



Full wwPDB EM Validation Report ⓘ

Aug 18, 2026 – 07:15 PM JST

PDB ID : 23FB / pdb_000023fb
EMDB ID : EMD-68918
Title : Cryo-EM structure of human ATR-ATRIP complex with ATPgammaS
Authors : Wang, L.; Wang, M.; Zhao, L.; Rao, Q.; Wu, H.; Ma, B.; Wang, J.; Zheng, J.;
Li, Y.; Xu, Y.; Guo, J.; Cheng, J.; Qiao, S.
Deposited on : 2026-02-04
Resolution : 3.00 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 ⓘ 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
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) : 2.50

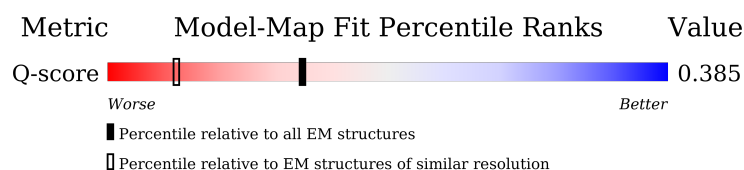
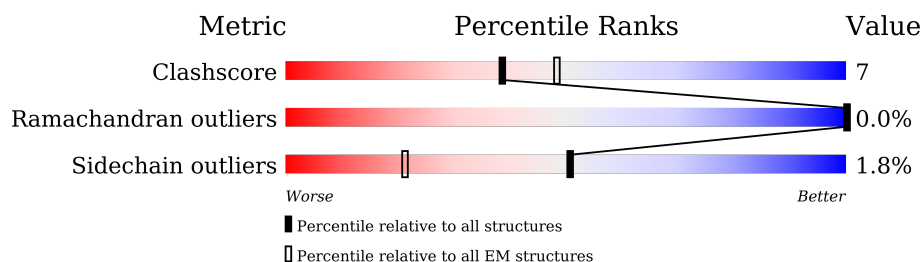
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	2644	
1	B	2644	
2	C	791	
2	D	791	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 45510 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.

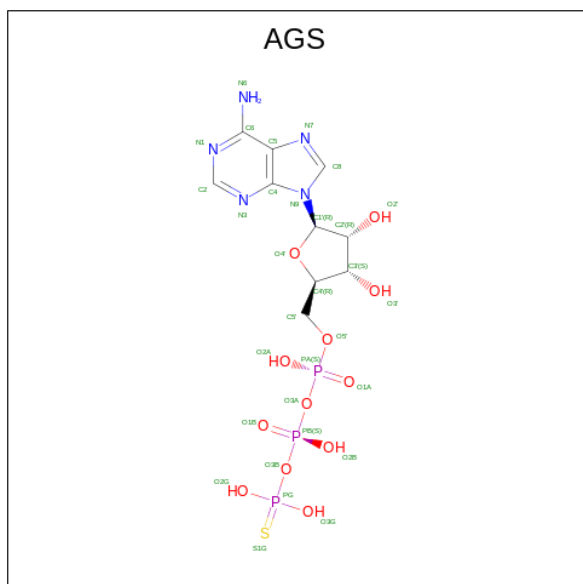
- Molecule 1 is a protein called Serine/threonine-protein kinase ATR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2492	Total	C	N	O	S	0	0
			19988	12826	3392	3630	140		
1	B	2480	Total	C	N	O	S	0	0
			19896	12774	3375	3607	140		

- Molecule 2 is a protein called ATR-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	361	Total	C	N	O	S	0	0
			2779	1776	484	494	25		
2	D	361	Total	C	N	O	S	0	0
			2779	1776	484	494	25		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Mg	0
			2	2	
4	B	2	Total	Mg	0
			2	2	

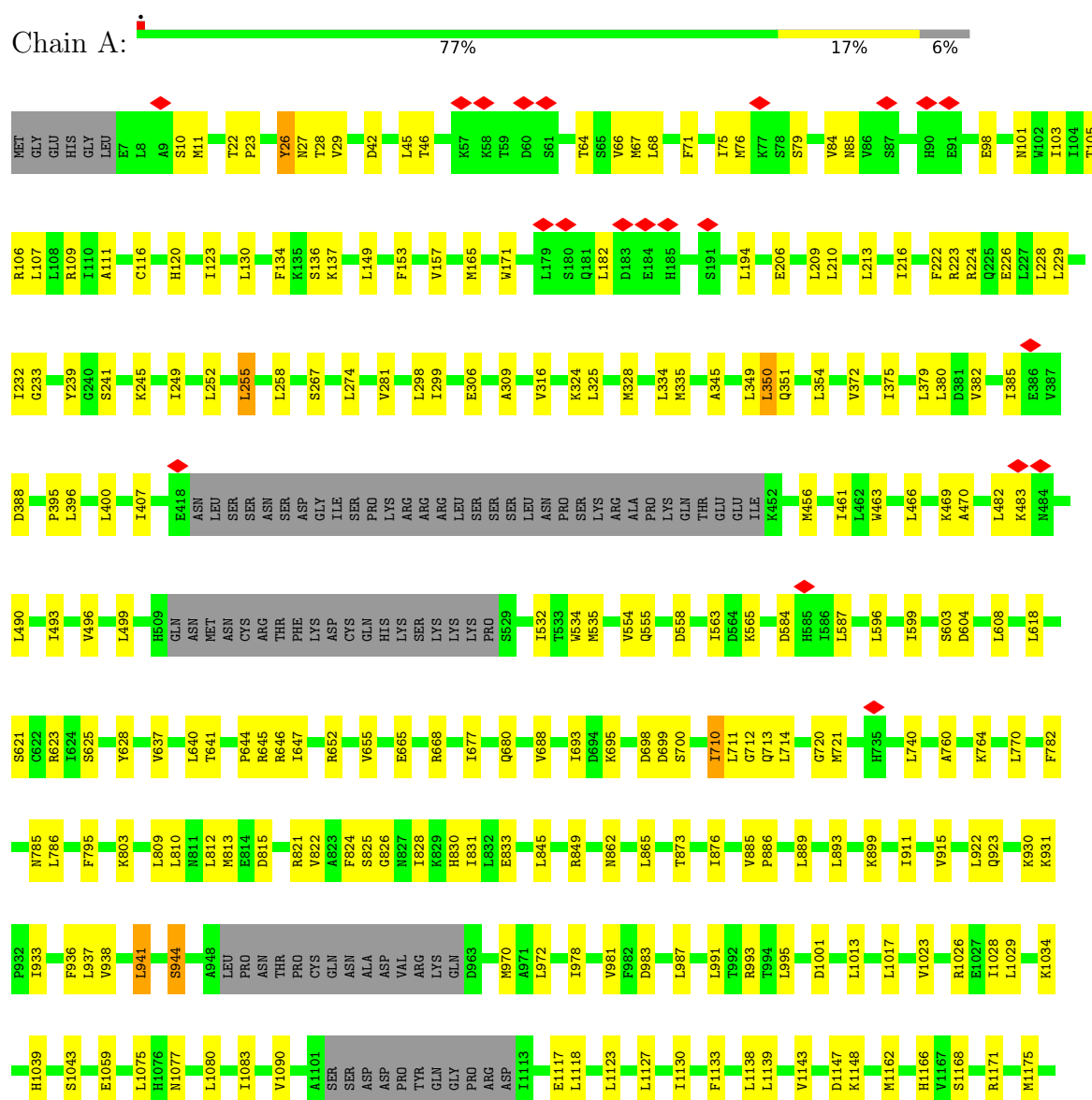
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

