83
3	B	901	AGS	PA-O3A-PB	-4.36	117.86	132.83
3	C	902	AGS	PA-O3A-PB	-4.22	118.33	132.83
3	D	901	AGS	PA-O3A-PB	-4.11	118.71	132.83
3	F	902	AGS	PA-O3A-PB	-4.09	118.80	132.83
4	E	901	ADP	PA-O3A-PB	-3.89	119.49	132.83
4	E	902	ADP	PA-O3A-PB	-3.70	120.13	132.83
3	F	901	AGS	PA-O3A-PB	-3.57	120.58	132.83
3	F	901	AGS	C3'-C2'-C1'	3.46	106.18	100.98
4	E	902	ADP	C3'-C2'-C1'	3.46	106.18	100.98
3	F	902	AGS	C3'-C2'-C1'	3.29	105.93	100.98
4	E	901	ADP	C3'-C2'-C1'	3.26	105.89	100.98
3	F	902	AGS	N3-C2-N1	-3.22	123.64	128.68
4	E	902	ADP	N3-C2-N1	-3.21	123.66	128.68
3	F	901	AGS	N3-C2-N1	-3.17	123.73	128.68
4	E	901	ADP	N3-C2-N1	-3.12	123.80	128.68
3	F	902	AGS	C4-C5-N7	-2.73	106.56	109.40
3	F	901	AGS	C4-C5-N7	-2.71	106.58	109.40
4	E	901	ADP	C4-C5-N7	-2.63	106.66	109.40
4	E	902	ADP	C4-C5-N7	-2.63	106.66	109.40
3	D	902	AGS	C5-C6-N6	2.31	123.87	120.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	901	AGS	C5-C6-N6	2.29	123.84	120.35
3	B	902	AGS	C5-C6-N6	2.28	123.82	120.35
3	B	901	AGS	C5-C6-N6	2.27	123.81	120.35
3	C	902	AGS	C5-C6-N6	2.27	123.80	120.35
3	A	902	AGS	C5-C6-N6	2.26	123.79	120.35
3	C	901	AGS	C5-C6-N6	2.26	123.78	120.35
3	A	901	AGS	C5-C6-N6	2.21	123.71	120.35

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	AGS	PB-O3B-PG-O2G
3	A	901	AGS	PB-O3B-PG-O3G
3	A	902	AGS	PB-O3B-PG-O3G
3	A	902	AGS	O4'-C4'-C5'-O5'
3	B	901	AGS	C5'-O5'-PA-O1A
3	B	901	AGS	O4'-C4'-C5'-O5'
3	B	902	AGS	PB-O3B-PG-O2G
3	B	902	AGS	PB-O3B-PG-O3G
3	B	902	AGS	C5'-O5'-PA-O2A
3	C	902	AGS	PB-O3B-PG-O2G
3	C	902	AGS	PB-O3B-PG-O3G
3	C	902	AGS	O4'-C4'-C5'-O5'
3	D	902	AGS	C5'-O5'-PA-O1A
3	D	902	AGS	C5'-O5'-PA-O2A
3	F	901	AGS	PB-O3B-PG-O3G
3	A	901	AGS	O4'-C4'-C5'-O5'
3	B	901	AGS	C3'-C4'-C5'-O5'
3	D	902	AGS	O4'-C4'-C5'-O5'
3	F	901	AGS	C4'-C5'-O5'-PA
3	B	902	AGS	O4'-C4'-C5'-O5'
3	D	902	AGS	C3'-C4'-C5'-O5'
3	C	902	AGS	PG-O3B-PB-O1B
3	B	901	AGS	C5'-O5'-PA-O3A
3	B	902	AGS	C5'-O5'-PA-O3A
3	D	902	AGS	C5'-O5'-PA-O3A
3	B	901	AGS	C5'-O5'-PA-O2A
3	B	902	AGS	C5'-O5'-PA-O1A
4	E	901	ADP	O4'-C4'-C5'-O5'
3	A	902	AGS	C3'-C4'-C5'-O5'
3	A	902	AGS	PB-O3B-PG-O2G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	901	AGS	PB-O3B-PG-O3G
3	F	901	AGS	PB-O3B-PG-O2G
3	F	902	AGS	O4'-C4'-C5'-O5'
4	E	901	ADP	PA-O3A-PB-O3B
3	C	902	AGS	PG-O3B-PB-O2B
4	E	902	ADP	O4'-C4'-C5'-O5'
3	C	901	AGS	O4'-C4'-C5'-O5'

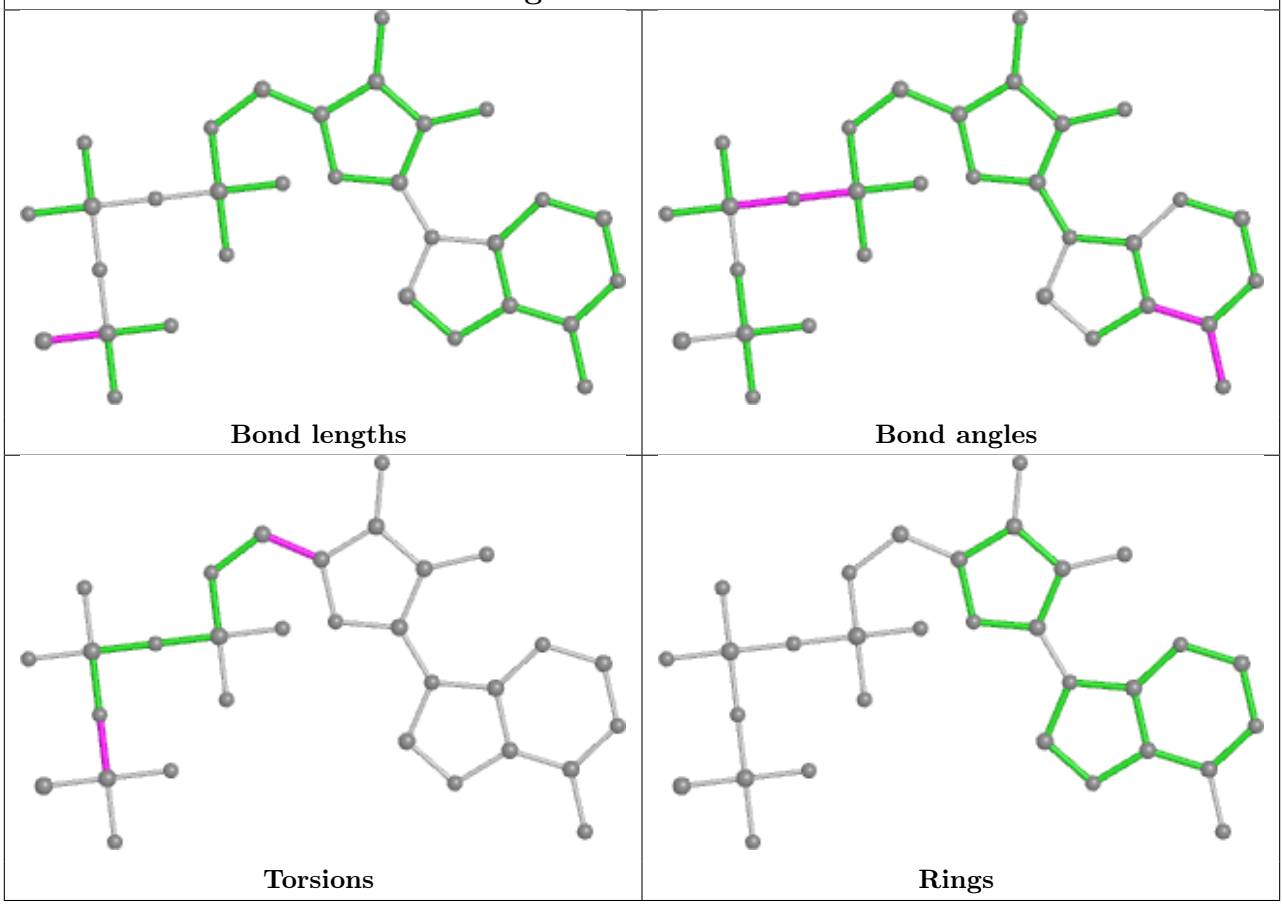
There are no ring outliers.

12 monomers are involved in 32 short contacts:

