



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:38 AM UTC

PDB ID : 6RN2 / pdb_00006rn2
EMDB ID : EMD-4940
Title : ClpB (DWB mutant) bound to casein in presence of ATPgammaS - state WT-1
Authors : Deville, C.; Saibil, H.R.
Deposited on : 2019-05-07
Resolution : 6.20 Å(reported)
Based on initial model : 1CIU

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

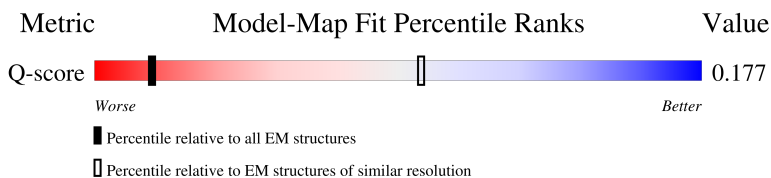
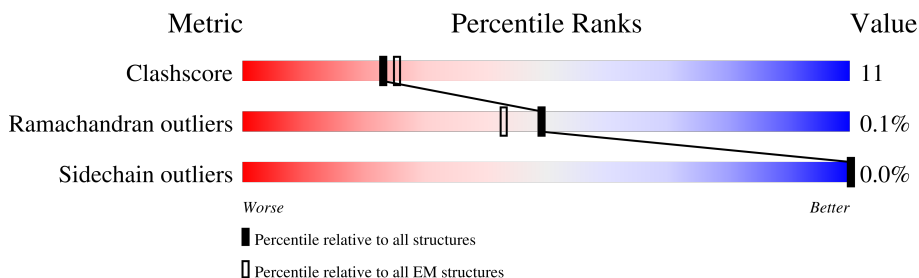
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	537 (5.70 - 6.70)

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

Mol	Chain	Length	Quality of chain
1	A	858	
1	B	858	
1	C	858	
1	D	858	

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Mol	Chain	Length	Quality of chain
1	E	858	
1	F	858	
2	S	24	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32937 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chaperone protein ClpB.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	B	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	C	689	Total	C	N	O	S	0	0
			5430	3400	981	1029	20		
1	D	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	E	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		
1	F	684	Total	C	N	O	S	0	0
			5406	3386	976	1024	20		

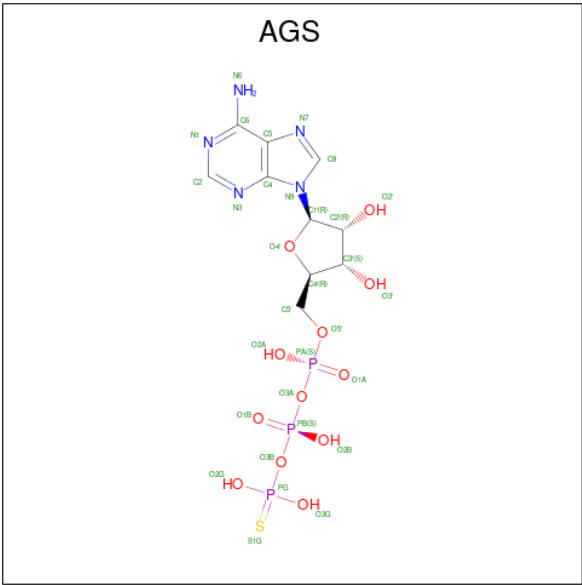
There are 18 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called casein.

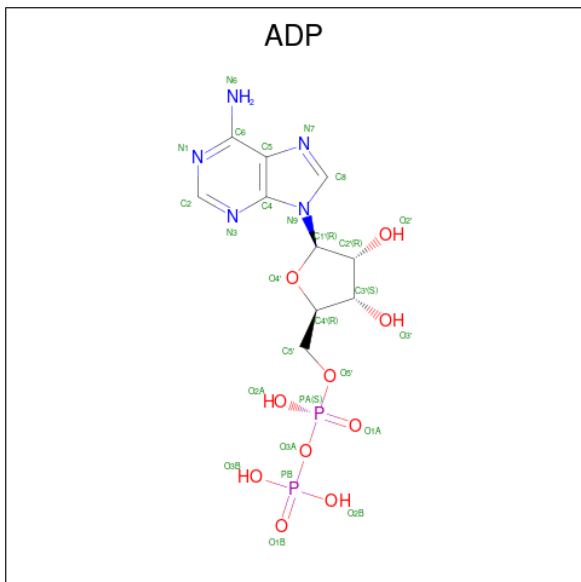
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	S	24	120	72	24	24	0	0

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



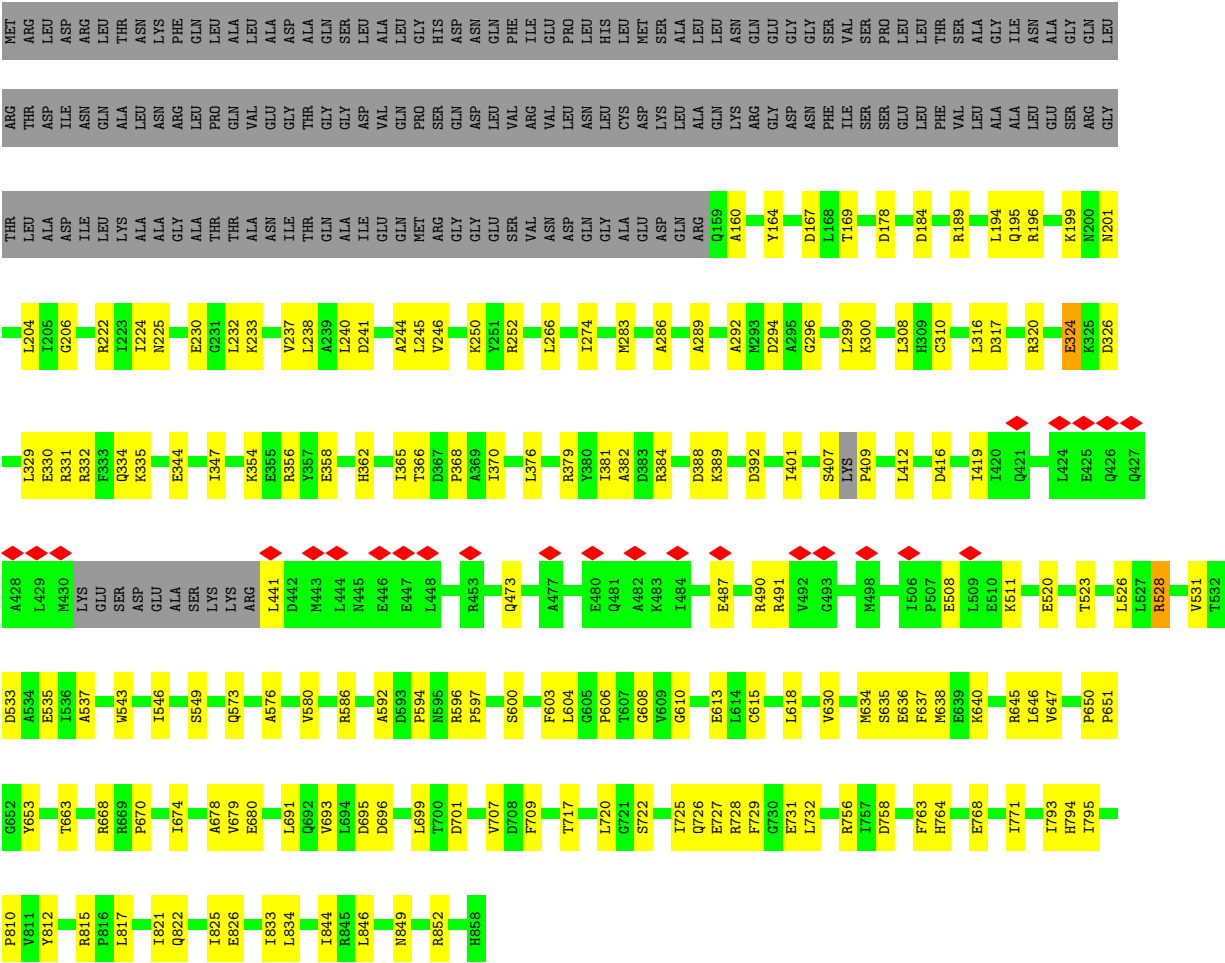
Mol	Chain	Residues	Atoms							AltConf
3	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0	
3	D	1	Total 31	C 10	N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

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

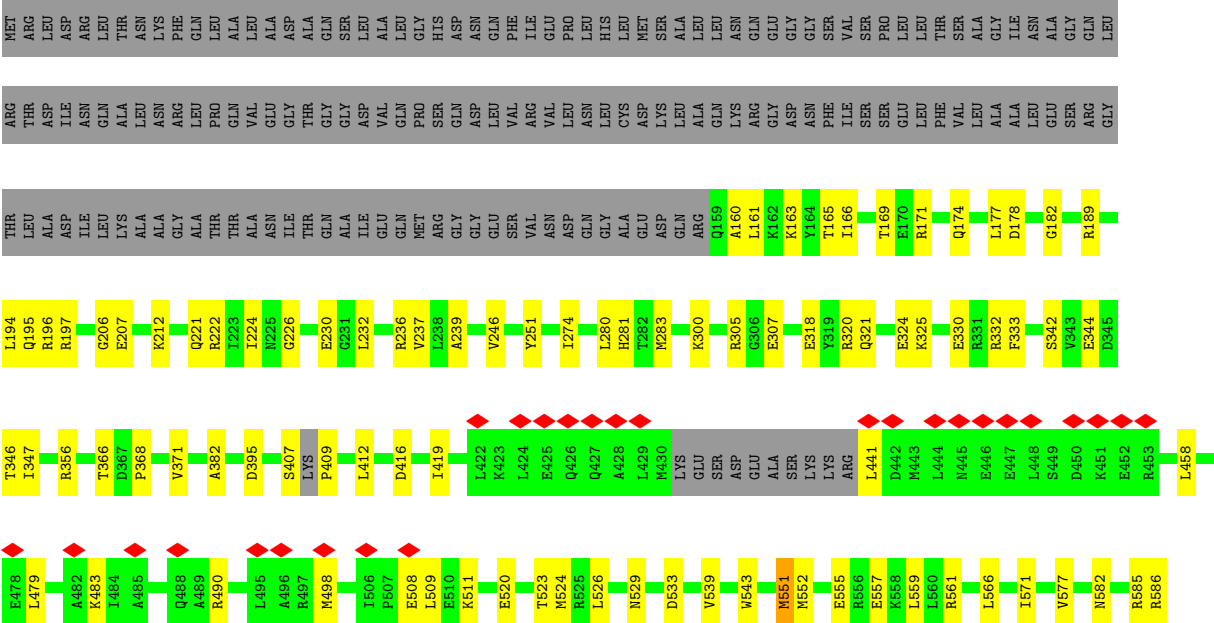


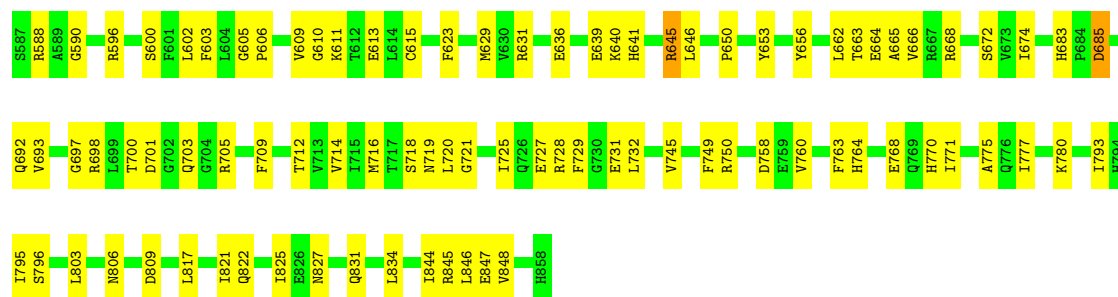
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	





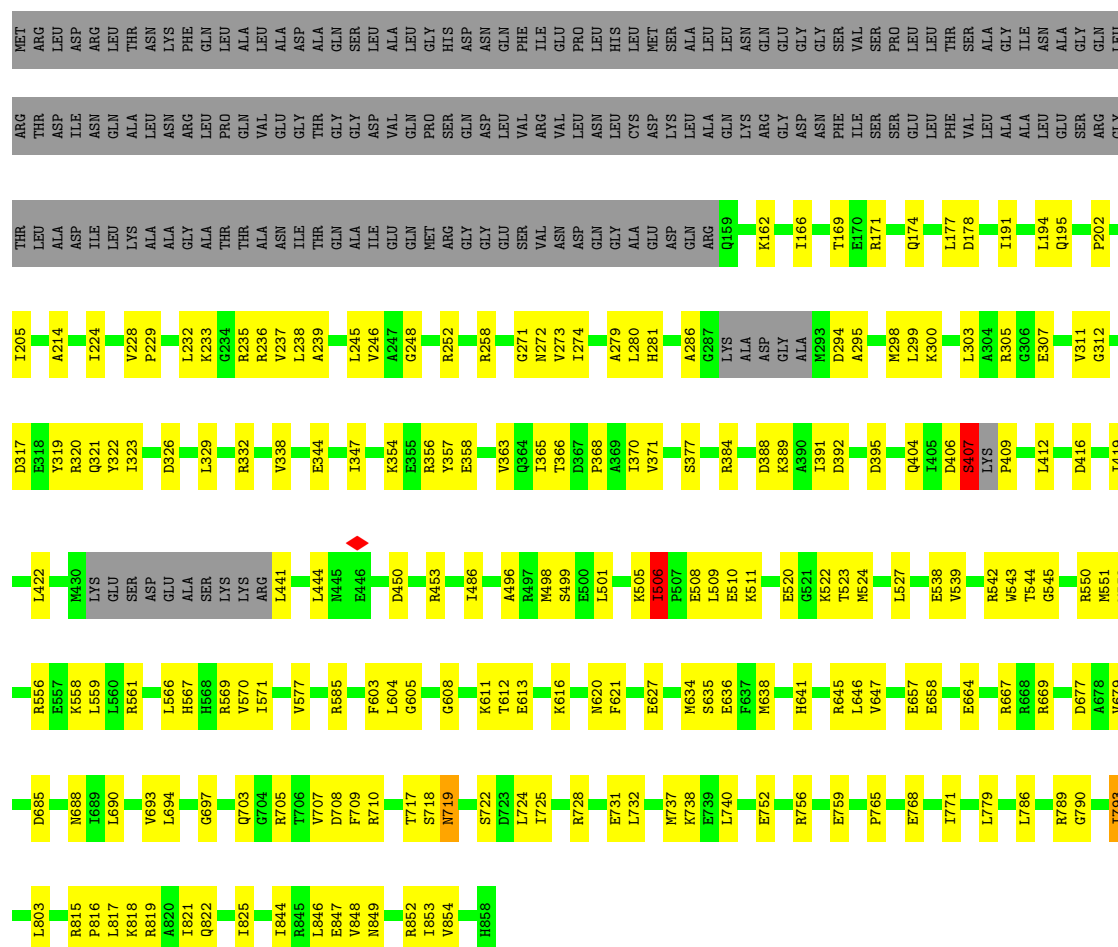
● Molecule 1: Chaperone protein ClpB





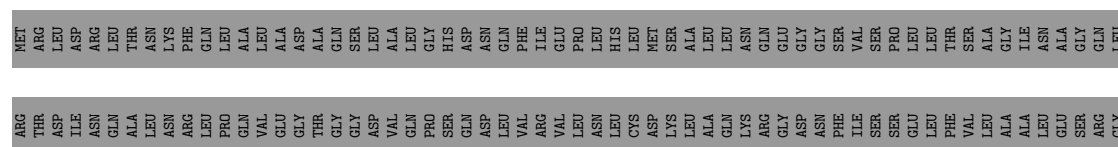
• Molecule 1: Chaperone protein ClpB

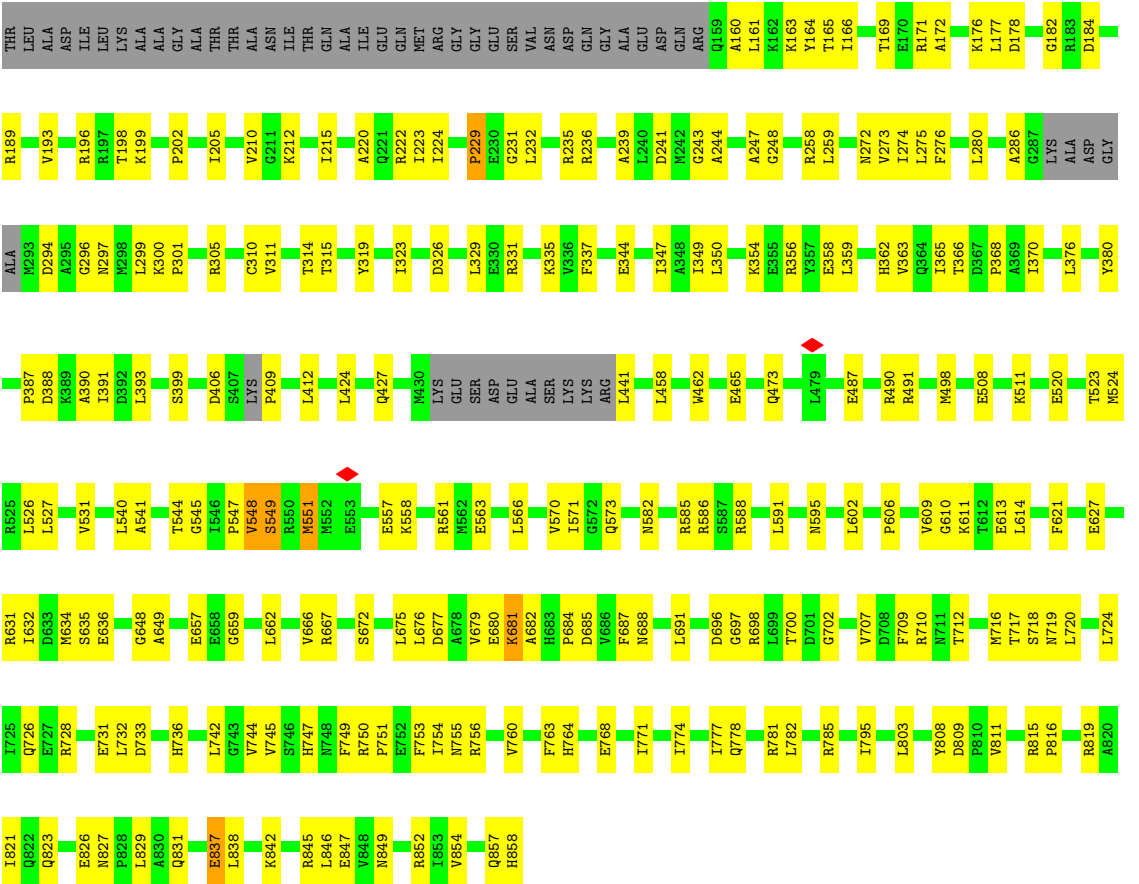
Chain D: 56% 23% 20%



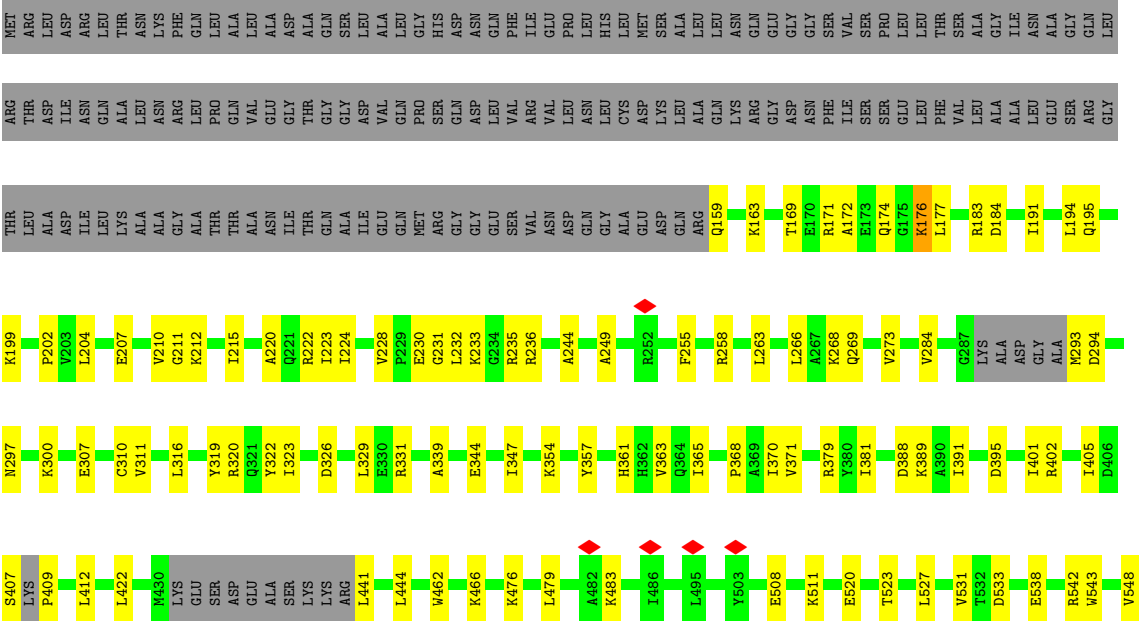
• Molecule 1: Chaperone protein ClpB

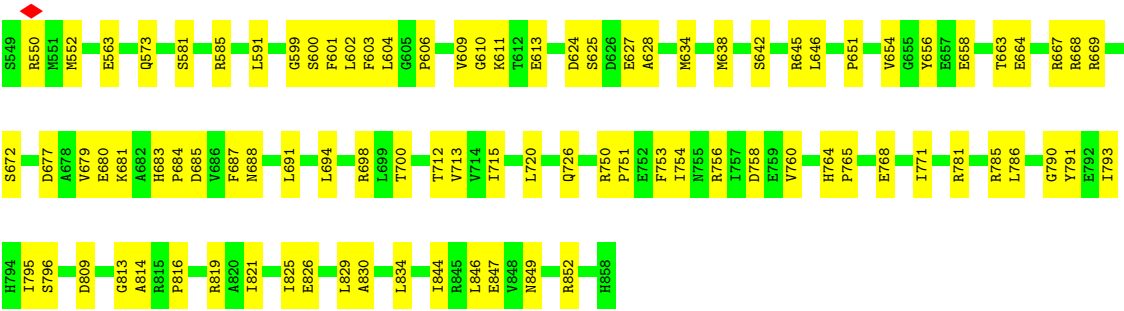
Chain E: 52% 27% 20%



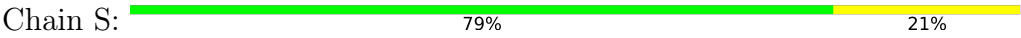


● Molecule 1: Chaperone protein ClpB





• Molecule 2: casein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21927	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	0.097	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/5479	0.65	0/7383
1	B	0.59	0/5504	0.76	3/7419 (0.0%)
1	C	0.61	0/5504	0.74	0/7419
1	D	0.54	0/5478	0.74	6/7380 (0.1%)
1	E	0.41	0/5477	0.65	0/7376
1	F	0.38	0/5478	0.61	0/7380
2	S	0.53	0/119	0.73	0/165
All	All	0.51	0/33039	0.69	9/44522 (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	10
1	B	0	11
1	C	0	15
1	D	0	13
1	E	0	12
1	F	0	6
All	All	0	67