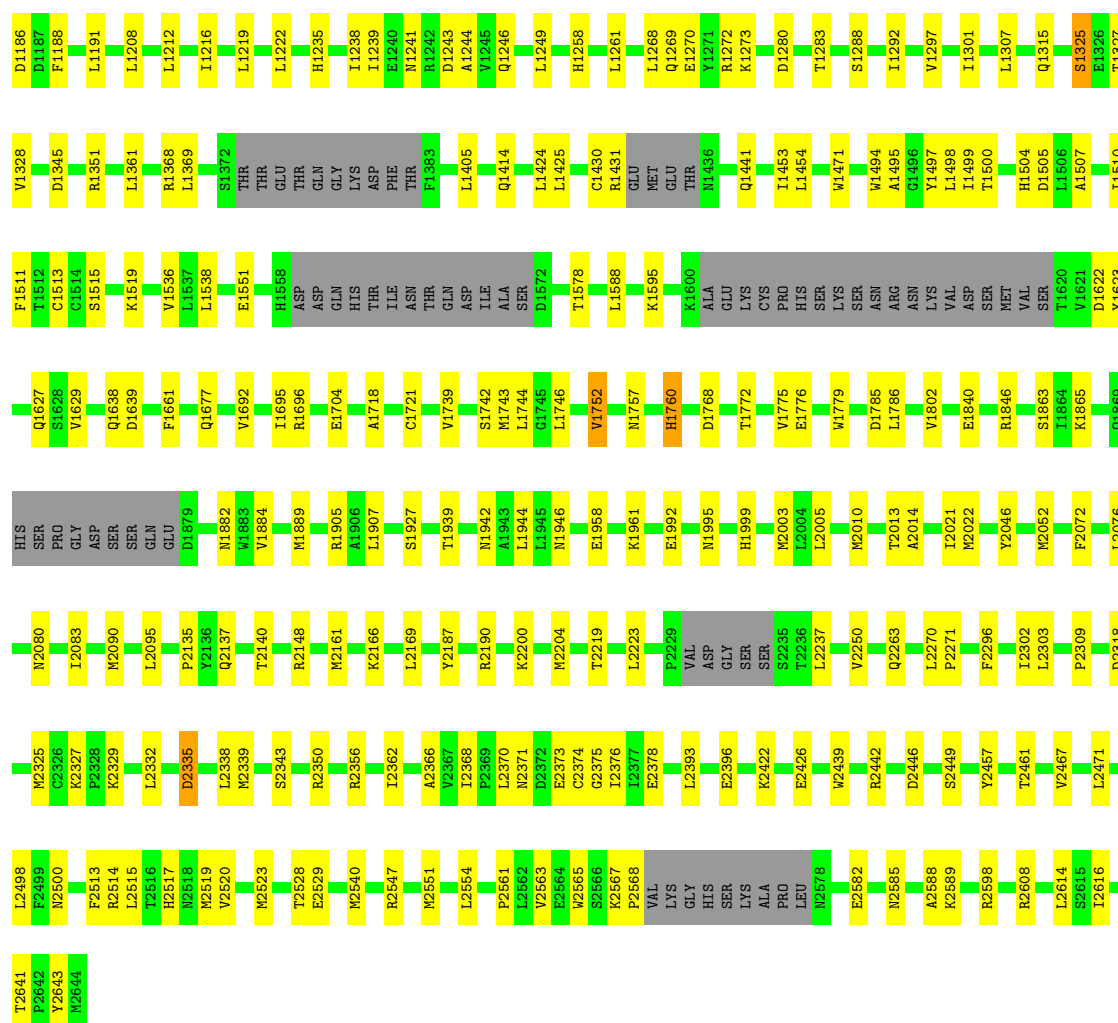
Mol	Chain	Residues	Atoms		AltConf
5	C	1	Total	Zn	0
			1	1	
5	D	1	Total	Zn	0
			1	1	