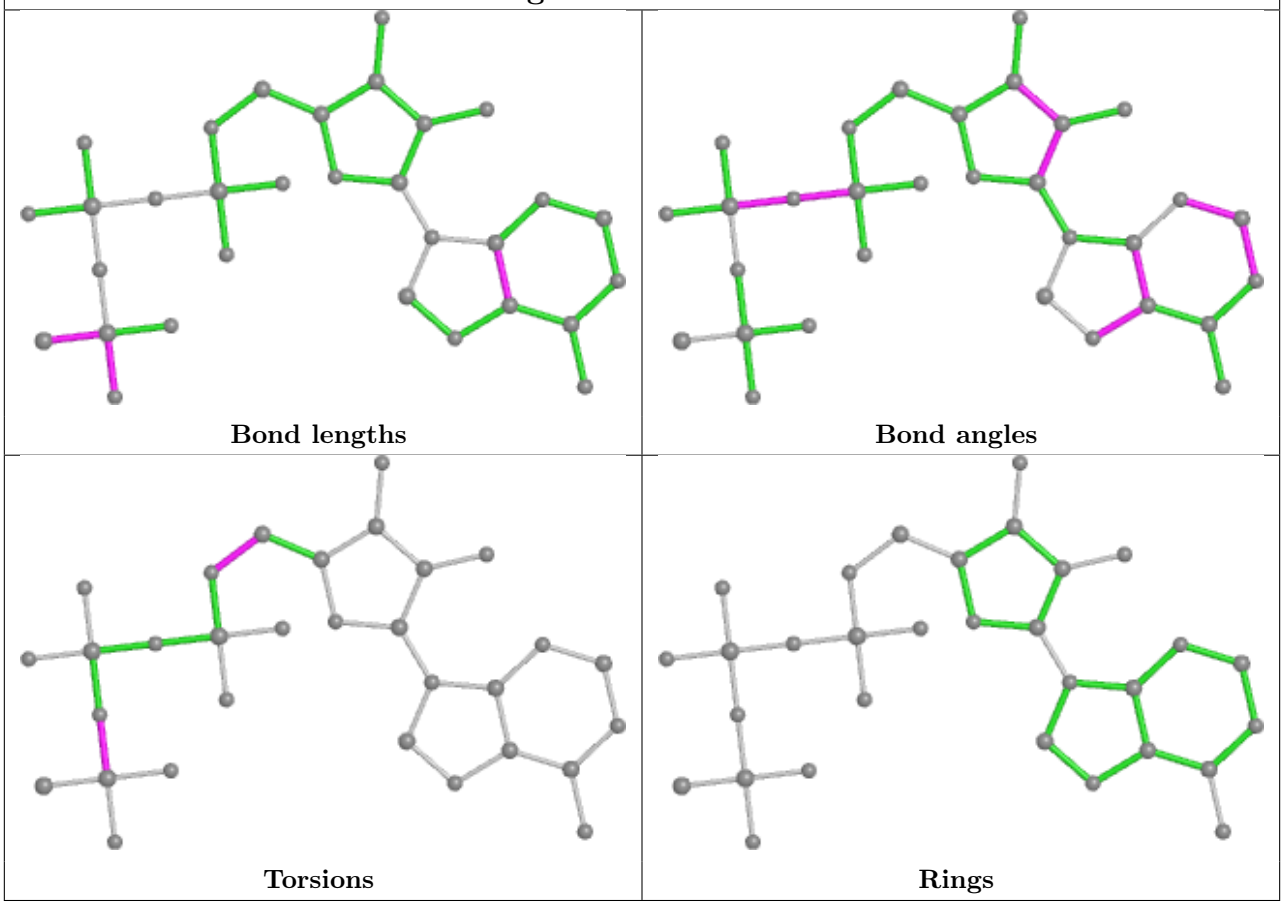
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	AGS	2	0
3	F	901	AGS	4	0
4	E	901	ADP	1	0
3	D	901	AGS	2	0
4	E	902	ADP	2	0
3	C	902	AGS	2	0
3	B	901	AGS	3	0
3	C	901	AGS	3	0
3	A	902	AGS	3	0
3	D	902	AGS	2	0
3	B	902	AGS	3	0
3	F	902	AGS	5	0

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 then 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.