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	407	SER	CA-C-N	8.94	148.46	127.00
1	D	407	SER	C-N-CA	8.94	148.46	127.00
1	D	407	SER	C-N-CD	-8.72	101.41	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	407	SER	CA-C-N	6.96	143.70	127.00
1	B	407	SER	C-N-CA	6.96	143.70	127.00
1	B	407	SER	C-N-CD	-6.60	106.08	120.60
1	D	694	LEU	CA-C-N	-5.36	112.52	122.60
1	D	694	LEU	C-N-CA	-5.36	112.52	122.60
1	D	506	ILE	CA-CB-CG1	5.08	119.05	110.40

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	SER	Peptide
1	A	441	LEU	Peptide
1	A	526	LEU	Peptide
1	A	528	ARG	Peptide
1	A	549	SER	Peptide
1	A	595	ASN	Peptide
1	A	624	ASP	Peptide
1	A	709	PHE	Peptide
1	A	727	GLU	Peptide
1	A	731	GLU	Peptide
1	B	206	GLY	Peptide
1	B	246	VAL	Peptide
1	B	324	GLU	Peptide
1	B	326	ASP	Peptide
1	B	382	ALA	Peptide
1	B	441	LEU	Peptide
1	B	526	LEU	Peptide
1	B	528	ARG	Peptide
1	B	597	PRO	Peptide
1	B	640	LYS	Peptide
1	B	678	ALA	Peptide
1	C	182	GLY	Peptide
1	C	207	GLU	Peptide
1	C	246	VAL	Peptide
1	C	325	LYS	Peptide
1	C	382	ALA	Peptide
1	C	441	LEU	Peptide
1	C	526	LEU	Peptide
1	C	551	MET	Peptide
1	C	636	GLU	Peptide
1	C	641	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	C	645	ARG	Peptide
1	C	650	PRO	Peptide
1	C	685	ASP	Peptide
1	C	834	LEU	Peptide
1	C	848	VAL	Peptide
1	D	246	VAL	Peptide
1	D	279	ALA	Peptide
1	D	441	LEU	Peptide
1	D	506	ILE	Peptide,Mainchain
1	D	522	LYS	Peptide
1	D	550	ARG	Peptide
1	D	552	MET	Peptide
1	D	627	GLU	Peptide
1	D	658	GLU	Peptide
1	D	719	ASN	Peptide
1	D	793	ILE	Peptide
1	D	848	VAL	Peptide
1	E	229	PRO	Peptide
1	E	275	LEU	Peptide
1	E	297	ASN	Peptide
1	E	441	LEU	Peptide
1	E	548	VAL	Peptide
1	E	549	SER	Peptide
1	E	551	MET	Peptide
1	E	627	GLU	Peptide
1	E	636	GLU	Peptide
1	E	681	LYS	Peptide
1	E	808	TYR	Peptide
1	E	837	GLU	Peptide
1	F	176	LYS	Peptide
1	F	294	ASP	Peptide
1	F	407	SER	Peptide
1	F	441	LEU	Peptide
1	F	624	ASP	Peptide
1	F	834	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5406	0	5486	137	0
1	B	5430	0	5507	119	0
1	C	5430	0	5505	118	0
1	D	5406	0	5486	134	0
1	E	5406	0	5484	156	0
1	F	5406	0	5487	116	0
2	S	120	0	122	5	0
3	A	31	0	10	4	0
3	B	62	0	23	9	0
3	C	62	0	24	6	0
3	D	62	0	24	10	0
3	E	62	0	21	10	0
4	A	27	0	10	4	0
4	E	27	0	8	1	0
All	All	32937	0	33197	733	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (733) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:VAL:O	1:D:543:TRP:HB2	1.65	0.97
1:A:618:LEU:O	1:A:622:MET:HB3	1.86	0.75
1:F:672:SER:H	1:F:712:THR:HG22	1.52	0.73
1:D:538:GLU:HB3	1:D:542:ARG:HH21	1.53	0.72
1:C:692:GLN:HE22	1:D:636:GLU:HG3	1.54	0.71
1:D:366:THR:HG22	1:D:368:PRO:HD2	1.72	0.70
1:E:160:ALA:HA	1:E:163:LYS:HB2	1.74	0.69
1:E:751:PRO:O	1:E:755:ASN:HB2	1.92	0.69
1:D:634:MET:HG3	1:D:679:VAL:HA	1.74	0.69
1:C:672:SER:H	1:C:712:THR:HG22	1.59	0.68
1:F:244:ALA:O	1:F:258:ARG:NH1	2.27	0.68
1:E:184:ASP:HA	1:E:222:ARG:HH12	1.59	0.67
1:E:205:ILE:HB	1:E:337:PHE:HA	1.76	0.67
1:F:249:ALA:HA	1:F:255:PHE:HB2	1.78	0.66
1:E:354:LYS:HD3	1:E:370:ILE:HD11	1.78	0.66
1:B:815:ARG:NH2	3:B:1002:AGS:O3A	2.29	0.66
1:A:409:PRO:HB2	1:A:412:LEU:HB2	1.78	0.65
1:A:692:GLN:HE22	1:B:636:GLU:HG3	1.61	0.65
1:E:815:ARG:NH1	3:E:1002:AGS:S1G	2.70	0.65
1:D:178:ASP:OD1	1:D:356:ARG:NH1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:GLN:OE1	1:C:705:ARG:NH2	2.31	0.65
1:C:321:GLN:NE2	1:D:657:GLU:O	2.30	0.64
1:A:195:GLN:HE21	1:A:232:LEU:HG	1.61	0.64
1:D:718:SER:OG	1:D:719:ASN:N	2.31	0.64
1:F:207:GLU:O	1:F:212:LYS:NZ	2.31	0.64
1:D:688:ASN:ND2	1:E:635:SER:O	2.31	0.64
1:E:595:ASN:HA	1:E:710:ARG:HH11	1.61	0.64
1:C:793:ILE:HG12	1:C:844:ILE:HB	1.80	0.64
1:E:586:ARG:HG2	1:E:591:LEU:HD22	1.80	0.64
1:F:691:LEU:O	1:F:756:ARG:NH1	2.31	0.63
1:A:331:ARG:NH1	3:B:1001:AGS:O3B	2.32	0.63
1:C:821:ILE:HG23	1:C:825:ILE:HD12	1.81	0.63
1:E:698:ARG:NH2	1:E:700:THR:OG1	2.31	0.63
1:F:601:PHE:HB2	1:F:715:ILE:HG12	1.81	0.63
1:B:701:ASP:O	1:C:645:ARG:NH2	2.31	0.63
1:D:236:ARG:HB2	1:D:273:VAL:HA	1.81	0.63
1:B:225:ASN:OD1	1:B:491:ARG:NH1	2.32	0.62
1:D:738:LYS:NZ	1:D:759:GLU:OE2	2.32	0.62
1:B:573:GLN:NE2	1:B:764:HIS:O	2.30	0.62
1:C:615:CYS:HB3	1:C:629:MET:HE1	1.82	0.62
1:B:663:THR:HB	1:B:707:VAL:HG21	1.82	0.61
1:E:366:THR:HG22	1:E:368:PRO:HD2	1.82	0.61
1:E:795:ILE:HA	1:E:846:LEU:HB2	1.81	0.61
1:E:610:GLY:HA2	1:E:613:GLU:HB3	1.80	0.61
1:F:726:GLN:HA	1:F:765:PRO:HG3	1.82	0.61
1:A:183:ARG:NH2	1:A:339:ALA:O	2.33	0.61
1:C:559:LEU:HD21	1:C:585:ARG:HG2	1.82	0.61
1:A:751:PRO:HA	1:A:754:ILE:HG12	1.82	0.61
1:C:605:GLY:O	1:C:611:LYS:NZ	2.31	0.61
1:A:189:ARG:HH21	1:B:543:TRP:HA	1.66	0.61
1:A:605:GLY:HA3	1:A:763:PHE:HB2	1.83	0.60
1:F:300:LYS:NZ	1:F:326:ASP:OD2	2.34	0.60
1:F:563:GLU:OE2	1:F:585:ARG:NH1	2.34	0.60
1:A:189:ARG:HH12	1:A:336:VAL:HA	1.67	0.60
1:A:573:GLN:NE2	1:A:764:HIS:O	2.33	0.60
1:B:252:ARG:NH1	1:C:251:TYR:O	2.34	0.60
1:C:539:VAL:O	1:C:543:TRP:HB2	2.02	0.60
1:E:611:LYS:NZ	1:E:718:SER:O	2.33	0.60
1:F:638:MET:HA	1:F:683:HIS:HB2	1.84	0.60
1:B:409:PRO:HG2	1:B:412:LEU:HD22	1.83	0.60
1:D:849:ASN:HD22	1:D:852:ARG:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:310:CYS:SG	1:F:311:VAL:N	2.75	0.60
1:F:548:VAL:HG12	1:F:550:ARG:H	1.66	0.60
1:A:693:VAL:O	1:A:697:GLY:N	2.34	0.60
1:A:755:ASN:ND2	1:B:812:TYR:O	2.32	0.60
1:E:815:ARG:NH2	3:E:1002:AGS:O2G	2.31	0.60
1:B:608:GLY:HA2	3:B:1002:AGS:H5'2	1.84	0.59
1:C:600:SER:OG	1:C:758:ASP:N	2.35	0.59
1:D:354:LYS:HD3	1:D:370:ILE:HD11	1.84	0.59
1:F:634:MET:HE1	1:F:646:LEU:HD22	1.85	0.59
1:A:556:ARG:NH2	1:B:833:ILE:O	2.36	0.59
3:A:1001:AGS:O3'	1:F:331:ARG:NH2	2.36	0.59
1:C:698:ARG:NH2	1:C:700:THR:OG1	2.35	0.59
1:A:193:VAL:HG13	1:A:196:ARG:HH11	1.68	0.59
3:B:1002:AGS:O2G	3:B:1002:AGS:O1B	2.20	0.59
1:C:803:LEU:HD23	1:C:806:ASN:HD22	1.67	0.59
1:B:821:ILE:HG23	1:B:825:ILE:HD12	1.84	0.58
1:E:490:ARG:HE	1:E:498:MET:HE1	1.66	0.58
1:C:305:ARG:NH1	1:C:307:GLU:OE2	2.36	0.58
1:C:366:THR:HG22	1:C:368:PRO:HD2	1.85	0.58
1:A:821:ILE:O	1:A:825:ILE:HB	2.04	0.58
1:C:160:ALA:HA	1:C:163:LYS:HD3	1.84	0.58
1:D:545:GLY:HA3	1:D:669:ARG:HH22	1.68	0.58
1:E:672:SER:H	1:E:712:THR:HG22	1.69	0.58
1:A:672:SER:H	1:A:712:THR:HG22	1.68	0.58
1:E:606:PRO:HG2	1:E:609:VAL:HG21	1.85	0.58
1:A:688:ASN:HB3	1:B:635:SER:HB2	1.85	0.58
1:B:600:SER:OG	1:B:758:ASP:N	2.35	0.58
1:C:674:ILE:HB	1:C:714:VAL:HG22	1.85	0.58
1:E:842:LYS:HD3	1:E:857:GLN:HB3	1.85	0.58
1:A:664:GLU:OE1	1:A:667:ARG:NH2	2.35	0.58
1:A:786:LEU:HD13	1:A:793:ILE:HD12	1.85	0.58
1:B:332:ARG:NH2	3:C:1001:AGS:S1G	2.70	0.58
1:E:196:ARG:HH21	1:E:199:LYS:HB2	1.68	0.58
1:E:676:LEU:HB2	1:E:716:MET:HG2	1.86	0.58
1:F:628:ALA:HB1	1:F:672:SER:HA	1.86	0.58
1:B:725:ILE:O	1:B:729:PHE:N	2.37	0.57
1:B:316:LEU:HD21	1:C:668:ARG:HD2	1.86	0.57
1:D:501:LEU:O	1:D:505:LYS:HB2	2.05	0.57
1:E:244:ALA:HA	1:E:247:ALA:HB3	1.86	0.57
1:B:366:THR:HG22	1:B:368:PRO:HD2	1.85	0.57
1:F:184:ASP:OD1	1:F:222:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:402:ARG:HD2	1:F:405:ILE:HD12	1.85	0.57
1:A:728:ARG:HB3	1:A:732:LEU:HD12	1.85	0.57
1:A:250:LYS:HB3	2:S:9:ALA:HA	1.86	0.57
1:A:384:ARG:HB2	1:A:389:LYS:HB3	1.87	0.57
1:B:586:ARG:HB3	1:B:592:ALA:HB2	1.87	0.57
1:C:692:GLN:NE2	1:D:635:SER:OG	2.38	0.57
1:D:752:GLU:OE2	1:E:719:ASN:ND2	2.36	0.57
1:F:809:ASP:OD1	1:F:813:GLY:N	2.37	0.57
1:B:189:ARG:HH22	1:C:543:TRP:HD1	1.52	0.57
1:C:320:ARG:NH1	1:D:664:GLU:OE1	2.37	0.57
1:C:718:SER:OG	1:C:719:ASN:N	2.33	0.57
1:D:728:ARG:HH11	1:D:740:LEU:HD21	1.68	0.57
1:E:677:ASP:OD1	1:E:717:THR:OG1	2.22	0.57
1:F:231:GLY:O	1:F:235:ARG:NH2	2.38	0.57
1:F:379:ARG:NH1	1:F:552:MET:SD	2.78	0.57
1:B:726:GLN:NE2	1:B:810:PRO:O	2.38	0.56
3:B:1002:AGS:O2A	3:B:1002:AGS:O2B	2.22	0.56
1:A:247:ALA:H	1:A:258:ARG:HH12	1.53	0.56
1:D:612:THR:HG22	1:D:616:LYS:HE3	1.87	0.56
3:B:1001:AGS:O1B	3:B:1001:AGS:O2G	2.22	0.56
1:E:296:GLY:O	1:E:300:LYS:N	2.37	0.56
1:E:731:GLU:HG2	1:E:732:LEU:HD12	1.86	0.56
1:A:834:LEU:HD13	1:F:585:ARG:HB3	1.86	0.56
1:D:756:ARG:HH21	1:E:815:ARG:HH12	1.53	0.56
1:C:827:ASN:O	1:C:831:GLN:HB2	2.05	0.56
1:A:688:ASN:ND2	1:B:638:MET:SD	2.74	0.56
1:A:344:GLU:HA	1:A:347:ILE:HD12	1.87	0.56
1:B:691:LEU:O	1:B:695:ASP:HB2	2.06	0.56
1:D:305:ARG:NH1	1:D:307:GLU:OE1	2.38	0.56
1:E:809:ASP:HB2	1:E:811:VAL:HG22	1.88	0.56
3:A:1001:AGS:O2A	3:A:1001:AGS:O1B	2.22	0.56
1:C:728:ARG:HB3	1:C:732:LEU:HD13	1.87	0.56
1:A:196:ARG:NH2	1:B:392:ASP:OD1	2.39	0.56
1:D:636:GLU:O	1:D:645:ARG:NH1	2.37	0.56
1:F:821:ILE:HG23	1:F:825:ILE:HD12	1.87	0.56
1:C:662:LEU:O	1:C:665:ALA:N	2.39	0.56
1:F:183:ARG:NH2	1:F:339:ALA:O	2.39	0.56
1:C:590:GLY:HA3	1:D:789:ARG:HH21	1.71	0.55
1:D:252:ARG:NH1	2:S:3:ALA:O	2.39	0.55
1:E:196:ARG:HA	1:F:361:HIS:HE1	1.71	0.55
1:F:520:GLU:HA	1:F:523:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:HG2	1:A:763:PHE:HE2	1.71	0.55
1:A:703:GLN:OE1	1:A:705:ARG:NH1	2.39	0.55
1:C:333:PHE:O	1:D:384:ARG:NH2	2.39	0.55
3:E:1001:AGS:O2G	3:E:1001:AGS:O1B	2.23	0.55
1:F:609:VAL:HG12	1:F:814:ALA:H	1.72	0.55
1:B:699:LEU:HB3	1:B:707:VAL:HB	1.86	0.55
1:C:685:ASP:OD2	1:C:750:ARG:NH2	2.38	0.55
1:F:363:VAL:O	1:F:476:LYS:NZ	2.39	0.55
1:D:422:LEU:HD22	1:D:444:LEU:HD11	1.88	0.55
1:E:487:GLU:OE2	1:E:490:ARG:NH1	2.40	0.55
1:C:768:GLU:HA	1:C:771:ILE:HD12	1.88	0.55
1:E:586:ARG:HA	1:E:591:LEU:HD13	1.87	0.55
1:D:725:ILE:HG22	1:D:765:PRO:HD3	1.89	0.55
1:D:786:LEU:O	1:D:790:GLY:N	2.39	0.55
1:A:645:ARG:HA	1:F:651:PRO:HD2	1.88	0.55
1:F:654:VAL:HG22	2:S:23:ALA:HB1	1.89	0.55
1:F:768:GLU:HA	1:F:771:ILE:HD12	1.88	0.55
1:D:613:GLU:HG3	3:D:1002:AGS:H2'	1.88	0.55
1:E:319:TYR:HA	1:E:323:ILE:HD12	1.89	0.55
1:E:827:ASN:O	1:E:831:GLN:HB2	2.07	0.55
1:F:388:ASP:HA	1:F:391:ILE:HD12	1.89	0.55
1:F:698:ARG:NH2	1:F:700:THR:OG1	2.36	0.55
1:F:781:ARG:HG3	1:F:785:ARG:HH22	1.71	0.55
1:A:401:ILE:HG13	1:A:531:VAL:HG22	1.89	0.54
1:C:582:ASN:OD1	1:C:585:ARG:NH2	2.31	0.54
1:E:388:ASP:HA	1:E:391:ILE:HD12	1.89	0.54
1:B:630:VAL:HB	1:B:674:ILE:HG12	1.88	0.54
1:F:361:HIS:NE2	1:F:395:ASP:OD1	2.40	0.54
1:A:212:LYS:NZ	3:A:1001:AGS:O2B	2.40	0.54
1:B:546:ILE:HD11	1:B:670:PRO:HB2	1.89	0.54
1:E:164:TYR:OH	1:E:258:ARG:NH1	2.41	0.54
1:A:593:ASP:OD1	1:A:595:ASN:ND2	2.41	0.54
1:A:815:ARG:HA	1:A:818:LYS:HD3	1.89	0.54
1:E:362:HIS:HD2	1:E:473:GLN:HG2	1.73	0.54
1:F:211:GLY:O	1:F:215:ILE:N	2.39	0.54
1:B:728:ARG:HB3	1:B:732:LEU:HD13	1.89	0.54
1:C:566:LEU:HD12	1:C:577:VAL:HG13	1.89	0.54
1:A:388:ASP:HA	1:A:391:ILE:HD12	1.89	0.54
1:F:202:PRO:HG2	1:F:311:VAL:HG13	1.89	0.54
1:E:551:MET:HE1	1:E:588:ARG:HD2	1.90	0.54
1:E:520:GLU:HA	1:E:523:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:520:GLU:O	1:F:523:THR:N	2.41	0.54
1:F:786:LEU:HD13	1:F:793:ILE:HD12	1.89	0.54
1:B:178:ASP:OD1	1:B:356:ARG:NH1	2.41	0.54
1:C:524:MET:HE2	1:C:529:ASN:HB3	1.91	0.54
1:E:280:LEU:HD21	1:E:329:LEU:HD11	1.89	0.54
3:E:1002:AGS:O2A	3:E:1002:AGS:O1B	2.25	0.54
1:A:786:LEU:O	1:A:790:GLY:N	2.39	0.53
1:F:786:LEU:HB3	1:F:791:TYR:HB2	1.89	0.53
1:C:557:GLU:O	1:C:561:ARG:N	2.40	0.53
1:D:816:PRO:HA	1:D:819:ARG:HG2	1.90	0.53
1:E:301:PRO:HB2	1:E:305:ARG:HH21	1.72	0.53
1:A:539:VAL:HG22	1:A:542:ARG:HH22	1.74	0.53
1:A:793:ILE:HG12	1:A:844:ILE:HB	1.90	0.53
1:B:409:PRO:HB2	1:B:412:LEU:HB2	1.90	0.53
1:D:252:ARG:HH22	2:S:2:ALA:HB3	1.71	0.53
1:E:632:ILE:HD12	1:E:662:LEU:HD13	1.89	0.53
1:C:344:GLU:HA	1:C:347:ILE:HD12	1.89	0.53
1:A:570:VAL:HA	4:A:1002:ADP:HN62	1.73	0.53
1:A:777:ILE:HA	1:A:780:LYS:HD2	1.90	0.53
1:D:245:LEU:O	1:D:258:ARG:NH1	2.36	0.53
1:F:663:THR:OG1	1:F:664:GLU:OE2	2.26	0.53
1:F:786:LEU:O	1:F:790:GLY:N	2.40	0.53
3:C:1002:AGS:O2B	3:C:1002:AGS:O2A	2.24	0.53
1:D:732:LEU:HD22	1:D:737:MET:HE2	1.90	0.53
1:F:220:ALA:HA	1:F:223:ILE:HD12	1.90	0.53
1:D:608:GLY:O	3:D:1002:AGS:H8	2.09	0.53
3:D:1001:AGS:O1B	3:D:1001:AGS:O2G	2.26	0.53
1:C:409:PRO:HG2	1:C:412:LEU:HD22	1.90	0.52
1:C:727:GLU:HG2	1:C:728:ARG:HG3	1.90	0.52
1:D:171:ARG:HA	1:D:174:GLN:HB2	1.91	0.52
1:A:608:GLY:HA2	4:A:1002:ADP:H5'2	1.90	0.52
1:B:164:TYR:HD1	1:B:244:ALA:HB1	1.73	0.52
1:D:169:THR:HB	1:D:224:ILE:HD11	1.90	0.52
3:E:1001:AGS:O2G	3:E:1001:AGS:O2A	2.25	0.52
1:E:196:ARG:HE	1:E:198:THR:HG23	1.74	0.52
1:E:376:LEU:O	1:E:380:TYR:N	2.33	0.52
1:F:685:ASP:HA	1:F:688:ASN:HD22	1.74	0.52
1:C:189:ARG:HH21	1:D:543:TRP:HA	1.74	0.52
1:D:300:LYS:HA	1:D:303:LEU:HB2	1.91	0.52
1:A:839:VAL:H	1:A:857:GLN:HE22	1.55	0.52
1:B:596:ARG:NH2	1:B:756:ARG:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ARG:HA	1:C:174:GLN:HB2	1.91	0.52
1:B:487:GLU:OE2	1:B:490:ARG:NH1	2.42	0.52
1:A:619:ALA:O	1:A:624:ASP:N	2.43	0.52
1:D:486:ILE:HG13	1:D:498:MET:HB2	1.92	0.52
1:E:202:PRO:HG2	1:E:311:VAL:HG13	1.92	0.52
1:E:566:LEU:O	1:E:570:VAL:N	2.43	0.52
1:F:816:PRO:HA	1:F:819:ARG:HG2	1.91	0.52
1:F:680:GLU:HG2	1:F:681:LYS:HG2	1.91	0.52
1:A:320:ARG:HA	1:A:324:GLU:HB2	1.91	0.52
1:D:520:GLU:HA	1:D:523:THR:HG22	1.92	0.52
1:D:319:TYR:HA	1:D:323:ILE:HD12	1.92	0.52
1:D:450:ASP:OD1	1:D:453:ARG:NH2	2.42	0.52
1:E:236:ARG:HB2	1:E:273:VAL:HA	1.90	0.52
1:F:688:ASN:OD1	1:F:750:ARG:NH1	2.42	0.52
1:A:559:LEU:HA	1:A:562:MET:HB2	1.91	0.51
1:C:237:VAL:HG22	1:C:274:ILE:HB	1.93	0.51
1:D:768:GLU:HA	1:D:771:ILE:HD12	1.91	0.51
1:A:726:GLN:NE2	1:A:810:PRO:O	2.42	0.51
1:D:847:GLU:O	1:D:854:VAL:N	2.40	0.51
1:C:552:MET:HG3	1:C:555:GLU:H	1.75	0.51
1:C:602:LEU:HB3	1:C:760:VAL:HG22	1.93	0.51
1:E:571:ILE:N	3:E:1002:AGS:HN62	2.08	0.51
1:A:487:GLU:OE2	1:A:490:ARG:NH1	2.43	0.51
1:A:632:ILE:HG12	1:A:661:TYR:HE2	1.76	0.51
1:E:205:ILE:HD11	1:E:335:LYS:HB3	1.91	0.51
1:F:600:SER:OG	1:F:758:ASP:N	2.42	0.51
1:A:334:GLN:OE1	1:B:384:ARG:NH2	2.43	0.51
1:A:838:LEU:HD23	1:A:844:ILE:HD13	1.93	0.51
1:B:696:ASP:OD2	1:C:631:ARG:NH1	2.28	0.51
1:D:295:ALA:HA	1:D:298:MET:HB2	1.92	0.51
1:D:295:ALA:O	1:D:299:LEU:N	2.44	0.51
1:D:368:PRO:HA	1:D:371:VAL:HG12	1.93	0.51
1:C:520:GLU:HA	1:C:523:THR:HG22	1.91	0.51
1:D:228:VAL:O	1:D:233:LYS:NZ	2.42	0.51
1:D:506:ILE:HG13	1:D:510:GLU:HG3	1.93	0.51
1:E:606:PRO:HB3	1:E:726:GLN:HE21	1.75	0.51
1:F:479:LEU:HG	1:F:483:LYS:HE3	1.93	0.51
1:A:333:PHE:O	1:B:384:ARG:NH2	2.44	0.51
1:B:196:ARG:HH21	1:C:395:ASP:HB3	1.76	0.51
1:B:699:LEU:N	1:B:707:VAL:O	2.43	0.51
1:E:310:CYS:SG	1:E:311:VAL:N	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:GLN:O	1:F:163:LYS:NZ	2.37	0.51
1:B:608:GLY:O	3:B:1002:AGS:H8	2.11	0.51
1:D:344:GLU:HA	1:D:347:ILE:HD12	1.93	0.51
1:E:595:ASN:OD1	1:E:710:ARG:NH1	2.44	0.51
1:E:666:VAL:HG13	1:E:712:THR:HG21	1.94	0.51
1:A:302:ALA:O	1:A:306:GLY:N	2.44	0.50
1:B:283:MET:HA	1:B:286:ALA:HB2	1.92	0.50
1:C:195:GLN:HE21	1:C:232:LEU:HG	1.75	0.50
1:E:547:PRO:HG2	1:E:549:SER:HB2	1.93	0.50
1:E:768:GLU:HA	1:E:771:ILE:HD12	1.93	0.50
1:A:200:ASN:ND2	1:A:306:GLY:O	2.44	0.50
1:E:719:ASN:N	1:E:719:ASN:OD1	2.43	0.50
1:F:236:ARG:HB3	1:F:273:VAL:HG22	1.92	0.50
1:D:724:LEU:HD21	1:D:740:LEU:HG	1.94	0.50
1:F:171:ARG:HE	1:F:177:LEU:HD21	1.76	0.50
1:D:214:ALA:HB2	3:D:1001:AGS:H2'	1.93	0.50
1:D:603:PHE:HB2	1:D:717:THR:HG22	1.92	0.50
1:E:611:LYS:N	3:E:1002:AGS:O2B	2.43	0.50
1:A:692:GLN:O	1:A:696:ASP:HB2	2.10	0.50
1:B:586:ARG:HH11	1:C:822:GLN:HG2	1.77	0.50
1:E:166:ILE:O	1:E:239:ALA:N	2.40	0.50
1:F:462:TRP:CE2	1:F:466:LYS:HD2	2.47	0.50
1:D:384:ARG:NH1	1:D:392:ASP:OD2	2.44	0.50
1:B:381:ILE:HD12	1:B:389:LYS:HD2	1.93	0.50
1:C:161:LEU:O	1:C:165:THR:OG1	2.25	0.50
1:E:220:ALA:HA	1:E:223:ILE:HD12	1.93	0.50
1:F:204:LEU:HB3	1:F:212:LYS:HD2	1.92	0.50
1:F:634:MET:N	1:F:677:ASP:O	2.42	0.50
1:A:235:ARG:O	1:A:236:ARG:NH1	2.42	0.50
1:D:815:ARG:NH2	3:D:1002:AGS:O2G	2.42	0.50
1:A:502:GLN:HG3	1:A:506:ILE:HD12	1.94	0.50
1:A:685:ASP:OD1	1:A:685:ASP:N	2.44	0.50
1:C:169:THR:HB	1:C:224:ILE:HD11	1.94	0.50
1:F:604:LEU:HD22	1:F:720:LEU:H	1.76	0.50
1:A:618:LEU:O	1:A:622:MET:CB	2.59	0.49
1:B:722:SER:HA	1:B:725:ILE:HD12	1.93	0.49
1:D:677:ASP:OD1	1:D:717:THR:OG1	2.22	0.49
1:E:696:ASP:HB3	1:E:698:ARG:HG2	1.94	0.49
1:A:375:THR:O	1:A:379:ARG:HB2	2.12	0.49
1:E:634:MET:HB2	1:E:679:VAL:HA	1.95	0.49
1:A:316:LEU:HG	1:A:320:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:745:VAL:O	1:E:749:PHE:N	2.42	0.49
1:D:693:VAL:HG22	1:D:709:PHE:HE2	1.77	0.49
1:D:759:GLU:OE1	1:E:823:GLN:NE2	2.45	0.49
1:E:540:LEU:O	1:E:544:THR:N	2.39	0.49
1:D:605:GLY:O	1:D:611:LYS:NZ	2.45	0.49
1:E:212:LYS:HA	1:E:215:ILE:HD12	1.95	0.49
1:E:212:LYS:N	3:E:1001:AGS:O2A	2.46	0.49
1:E:557:GLU:O	1:E:561:ARG:N	2.44	0.49
1:A:180:VAL:HG21	1:A:214:ALA:HB1	1.94	0.49
1:A:402:ARG:HD2	1:A:405:ILE:HD12	1.93	0.49
1:F:599:GLY:HA3	1:F:713:VAL:HG13	1.94	0.49
1:A:199:LYS:NZ	1:B:388:ASP:OD1	2.46	0.49
1:B:324:GLU:OE2	1:B:335:LYS:NZ	2.41	0.49
1:E:718:SER:OG	1:E:719:ASN:N	2.43	0.49
1:F:625:SER:OG	1:F:627:GLU:OE1	2.28	0.49
1:D:708:ASP:OD1	1:D:710:ARG:N	2.35	0.49
1:A:756:ARG:HE	1:B:815:ARG:NH2	2.11	0.48
1:C:720:LEU:HD12	1:C:745:VAL:HG22	1.96	0.48
1:D:558:LYS:HA	1:D:561:ARG:HH21	1.79	0.48
1:E:508:GLU:HA	1:E:511:LYS:HE3	1.95	0.48
1:F:344:GLU:HA	1:F:347:ILE:HD12	1.95	0.48
1:F:684:PRO:HA	1:F:687:PHE:HD2	1.77	0.48
1:E:171:ARG:NH2	1:E:176:LYS:O	2.46	0.48
1:A:547:PRO:HG2	1:A:588:ARG:HH12	1.79	0.48
1:B:289:ALA:HB3	1:B:292:ALA:HB3	1.95	0.48
1:C:653:TYR:CZ	1:D:641:HIS:HB2	2.48	0.48
1:A:253:GLY:O	1:A:257:GLU:N	2.43	0.48
1:D:358:GLU:OE2	1:D:365:ILE:N	2.42	0.48
1:D:496:ALA:HB1	1:E:427:GLN:HG2	1.95	0.48
1:B:416:ASP:HA	1:B:419:ILE:HG12	1.95	0.48
1:C:222:ARG:O	1:C:226:GLY:N	2.45	0.48
1:E:582:ASN:OD1	1:E:585:ARG:NH2	2.37	0.48
1:F:573:GLN:HB2	1:F:764:HIS:CD2	2.48	0.48
1:A:165:THR:HG22	1:A:240:LEU:HB2	1.95	0.48
1:A:625:SER:OG	1:A:627:GLU:OE1	2.24	0.48
1:B:610:GLY:HA2	3:B:1002:AGS:H5'1	1.95	0.48
1:C:177:LEU:HB2	1:C:221:GLN:HE21	1.78	0.48
1:D:567:HIS:ND1	1:D:570:VAL:O	2.47	0.48
1:F:191:ILE:HA	1:F:194:LEU:HB2	1.95	0.48
1:A:622:MET:HE3	1:A:623:PHE:HB2	1.96	0.48