3 Residue-property plots

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

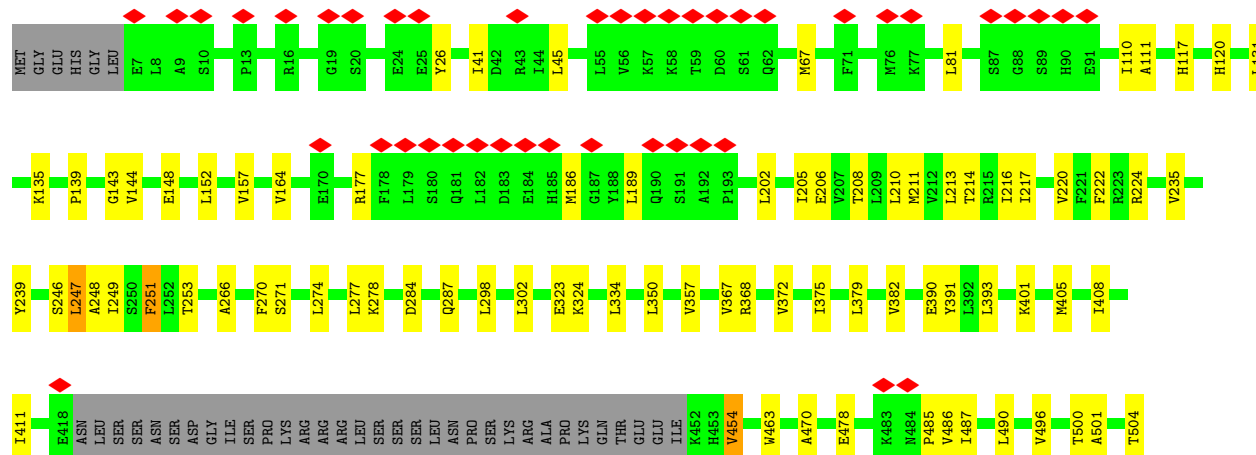
- Molecule 1: Serine/threonine-protein kinase ATR



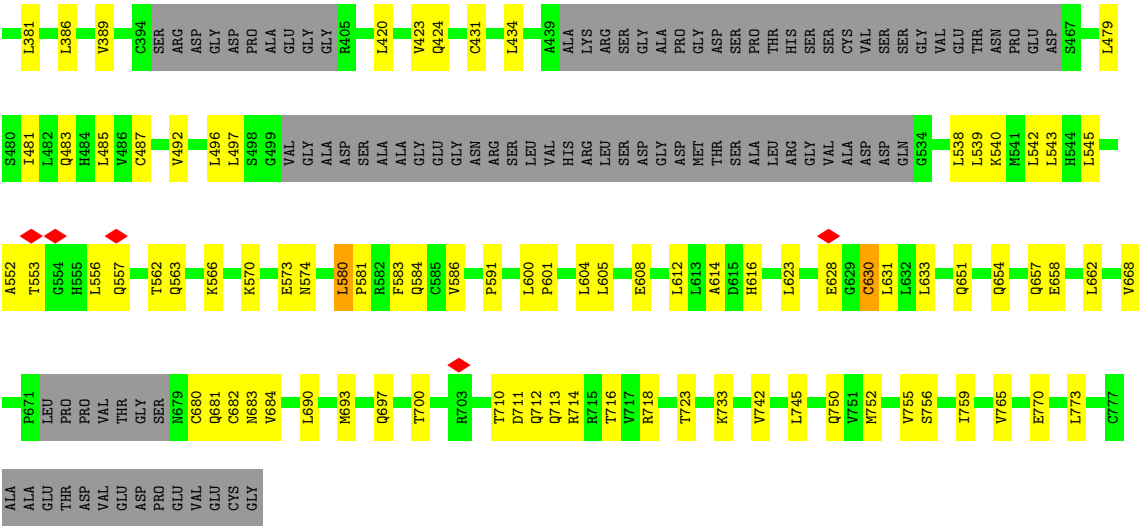


- Molecule 1: Serine/threonine-protein kinase ATR

Chain B:







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382415	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.934	Depositor
Minimum map value	-1.187	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	401.76, 401.76, 401.76	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.93, 0.93, 0.93	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/20402	0.44	0/27571
1	B	0.19	0/20306	0.43	0/27439
2	C	0.28	0/2826	0.64	1/3837 (0.0%)
2	D	0.35	1/2826 (0.0%)	0.74	2/3837 (0.1%)
All	All	0.21	1/46360 (0.0%)	0.47	3/62684 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	580	LEU	C-N	5.59	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	316	LEU	CA-CB-CG	5.90	136.94	116.30
2	D	684	VAL	N-CA-C	-5.62	107.33	112.96
2	C	743	GLU	N-CA-C	-5.14	107.01	113.28

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	TRP	Peptide
1	B	1476	LYS	Peptide
2	C	319	GLN	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	19988	0	20280	306	0
1	B	19896	0	20201	253	0
2	C	2779	0	2873	62	0
2	D	2779	0	2872	65	0
3	A	31	0	12	1	0
3	B	31	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	45510	0	46250	667	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 7.