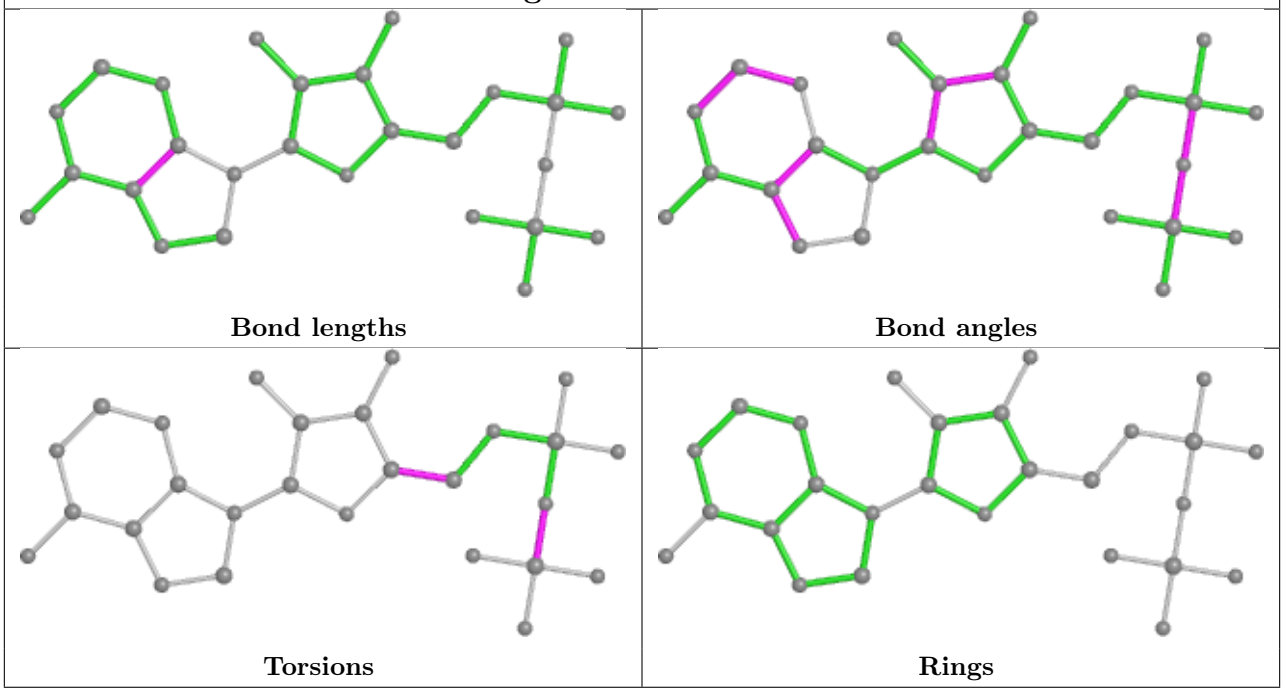
Ligand AGS A 901



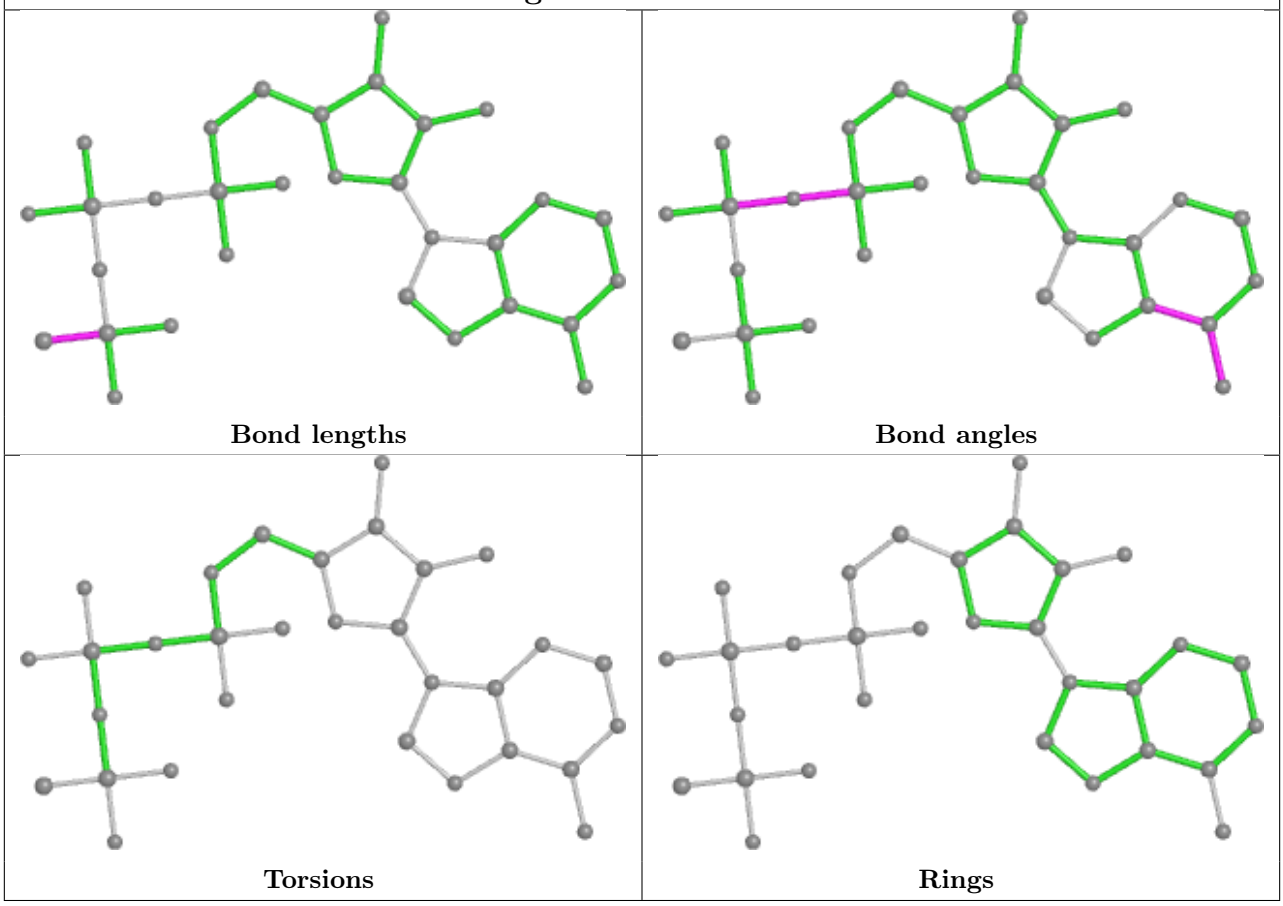
Ligand AGS F 901



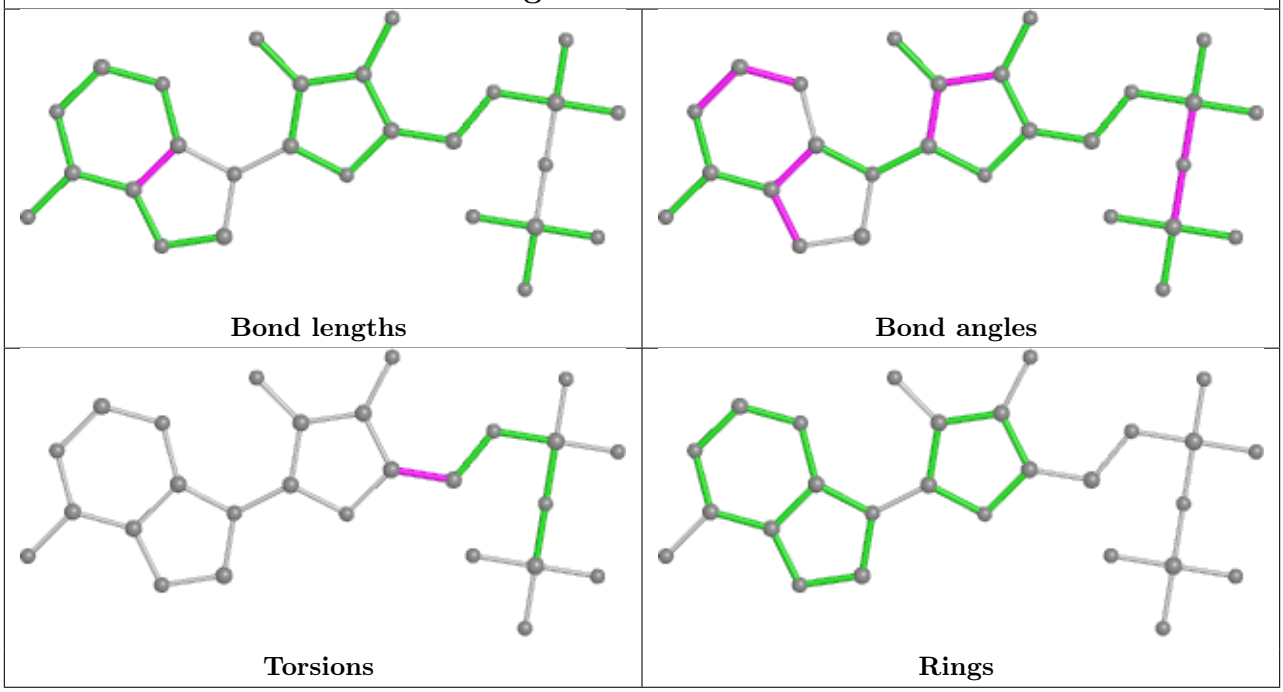
Ligand ADP E 901



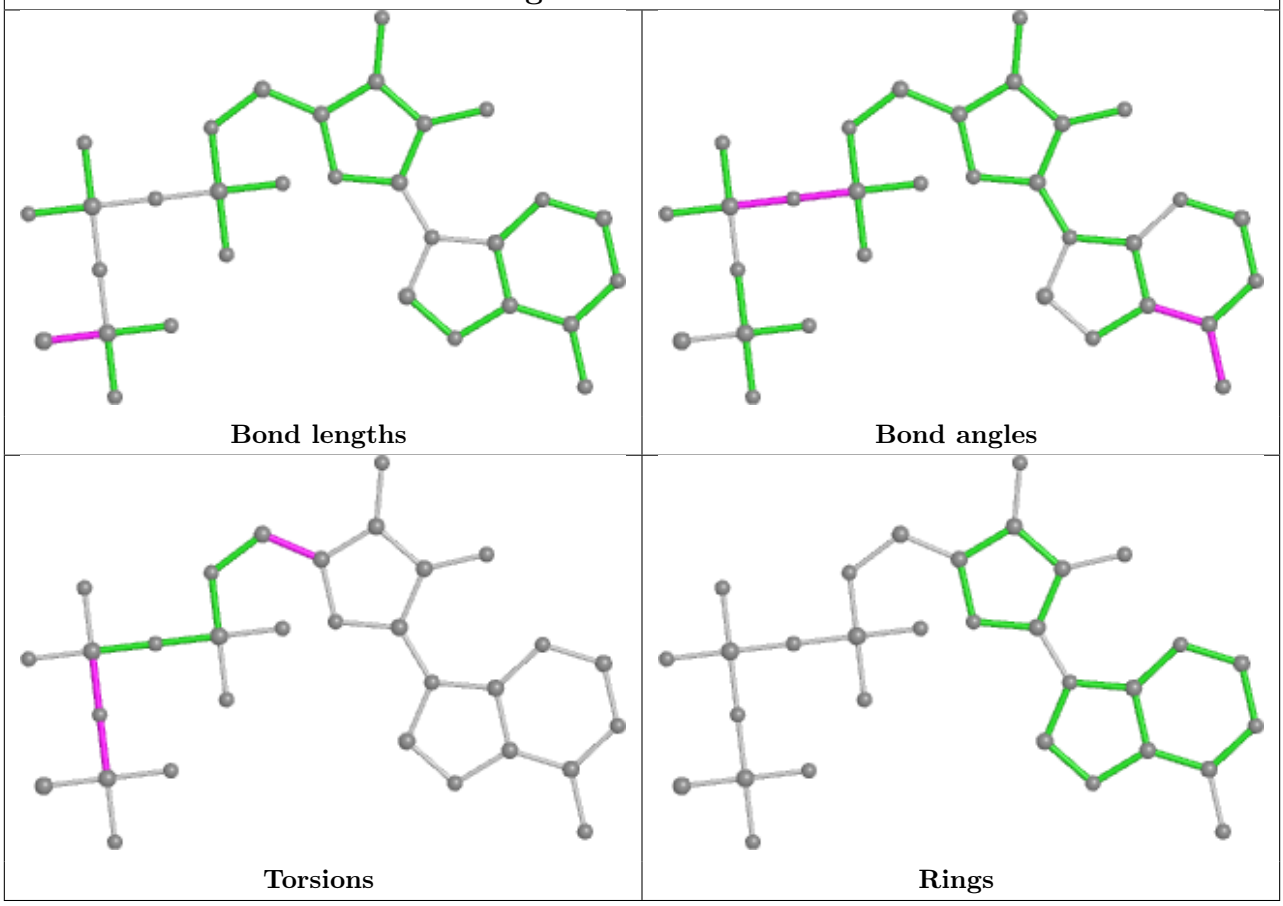
Ligand AGS D 901



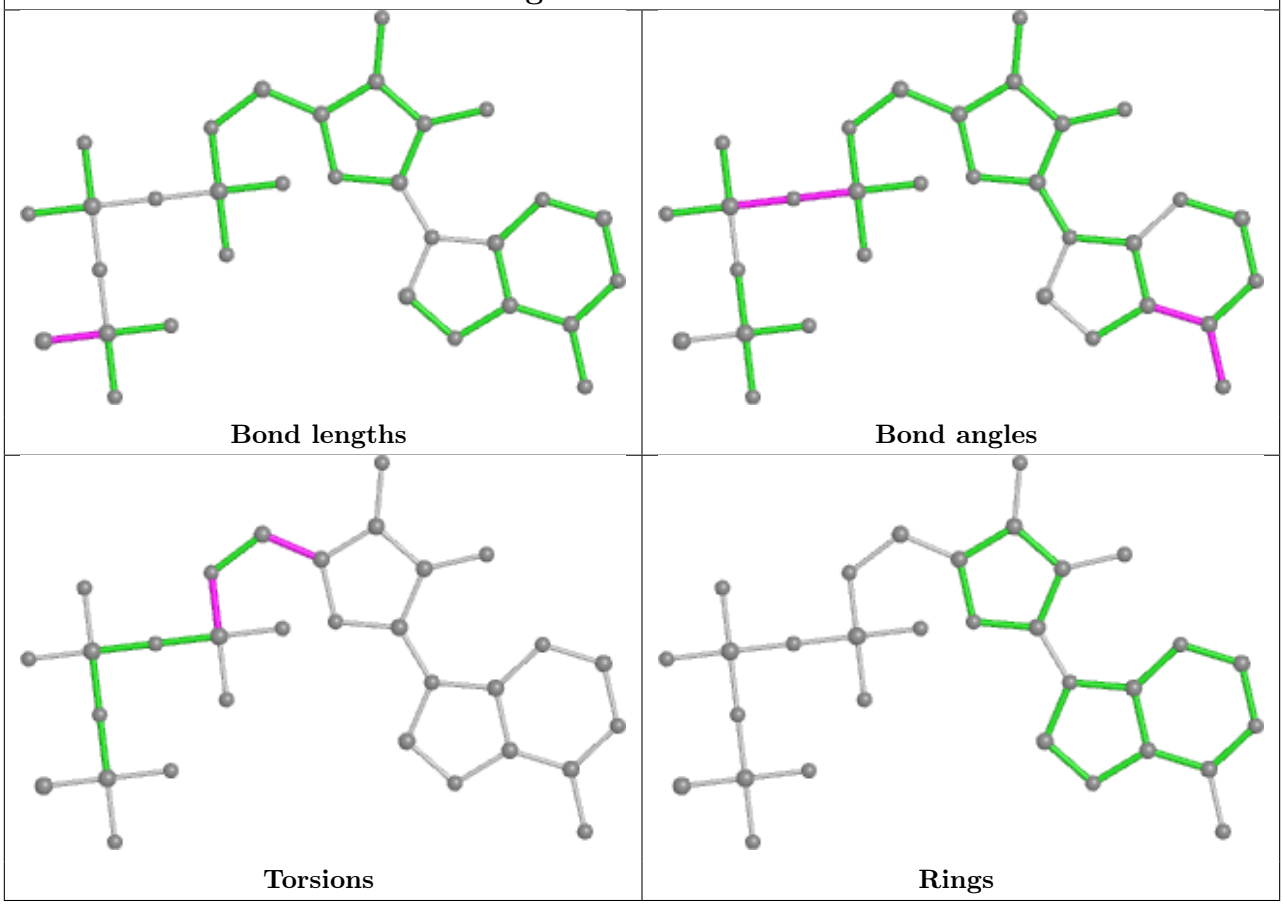
Ligand ADP E 902