1:D:235:ARG:NH1	1:D:271:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:GLU:HA	1:D:511:LYS:HE3	1.96	0.48
1:D:646:LEU:HD12	1:D:647:VAL:HG23	1.95	0.48
4:E:1003:ADP:O1B	1:F:210:VAL:N	2.44	0.48
1:A:181:ILE:HD12	1:A:349:ILE:HA	1.95	0.48
1:C:719:ASN:N	1:C:719:ASN:OD1	2.46	0.48
1:D:237:VAL:HG22	1:D:274:ILE:HB	1.94	0.48
1:D:818:LYS:NZ	3:D:1002:AGS:O3'	2.39	0.48
1:E:229:PRO:HD2	1:E:232:LEU:HD12	1.95	0.48
1:A:362:HIS:CD2	1:A:473:GLN:HG2	2.49	0.47
1:B:199:LYS:NZ	1:B:331:ARG:O	2.47	0.47
1:D:685:ASP:OD1	1:D:685:ASP:N	2.46	0.47
1:F:326:ASP:OD2	1:F:329:LEU:N	2.44	0.47
1:A:849:ASN:N	1:A:852:ARG:O	2.43	0.47
1:C:189:ARG:NE	1:D:542:ARG:O	2.48	0.47
1:D:697:GLY:O	1:D:709:PHE:N	2.46	0.47
1:E:326:ASP:OD2	1:E:329:LEU:N	2.44	0.47
1:E:680:GLU:OE2	1:E:681:LYS:NZ	2.47	0.47
1:A:236:ARG:O	1:A:274:ILE:N	2.40	0.47
1:A:469:LEU:HD21	1:A:529:ASN:HB3	1.97	0.47
1:E:182:GLY:O	1:E:222:ARG:NH2	2.47	0.47
1:E:685:ASP:HA	1:E:688:ASN:HD22	1.78	0.47
1:F:319:TYR:HA	1:F:323:ILE:HD12	1.96	0.47
1:F:422:LEU:HD22	1:F:444:LEU:HD11	1.97	0.47
1:C:571:ILE:HG12	1:C:770:HIS:HA	1.95	0.47
1:E:365:ILE:HA	1:E:531:VAL:HB	1.97	0.47
1:F:195:GLN:HE21	1:F:232:LEU:HG	1.80	0.47
1:A:692:GLN:NE2	1:B:635:SER:OG	2.48	0.47
1:B:520:GLU:HA	1:B:523:THR:HG22	1.96	0.47
1:B:603:PHE:HB2	1:B:717:THR:HA	1.97	0.47
1:E:837:GLU:HB3	1:E:838:LEU:HD12	1.97	0.47
1:C:479:LEU:HG	1:C:483:LYS:HE3	1.97	0.47
1:D:388:ASP:HA	1:D:391:ILE:HD12	1.96	0.47
1:A:406:ASP:HB2	1:F:230:GLU:HG2	1.97	0.47
1:A:520:GLU:HA	1:A:523:THR:HG22	1.97	0.47
1:B:189:ARG:NH2	1:C:543:TRP:HD1	2.11	0.47
1:B:195:GLN:HE21	1:B:232:LEU:HG	1.79	0.47
1:C:368:PRO:HA	1:C:371:VAL:HG12	1.96	0.47
1:D:544:THR:OG1	1:D:545:GLY:N	2.46	0.47
1:D:551:MET:HB3	1:D:556:ARG:HB2	1.95	0.47
1:E:286:ALA:N	1:E:294:ASP:OD2	2.42	0.47
1:F:172:ALA:HB2	1:F:177:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:849:ASN:HD22	1:F:852:ARG:HB2	1.80	0.47
1:B:300:LYS:NZ	1:B:329:LEU:HB2	2.30	0.47
1:A:368:PRO:HA	1:A:371:VAL:HG12	1.97	0.47
1:B:401:ILE:HG13	1:B:531:VAL:HG22	1.96	0.47
1:E:684:PRO:HA	1:E:687:PHE:HD2	1.80	0.47
1:F:293:MET:N	1:F:297:ASN:H	2.13	0.47
1:A:582:ASN:OD1	1:A:585:ARG:NH2	2.38	0.47
1:A:722:SER:HA	1:A:725:ILE:HD12	1.96	0.47
1:B:646:LEU:HD12	1:B:647:VAL:HG13	1.96	0.47
1:B:693:VAL:HG13	1:B:709:PHE:HD2	1.80	0.47
1:C:342:SER:O	1:C:346:THR:OG1	2.29	0.47
1:D:771:ILE:HG23	1:D:817:LEU:HD22	1.96	0.47
1:A:775:ALA:HB2	1:A:817:LEU:HD21	1.96	0.46
1:D:731:GLU:HG2	1:D:732:LEU:HD12	1.97	0.46
1:D:852:ARG:HG2	1:D:853:ILE:H	1.78	0.46
1:D:281:HIS:HB2	1:D:322:TYR:HD2	1.79	0.46
1:D:569:ARG:HH11	1:D:620:ASN:HD22	1.63	0.46
1:E:193:VAL:HG22	1:E:196:ARG:HH12	1.80	0.46
1:F:683:HIS:ND1	1:F:685:ASP:OD1	2.49	0.46
1:C:281:HIS:CE1	1:C:318:GLU:HG2	2.50	0.46
1:A:184:ASP:HA	1:A:187:ILE:HD12	1.96	0.46
1:A:358:GLU:OE2	1:A:365:ILE:N	2.48	0.46
1:A:611:LYS:HG2	1:A:763:PHE:CE2	2.49	0.46
1:C:206:GLY:HA3	1:C:212:LYS:HD3	1.97	0.46
1:C:212:LYS:NZ	3:C:1001:AGS:O3B	2.46	0.46
1:C:551:MET:HE1	1:C:588:ARG:HH11	1.80	0.46
1:C:693:VAL:HG13	1:C:709:PHE:HD2	1.81	0.46
1:A:396:GLU:OE1	1:A:543:TRP:NE1	2.38	0.46
1:D:508:GLU:HG3	1:D:509:LEU:HD12	1.96	0.46
1:E:314:THR:OG1	1:E:315:THR:N	2.48	0.46
1:B:822:GLN:O	1:B:826:GLU:HB2	2.15	0.46
1:E:390:ALA:HA	1:E:393:LEU:HD12	1.97	0.46
1:E:236:ARG:O	1:E:274:ILE:N	2.44	0.46
1:F:263:LEU:HD23	1:F:266:LEU:HD12	1.97	0.46
1:B:362:HIS:CD2	1:B:473:GLN:HG2	2.50	0.46
1:B:794:HIS:N	1:B:844:ILE:O	2.49	0.46
1:B:533:ASP:N	1:B:533:ASP:OD1	2.49	0.46
1:E:358:GLU:OE2	1:E:365:ILE:N	2.49	0.46
1:F:266:LEU:HB3	1:F:307:GLU:HB3	1.97	0.46
1:A:462:TRP:CE2	1:A:466:LYS:HD2	2.51	0.46
1:C:324:GLU:HG2	1:C:330:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:HD2	1:E:272:ASN:HA	1.98	0.46
1:E:558:LYS:HA	1:E:561:ARG:HB2	1.97	0.46
1:E:570:VAL:HG21	1:E:614:LEU:HD13	1.98	0.46
1:A:847:GLU:O	1:A:854:VAL:N	2.43	0.45
1:B:344:GLU:HA	1:B:347:ILE:HD12	1.98	0.45
1:C:533:ASP:OD1	1:C:533:ASP:N	2.48	0.45
1:D:195:GLN:HE21	1:D:232:LEU:HG	1.82	0.45
1:D:821:ILE:HG23	1:D:825:ILE:HD12	1.98	0.45
1:E:648:GLY:HA3	1:E:702:GLY:H	1.80	0.45
1:F:691:LEU:HD21	1:F:753:PHE:HA	1.98	0.45
1:B:201:ASN:OD1	1:B:310:CYS:N	2.49	0.45
1:B:240:LEU:HD11	1:B:245:LEU:HD11	1.97	0.45
1:C:809:ASP:OD1	1:C:809:ASP:N	2.46	0.45
1:B:613:GLU:HG3	3:B:1002:AGS:H2'	1.98	0.45
1:B:727:GLU:HG2	1:B:728:ARG:HG3	1.98	0.45
1:D:559:LEU:HD21	1:D:585:ARG:HG2	1.97	0.45
1:E:816:PRO:HA	1:E:819:ARG:HG2	1.97	0.45
1:F:581:SER:HB3	1:F:585:ARG:HH12	1.81	0.45
1:A:204:LEU:HB2	1:A:313:ALA:HA	1.99	0.45
1:A:508:GLU:HA	1:A:511:LYS:HE3	1.98	0.45
1:A:613:GLU:CD	4:A:1002:ADP:H2'	2.41	0.45
1:C:490:ARG:HE	1:C:498:MET:HE1	1.82	0.45
1:E:199:LYS:HE2	1:E:331:ARG:HA	1.99	0.45
1:E:845:ARG:HH21	1:E:858:HIS:CD2	2.35	0.45
1:A:693:VAL:O	1:A:696:ASP:N	2.49	0.45
1:B:354:LYS:HD3	1:B:370:ILE:HD11	1.99	0.45
1:C:416:ASP:HA	1:C:419:ILE:HG12	1.98	0.45
1:C:596:ARG:NH2	1:C:600:SER:OG	2.50	0.45
1:D:793:ILE:HG12	1:D:844:ILE:HB	1.98	0.45
1:A:673:VAL:HG22	1:A:713:VAL:HB	1.97	0.45
1:D:317:ASP:O	1:D:321:GLN:N	2.45	0.45
1:D:499:SER:HB3	1:E:424:LEU:HD22	1.99	0.45
1:D:506:ILE:O	1:D:510:GLU:HB2	2.17	0.45
1:E:161:LEU:O	1:E:165:THR:OG1	2.34	0.45
1:E:558:LYS:HG2	1:E:621:PHE:HE1	1.82	0.45
1:B:334:GLN:NE2	1:C:543:TRP:HE1	2.14	0.45
1:C:729:PHE:CE1	1:C:764:HIS:HB2	2.52	0.45
1:C:745:VAL:O	1:C:749:PHE:N	2.40	0.45
1:D:191:ILE:HA	1:D:194:LEU:HD12	1.99	0.45
1:A:632:ILE:HD11	1:A:662:LEU:HD13	1.99	0.45
1:A:637:PHE:CD1	1:A:642:SER:HB3	2.53	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASP:HA	1:B:222:ARG:HH22	1.81	0.45
1:B:283:MET:HE3	1:B:299:LEU:HD22	1.99	0.45
1:B:637:PHE:HE1	1:B:645:ARG:HD2	1.82	0.45
1:E:241:ASP:OD1	1:E:243:GLY:N	2.50	0.45
1:F:642:SER:HA	1:F:645:ARG:HH21	1.82	0.45
1:B:379:ARG:CZ	1:B:594:PRO:HB3	2.47	0.44
1:B:606:PRO:HB3	1:B:722:SER:HB3	1.98	0.44
1:B:615:CYS:HA	1:B:618:LEU:HD12	1.99	0.44
1:D:229:PRO:HB3	1:E:406:ASP:HB3	1.98	0.44
1:D:846:LEU:HD23	1:D:846:LEU:HA	1.83	0.44
1:F:174:GLN:HB2	1:F:176:LYS:HZ2	1.82	0.44
1:F:691:LEU:HD23	1:F:694:LEU:HD12	2.00	0.44
1:C:412:LEU:HD11	1:C:458:LEU:HB3	1.97	0.44
1:C:845:ARG:HB3	1:C:847:GLU:HG3	1.98	0.44
1:D:303:LEU:HB3	1:D:332:ARG:HG3	1.98	0.44
1:F:602:LEU:HB3	1:F:760:VAL:HG13	1.99	0.44
1:C:697:GLY:HA2	1:C:709:PHE:HB2	1.99	0.44
1:C:721:GLY:O	1:C:725:ILE:N	2.45	0.44
1:C:795:ILE:HA	1:C:846:LEU:HB2	1.99	0.44
1:E:178:ASP:OD1	1:E:356:ARG:NH1	2.37	0.44
1:E:276:PHE:HD1	1:E:311:VAL:HB	1.82	0.44
1:E:563:GLU:HA	1:E:566:LEU:HD12	2.00	0.44
1:E:847:GLU:O	1:E:854:VAL:N	2.49	0.44
1:A:799:ALA:HB2	1:A:848:VAL:HG12	1.99	0.44
1:A:816:PRO:HA	1:A:819:ARG:HG2	1.99	0.44
1:B:237:VAL:HG22	1:B:274:ILE:HB	1.98	0.44
1:C:697:GLY:O	1:C:709:PHE:N	2.51	0.44
1:F:368:PRO:HA	1:F:371:VAL:HG12	1.99	0.44
1:B:793:ILE:HA	1:B:844:ILE:HB	1.98	0.44
1:E:742:LEU:HD11	1:E:754:ILE:HD12	2.00	0.44
1:A:528:ARG:HH22	1:A:532:THR:H	1.66	0.44
1:C:166:ILE:HB	1:C:239:ALA:HB3	2.00	0.44
1:E:667:ARG:HD3	1:E:707:VAL:HG22	2.00	0.44
1:A:367:ASP:HA	1:A:370:ILE:HD12	2.00	0.44
1:D:191:ILE:HG23	1:D:232:LEU:HD12	1.99	0.44
1:D:286:ALA:HB3	1:D:294:ASP:HB2	1.99	0.44
1:C:169:THR:OG1	1:C:236:ARG:NH1	2.49	0.44
1:C:775:ALA:HB2	1:C:817:LEU:HD21	1.98	0.44
1:E:680:GLU:HG3	1:E:720:LEU:HD21	1.99	0.44
1:A:251:TYR:HB3	1:B:250:LYS:HB2	2.00	0.44
1:A:733:ASP:CG	1:A:736:HIS:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:604:LEU:O	1:B:763:PHE:N	2.45	0.44
1:B:634:MET:HG3	1:B:679:VAL:HG23	2.00	0.44
1:C:197:ARG:HE	1:D:357:TYR:HE1	1.66	0.44
1:C:796:SER:HB2	1:C:847:GLU:HA	2.00	0.44
1:E:358:GLU:HG2	1:E:363:VAL:HG23	2.00	0.44
1:E:359:LEU:HA	1:E:473:GLN:HE22	1.82	0.44
1:E:778:GLN:HA	1:E:781:ARG:HG2	2.00	0.44
1:A:189:ARG:NH2	1:B:543:TRP:HA	2.31	0.43
1:E:774:ILE:HA	1:E:777:ILE:HD12	1.99	0.43
1:A:293:MET:N	1:A:297:ASN:OD1	2.50	0.43
1:B:324:GLU:HG2	1:B:330:GLU:HG3	1.99	0.43
1:D:416:ASP:HA	1:D:419:ILE:HG12	2.00	0.43
1:D:566:LEU:HD12	1:D:577:VAL:HG13	1.99	0.43
1:E:189:ARG:HH21	1:F:543:TRP:NE1	2.16	0.43
1:E:344:GLU:HA	1:E:347:ILE:HD12	2.00	0.43
1:E:520:GLU:O	1:E:523:THR:N	2.52	0.43
1:F:169:THR:HB	1:F:224:ILE:HD11	1.99	0.43
1:F:401:ILE:HG13	1:F:531:VAL:HG22	1.99	0.43
1:A:553:GLU:HA	1:A:556:ARG:HB3	1.99	0.43
1:D:166:ILE:N	1:D:239:ALA:O	2.47	0.43
1:A:278:ASP:N	1:A:278:ASP:OD1	2.51	0.43
1:B:731:GLU:HG2	1:B:732:LEU:HD12	1.99	0.43
1:C:230:GLU:N	1:D:406:ASP:OD2	2.46	0.43
1:D:803:LEU:HD13	1:D:821:ILE:HG12	2.01	0.43
1:E:631:ARG:HA	1:E:675:LEU:HB3	2.01	0.43
1:F:357:TYR:O	1:F:361:HIS:N	2.31	0.43
1:A:610:GLY:O	1:A:614:LEU:N	2.48	0.43
1:A:809:ASP:OD1	1:A:813:GLY:N	2.49	0.43
1:B:604:LEU:HD23	1:B:604:LEU:HA	1.85	0.43
1:D:236:ARG:HB3	1:D:238:LEU:HD13	2.00	0.43
1:D:409:PRO:HD2	1:D:412:LEU:HD22	2.00	0.43
1:A:236:ARG:HB2	1:A:273:VAL:HA	2.01	0.43
1:B:768:GLU:HA	1:B:771:ILE:HD12	1.99	0.43
1:C:586:ARG:CZ	1:D:822:GLN:HE21	2.32	0.43
1:C:731:GLU:HG2	1:C:732:LEU:HD12	1.99	0.43
1:F:381:ILE:HB	1:F:389:LYS:HD2	2.01	0.43
1:F:634:MET:HB2	1:F:679:VAL:HA	2.00	0.43
1:A:404:GLN:HA	1:A:407:SER:HB3	2.00	0.43
1:B:693:VAL:HG13	1:B:709:PHE:CD2	2.53	0.43
1:E:347:ILE:HA	1:E:350:LEU:HD12	2.00	0.43
1:F:533:ASP:OD1	1:F:533:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:691:LEU:HD22	1:F:756:ARG:HG3	2.01	0.43
1:A:546:ILE:HG12	1:A:671:TYR:CG	2.54	0.43
1:D:779:LEU:HD23	1:D:779:LEU:HA	1.90	0.43
1:E:611:LYS:HA	1:E:763:PHE:HE2	1.84	0.43
1:E:634:MET:HB3	1:E:682:ALA:HB2	1.99	0.43
1:E:744:VAL:HA	1:E:747:HIS:HD2	1.84	0.43
1:A:294:ASP:OD1	1:A:295:ALA:N	2.51	0.43
1:C:666:VAL:HG21	1:C:709:PHE:HE1	1.83	0.43
1:D:703:GLN:OE1	1:D:705:ARG:NH1	2.52	0.43
1:E:649:ALA:HB3	1:E:659:GLY:HA2	2.00	0.43
1:B:358:GLU:OE2	1:B:365:ILE:N	2.40	0.43
1:C:656:TYR:O	1:C:703:GLN:NE2	2.51	0.43
1:E:782:LEU:HD13	1:E:785:ARG:HH21	1.84	0.43
1:C:280:LEU:HD21	1:C:333:PHE:CZ	2.53	0.42
1:E:171:ARG:HE	1:E:177:LEU:HD21	1.84	0.42
1:E:803:LEU:HD22	1:E:821:ILE:HG12	2.00	0.42
1:A:610:GLY:N	4:A:1002:ADP:H5'1	2.33	0.42
1:B:849:ASN:HB2	1:B:852:ARG:H	1.84	0.42
1:C:196:ARG:HE	1:D:395:ASP:CG	2.27	0.42
1:C:603:PHE:N	1:C:716:MET:O	2.43	0.42
1:C:610:GLY:O	1:C:613:GLU:N	2.52	0.42
1:E:749:PHE:HB3	1:E:750:ARG:H	1.64	0.42
1:F:793:ILE:HG12	1:F:844:ILE:HB	2.01	0.42
1:A:675:LEU:HD21	1:A:677:ASP:HB2	2.02	0.42
1:B:167:ASP:HA	1:B:238:LEU:HG	2.01	0.42
1:C:606:PRO:HD3	1:C:725:ILE:HG21	2.01	0.42
1:D:280:LEU:HD22	1:D:312:GLY:HA3	2.01	0.42
1:D:321:GLN:NE2	1:E:657:GLU:OE2	2.52	0.42
1:D:690:LEU:HD23	1:D:693:VAL:HG21	2.01	0.42
1:E:169:THR:HB	1:E:224:ILE:HD11	2.01	0.42
1:E:409:PRO:HB2	1:E:412:LEU:HB2	2.02	0.42
1:E:756:ARG:HA	1:E:756:ARG:HD3	1.86	0.42
1:E:815:ARG:NH2	3:E:1002:AGS:O3A	2.52	0.42
1:F:606:PRO:HG2	1:F:609:VAL:HG21	2.01	0.42
1:F:667:ARG:NH2	1:F:668:ARG:HE	2.18	0.42
1:D:604:LEU:HD23	1:D:718:SER:HB3	2.02	0.42
1:C:664:GLU:O	1:C:668:ARG:HG2	2.19	0.42
3:D:1001:AGS:O1B	3:D:1001:AGS:O2A	2.36	0.42
1:E:465:GLU:HB3	1:E:524:MET:HE1	2.00	0.42
1:F:284:VAL:HG11	1:F:322:TYR:HB3	2.00	0.42
1:F:354:LYS:HG3	1:F:365:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:HA3	3:A:1001:AGS:H8	2.02	0.42
1:C:640:LYS:NZ	1:D:638:MET:SD	2.93	0.42
1:A:654:VAL:HG11	1:F:656:TYR:HB3	2.02	0.42
1:A:768:GLU:HA	1:A:771:ILE:HD12	2.00	0.42
1:D:205:ILE:O	1:D:338:VAL:N	2.46	0.42
3:D:1002:AGS:O1B	3:D:1002:AGS:O2A	2.32	0.42
1:E:573:GLN:HE22	1:E:764:HIS:H	1.67	0.42
1:F:199:LYS:HE2	1:F:331:ARG:HG2	2.02	0.42
1:F:751:PRO:HA	1:F:754:ILE:HG12	2.01	0.42
1:A:362:HIS:HD2	1:A:473:GLN:HG2	1.84	0.42
1:D:248:GLY:HA3	1:D:258:ARG:HH22	1.84	0.42
1:E:362:HIS:CD2	1:E:473:GLN:HG2	2.54	0.42
1:F:603:PHE:HB3	1:F:611:LYS:HE2	2.02	0.42
1:A:606:PRO:HG2	1:A:609:VAL:HG11	2.02	0.42
1:C:640:LYS:HG3	1:C:683:HIS:CE1	2.55	0.42
1:E:164:TYR:HD1	1:E:241:ASP:HB3	1.83	0.42
1:E:196:ARG:HH11	1:E:196:ARG:HD3	1.73	0.42
1:E:458:LEU:HD22	1:E:526:LEU:HD21	2.02	0.42
1:F:849:ASN:N	1:F:852:ARG:O	2.41	0.42
1:A:602:LEU:HB3	1:A:760:VAL:HG13	2.01	0.42
1:C:571:ILE:N	3:C:1002:AGS:HN62	2.18	0.42
1:E:248:GLY:HA3	1:E:258:ARG:HH12	1.85	0.42
1:E:541:ALA:O	1:E:545:GLY:N	2.44	0.42
1:E:566:LEU:HD23	1:E:566:LEU:HA	1.91	0.42
1:E:826:GLU:HA	1:E:829:LEU:HB3	2.01	0.42
1:A:316:LEU:HD11	1:B:668:ARG:HE	1.85	0.41
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.92	0.41
1:B:266:LEU:HD13	1:B:308:LEU:HD11	2.02	0.41
1:C:300:LYS:HG3	1:C:332:ARG:HG3	2.02	0.41
3:C:1001:AGS:O1B	3:C:1001:AGS:O2A	2.36	0.41
1:D:171:ARG:HE	1:D:177:LEU:HD21	1.85	0.41
1:D:202:PRO:HG2	1:D:311:VAL:HG13	2.01	0.41
1:E:733:ASP:CG	1:E:736:HIS:H	2.27	0.41
1:E:744:VAL:HA	1:E:747:HIS:CD2	2.55	0.41
1:B:225:ASN:HA	1:B:491:ARG:HD2	2.03	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.84	0.41
1:B:651:PRO:HD3	1:C:645:ARG:HB3	2.02	0.41
1:B:834:LEU:HD23	1:B:834:LEU:HA	1.90	0.41
1:D:162:LYS:HA	1:D:162:LYS:HD2	1.90	0.41
1:D:236:ARG:N	1:D:272:ASN:O	2.49	0.41
1:D:508:GLU:HA	1:D:511:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:608:GLY:HA2	3:D:1002:AGS:H5'2	2.03	0.41
1:E:724:LEU:O	1:E:728:ARG:HB2	2.20	0.41
1:F:508:GLU:HA	1:F:511:LYS:HG2	2.01	0.41
1:A:604:LEU:HD23	1:A:604:LEU:HA	1.90	0.41
1:B:771:ILE:HG23	1:B:817:LEU:HD22	2.01	0.41
1:C:178:ASP:OD1	1:C:356:ARG:NH1	2.54	0.41
1:C:508:GLU:HA	1:C:511:LYS:HE3	2.02	0.41
1:C:663:THR:HG21	1:C:701:ASP:HB3	2.00	0.41
1:C:701:ASP:OD1	1:C:701:ASP:N	2.48	0.41
1:C:777:ILE:HA	1:C:780:LYS:HD2	2.01	0.41
1:D:248:GLY:H	1:D:258:ARG:HH12	1.69	0.41
1:E:210:VAL:HA	1:E:387:PRO:HD2	2.02	0.41
1:E:602:LEU:HB3	1:E:760:VAL:HG13	2.01	0.41
1:E:691:LEU:HD21	1:E:753:PHE:HA	2.01	0.41
1:B:680:GLU:HG3	1:B:720:LEU:HD21	2.03	0.41
1:B:795:ILE:HG13	1:B:846:LEU:HB2	2.01	0.41
1:A:821:ILE:HG23	1:A:825:ILE:HD12	2.02	0.41
1:B:160:ALA:HB1	1:B:164:TYR:HD2	1.84	0.41
1:D:358:GLU:HG2	1:D:363:VAL:HG23	2.02	0.41
1:E:259:LEU:HD11	1:E:299:LEU:HD11	2.02	0.41
1:E:462:TRP:HD1	1:E:527:LEU:HD21	1.85	0.41
1:A:220:ALA:HA	1:A:223:ILE:HD12	2.01	0.41
1:C:409:PRO:HB2	1:C:412:LEU:HB2	2.02	0.41
1:D:317:ASP:OD1	1:D:320:ARG:NH2	2.43	0.41
1:D:404:GLN:O	1:D:407:SER:OG	2.35	0.41
1:D:409:PRO:HB2	1:D:412:LEU:HD13	2.01	0.41
1:E:684:PRO:HG2	1:F:658:GLU:HG2	2.01	0.41
1:E:697:GLY:O	1:E:709:PHE:N	2.37	0.41
1:F:268:LYS:HE3	1:F:269:GLN:HE21	1.86	0.41
1:C:623:PHE:CZ	1:C:672:SER:HA	2.55	0.41
1:D:524:MET:HE3	1:D:527:LEU:HB3	2.01	0.41
1:F:628:ALA:HB2	1:F:669:ARG:HE	1.85	0.41
1:F:795:ILE:HA	1:F:846:LEU:HB2	2.01	0.41
1:F:796:SER:HB3	1:F:847:GLU:HA	2.02	0.41
1:A:247:ALA:N	1:A:258:ARG:HH12	2.18	0.41
1:A:350:LEU:HD23	1:A:350:LEU:HA	1.89	0.41
1:A:786:LEU:HD21	1:F:591:LEU:HG	2.02	0.41
1:B:169:THR:HB	1:B:224:ILE:HD11	2.03	0.41
1:B:317:ASP:OD1	1:B:320:ARG:NH1	2.34	0.41
1:D:667:ARG:HD3	1:D:707:VAL:HG22	2.03	0.41
1:A:702:GLY:HA2	1:B:645:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:N	2:S:6:ALA:O	2.54	0.41
1:B:331:ARG:NH1	3:C:1001:AGS:S1G	2.94	0.41
1:B:528:ARG:NH2	1:B:535:GLU:OE2	2.54	0.41
1:B:580:VAL:HG11	1:B:618:LEU:HD11	2.01	0.41
1:B:650:PRO:HG2	1:B:653:TYR:CD2	2.56	0.41
1:C:407:SER:HA	1:C:409:PRO:HD3	1.88	0.41
1:D:326:ASP:HB3	1:D:329:LEU:HB3	2.02	0.41
1:E:172:ALA:O	1:E:491:ARG:NH1	2.54	0.41
1:E:547:PRO:HB2	1:E:548:VAL:H	1.71	0.41
1:C:693:VAL:HG13	1:C:709:PHE:CD2	2.56	0.41
1:F:316:LEU:HG	1:F:320:ARG:HH11	1.86	0.41
1:F:354:LYS:HD3	1:F:370:ILE:HD11	2.03	0.41
1:A:837:GLU:HB3	1:A:838:LEU:HD12	2.02	0.40
1:B:576:ALA:HB2	1:B:763:PHE:CE1	2.57	0.40
1:E:231:GLY:O	1:E:235:ARG:NE	2.53	0.40
1:F:826:GLU:HA	1:F:829:LEU:HB3	2.03	0.40
1:A:204:LEU:HD23	1:A:336:VAL:HB	2.03	0.40
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.90	0.40
1:A:392:ASP:OD2	1:F:199:LYS:NZ	2.49	0.40
1:B:241:ASP:CG	1:B:244:ALA:H	2.29	0.40
1:B:508:GLU:HA	1:B:511:LYS:HG2	2.02	0.40
1:C:508:GLU:HG3	1:C:509:LEU:HD12	2.03	0.40
1:D:377:SER:HB2	1:D:389:LYS:HD3	2.02	0.40
1:D:719:ASN:O	1:D:722:SER:OG	2.29	0.40
1:E:161:LEU:HD23	1:E:165:THR:HG21	2.03	0.40
1:F:409:PRO:HB3	1:F:412:LEU:HD13	2.02	0.40
1:A:212:LYS:HA	1:A:215:ILE:HD12	2.03	0.40
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.90	0.40
1:C:283:MET:HE2	1:C:283:MET:HB3	1.94	0.40
1:C:639:GLU:HA	1:C:683:HIS:HD2	1.87	0.40
1:C:645:ARG:H	1:C:645:ARG:HG2	1.68	0.40
1:D:195:GLN:O	1:E:399:SER:OG	2.38	0.40
1:F:610:GLY:HA2	1:F:613:GLU:HB2	2.02	0.40
1:F:786:LEU:O	1:F:791:TYR:N	2.44	0.40
1:B:204:LEU:HD23	1:B:204:LEU:HA	1.85	0.40
1:B:230:GLU:HA	1:B:233:LYS:HG3	2.02	0.40
1:B:294:ASP:OD1	1:B:294:ASP:N	2.51	0.40
1:C:609:VAL:HG23	1:C:763:PHE:HD2	1.87	0.40
1:D:558:LYS:HG2	1:D:621:PHE:HE1	1.87	0.40
1:D:571:ILE:N	3:D:1002:AGS:HN62	2.19	0.40
1:E:349:ILE:HG21	3:E:1001:AGS:N1	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:573:GLN:NE2	1:E:764:HIS:O	2.54	0.40
1:E:585:ARG:HB3	1:F:830:ALA:HB1	2.03	0.40
1:E:849:ASN:HD22	1:E:852:ARG:HB2	1.86	0.40
1:F:228:VAL:O	1:F:233:LYS:NZ	2.40	0.40
1:F:462:TRP:HD1	1:F:527:LEU:HD21	1.86	0.40
1:F:538:GLU:HB3	1:F:542:ARG:NH1	2.37	0.40
1:A:299:LEU:HB3	1:A:303:LEU:HD13	2.02	0.40
1:A:340:GLU:HG3	1:A:341:PRO:HD2	2.03	0.40
1:A:671:TYR:CE1	1:A:711:ASN:HB3	2.57	0.40
1:A:768:GLU:HG2	1:A:771:ILE:HD12	2.02	0.40
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.83	0.40
1:B:296:GLY:O	1:B:300:LYS:HG3	2.21	0.40
1:B:537:ALA:HB1	1:B:549:SER:HA	2.02	0.40
1:C:194:LEU:HD13	1:C:274:ILE:HD13	2.03	0.40
1:C:803:LEU:HD23	1:C:803:LEU:HA	1.95	0.40
1:E:409:PRO:HB3	1:E:412:LEU:HD13	2.02	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	678/858 (79%)	614 (91%)	63 (9%)	1 (0%)	48	83
1	B	685/858 (80%)	627 (92%)	58 (8%)	0	100	100
1	C	685/858 (80%)	621 (91%)	64 (9%)	0	100	100
1	D	676/858 (79%)	624 (92%)	50 (7%)	2 (0%)	36	72
1	E	674/858 (79%)	615 (91%)	59 (9%)	0	100	100
1	F	676/858 (79%)	617 (91%)	59 (9%)	0	100	100
2	S	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
All	All	4096/5172 (79%)	3735 (91%)	358 (9%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	527	LEU
1	D	407	SER
1	D	506	ILE