All (667) 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:A:11:MET:HG3	1:A:71:PHE:CZ	1.87	1.08
2:D:424:GLN:CB	2:D:538:LEU:HD21	1.83	1.07
1:A:456:MET:HG2	1:A:532:ILE:HD11	1.36	1.05
1:A:335:MET:CG	1:A:382:VAL:HG12	1.86	1.05
1:B:206:GLU:O	1:B:210:LEU:HB2	1.59	1.02
2:D:424:GLN:HB2	2:D:538:LEU:HD21	1.06	1.01
1:A:11:MET:HG3	1:A:71:PHE:HZ	1.24	0.99
2:C:636:TYR:HA	2:C:639:ILE:HG22	1.50	0.94
1:A:456:MET:CG	1:A:532:ILE:HD11	1.98	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:424:GLN:HB2	2:D:538:LEU:CD2	1.97	0.93
1:A:11:MET:HE2	1:A:71:PHE:CZ	2.05	0.91
1:A:11:MET:HE2	1:A:75:ILE:HD11	1.54	0.89
2:C:422:LEU:O	2:C:425:PHE:HB3	1.75	0.86
1:A:335:MET:HG3	1:A:382:VAL:CG1	2.05	0.86
1:A:335:MET:HG2	1:A:382:VAL:HG12	1.56	0.85
1:A:84:VAL:HG12	1:A:85:ASN:N	1.90	0.83
1:A:11:MET:CG	1:A:71:PHE:HZ	1.92	0.83
1:A:456:MET:HG2	1:A:532:ILE:CD1	2.08	0.82
2:C:636:TYR:HA	2:C:639:ILE:CG2	2.11	0.80
1:A:335:MET:CG	1:A:382:VAL:CG1	2.58	0.79
2:C:636:TYR:CA	2:C:639:ILE:HG22	2.12	0.79
1:A:456:MET:SD	1:A:532:ILE:HD11	2.23	0.79
1:A:84:VAL:HG12	1:A:85:ASN:H	1.47	0.78
1:A:645:ARG:NH2	1:A:720:GLY:O	2.17	0.77
1:B:486:VAL:O	1:B:490:LEU:HB2	1.85	0.75
2:C:756:SER:HA	2:C:773:LEU:HD13	1.69	0.74
1:A:84:VAL:CG1	1:A:85:ASN:H	2.01	0.73
2:C:636:TYR:O	2:C:639:ILE:HG22	1.90	0.71
1:B:850:MET:HE3	1:B:869:LEU:HD12	1.73	0.70
1:B:211:MET:HA	1:B:214:THR:HG23	1.74	0.70
2:C:636:TYR:C	2:C:639:ILE:HG22	2.16	0.70
2:D:630:CYS:HB3	2:D:633:LEU:HD12	1.73	0.70
1:A:84:VAL:CG1	1:A:85:ASN:N	2.55	0.69
1:B:390:GLU:HA	1:B:393:LEU:HD12	1.74	0.69
1:A:23:PRO:HA	1:A:26:TYR:HB3	1.74	0.69
1:A:944:SER:OG	1:A:970:MET:HE1	1.93	0.69
1:B:274:LEU:O	1:B:324:LYS:NZ	2.26	0.69
1:B:1355:GLY:HA3	1:B:1831:ILE:HD11	1.75	0.68
1:A:810:LEU:HB3	1:A:849:ARG:HG2	1.76	0.68
1:A:944:SER:OG	1:A:970:MET:CE	2.42	0.68
2:D:566:LYS:HG3	2:D:605:LEU:CD1	2.23	0.67
2:D:424:GLN:CA	2:D:538:LEU:HD21	2.24	0.67
1:B:850:MET:CE	1:B:869:LEU:HD12	2.26	0.65
1:B:1992:GLU:HB2	1:B:1995:ASN:HB2	1.79	0.65
1:B:504:THR:HG21	1:B:576:MET:HE3	1.79	0.65
1:B:673:SER:HA	1:B:710:ILE:HG21	1.80	0.64
1:A:26:TYR:HA	1:A:29:VAL:HB	1.80	0.64
1:A:641:THR:HA	1:A:677:ILE:CD1	2.28	0.64
1:A:456:MET:SD	1:A:532:ILE:CD1	2.86	0.64
1:B:131:LEU:HD12	1:B:216:ILE:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:584:GLN:HA	2:C:619:LEU:HD11	1.81	0.63
1:B:707:PHE:O	1:B:711:LEU:HB2	1.98	0.63
2:D:424:GLN:HA	2:D:538:LEU:CD2	2.29	0.63
1:B:2303:LEU:HB2	1:B:2309:PRO:HD2	1.80	0.63
1:A:915:VAL:HG11	1:A:922:LEU:HG	1.81	0.62
1:B:679:LEU:HD11	1:B:714:LEU:HD12	1.81	0.62
1:A:2608:ARG:NH2	1:B:2013:THR:O	2.33	0.61
2:C:553:THR:HA	2:C:557:GLN:HB2	1.82	0.61
1:B:799:GLU:HG2	1:B:841:PHE:CZ	2.35	0.61
1:A:165:MET:SD	1:A:239:TYR:CE1	2.94	0.61
1:B:152:LEU:HD12	1:B:177:ARG:HB2	1.83	0.61
1:B:2393:LEU:HD11	1:B:2439:TRP:HB2	1.81	0.61
1:A:1241:ASN:HD21	1:A:1244:ALA:HB3	1.65	0.60
1:A:2393:LEU:HD11	1:A:2439:TRP:HB2	1.82	0.60
1:B:710:ILE:O	1:B:714:LEU:HB2	2.02	0.60
1:A:2303:LEU:HB2	1:A:2309:PRO:HD2	1.82	0.60
2:D:424:GLN:CB	2:D:538:LEU:CD2	2.68	0.60
1:A:42:ASP:OD1	1:A:106:ARG:NH2	2.34	0.60
1:B:246:SER:HA	1:B:249:ILE:HD12	1.83	0.60
1:A:11:MET:CE	1:A:71:PHE:HZ	2.15	0.60
1:A:645:ARG:HH22	1:A:721:MET:HA	1.66	0.60
1:B:786:LEU:HA	1:B:789:LEU:HB3	1.83	0.59
1:B:1677:GLN:HB2	1:B:1692:VAL:HG11	1.83	0.59