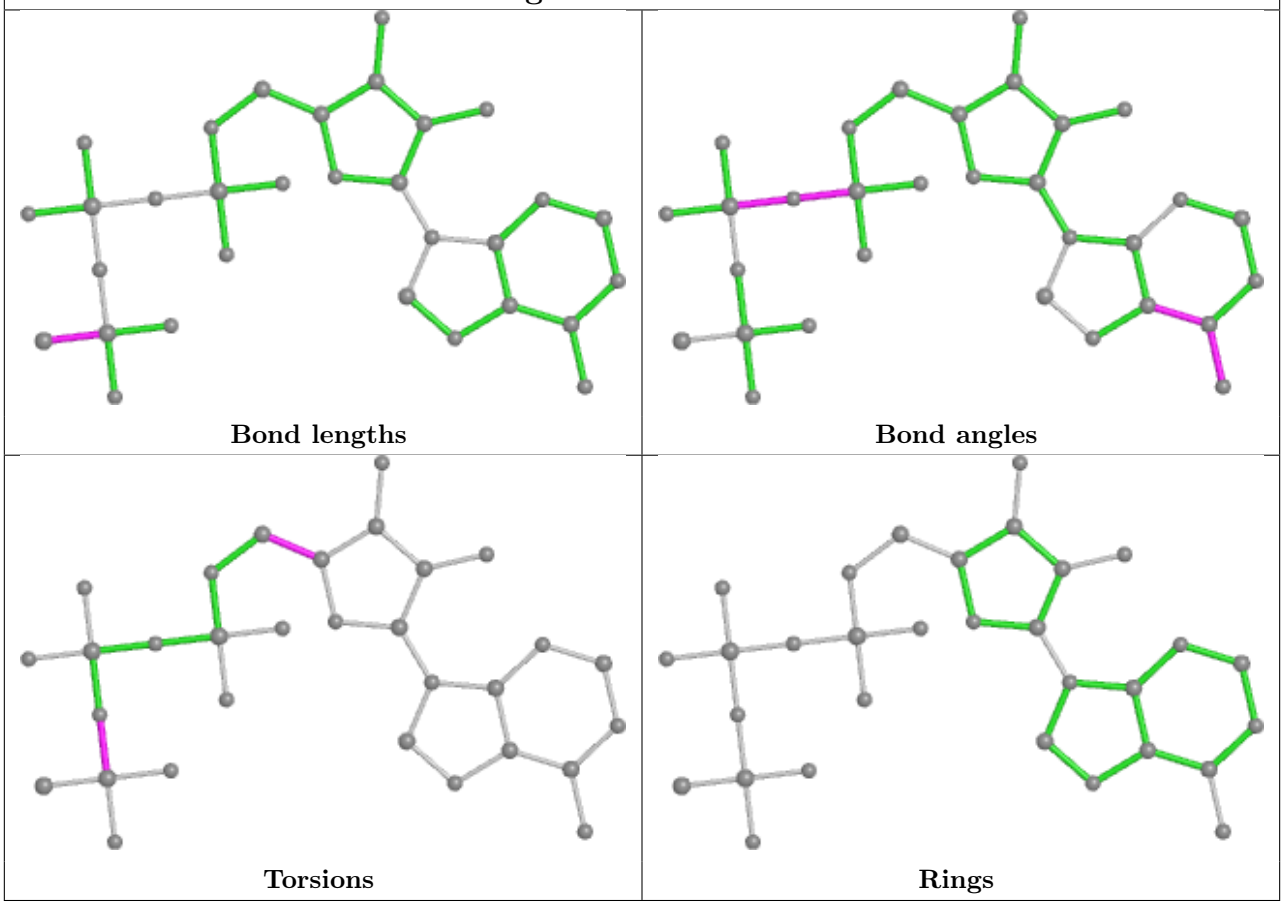
Ligand AGS C 902



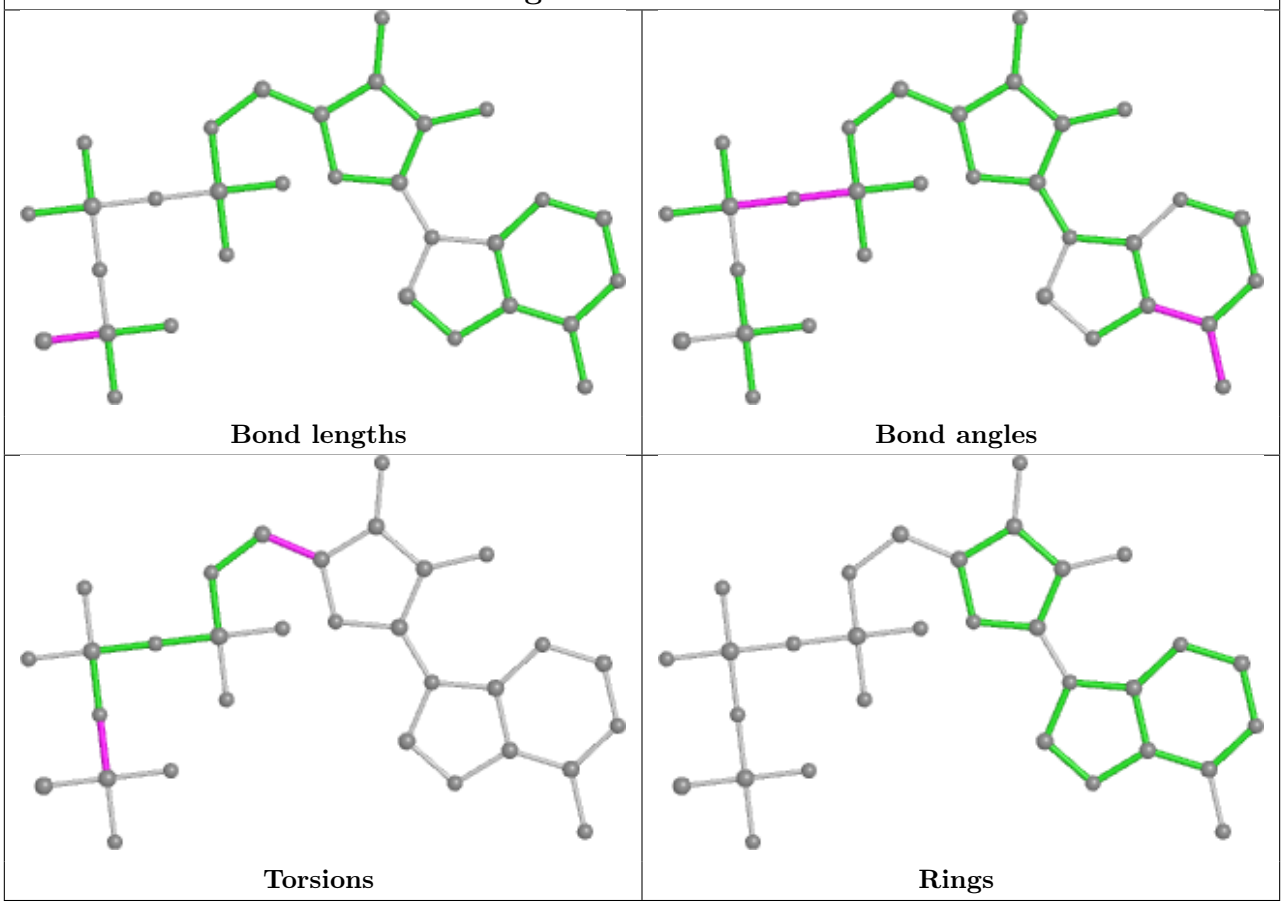
Ligand AGS B 901



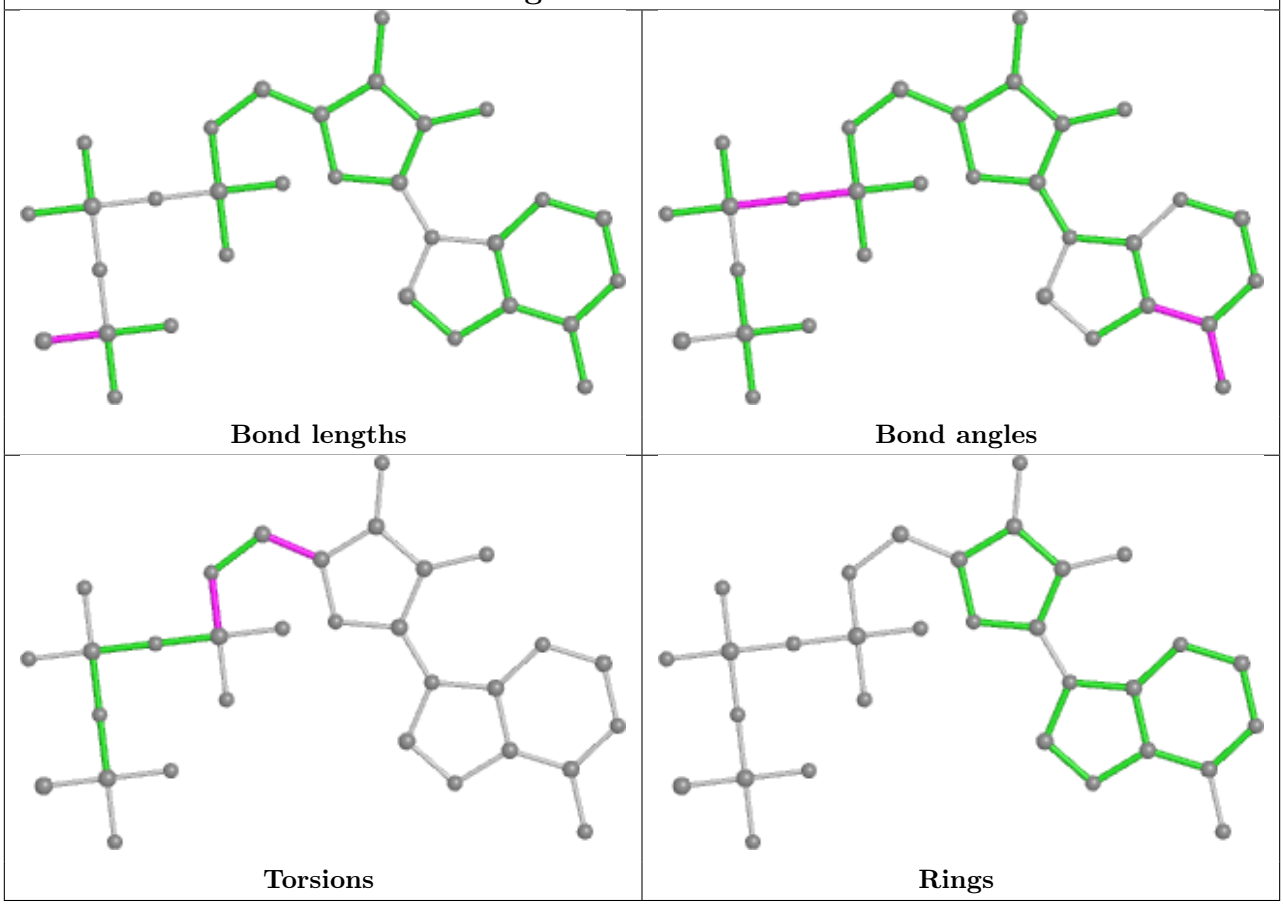
Ligand AGS C 901



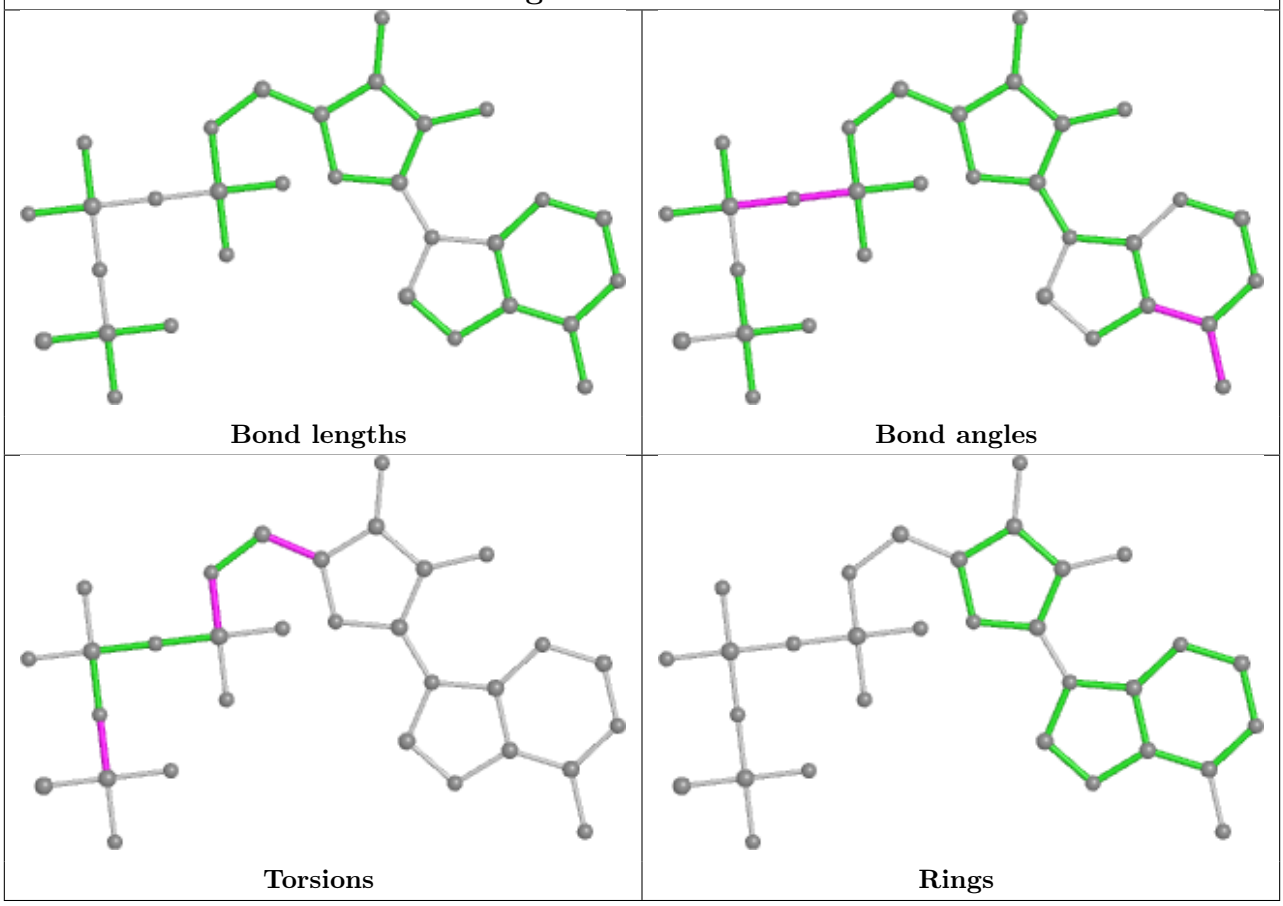
Ligand AGS A 902

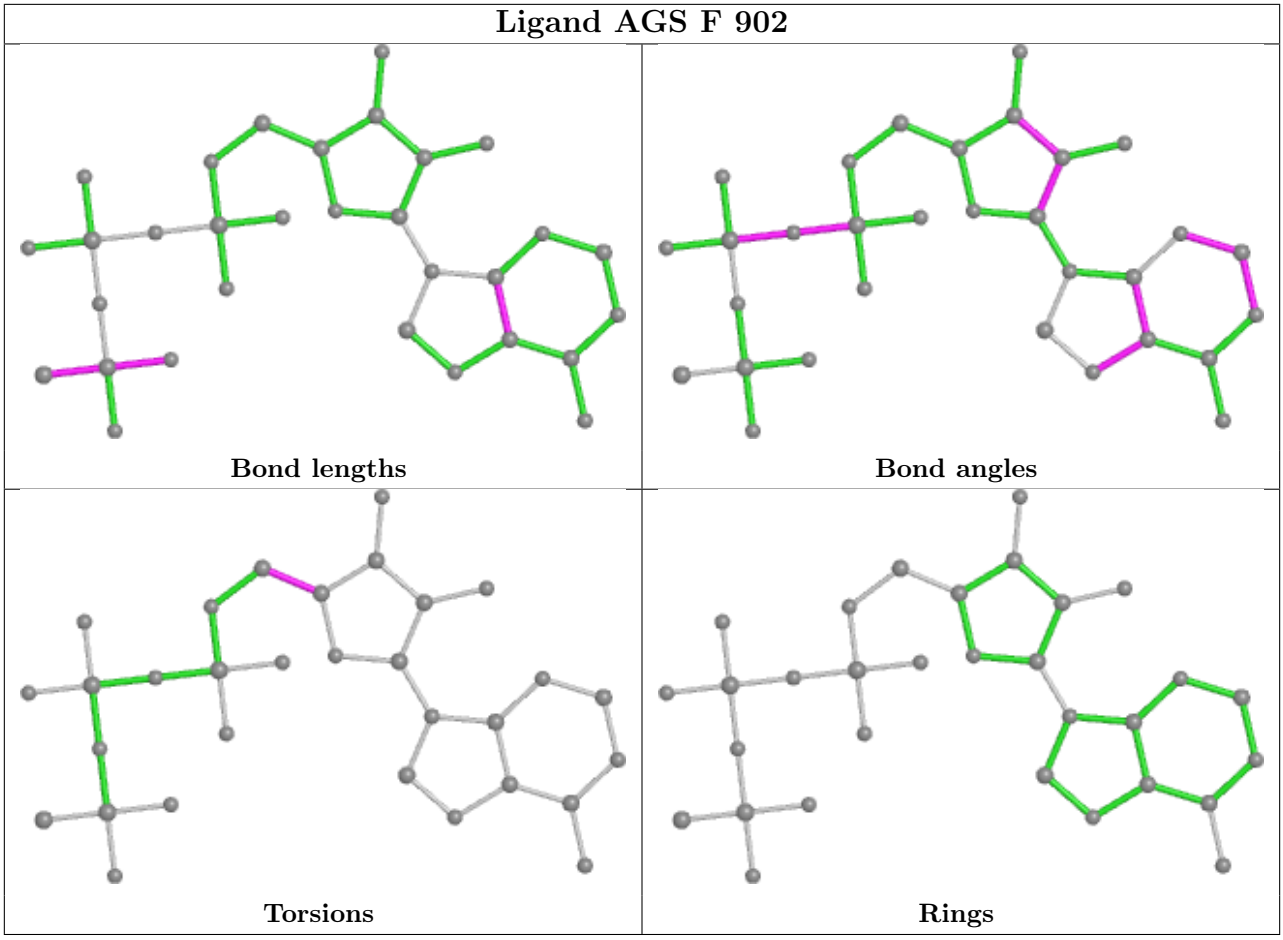


Ligand AGS D 902



Ligand AGS B 902





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

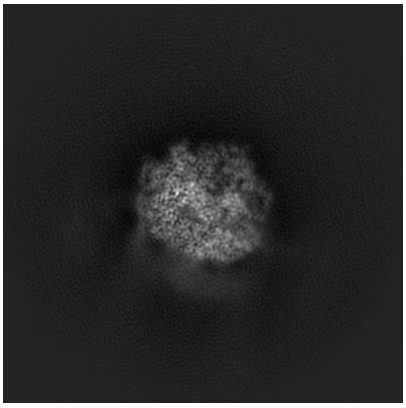
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21555. These allow visual inspection of the internal detail of the map and identification of artifacts.