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	574/714 (80%)	574 (100%)	0	100	100
1	B	574/714 (80%)	574 (100%)	0	100	100
1	C	574/714 (80%)	573 (100%)	1 (0%)	87	87
1	D	574/714 (80%)	574 (100%)	0	100	100
1	E	574/714 (80%)	574 (100%)	0	100	100
1	F	574/714 (80%)	574 (100%)	0	100	100
All	All	3444/4284 (80%)	3443 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	646	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	281	HIS
1	A	309	HIS
1	A	362	HIS
1	A	378	HIS
1	A	512	GLN
1	A	595	ASN
1	A	692	GLN

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Mol	Chain	Res	Type
1	A	857	GLN
1	A	858	HIS
1	B	195	GLN
1	B	264	ASN
1	B	297	ASN
1	B	309	HIS
1	B	334	GLN
1	B	362	HIS
1	B	794	HIS
1	B	806	ASN
1	B	827	ASN
1	B	858	HIS
1	C	195	GLN
1	C	221	GLN
1	C	281	HIS
1	C	334	GLN
1	C	360	HIS
1	C	378	HIS
1	C	473	GLN
1	C	688	ASN
1	C	692	GLN
1	C	726	GLN
1	C	778	GLN
1	C	806	ASN
1	C	831	GLN
1	C	858	HIS
1	D	195	GLN
1	D	264	ASN
1	D	297	ASN
1	D	321	GLN
1	D	378	HIS
1	D	421	GLN
1	D	574	ASN
1	D	620	ASN
1	D	688	ASN
1	D	806	ASN
1	D	831	GLN
1	D	849	ASN
1	D	857	GLN
1	D	858	HIS
1	E	225	ASN
1	E	264	ASN