1:B:1827:ARG:HG2	1:B:1857:LEU:HD13	1.84	0.59
1:A:11:MET:HE2	1:A:71:PHE:HZ	1.60	0.59
2:D:752:MET:HA	2:D:755:VAL:HG22	1.83	0.59
1:B:270:PHE:O	1:B:274:LEU:N	2.33	0.59
1:B:164:VAL:HG21	1:B:239:TYR:HB3	1.85	0.59
1:B:1499:ILE:HG12	1:B:1511:PHE:HB3	1.84	0.59
1:B:1639:ASP:OD1	1:B:1639:ASP:N	2.36	0.59
1:A:711:LEU:HD23	1:A:714:LEU:HD23	1.85	0.59
1:B:1127:LEU:HA	1:B:1130:ILE:HD12	1.84	0.59
2:C:312:LEU:HD23	2:C:389:VAL:HG21	1.84	0.59
1:A:267:SER:HB2	2:C:311:ILE:HD13	1.85	0.58
1:A:1498:LEU:HB3	1:A:1536:VAL:HG21	1.84	0.58
1:B:1360:GLU:OE1	1:B:1862:HIS:NE2	2.37	0.58
1:B:1652:THR:HG21	1:B:2448:THR:HA	1.85	0.58
2:C:317:LEU:HD11	2:D:386:LEU:HD22	1.84	0.58
1:A:11:MET:CE	1:A:71:PHE:CZ	2.84	0.58
2:D:742:VAL:HA	2:D:745:LEU:HG	1.86	0.58
1:B:815:ASP:O	1:B:821:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:VAL:HG21	1:A:1001:ASP:HB2	1.85	0.58
1:A:1127:LEU:HD22	1:A:1162:MET:HE2	1.86	0.57
1:B:411:ILE:HD13	1:B:454:VAL:HG22	1.86	0.57
1:B:2585:ASN:HB3	1:B:2588:ALA:HB2	1.86	0.57
1:B:2217:ARG:HB3	1:B:2249:LEU:HD11	1.85	0.57
1:A:2547:ARG:O	1:A:2551:MET:HB2	2.05	0.57
1:B:139:PRO:HG2	2:D:733:LYS:HE3	1.85	0.57
1:A:233:GLY:HA3	1:A:252:LEU:HD21	1.85	0.57
1:A:2561:PRO:HB3	1:A:2582:GLU:HG3	1.86	0.57
1:A:11:MET:CE	1:A:75:ILE:HD11	2.30	0.57
1:B:799:GLU:HG2	1:B:841:PHE:CE1	2.39	0.57
1:B:803:LYS:HG2	1:B:845:LEU:HD11	1.85	0.57
1:B:1832:VAL:HG13	1:B:1833:PRO:HD3	1.87	0.57
1:A:652:ARG:NH1	1:A:677:ILE:HD11	2.19	0.57
1:B:501:ALA:HA	1:B:576:MET:CG	2.35	0.57
1:A:64:THR:HA	1:A:67:MET:HE2	1.87	0.57
1:A:456:MET:SD	1:A:532:ILE:HG12	2.45	0.57
2:C:660:VAL:HG11	2:C:722:ASP:HB3	1.87	0.57
1:A:2223:LEU:HD11	1:A:2371:ASN:HB2	1.87	0.56
1:B:1079:LEU:HG	1:B:1090:VAL:HG13	1.87	0.56
2:D:487:CYS:HB3	2:D:570:LYS:HD3	1.86	0.56
2:C:725:LEU:HD11	2:C:768:CYS:HB3	1.85	0.56
1:A:335:MET:HE3	1:A:385:ILE:HD13	1.88	0.56
1:A:698:ASP:OD1	1:A:698:ASP:N	2.38	0.56
1:A:1325:SER:HA	1:A:2271:PRO:HA	1.87	0.56
1:B:372:VAL:HA	1:B:375:ILE:HG12	1.86	0.56
2:D:424:GLN:CA	2:D:538:LEU:CD2	2.83	0.56
1:A:1039:HIS:O	1:A:1043:SER:HB2	2.05	0.56
1:B:1677:GLN:HG2	1:B:1707:LEU:HD23	1.87	0.56
2:D:434:LEU:HD11	2:D:556:LEU:HD21	1.88	0.56
1:A:825:SER:HA	1:A:828:ILE:HG12	1.88	0.56
1:A:2250:VAL:HG21	1:A:2296:PHE:HE1	1.71	0.56
1:A:822:VAL:O	2:C:703:ARG:NH1	2.39	0.56
1:B:770:LEU:HD22	1:B:812:LEU:HD11	1.86	0.56
1:A:873:THR:HA	1:A:876:ILE:HG22	1.88	0.56
1:A:1430:CYS:O	1:A:1431:ARG:NH1	2.38	0.56
1:B:1023:VAL:HB	1:B:1028:ILE:HD11	1.88	0.56
1:B:1079:LEU:HD23	1:B:1094:LEU:HG	1.88	0.56
2:C:717:VAL:HA	2:C:720:LEU:HD12	1.87	0.56
1:A:937:LEU:HD21	1:A:978:ILE:HG13	1.88	0.56
1:A:2540:MET:HB3	1:A:2616:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:566:LYS:CG	2:D:605:LEU:CD1	2.84	0.56
1:A:641:THR:HA	1:A:677:ILE:HD11	1.88	0.55
2:D:543:LEU:HD21	2:D:586:VAL:HA	1.88	0.55
2:D:628:GLU:OE2	2:D:681:GLN:NE2	2.39	0.55
1:B:1518:MET:HG3	1:B:1525:THR:HG22	1.88	0.55
1:B:1746:LEU:HA	1:B:1939:THR:HG22	1.88	0.55
1:A:1246:GLN:HA	1:A:1249:LEU:HD23	1.89	0.55
1:A:2072:PHE:HB3	1:A:2090:MET:HE2	1.89	0.55
1:B:334:LEU:HD12	1:B:391:TYR:HE2	1.72	0.55
1:A:2135:PRO:HG3	1:A:2166:LYS:HE3	1.89	0.55
1:B:139:PRO:HG2	2:D:733:LYS:CE	2.37	0.55
1:A:1515:SER:O	1:A:1519:LYS:NZ	2.40	0.55
1:B:284:ASP:OD1	1:B:287:GLN:OE1	2.24	0.55
1:B:783:ILE:HD11	1:B:824:PHE:HA	1.89	0.55
1:B:2422:LYS:O	1:B:2426:GLU:HB2	2.07	0.55