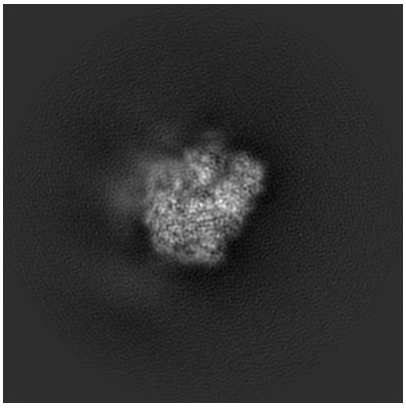
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

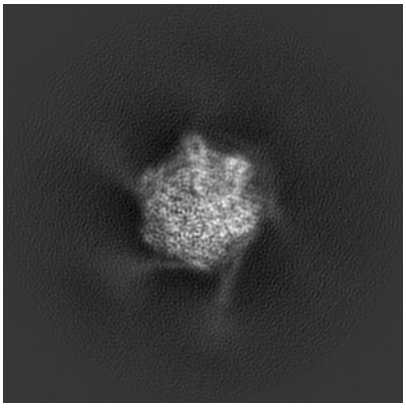
6.1.1 Primary map



X



Y

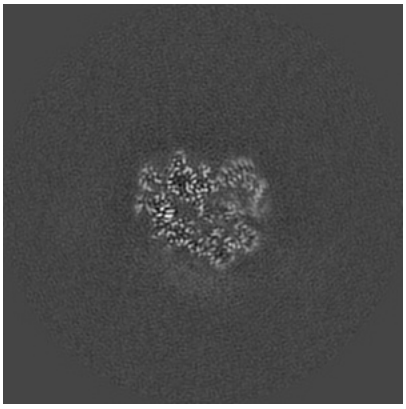


Z

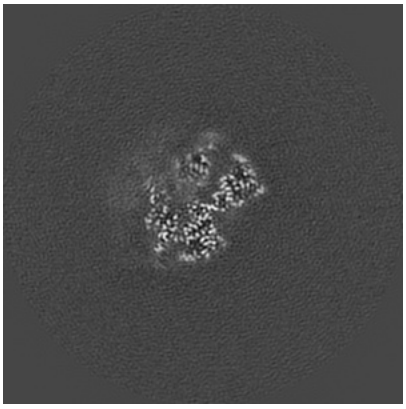
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

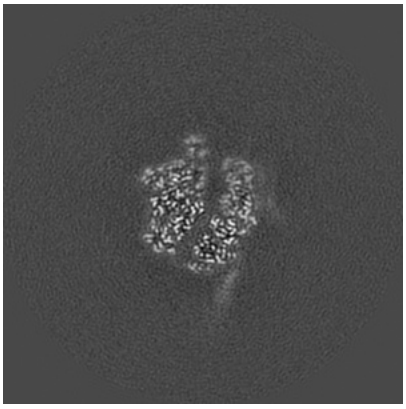
6.2.1 Primary map



X Index: 180



Y Index: 180

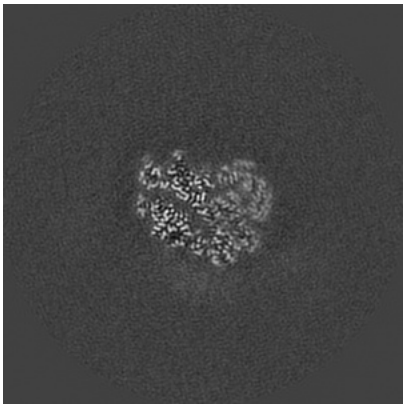


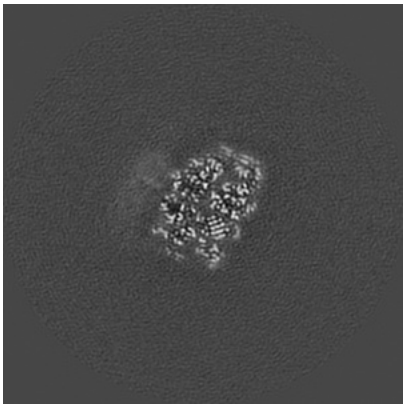
Z Index: 180

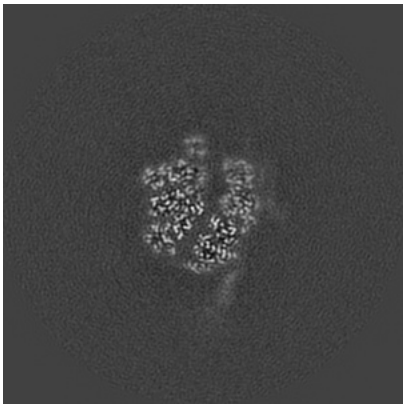
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 177

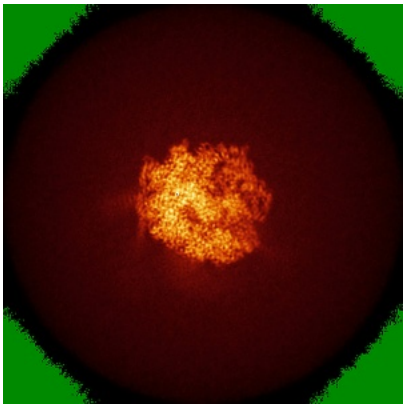

Y Index: 157

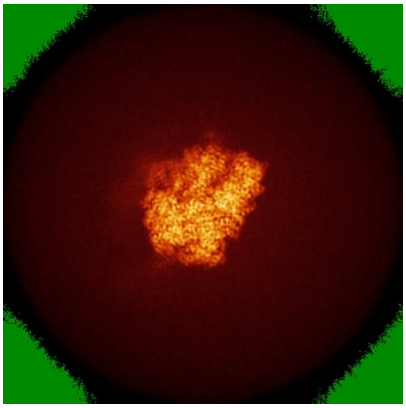

Z Index: 179

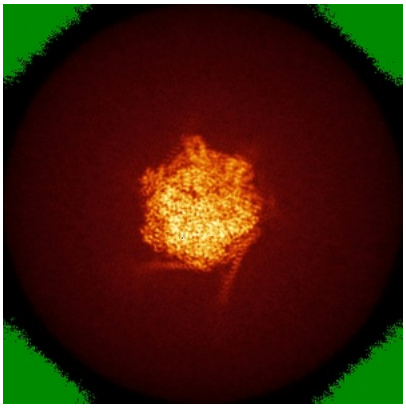
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0131. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

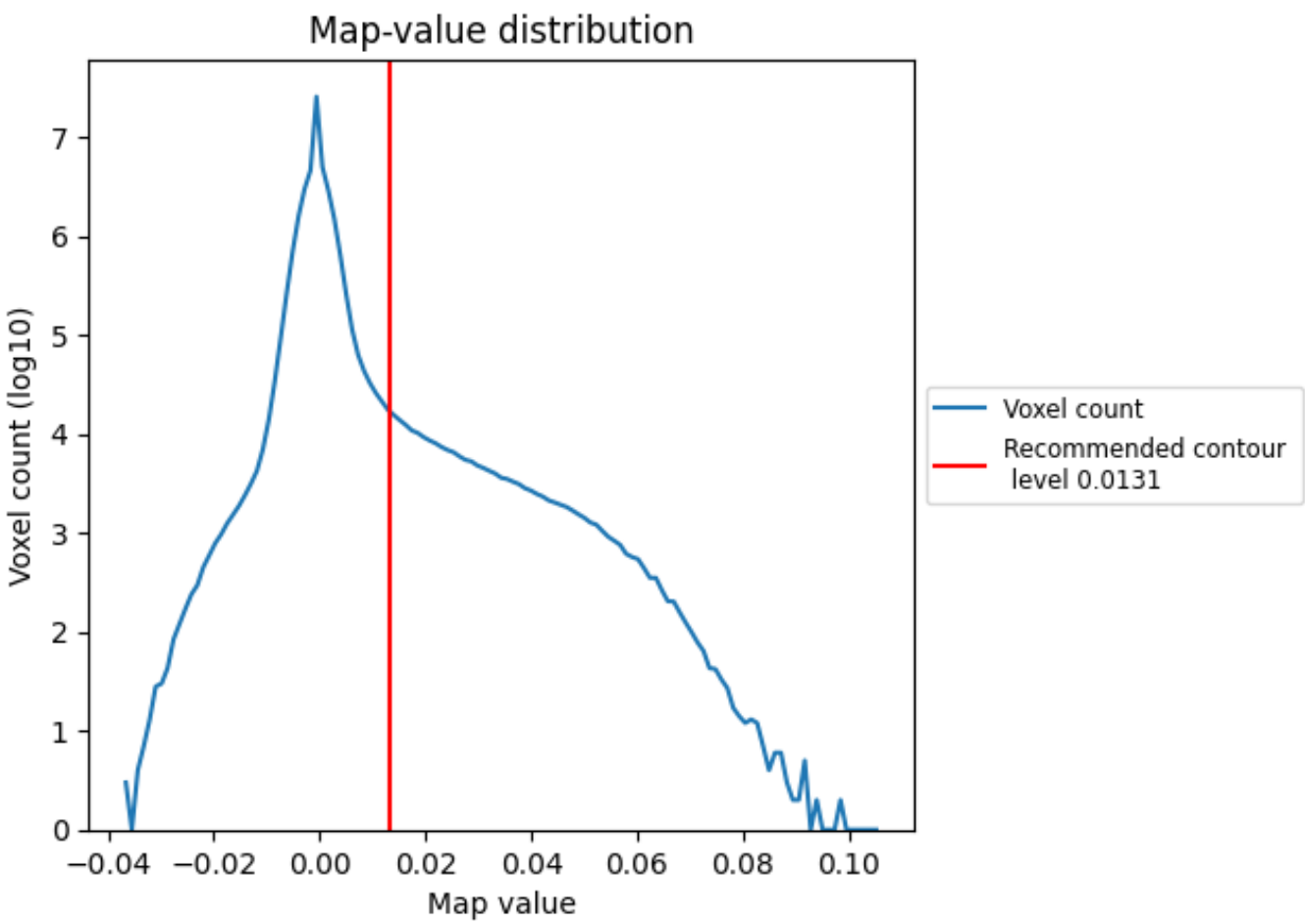
6.6 Mask visualisation (i)