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Mol	Chain	Res	Type
1	E	334	GLN
1	E	362	HIS
1	E	421	GLN
1	E	473	GLN
1	E	726	GLN
1	E	747	HIS
1	E	858	HIS
1	F	269	GLN
1	F	385	GLN
1	F	421	GLN
1	F	473	GLN
1	F	755	ASN
1	F	827	ASN
1	F	857	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	C	1002	-	32,33,33	2.21	4 (12%)	45,52,52	1.42	1 (2%)
4	ADP	A	1002	-	28,29,29	1.53	4 (14%)	43,45,45	3.25	14 (32%)
3	AGS	C	1001	-	32,33,33	1.38	3 (9%)	45,52,52	1.21	3 (6%)
3	AGS	E	1002	-	32,33,33	1.26	1 (3%)	45,52,52	1.02	2 (4%)
3	AGS	A	1001	-	32,33,33	1.32	3 (9%)	45,52,52	1.00	1 (2%)
3	AGS	B	1001	-	32,33,33	1.48	3 (9%)	45,52,52	0.90	1 (2%)
3	AGS	D	1002	-	32,33,33	1.71	3 (9%)	45,52,52	0.98	1 (2%)
3	AGS	D	1001	-	32,33,33	1.43	3 (9%)	45,52,52	1.03	1 (2%)
3	AGS	E	1001	-	32,33,33	0.93	2 (6%)	45,52,52	0.76	1 (2%)
3	AGS	B	1002	-	32,33,33	1.74	3 (9%)	45,52,52	0.94	1 (2%)
4	ADP	E	1003	-	28,29,29	1.39	4 (14%)	43,45,45	2.21	10 (23%)

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	C	1002	-	-	4/21/38/38	0/3/3/3
4	ADP	A	1002	-	-	6/16/32/32	0/3/3/3
3	AGS	C	1001	-	-	0/21/38/38	0/3/3/3
3	AGS	E	1002	-	-	8/21/38/38	0/3/3/3
3	AGS	A	1001	-	-	4/21/38/38	0/3/3/3
3	AGS	B	1001	-	-	2/21/38/38	0/3/3/3
3	AGS	D	1002	-	-	2/21/38/38	0/3/3/3
3	AGS	D	1001	-	-	5/21/38/38	0/3/3/3
3	AGS	E	1001	-	-	5/21/38/38	0/3/3/3
3	AGS	B	1002	-	-	3/21/38/38	0/3/3/3
4	ADP	E	1003	-	-	4/16/32/32	0/3/3/3

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	AGS	PB-O3B	-7.67	1.51	1.59
3	C	1002	AGS	PA-O3A	-7.11	1.51	1.59
3	B	1002	AGS	PB-O3A	-7.06	1.51	1.59
3	E	1002	AGS	PB-O3A	-6.13	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	AGS	PB-O3A	-5.97	1.53	1.59
3	D	1002	AGS	PB-O3B	-5.82	1.53	1.59
3	D	1002	AGS	PB-O3A	-5.72	1.53	1.59
3	D	1001	AGS	PB-O3B	-5.37	1.53	1.59
4	A	1002	ADP	C5-C4	5.27	1.48	1.39
3	B	1001	AGS	PA-O3A	-4.64	1.54	1.59
3	C	1001	AGS	PB-O3A	-4.59	1.54	1.59
3	B	1001	AGS	PB-O3A	-4.58	1.54	1.59
3	B	1002	AGS	PA-O3A	-4.56	1.54	1.59
3	C	1001	AGS	PA-O3A	-4.39	1.54	1.59
4	E	1003	ADP	C5-C4	4.37	1.46	1.39
3	B	1002	AGS	PB-O3B	-4.30	1.54	1.59
3	B	1001	AGS	PB-O3B	-4.28	1.54	1.59
3	A	1001	AGS	PB-O3B	-4.07	1.55	1.59
3	A	1001	AGS	PB-O3A	-4.03	1.55	1.59
3	A	1001	AGS	PA-O3A	-3.87	1.55	1.59
3	D	1001	AGS	PB-O3A	-3.79	1.55	1.59
3	D	1002	AGS	PA-O3A	-3.78	1.55	1.59
3	D	1001	AGS	PA-O3A	-3.59	1.55	1.59
3	C	1001	AGS	PB-O3B	-3.31	1.55	1.59
3	E	1001	AGS	PB-O3A	-3.27	1.56	1.59
4	E	1003	ADP	C5-C6	2.76	1.48	1.41
4	A	1002	ADP	C5-N7	-2.76	1.34	1.39
4	A	1002	ADP	C5-C6	2.66	1.48	1.41
4	E	1003	ADP	C5-N7	-2.60	1.34	1.39
3	E	1001	AGS	PB-O3B	-2.55	1.56	1.59
4	A	1002	ADP	C1'-N9	2.11	1.52	1.46
3	C	1002	AGS	PA-O1A	-2.03	1.43	1.50
4	E	1003	ADP	C8-N7	2.02	1.35	1.31

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	C5-C4-N3	-11.39	111.03	126.72
4	A	1002	ADP	N3-C4-N9	10.29	144.67	127.17
3	C	1002	AGS	PB-O3B-PG	-8.12	103.44	133.17
4	E	1003	ADP	C5-C4-N3	-6.67	117.53	126.72
4	A	1002	ADP	C1'-N9-C8	-6.44	112.81	127.09
4	E	1003	ADP	N3-C2-N1	-6.21	119.18	128.58
3	D	1001	AGS	PB-O3B-PG	-6.01	111.19	133.17
3	C	1001	AGS	PB-O3B-PG	-6.00	111.22	133.17
4	A	1002	ADP	C2-N3-C4	5.90	126.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	ADP	C4-N9-C1'	5.58	139.68	126.63
3	A	1001	AGS	PB-O3B-PG	-5.51	113.02	133.17
4	E	1003	ADP	C2-N3-C4	5.23	124.61	111.83
4	E	1003	ADP	N3-C4-N9	5.20	136.02	127.17
3	B	1001	AGS	PB-O3B-PG	-5.17	114.23	133.17
4	A	1002	ADP	C3'-C2'-C1'	4.40	109.79	101.46
3	E	1001	AGS	PB-O3B-PG	-4.34	117.28	133.17
3	E	1002	AGS	PB-O3B-PG	-4.26	117.58	133.17
4	A	1002	ADP	C2'-C1'-N9	4.08	123.44	113.30
3	B	1002	AGS	PB-O3B-PG	-4.07	118.28	133.17
3	D	1002	AGS	PB-O3B-PG	-3.86	119.04	133.17
4	E	1003	ADP	C4-C5-N7	-3.29	106.82	110.58
4	E	1003	ADP	C2-N1-C6	3.22	124.02	118.73
4	A	1002	ADP	C5-C6-N6	-3.20	115.37	123.29
3	C	1001	AGS	O3G-PG-O3B	3.06	114.84	104.64
4	A	1002	ADP	N3-C2-N1	-2.72	124.47	128.58
4	E	1003	ADP	C3'-C2'-C1'	2.55	106.28	101.46
3	E	1002	AGS	O2A-PA-O3A	2.35	113.61	107.27
3	C	1001	AGS	O2A-PA-O3A	-2.35	100.93	107.27
4	A	1002	ADP	C5-N7-C8	2.28	107.03	103.45
4	E	1003	ADP	C6-C5-N7	2.24	136.40	132.09
4	E	1003	ADP	C5-N7-C8	2.20	106.90	103.45
4	A	1002	ADP	C5-C4-N9	-2.19	103.42	105.81
4	A	1002	ADP	N6-C6-N1	2.15	123.17	118.38
4	E	1003	ADP	C5'-C4'-C3'	-2.12	107.57	115.21
4	A	1002	ADP	C6-C5-C4	2.09	120.03	117.18
4	A	1002	ADP	O4'-C1'-C2'	-2.00	102.33	106.62

There are no chirality outliers.

All (43) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	E	1001	AGS	O4'-C4'-C5'-O5'
3	E	1002	AGS	PB-O3B-PG-O2G
3	E	1002	AGS	C5'-O5'-PA-O2A
3	E	1002	AGS	C5'-O5'-PA-O3A
4	A	1002	ADP	C5'-O5'-PA-O1A
4	A	1002	ADP	C5'-O5'-PA-O3A
4	E	1003	ADP	C5'-O5'-PA-O1A
3	C	1002	AGS	O4'-C4'-C5'-O5'
3	C	1002	AGS	C3'-C4'-C5'-O5'
3	E	1001	AGS	C3'-C4'-C5'-O5'
3	E	1002	AGS	O4'-C4'-C5'-O5'
4	A	1002	ADP	O4'-C4'-C5'-O5'
4	E	1003	ADP	O4'-C4'-C5'-O5'
3	E	1001	AGS	C4'-C5'-O5'-PA
3	A	1001	AGS	PA-O3A-PB-O1B
4	A	1002	ADP	C3'-C4'-C5'-O5'
3	A	1001	AGS	C5'-O5'-PA-O3A
3	B	1001	AGS	C5'-O5'-PA-O3A
3	D	1001	AGS	C5'-O5'-PA-O1A
3	D	1001	AGS	C5'-O5'-PA-O2A
3	D	1001	AGS	C5'-O5'-PA-O3A
3	E	1002	AGS	C5'-O5'-PA-O1A
4	A	1002	ADP	C5'-O5'-PA-O2A
4	E	1003	ADP	C5'-O5'-PA-O2A
4	E	1003	ADP	C5'-O5'-PA-O3A
3	E	1002	AGS	PB-O3A-PA-O2A
3	E	1002	AGS	C3'-C4'-C5'-O5'
3	A	1001	AGS	C4'-C5'-O5'-PA
3	D	1002	AGS	PB-O3B-PG-O3G
3	E	1002	AGS	PB-O3B-PG-O3G
3	B	1001	AGS	O4'-C4'-C5'-O5'
3	B	1002	AGS	C2'-C1'-N9-C8
4	A	1002	ADP	PB-O3A-PA-O2A

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1002	AGS	2	0
4	A	1002	ADP	4	0
3	C	1001	AGS	4	0
3	E	1002	AGS	6	0

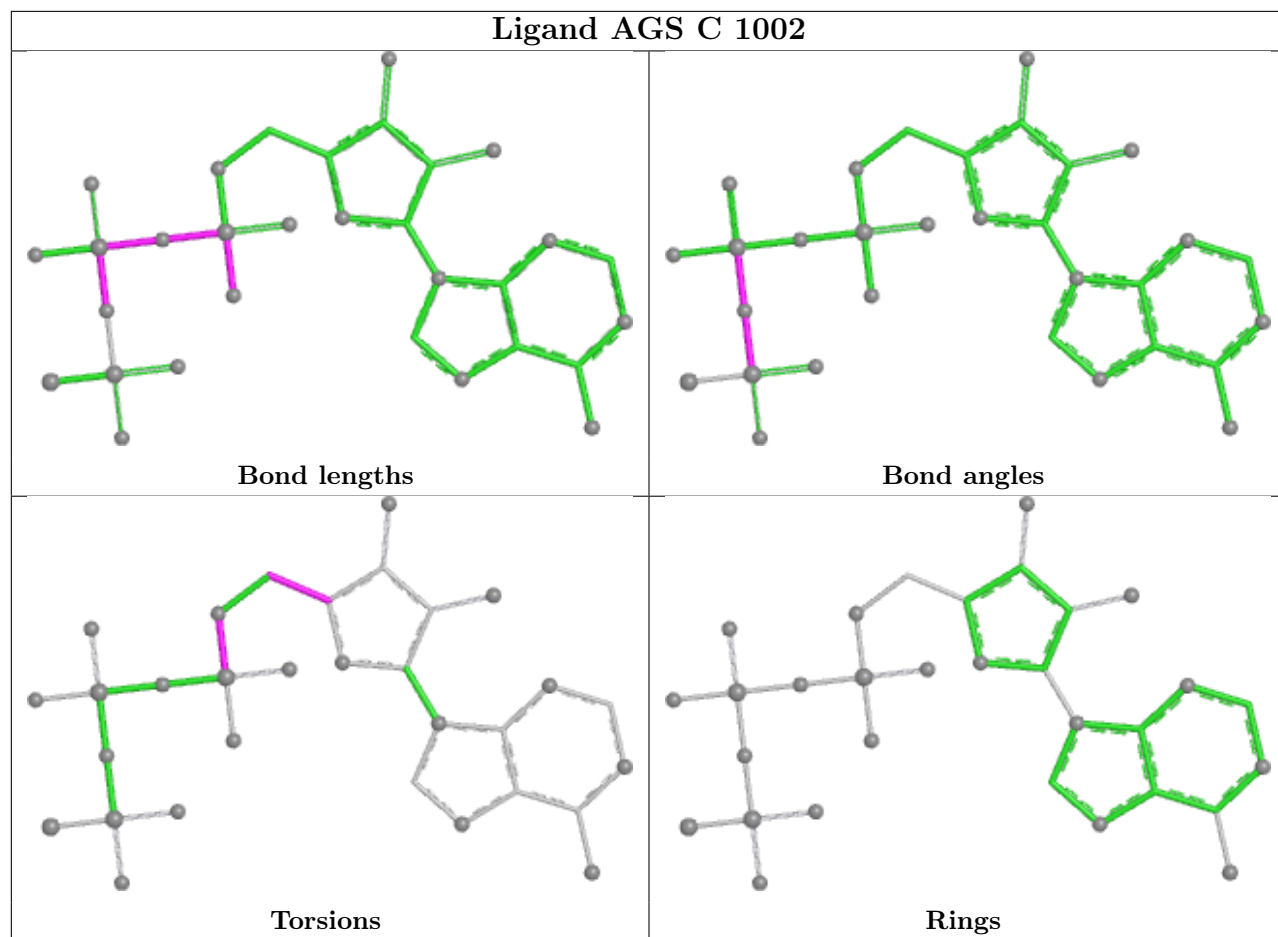
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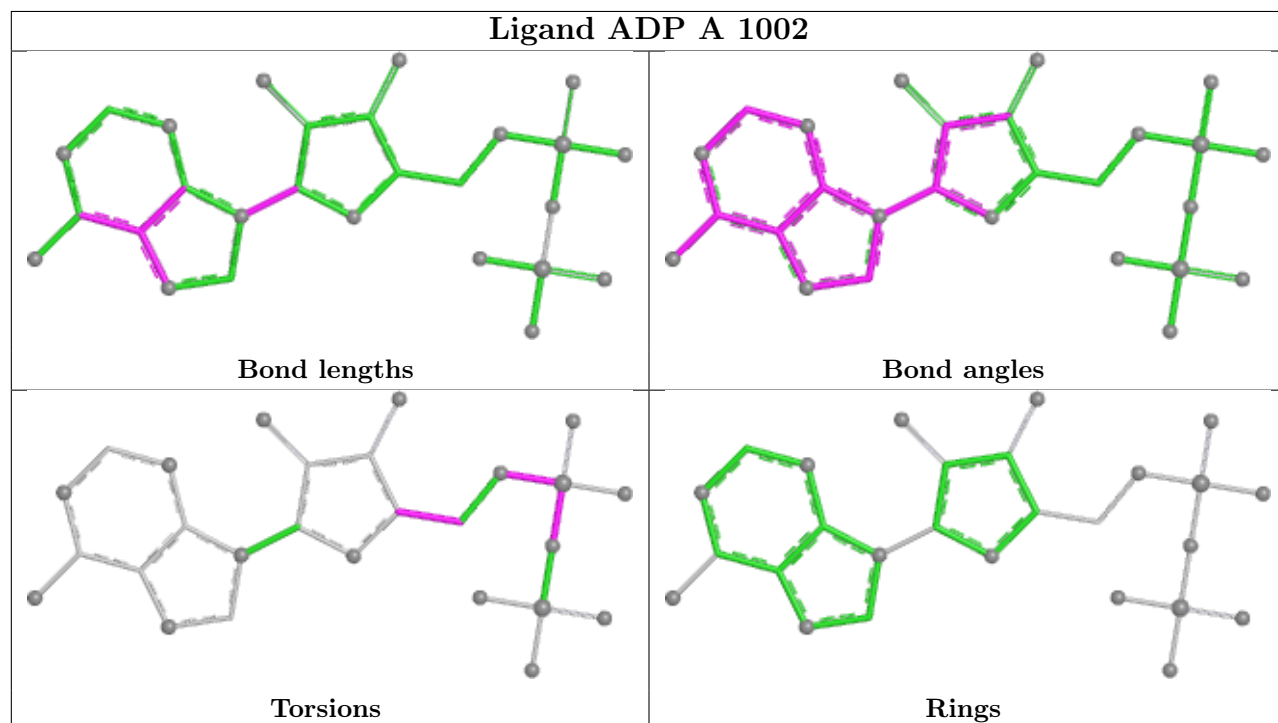
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	AGS	4	0
3	B	1001	AGS	2	0
3	D	1002	AGS	7	0
3	D	1001	AGS	3	0
3	E	1001	AGS	4	0
3	B	1002	AGS	7	0
4	E	1003	ADP	1	0

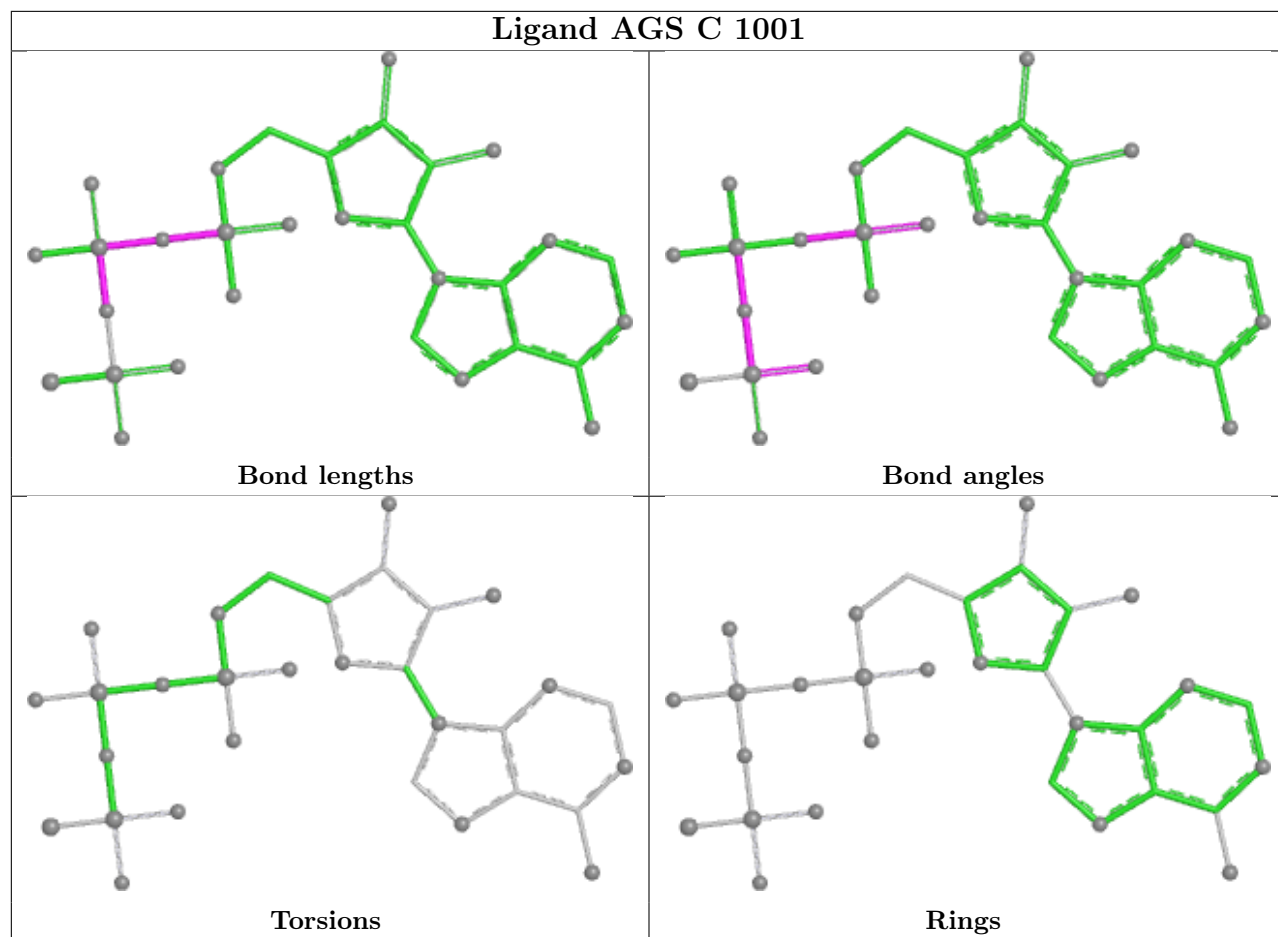
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