1:A:554:VAL:O	1:A:623:ARG:NH2	2.36	0.54
1:A:1942:ASN:O	1:A:1946:ASN:ND2	2.40	0.54
2:C:698:TRP:O	2:C:702:ARG:HB2	2.06	0.54
1:A:153:PHE:HD2	1:A:232:ILE:HD13	1.72	0.54
1:A:1718:ALA:HB1	1:A:1742:SER:HB3	1.88	0.54
1:B:2200:LYS:HE3	1:B:2204:MET:HE3	1.89	0.54
1:B:909:THR:OG1	2:D:750:GLN:OE1	2.20	0.54
1:A:604:ASP:OD1	1:A:604:ASP:N	2.38	0.54
1:A:1143:VAL:HG13	1:A:1147:ASP:HB3	1.89	0.54
1:A:2396:GLU:OE1	1:A:2442:ARG:NH1	2.40	0.54
1:B:1390:SER:HB2	1:B:1442:LEU:HD13	1.90	0.54
1:A:2014:ALA:HA	1:B:2608:ARG:HH21	1.72	0.54
1:B:862:ASN:HB3	1:B:865:LEU:HD12	1.89	0.54
2:C:601:PRO:HA	2:C:604:LEU:HG	1.89	0.54
1:B:45:LEU:HB3	1:B:110:ILE:HD11	1.90	0.54
1:B:277:LEU:HB3	1:B:324:LYS:NZ	2.23	0.54
1:A:335:MET:HE3	1:A:385:ILE:HG21	1.89	0.54
1:A:2514:ARG:NH2	1:A:2641:THR:O	2.41	0.54
1:B:2330:ASP:N	1:B:2330:ASP:OD1	2.39	0.54
2:D:712:GLN:O	2:D:716:THR:OG1	2.19	0.54
1:A:226:GLU:HA	1:A:229:LEU:HD12	1.88	0.54
1:A:490:LEU:HD12	1:A:493:ILE:HD11	1.90	0.54
1:A:886:PRO:O	1:A:889:LEU:HB3	2.08	0.54
1:A:46:THR:O	1:A:109:ARG:NH2	2.41	0.53
1:A:810:LEU:HB3	1:A:849:ARG:CG	2.37	0.53
1:A:1495:ALA:O	1:A:1499:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2318:ASP:OD1	1:A:2318:ASP:N	2.40	0.53
1:A:456:MET:HE2	1:A:534:TRP:CH2	2.43	0.53
1:B:298:LEU:O	1:B:302:LEU:HB2	2.07	0.53
2:D:580:LEU:HD23	2:D:616:HIS:HB2	1.89	0.53
1:A:2585:ASN:HB3	1:A:2588:ALA:HB2	1.90	0.53
1:A:815:ASP:O	1:A:821:ARG:NH1	2.40	0.53
1:B:1292:ILE:HD11	1:B:1307:LEU:HD22	1.90	0.53
2:C:649:GLU:OE1	2:C:712:GLN:NE2	2.40	0.53
1:B:266:ALA:O	1:B:270:PHE:N	2.30	0.53
2:C:650:THR:HA	2:C:712:GLN:HE22	1.73	0.53
1:A:2095:LEU:HD13	1:A:2148:ARG:HG3	1.90	0.53
1:A:2520:VAL:HG13	1:A:2528:THR:HG23	1.90	0.53
1:B:1922:GLU:HG3	1:B:1951:ARG:HH22	1.74	0.53
1:A:677:ILE:HG22	1:A:677:ILE:O	2.09	0.53
1:A:809:LEU:HB3	1:A:824:PHE:HZ	1.74	0.53
1:A:1638:GLN:HB2	1:A:1661:PHE:HB2	1.91	0.53
2:D:479:LEU:HD12	2:D:563:GLN:HB3	1.89	0.53
1:B:1807:LEU:HD11	1:B:1826:VAL:HG21	1.91	0.52
1:A:400:LEU:HD22	1:A:499:LEU:HD22	1.91	0.52
1:B:1673:LEU:HD22	1:B:1692:VAL:HG13	1.90	0.52
1:A:1292:ILE:HD11	1:A:1307:LEU:HD22	1.91	0.52
1:B:1209:GLY:HA2	1:B:1245:VAL:HG12	1.92	0.52
2:C:636:TYR:O	2:C:639:ILE:CG2	2.57	0.52
2:C:468:VAL:O	2:C:472:GLU:HB2	2.10	0.52
2:C:695:HIS:CD2	2:C:747:GLN:HG3	2.45	0.52
1:A:456:MET:CG	1:A:532:ILE:CD1	2.79	0.52
1:B:1673:LEU:HD11	1:B:1695:ILE:HG22	1.92	0.52
1:B:1212:LEU:HD13	1:B:1237:LEU:HD22	1.91	0.52
1:A:862:ASN:HB3	1:A:865:LEU:HB3	1.92	0.52
1:A:1139:LEU:O	1:A:1414:GLN:NE2	2.43	0.51
1:A:1328:VAL:HG13	1:A:1368:ARG:HB3	1.91	0.51
1:A:325:LEU:HA	1:A:328:MET:HG2	1.92	0.51
1:A:2517:HIS:NE2	1:A:2643:TYR:O	2.38	0.51
2:C:680:CYS:SG	2:C:681:GLN:N	2.83	0.51
2:D:591:PRO:HD3	2:D:631:LEU:HD11	1.92	0.51
1:A:695:LYS:NZ	1:A:699:ASP:OD2	2.42	0.51
1:A:1280:ASP:OD1	1:A:1283:THR:OG1	2.28	0.51
1:A:299:ILE:HG21	1:A:345:ALA:HB1	1.91	0.51
1:A:2332:LEU:HD12	1:A:2375:GLY:HA3	1.93	0.51
1:B:271:SER:HA	1:B:274:LEU:HD12	1.92	0.51
1:B:1323:THR:O	1:B:2272:SER:OG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1944:LEU:HD21	1:B:1958:GLU:HG3	1.92	0.51
2:C:752:MET:HG3	2:C:777:CYS:HB2	1.91	0.51
2:C:571:LEU:O	2:C:575:THR:OG1	2.28	0.51
1:B:2540:MET:HB3	1:B:2616:ILE:HG23	1.92	0.51
2:C:549:SER:HA	2:C:556:LEU:HG	1.93	0.51
2:C:759:ILE:HA	2:C:762:LEU:HG	1.93	0.51