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

7 Map analysis (i)

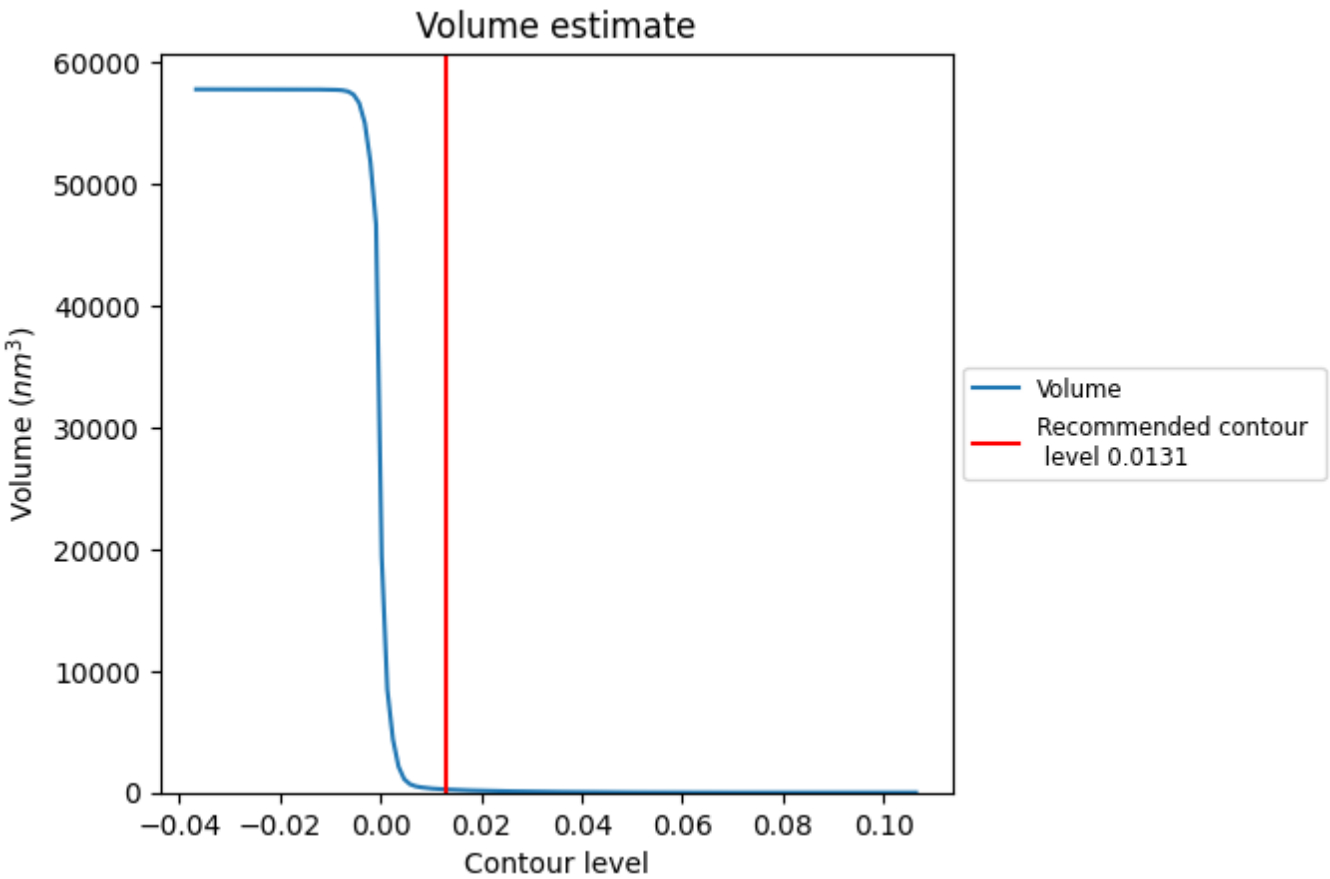
This section contains the results of statistical analysis of the map.

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.

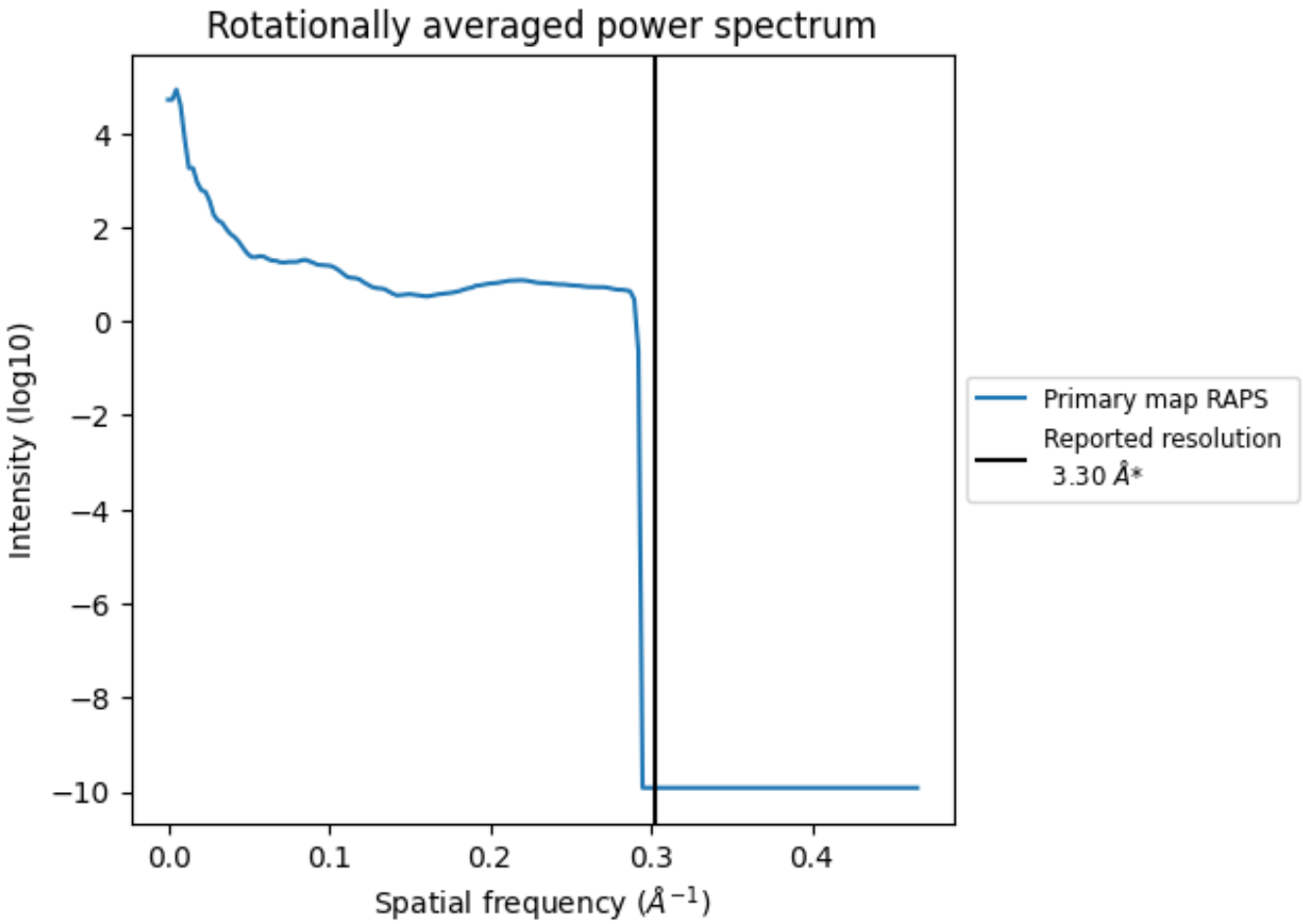
7.2 Volume estimate (i)



The volume at the recommended contour level is 255 nm^3; this corresponds to an approximate mass of 230 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)