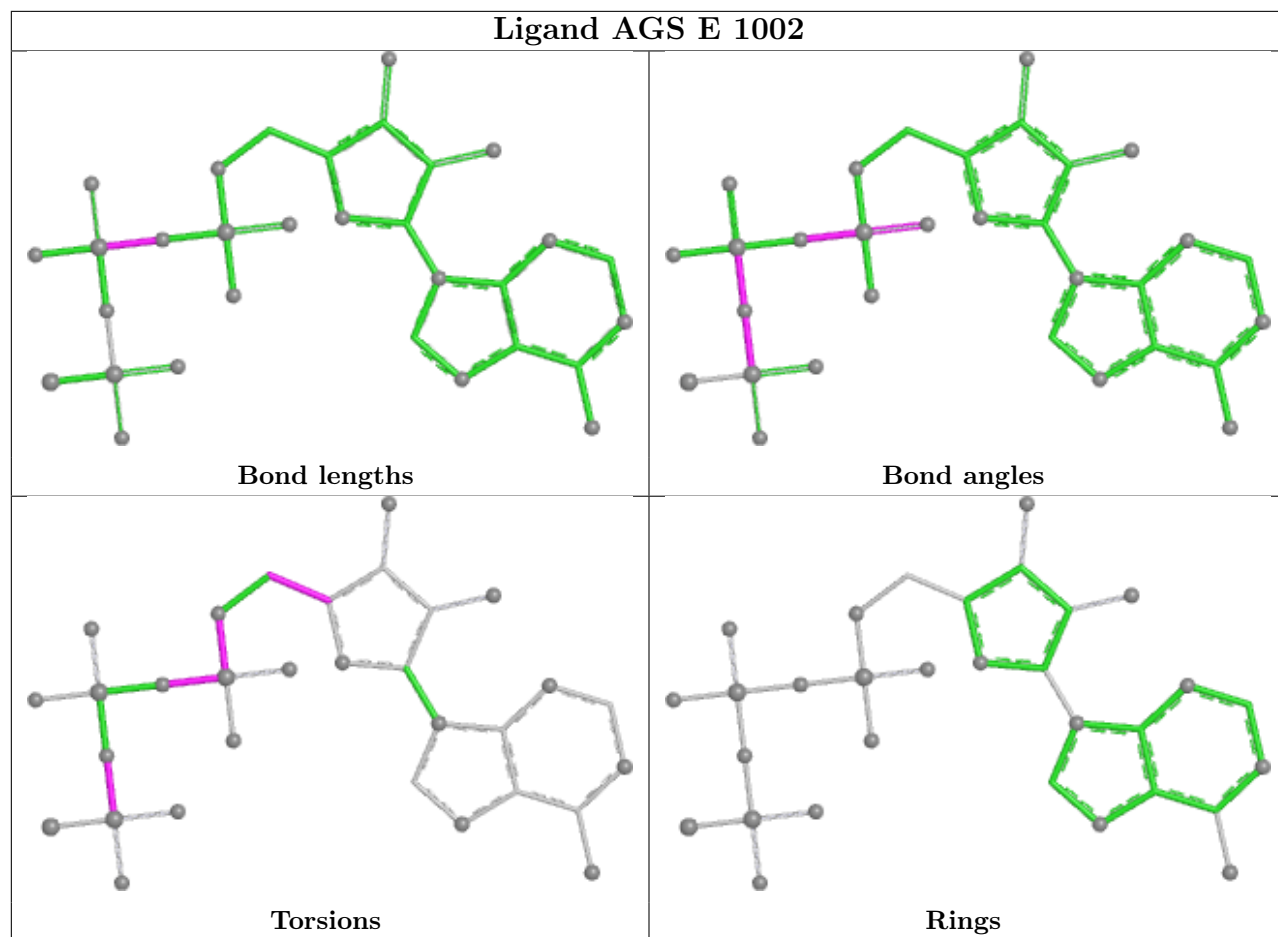
Ligand AGS C 1002

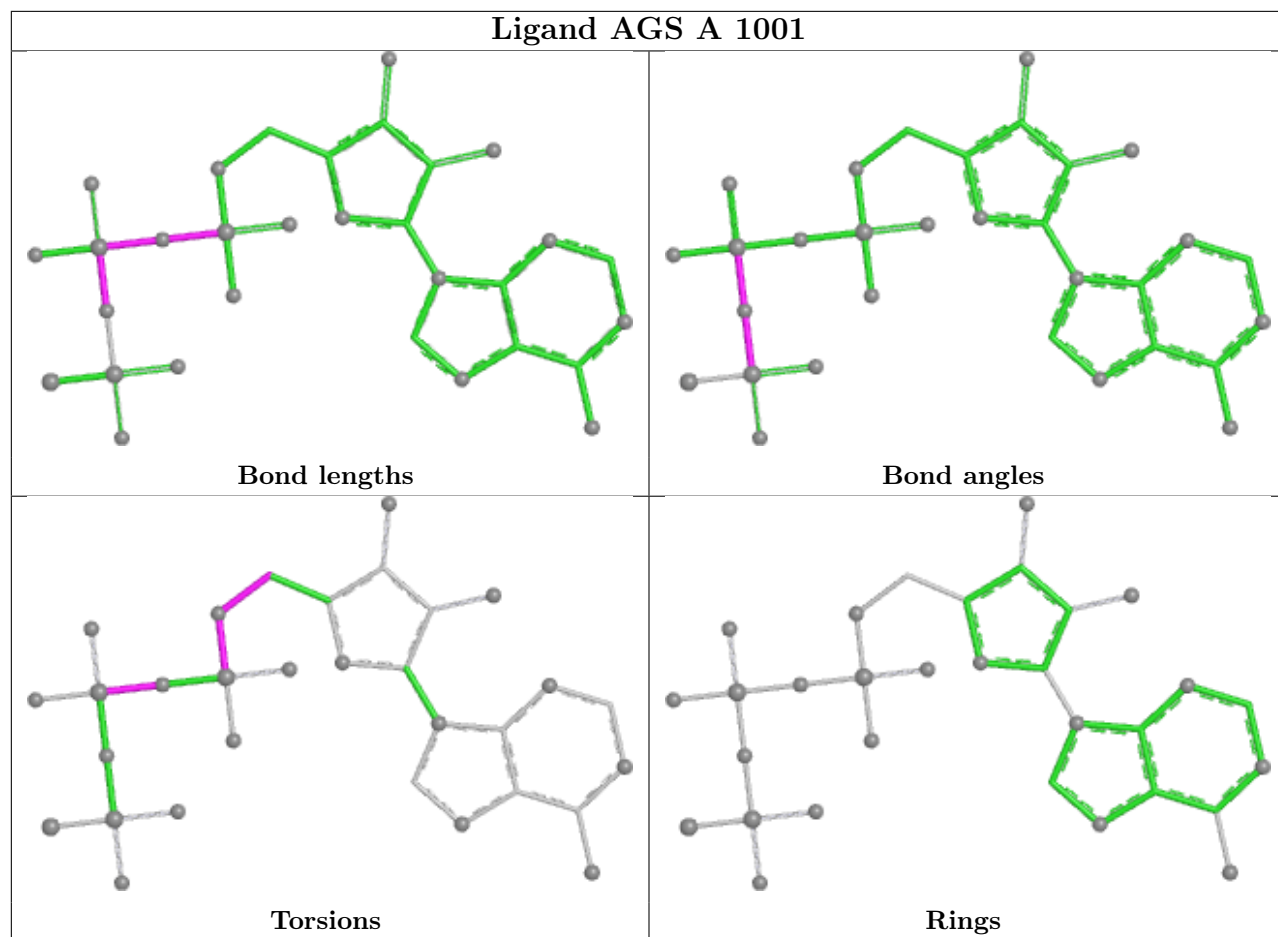


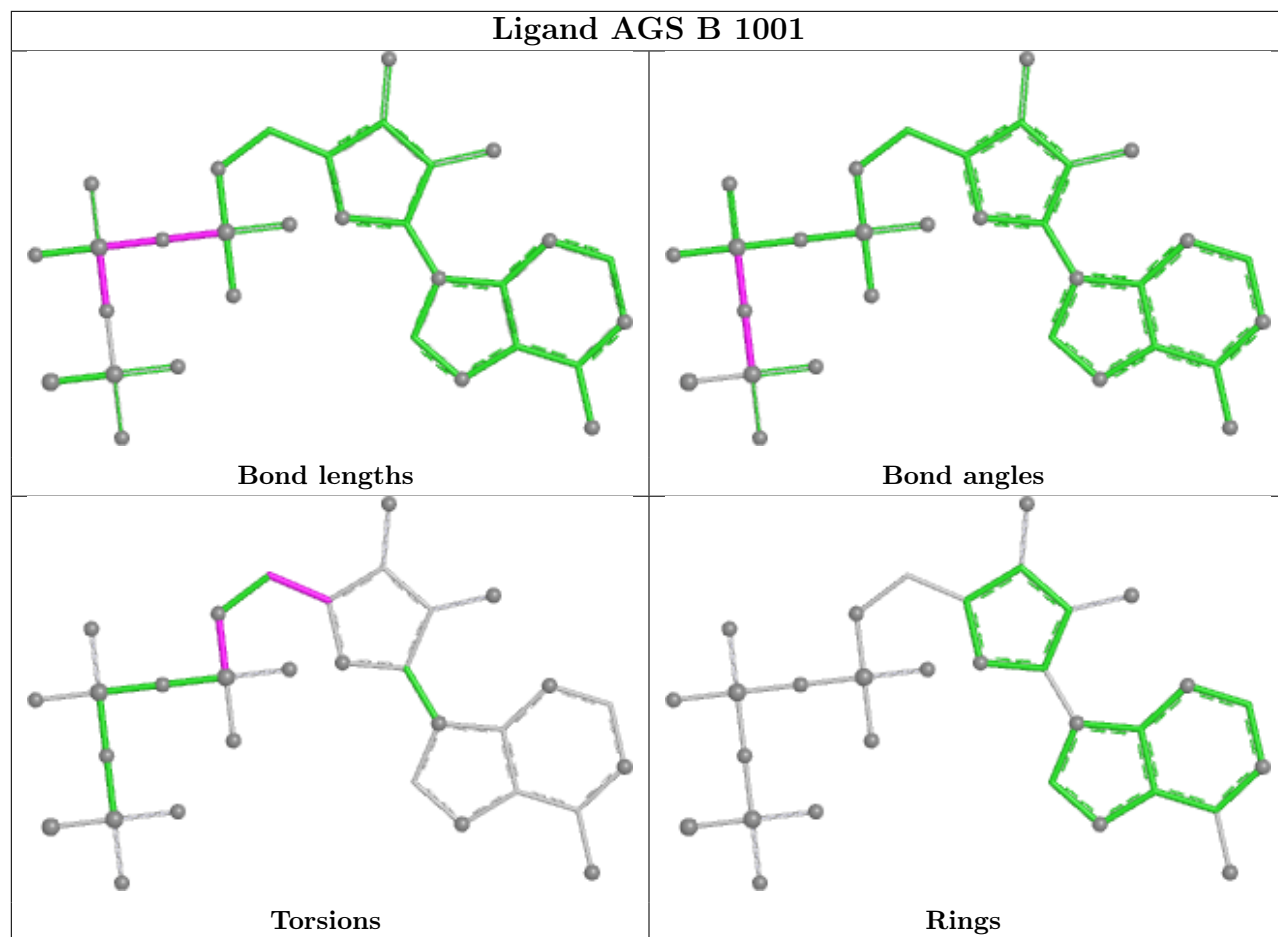
Ligand ADP A 1002

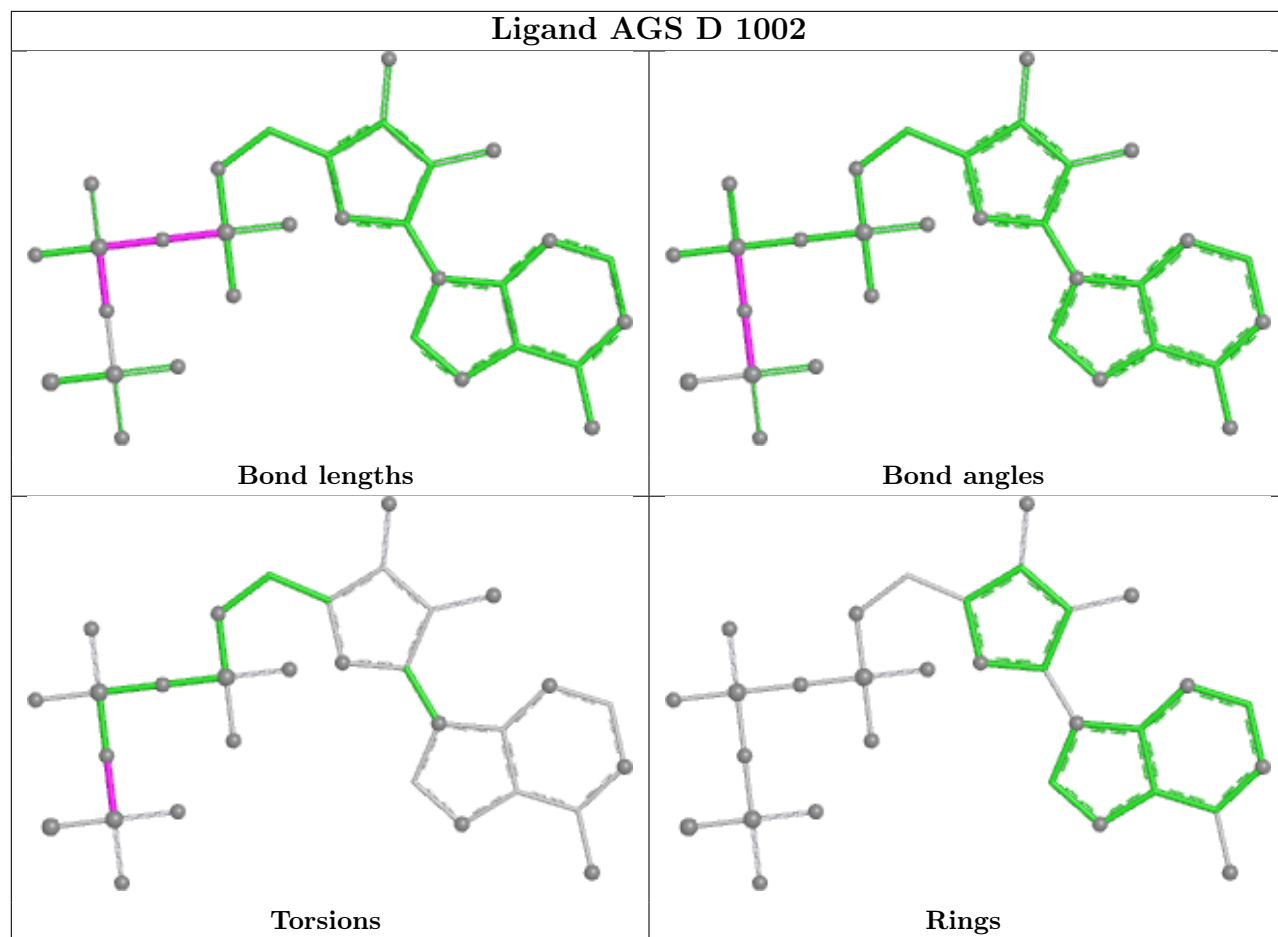


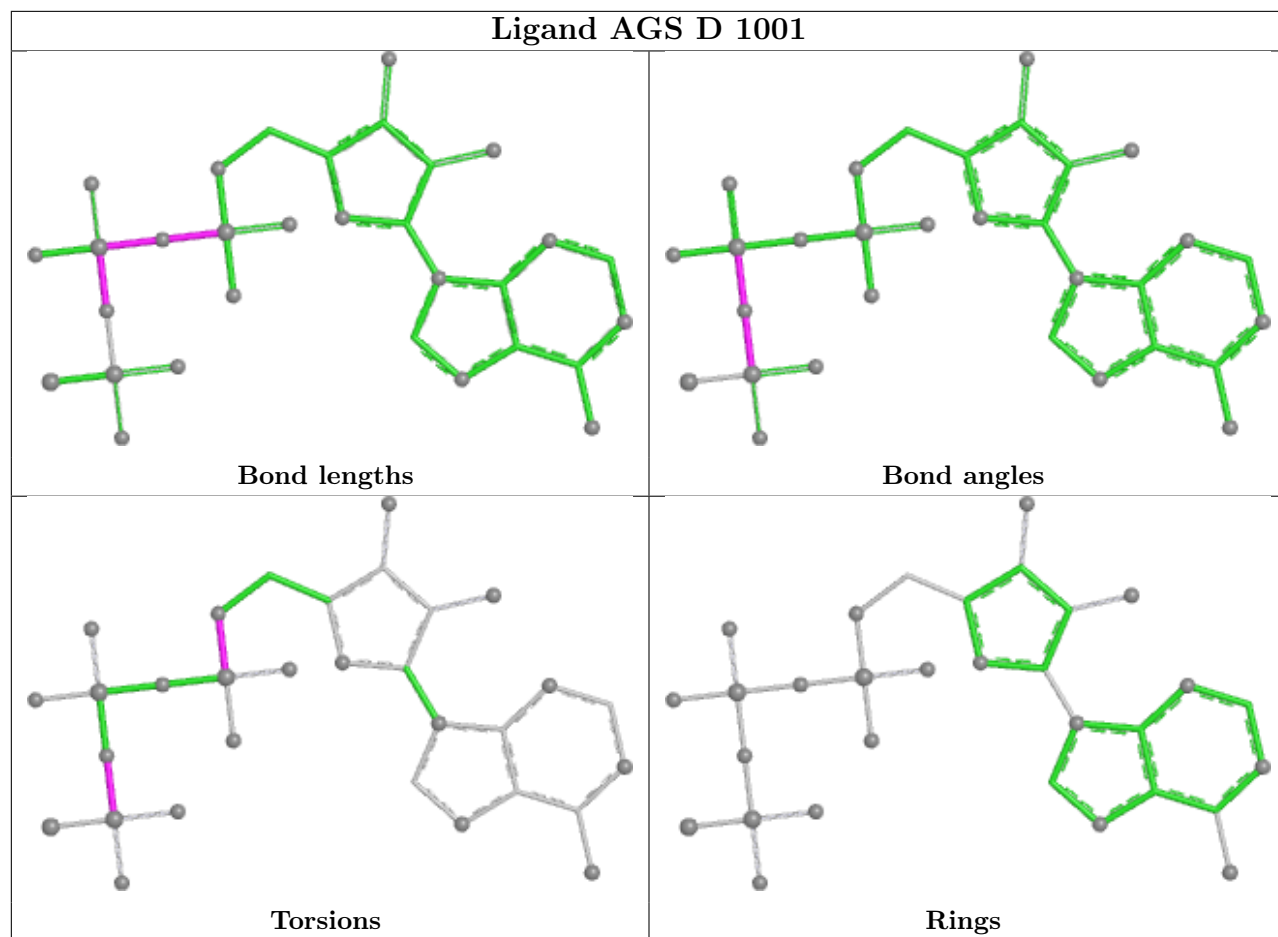


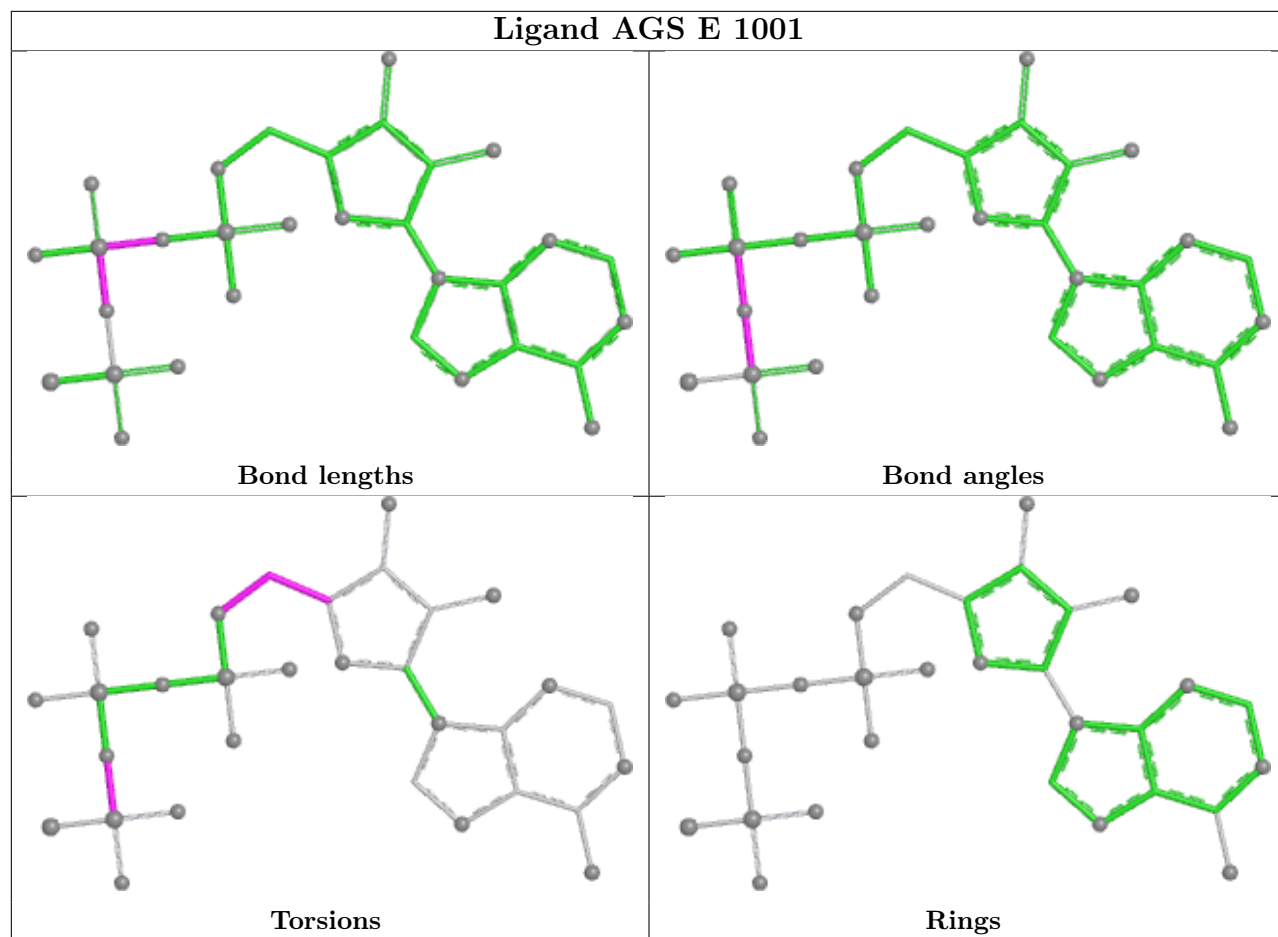




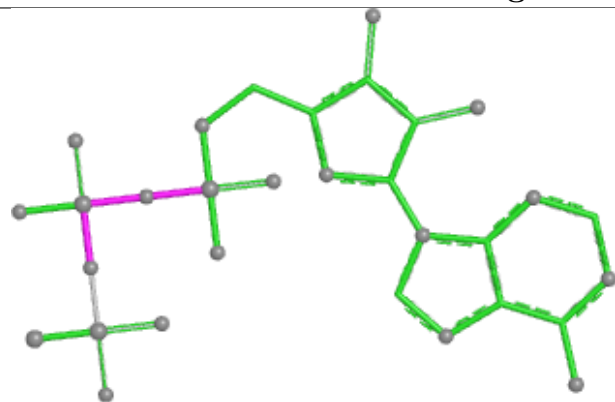




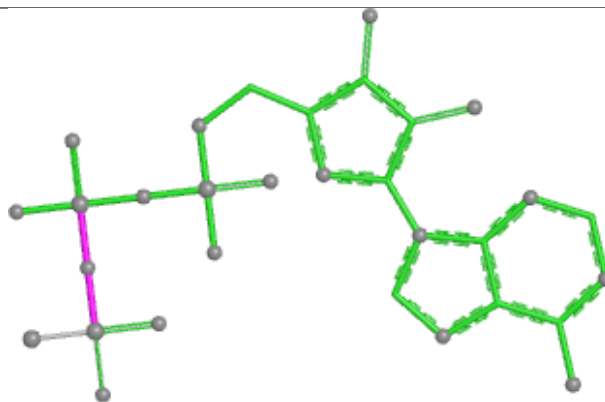




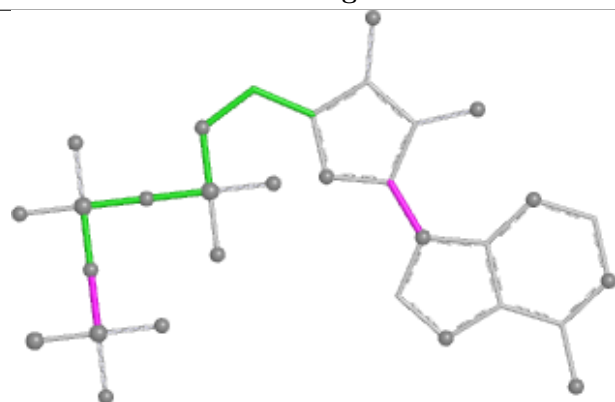
Ligand AGS B 1002



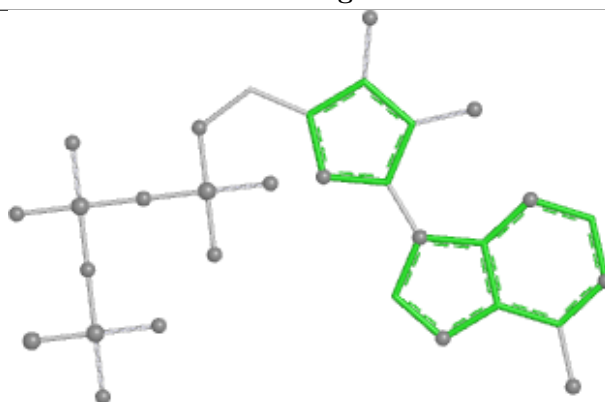
Bond lengths



Bond angles

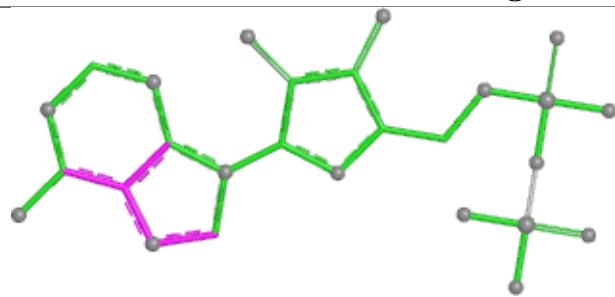


Torsions

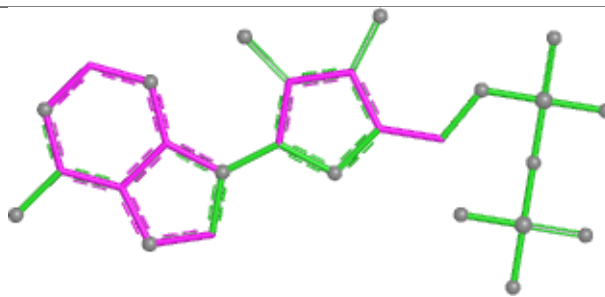


Rings

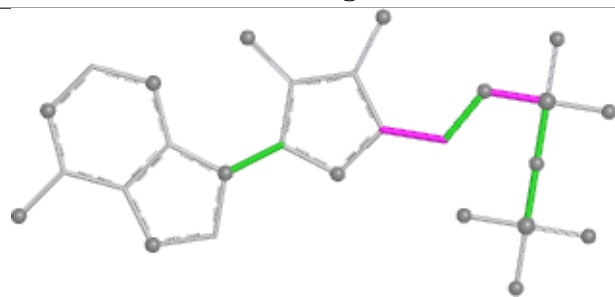
Ligand ADP E 1003



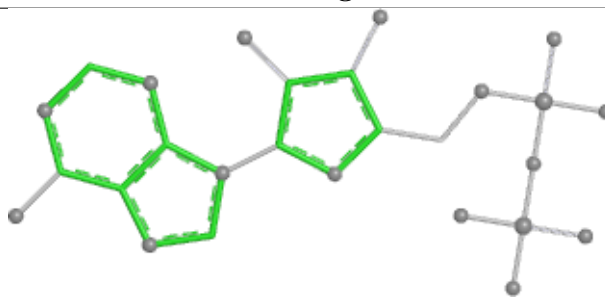
Bond lengths



Bond angles



Torsions



Rings

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	E	2
1	F	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	546:ILE	C	547:PRO	N	7.97
1	E	526:LEU	C	527:LEU	N	5.85
1	F	526:LEU	C	527:LEU	N	5.69
1	D	526:LEU	C	527:LEU	N	4.02

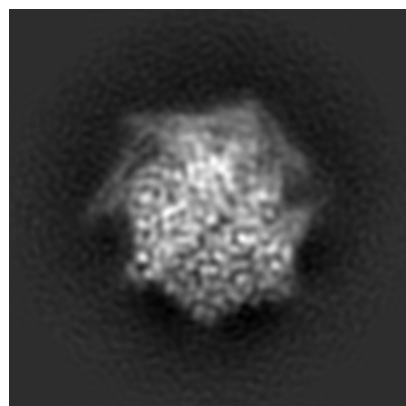
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4940. These allow visual inspection of the internal detail of the map and identification of artifacts.

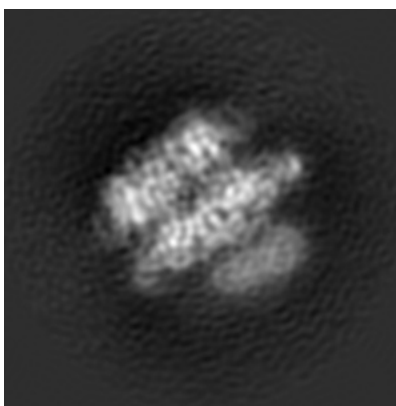
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

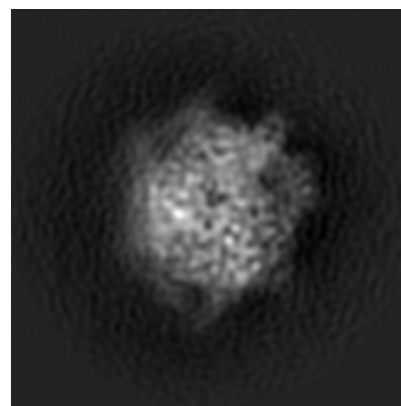
6.1.1 Primary map



X

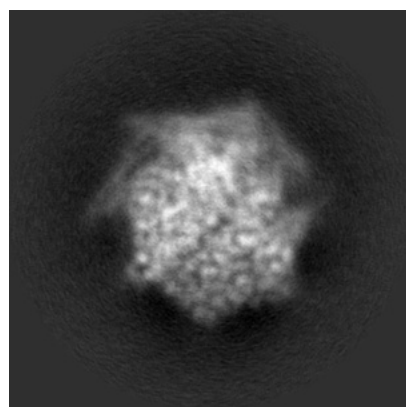


Y

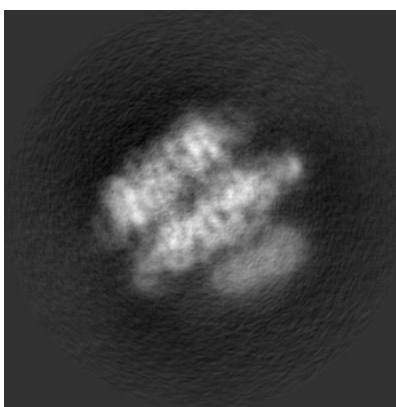


Z

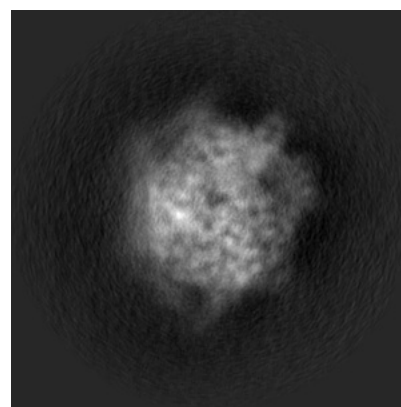
6.1.2 Raw map



X



Y

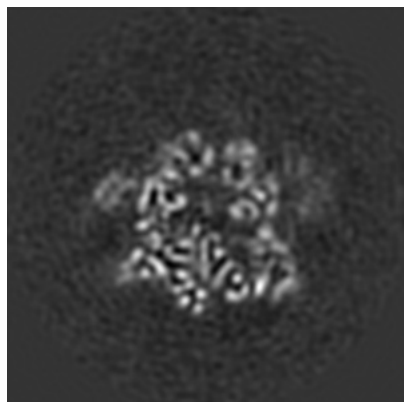


Z

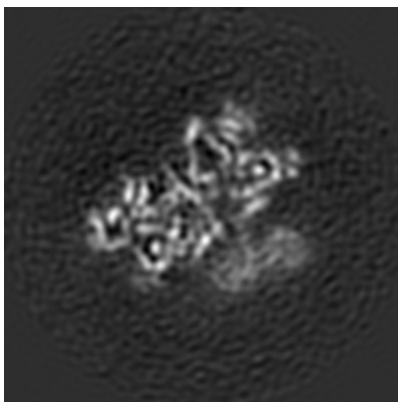
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

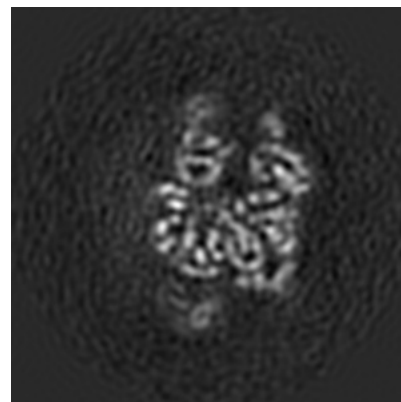
6.2.1 Primary map



X Index: 128