1:A:456:MET:SD	1:A:532:ILE:CG1	2.99	0.51
1:A:2614:LEU:HD11	1:B:2015:ASN:HB3	1.93	0.51
1:B:1220:LEU:HD23	1:B:1223:ILE:HD12	1.93	0.51
2:D:553:THR:HA	2:D:557:GLN:HB2	1.92	0.51
2:D:755:VAL:O	2:D:759:ILE:HD12	2.11	0.51
2:D:566:LYS:CG	2:D:605:LEU:HD13	2.40	0.51
1:A:299:ILE:HD11	1:A:349:LEU:HD22	1.92	0.51
1:A:2161:MET:HG2	1:A:2200:LYS:HD3	1.93	0.51
1:B:1247:ASP:OD1	1:B:1247:ASP:N	2.42	0.51
1:A:380:LEU:HD13	1:A:469:LYS:HZ1	1.76	0.50
1:A:645:ARG:HE	1:A:680:GLN:HG2	1.76	0.50
1:A:2362:ILE:HD11	1:A:2467:VAL:HG21	1.93	0.50
1:B:2362:ILE:HD11	1:B:2467:VAL:HG21	1.93	0.50
2:D:633:LEU:HG	2:D:682:CYS:HB3	1.92	0.50
2:C:482:LEU:HD21	2:C:538:LEU:HD21	1.92	0.50
1:A:157:VAL:HG11	1:A:232:ILE:HG23	1.93	0.50
1:A:1961:LYS:HG3	1:A:2005:LEU:HD21	1.94	0.50
1:A:2140:THR:HG21	1:A:2270:LEU:HD21	1.93	0.50
2:C:694:LEU:HD12	2:C:720:LEU:HD23	1.92	0.50
1:A:11:MET:SD	1:A:71:PHE:HZ	2.34	0.50
1:A:388:ASP:OD1	1:A:388:ASP:N	2.44	0.50
1:A:991:LEU:HD23	1:A:1017:LEU:HD23	1.93	0.50
1:A:1739:VAL:O	1:A:1743:MET:HG3	2.12	0.50
1:B:1484:GLY:HA2	1:B:1490:TRP:HB2	1.94	0.50
1:A:223:ARG:NH1	1:A:226:GLU:OE1	2.45	0.50
1:A:2515:LEU:HD11	1:A:2523:MET:HE1	1.94	0.50
1:B:1556:LEU:O	1:B:1647:ARG:NH2	2.40	0.50
2:D:562:THR:O	2:D:566:LYS:HG3	2.12	0.49
1:A:641:THR:HA	1:A:677:ILE:HD12	1.93	0.49
1:A:2446:ASP:HB3	1:A:2449:SER:HB2	1.94	0.49
2:C:616:HIS:CE1	2:C:618:GLN:HB3	2.46	0.49
2:D:570:LYS:NZ	2:D:573:GLU:OE1	2.45	0.49
1:A:222:PHE:HB3	2:C:665:LYS:HE2	1.94	0.49
1:A:1127:LEU:HA	1:A:1130:ILE:HB	1.94	0.49
1:A:2396:GLU:OE2	1:A:2442:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:CYS:HA	1:B:793:LEU:HG	1.95	0.49
1:B:2000:GLY:HA3	1:B:2032:LEU:HD12	1.93	0.49
1:B:2366:ALA:H	1:B:2378:GLU:HB3	1.78	0.49
1:A:1117:GLU:N	1:A:1117:GLU:OE1	2.45	0.49
1:B:350:LEU:HD23	1:B:379:LEU:HD11	1.93	0.49
2:C:570:LYS:O	2:C:574:ASN:ND2	2.45	0.49
2:D:604:LEU:O	2:D:608:GLU:HG2	2.13	0.49
1:A:2422:LYS:O	1:A:2426:GLU:HB2	2.13	0.49
1:B:783:ILE:HD12	1:B:786:LEU:HD21	1.94	0.49
1:B:1169:SER:O	1:B:1171:ARG:NH1	2.46	0.49
1:A:584:ASP:OD1	1:A:646:ARG:NH1	2.46	0.49
1:A:677:ILE:O	1:A:677:ILE:CG2	2.61	0.49
1:B:2315:LYS:HE2	1:B:2319:GLY:HA2	1.94	0.49
2:C:545:LEU:HD11	2:C:564:CYS:HB2	1.95	0.49
2:C:656:GLU:HG2	2:C:693:MET:HE2	1.94	0.49
1:A:1026:ARG:NH2	1:A:1059:GLU:OE2	2.45	0.49
1:B:41:ILE:HG23	1:B:45:LEU:HB2	1.95	0.49
1:B:334:LEU:HD11	1:B:382:VAL:HG21	1.94	0.49
2:C:334:SER:HG	2:D:330:CYS:HG	1.57	0.49
2:D:600:LEU:HD22	2:D:651:GLN:HB3	1.94	0.49
1:B:1731:ASP:OD1	1:B:1763:ARG:NH2	2.45	0.49
1:B:1574:CYS:SG	1:B:1647:ARG:NH1	2.86	0.49
1:B:2547:ARG:O	1:B:2551:MET:HB2	2.13	0.49
1:A:463:TRP:HZ2	1:A:535:MET:HG3	1.78	0.48
1:A:760:ALA:HB2	1:A:795:PHE:HA	1.94	0.48
1:B:248:ALA:HA	1:B:251:PHE:CD2	2.48	0.48
1:B:672:VAL:HG21	1:B:703:VAL:HG13	1.94	0.48
1:B:1768:ASP:O	1:B:1771:ASN:HB3	2.12	0.48
1:A:165:MET:SD	1:A:239:TYR:CZ	3.06	0.48
1:A:944:SER:OG	1:A:970:MET:HE2	2.12	0.48
1:A:2076:LEU:HD22	1:A:2083:ILE:HD12	1.94	0.48
1:B:247:LEU:HD22	1:B:251:PHE:CE1	2.48	0.48
1:A:2500:ASN:OD1	1:A:2598:ARG:NH1	2.42	0.48
1:B:1352:LEU:HA	1:B:1831:ILE:HD13	1.95	0.48
1:B:1446:PHE:HB2	1:B:1451:ARG:HG3	1.94	0.48
1:B:1701:SER:OG	1:B:1702:LEU:N	2.45	0.48
1:A:596:LEU:O	1:A:621:SER:OG	2.28	0.48
2:D:759:ILE:HG22	2:D:765:VAL:HG23	1.95	0.48
1:B:656:TYR:HE2	1:B:677:ILE:HG12	1.78	0.48