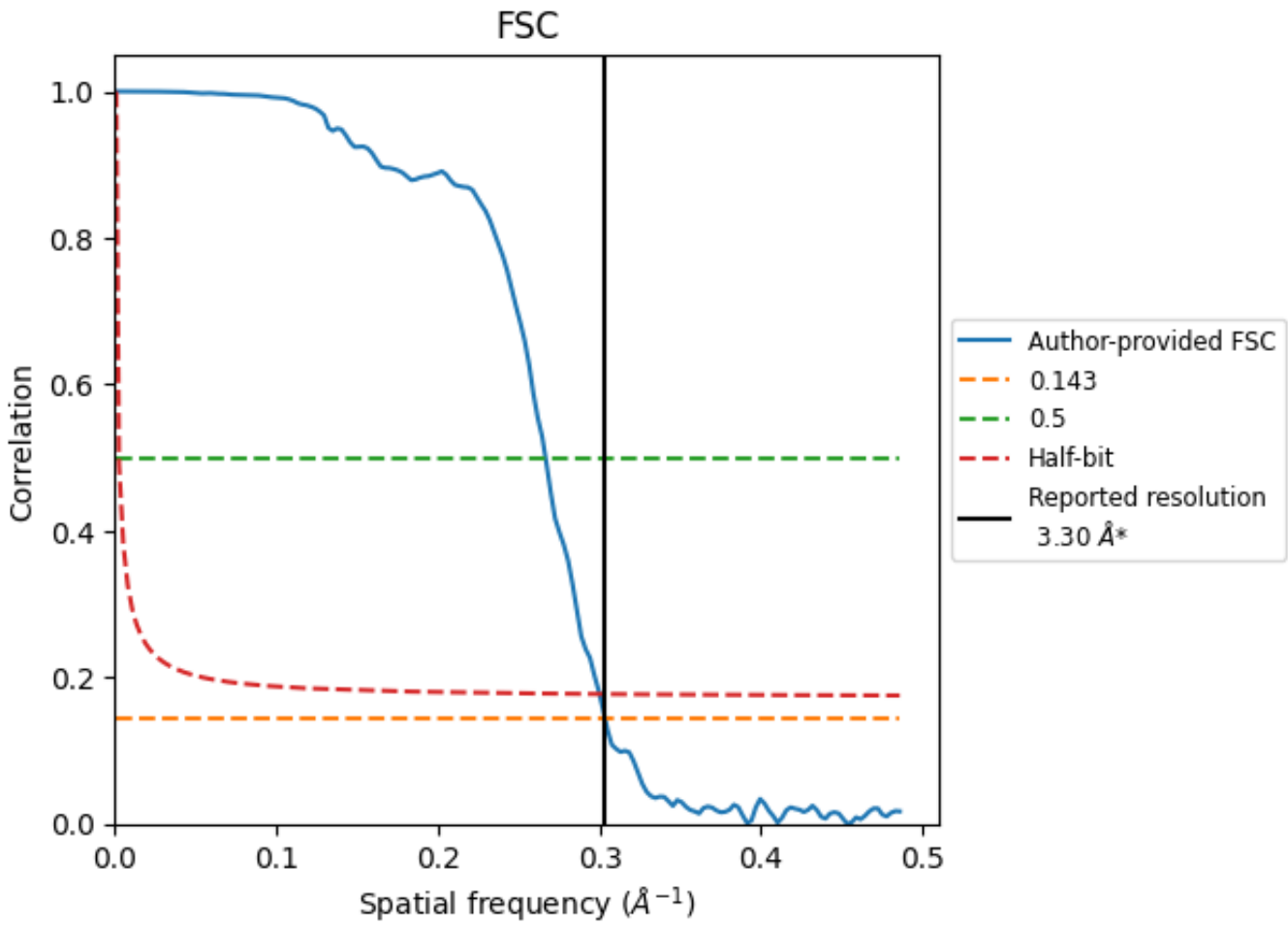


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

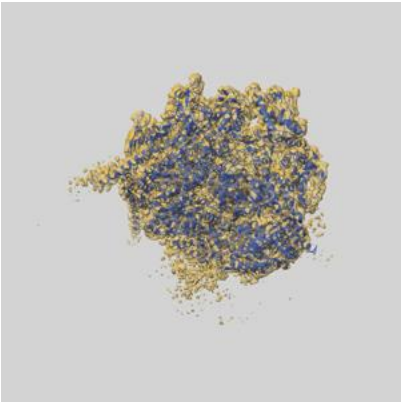
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.75	3.33
Unmasked-calculated*	-	-	-

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

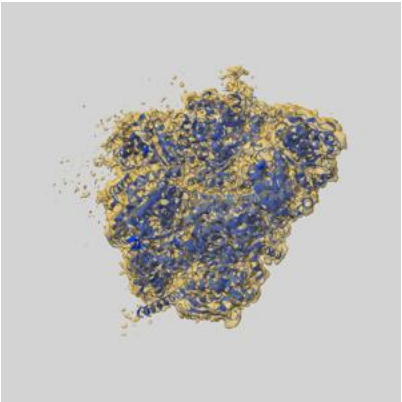
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21555 and PDB model 6W6H. Per-residue inclusion information can be found in section 3 on page 6.

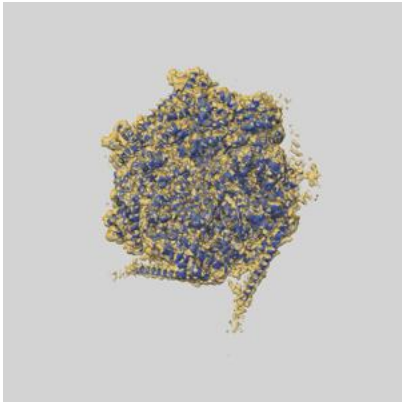
9.1 Map-model overlay (i)



X



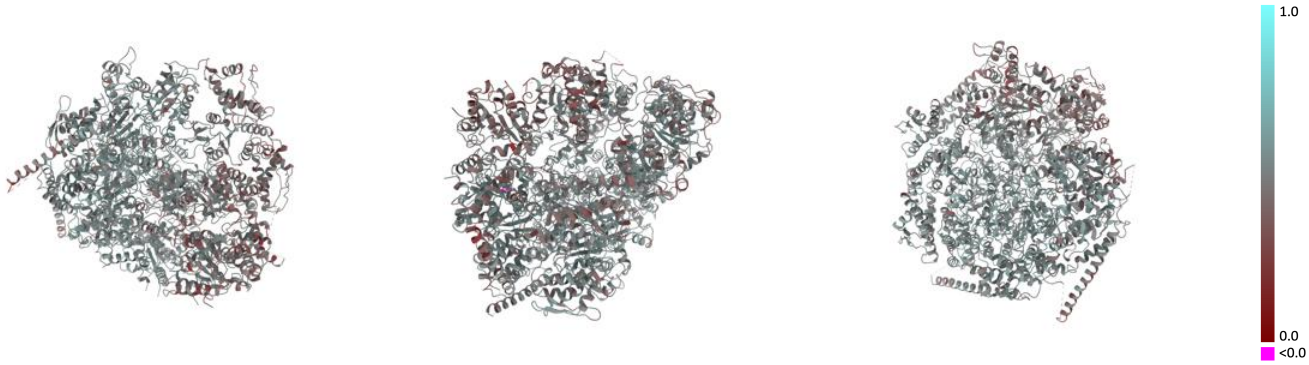
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0131 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.

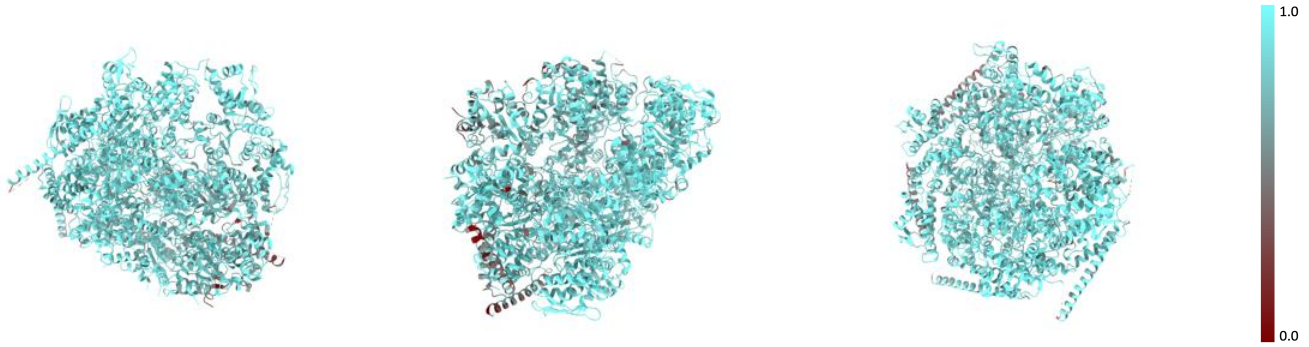
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

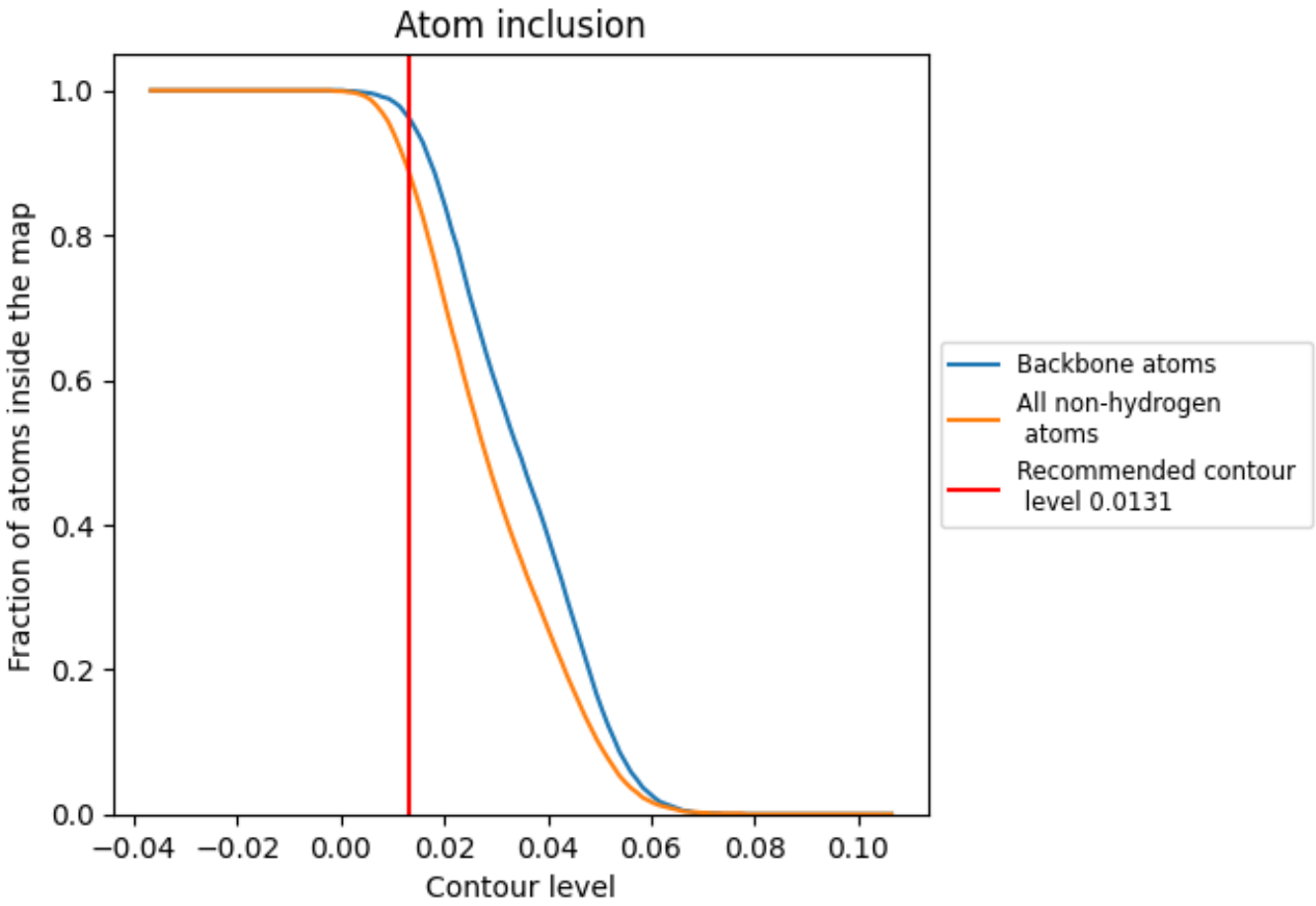
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0131).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8900	0.4940
A	0.8930	0.5140
B	0.9240	0.5270
C	0.9290	0.5240
D	0.9240	0.5090
E	0.8670	0.4360
F	0.7980	0.4480
N	0.9460	0.5200