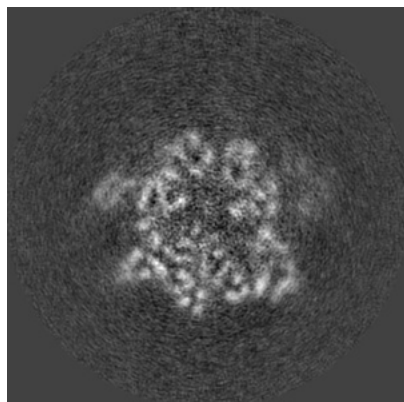


Y Index: 128

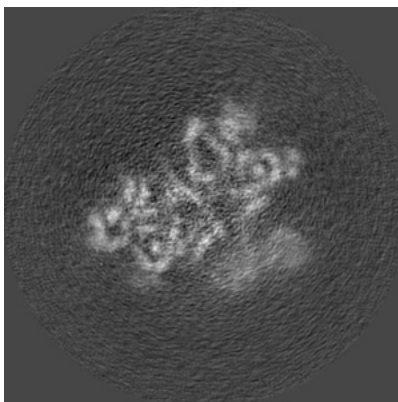


Z Index: 128

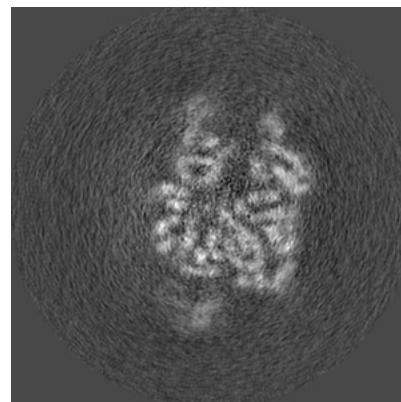
6.2.2 Raw map



X Index: 128



Y Index: 128

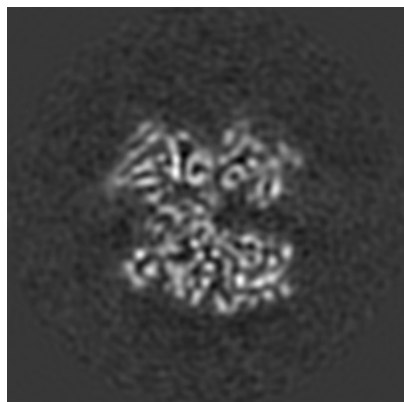


Z Index: 128

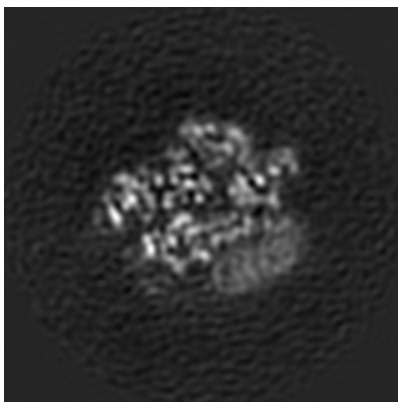
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

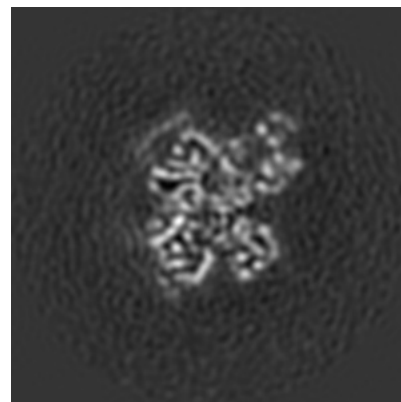
6.3.1 Primary map



X Index: 138

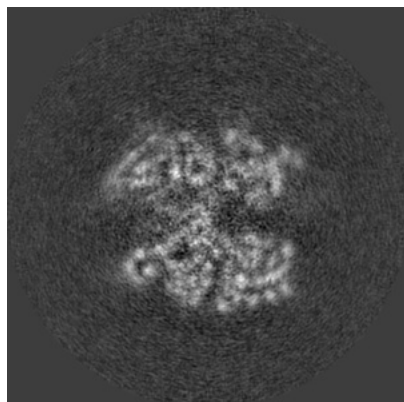


Y Index: 116

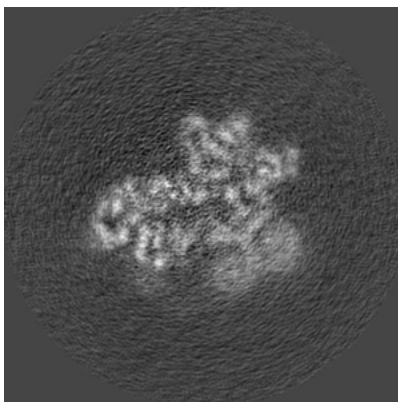


Z Index: 108

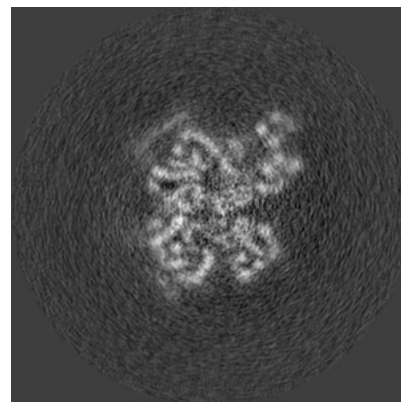
6.3.2 Raw map



X Index: 136



Y Index: 124

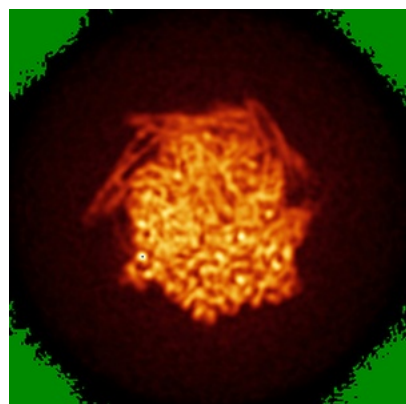


Z Index: 108

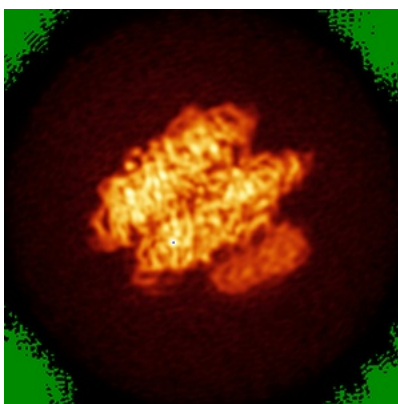
The images above show the largest variance slices of the map in three orthogonal directions.

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

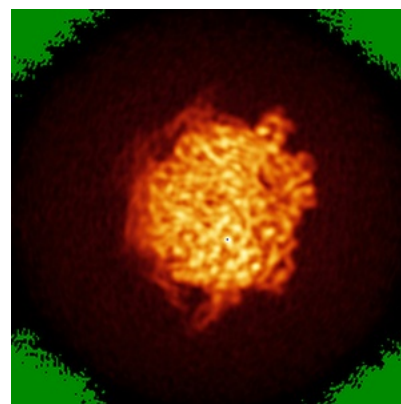
6.4.1 Primary map



X

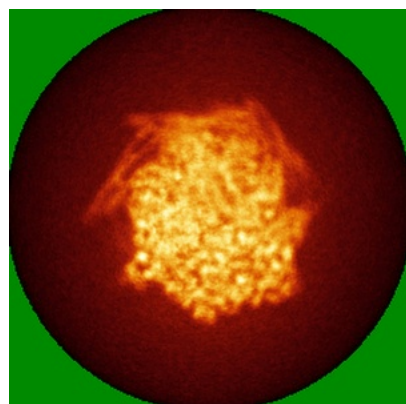


Y

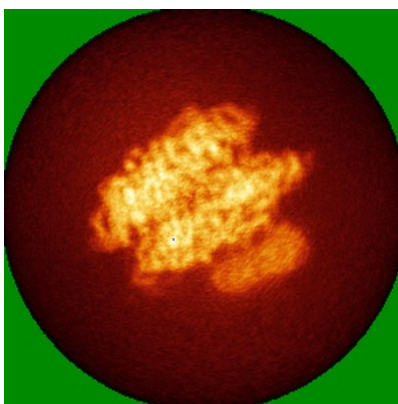


Z

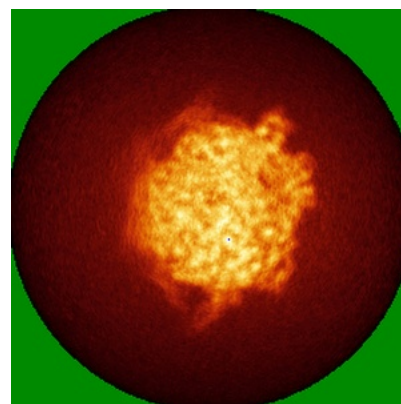
6.4.2 Raw map



X



Y

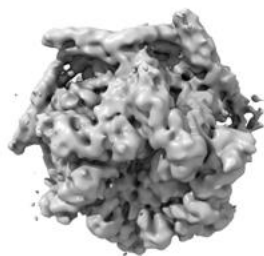


Z

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

6.5 Orthogonal surface views [i](#)

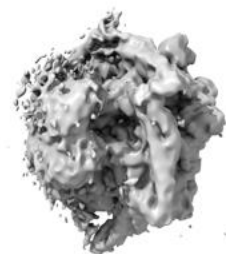
6.5.1 Primary map



X



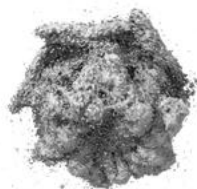
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

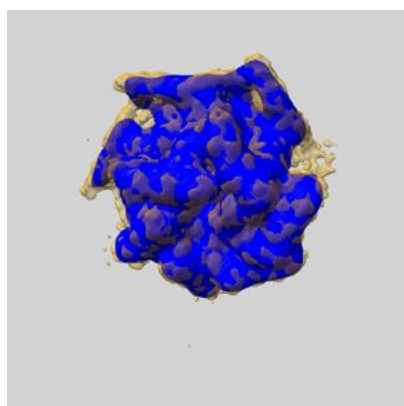
6.6 Mask visualisation [i](#)

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

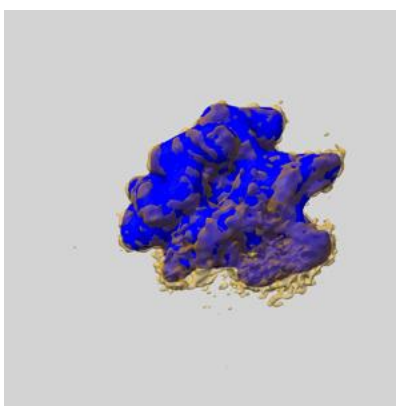
A mask typically either:

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

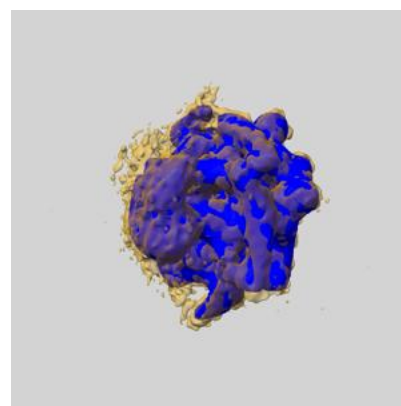
6.6.1 emd_4940_msk_1.map [i](#)



X



Y

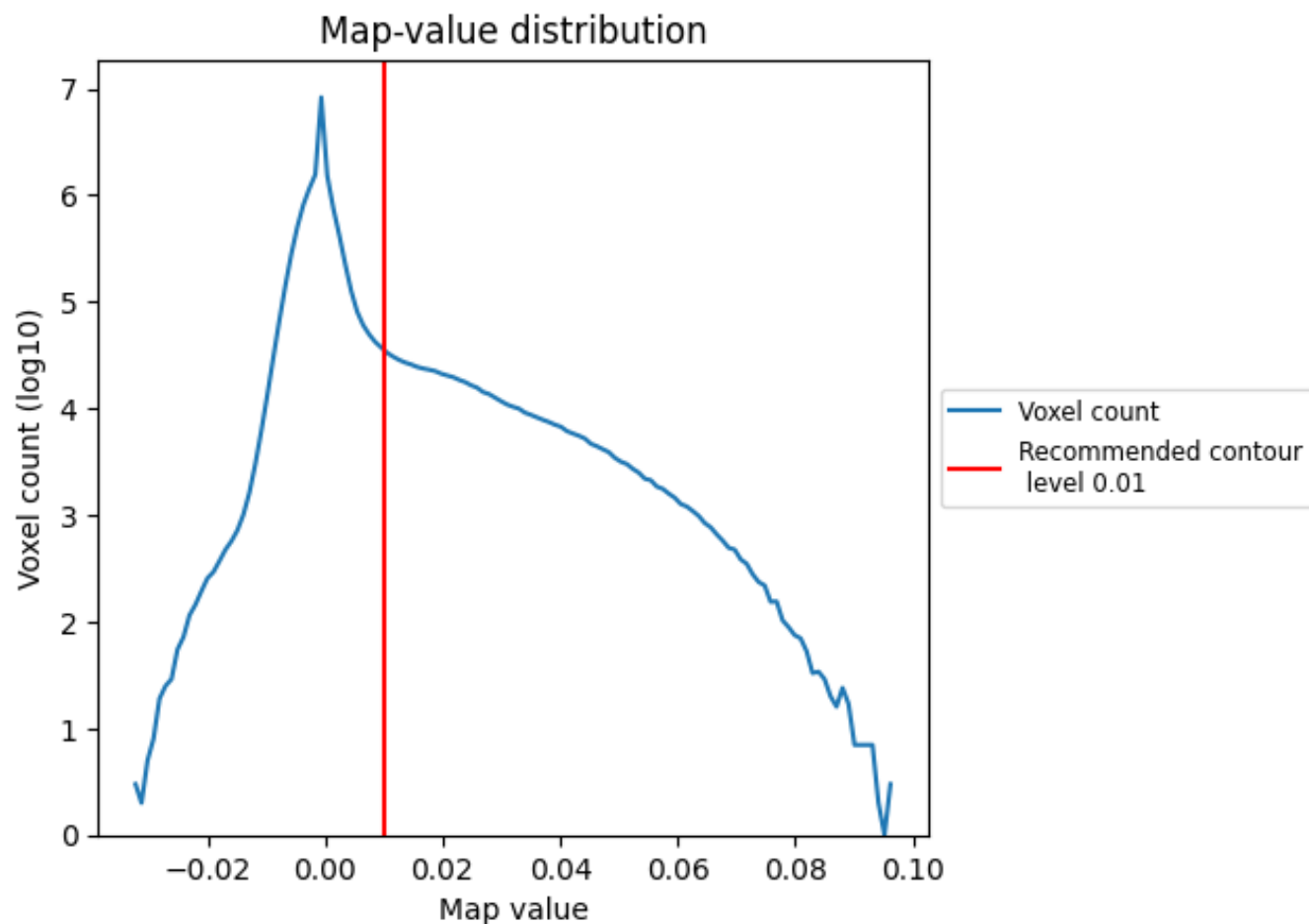


Z

7 Map analysis [i](#)

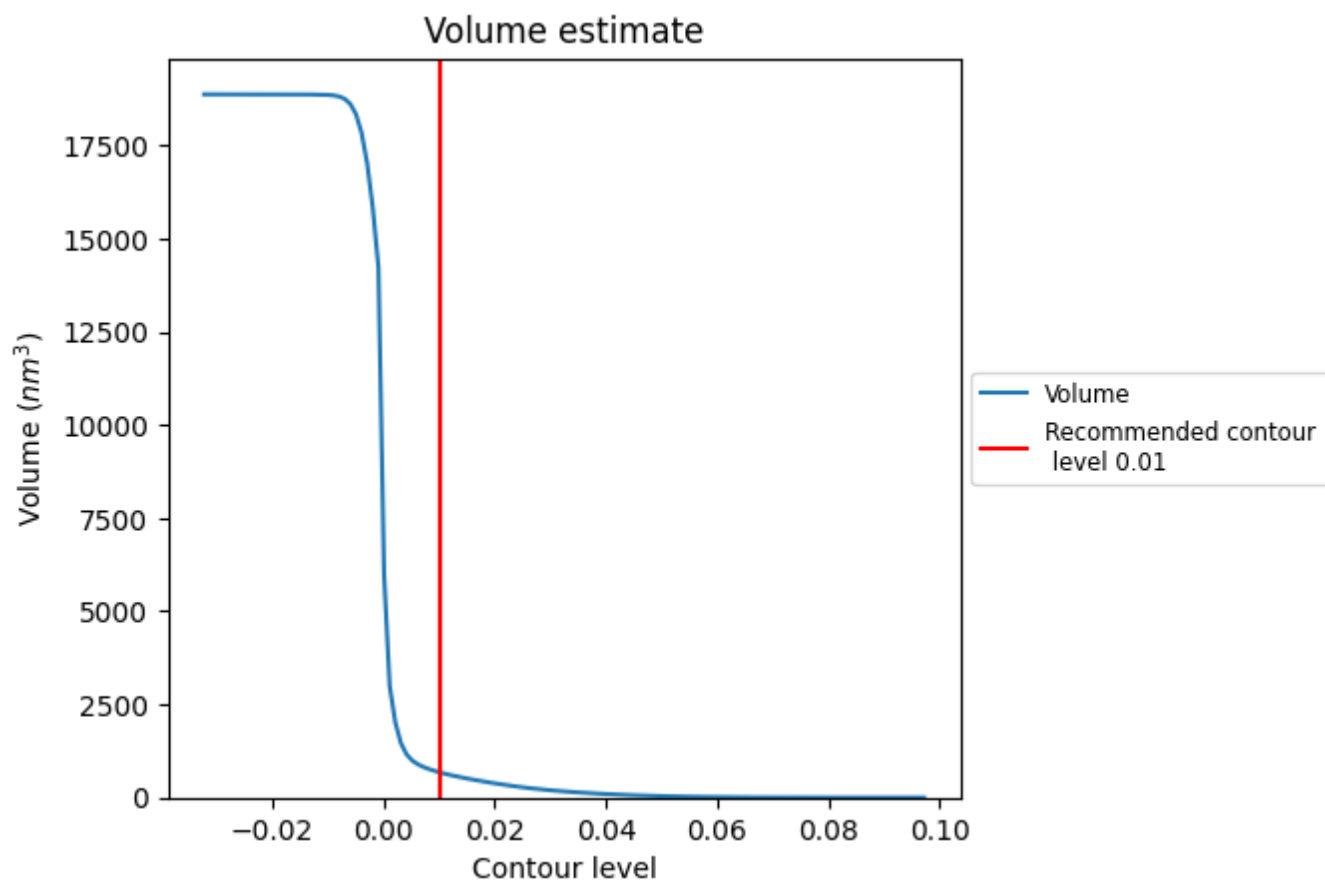
This section contains the results of statistical analysis of the map.

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.

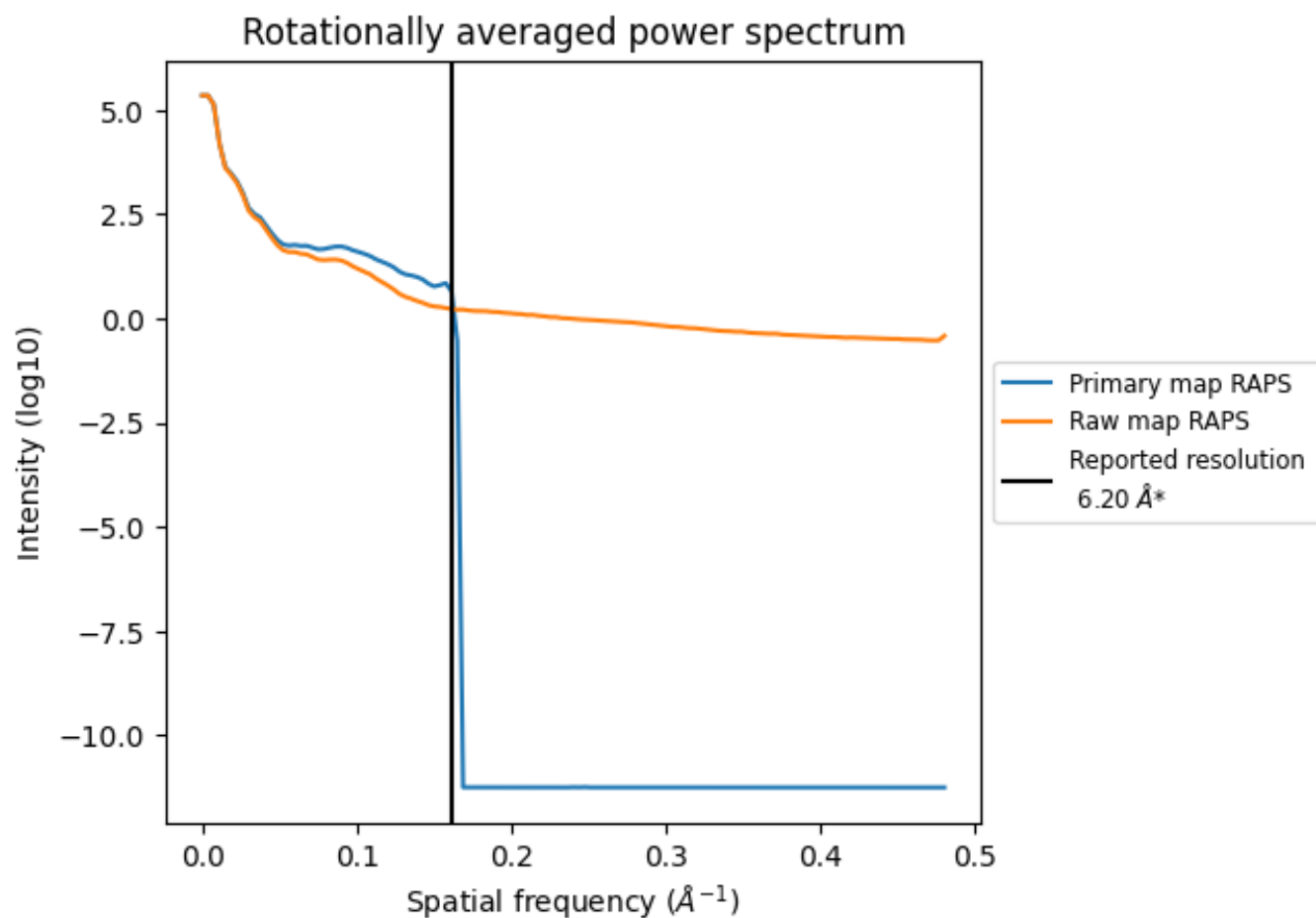
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 680 nm^3 ; this corresponds to an approximate mass of 614 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

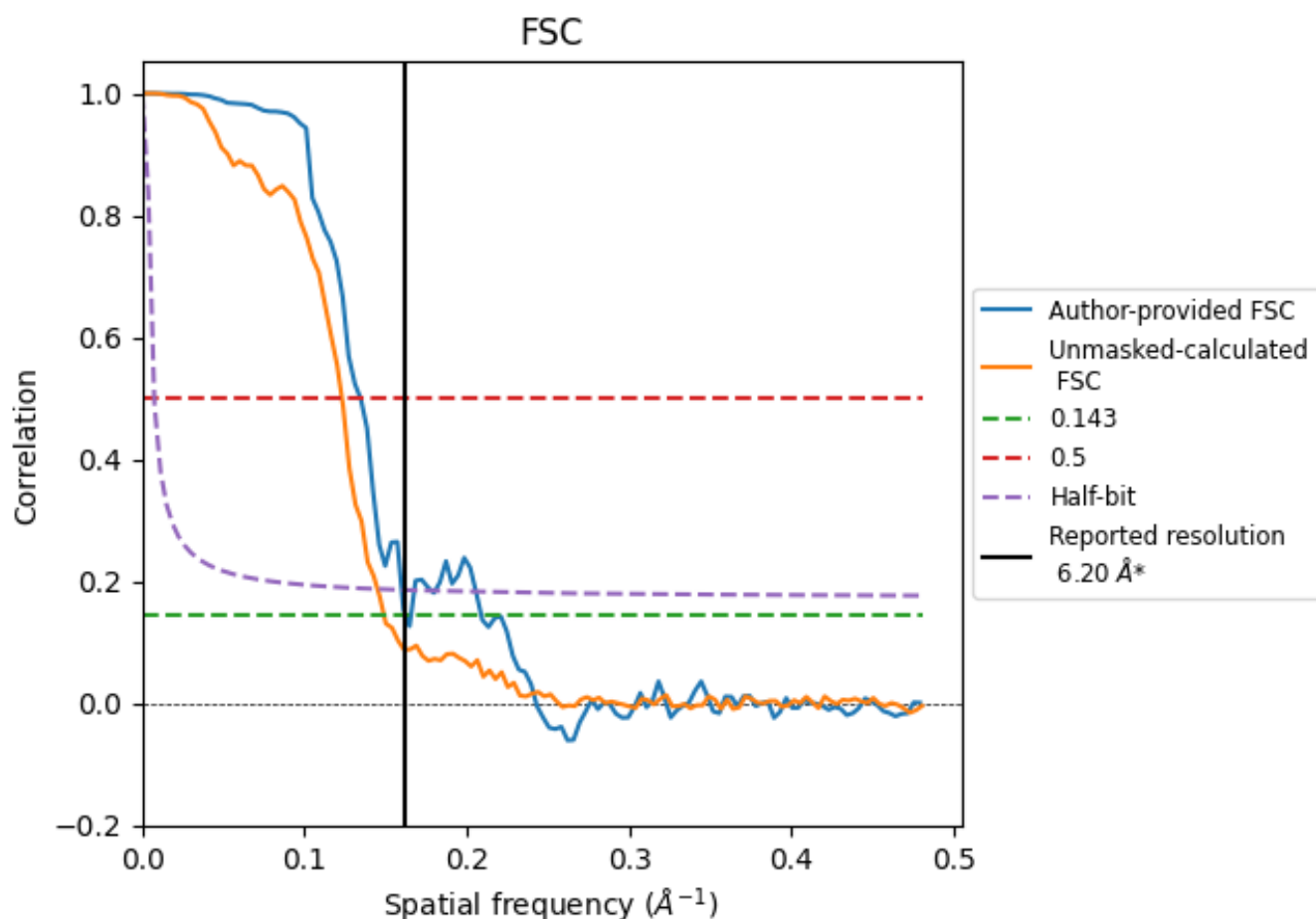


*Reported resolution corresponds to spatial frequency of 0.161 Å⁻¹

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 0.161 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

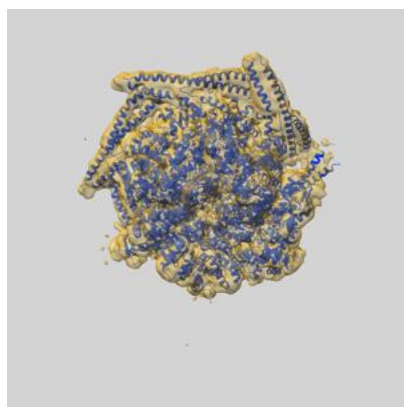
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.20	-	-
Author-provided FSC curve	6.15	7.43	6.25
Unmasked-calculated*	6.71	8.12	6.90

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

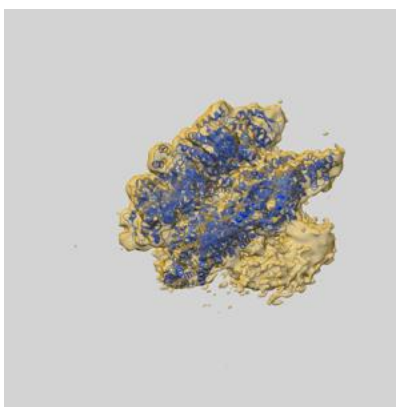
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4940 and PDB model 6RN2. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

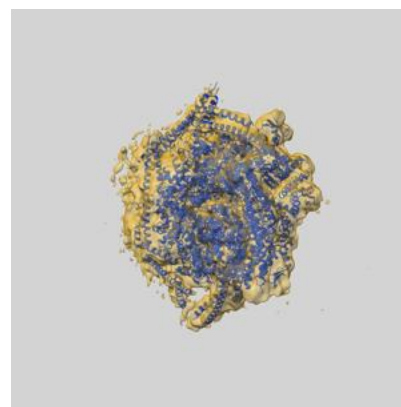
9.1 Map-model overlay [i](#)



X



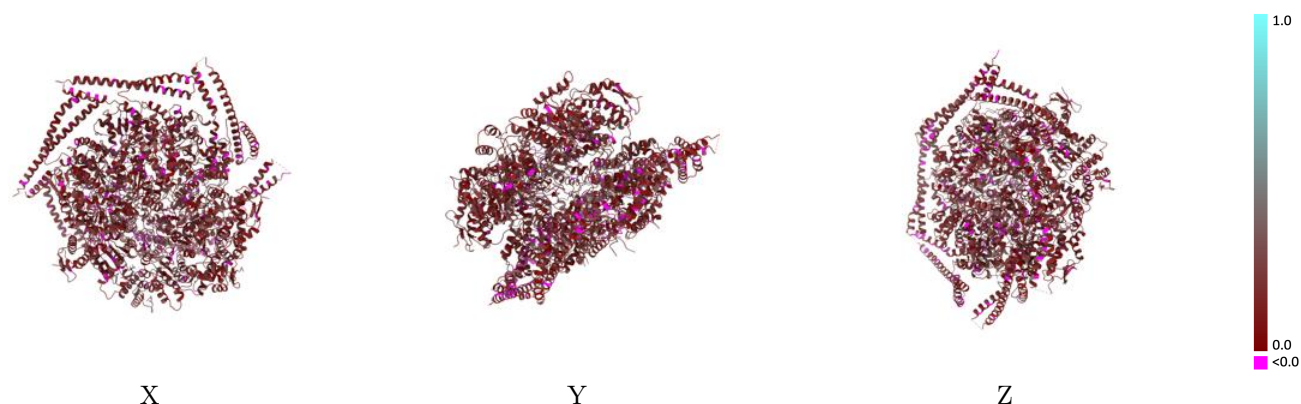
Y



Z

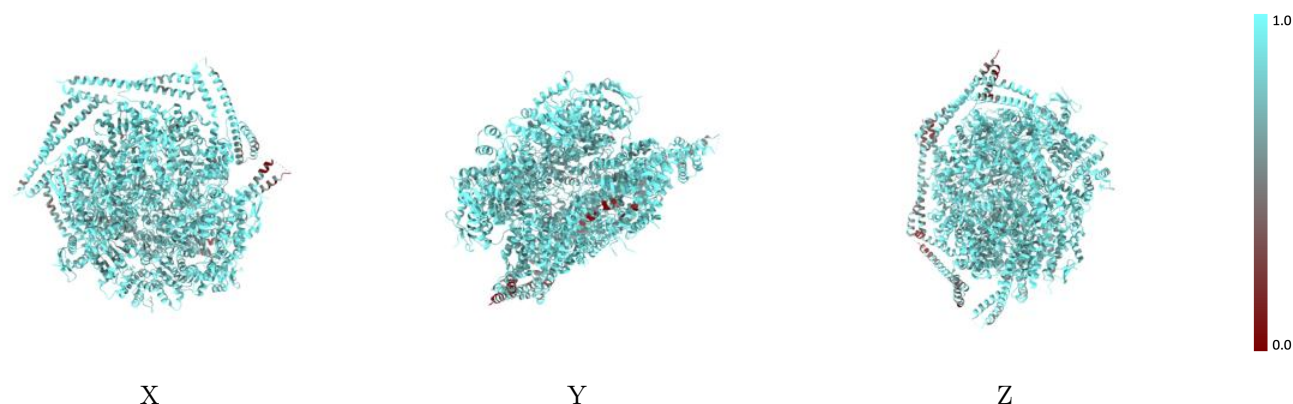
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



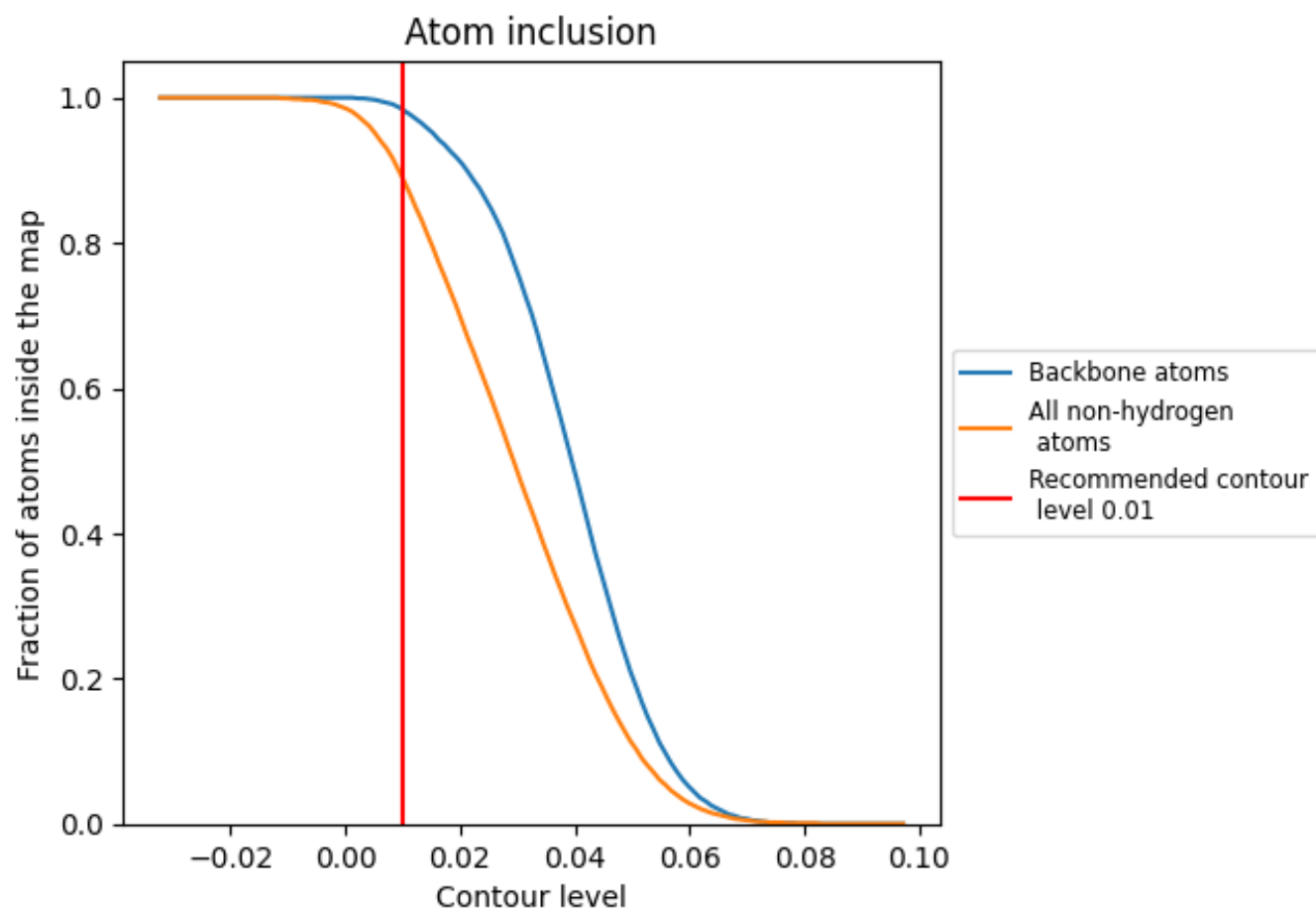
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.1770
A	0.8780	0.1790
B	0.8690	0.1730
C	0.8570	0.1700
D	0.8970	0.1810
E	0.9170	0.1800
F	0.9160	0.1740
S	0.9920	0.2870

1.0

0.0

<0.0