2:D:492:VAL:O	2:D:496:LEU:HB2	2.13	0.48
1:B:217:ILE:HA	1:B:220:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:LEU:HD21	1:B:977:GLU:HG2	1.95	0.48
1:B:1997:LEU:HA	1:B:2032:LEU:HD11	1.96	0.48
1:A:350:LEU:HD21	1:A:379:LEU:HD11	1.96	0.48
1:A:1315:GLN:HE22	1:A:1882:ASN:H	1.61	0.48
1:A:2325:MET:HE3	1:A:2327:LYS:HB2	1.96	0.48
1:B:111:ALA:HB1	1:B:208:THR:HG21	1.95	0.48
2:C:760:ARG:HG3	2:C:773:LEU:HD12	1.96	0.48
1:A:306:GLU:HB2	1:A:309:ALA:HB2	1.96	0.47
1:B:496:VAL:O	1:B:500:THR:HG23	2.14	0.47
3:B:5001:AGS:O2B	3:B:5001:AGS:O1A	2.32	0.47
1:A:941:LEU:HB3	1:A:1013:LEU:HD13	1.96	0.47
1:A:1840:GLU:HB3	1:A:1846:ARG:HH22	1.78	0.47
1:B:1004:ALA:HA	1:B:1040:LEU:HD11	1.95	0.47
2:C:769:GLU:O	2:C:773:LEU:HG	2.13	0.47
1:A:688:VAL:HG13	1:A:693:ILE:HD11	1.97	0.47
1:B:821:ARG:HE	1:B:868:THR:HG21	1.79	0.47
1:A:652:ARG:NH1	1:A:677:ILE:CD1	2.77	0.47
1:A:813:MET:HE3	1:A:813:MET:HB2	1.81	0.47
1:B:357:VAL:O	1:B:368:ARG:NH2	2.41	0.47
1:B:791:LYS:HB3	1:B:791:LYS:HE2	1.71	0.47
1:B:2095:LEU:HD13	1:B:2148:ARG:HG3	1.95	0.47
1:A:2338:LEU:HD22	1:A:2498:LEU:HD11	1.96	0.47
1:B:1255:LEU:HD13	1:B:1256:PRO:HD2	1.96	0.47
1:B:1837:ALA:O	1:B:1846:ARG:NH1	2.48	0.47
1:A:699:ASP:OD1	1:A:700:SER:N	2.38	0.47
1:B:975:LEU:HD22	1:B:991:LEU:HD21	1.97	0.47
1:A:1623:TYR:O	1:A:1627:GLN:HG2	2.14	0.47
1:A:1677:GLN:HB2	1:A:1692:VAL:HG11	1.97	0.47
1:A:1746:LEU:HA	1:A:1939:THR:HG22	1.97	0.47
1:A:1775:VAL:HG11	1:A:1802:VAL:HA	1.97	0.47
1:B:157:VAL:HG13	1:B:235:VAL:HG11	1.95	0.47
1:B:688:VAL:O	1:B:690:LYS:NZ	2.39	0.47
2:C:485:LEU:HB3	2:C:492:VAL:HG21	1.96	0.47
1:A:2237:LEU:HG	1:A:2302:ILE:HD11	1.95	0.47
1:A:2366:ALA:H	1:A:2378:GLU:HB3	1.78	0.47
1:B:1242:ARG:NH2	1:B:1270:GLU:OE2	2.47	0.47
1:A:22:THR:O	1:A:26:TYR:N	2.47	0.47
1:A:1328:VAL:HG21	1:A:1369:LEU:HD23	1.96	0.47
1:A:1863:SER:HB3	1:A:1907:LEU:HD22	1.97	0.47
1:B:501:ALA:HA	1:B:576:MET:HG3	1.97	0.47
1:B:2387:ARG:HB2	1:B:2478:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:TRP:CE2	1:A:1551:GLU:HG2	2.49	0.46
1:A:2010:MET:HB3	1:A:2021:ILE:HG12	1.96	0.46
1:A:2080:ASN:OD1	1:A:2137:GLN:NE2	2.48	0.46
1:B:1242:ARG:NH1	1:B:1246:GLN:OE1	2.46	0.46
1:B:2276:THR:OG1	1:B:2280:HIS:ND1	2.46	0.46
1:A:1168:SER:O	1:A:1171:ARG:NH1	2.48	0.46
1:A:1288:SER:O	1:A:1292:ILE:HG13	2.15	0.46
1:B:1238:ILE:HG23	1:B:1249:LEU:HD21	1.97	0.46
1:B:1522:PHE:O	1:B:1525:THR:OG1	2.26	0.46
1:B:1767:THR:O	1:B:1771:ASN:N	2.46	0.46
1:A:98:GLU:OE1	1:A:101:ASN:ND2	2.41	0.46
1:B:2076:LEU:HD13	1:B:2087:MET:HE3	1.95	0.46
2:D:483:GLN:HE22	2:D:570:LYS:HG3	1.79	0.46
1:A:640:LEU:HD22	1:A:652:ARG:HG2	1.97	0.46
1:B:999:LEU:HB2	1:B:1032:ASN:HD21	1.79	0.46
2:C:420:LEU:HD21	2:C:492:VAL:HG22	1.97	0.46
1:A:1497:TYR:O	1:A:1500:THR:OG1	2.30	0.46
1:B:405:MET:HA	1:B:408:ILE:HG12	1.96	0.46
1:B:463:TRP:HH2	1:B:500:THR:HG22	1.81	0.46
1:B:799:GLU:OE2	1:B:841:PHE:CE1	2.69	0.46
1:B:2110:SER:OG	1:B:2111:ASP:OD1	2.27	0.46
2:D:756:SER:HA	2:D:773:LEU:HD22	1.98	0.46
1:A:1083:ILE:HB	1:A:1090:VAL:HG11	1.97	0.46
1:B:761:SER:HA	1:B:764:LYS:HE2	1.97	0.46
1:B:1318:LEU:HA	1:B:1321:TYR:HB2	1.97	0.46
2:C:387:ASN:ND2	2:D:314:ASN:OD1	2.44	0.46
1:A:407:ILE:HD11	1:A:456:MET:SD	2.56	0.46
1:A:677:ILE:HA	1:A:680:GLN:HB2	1.98	0.46
1:A:972:LEU:HD22	1:A:987:LEU:HD21	1.96	0.46
1:A:1944:LEU:HD21	1:A:1958:GLU:HG3	1.97	0.46
1:B:1057:LYS:HE3	1:B:1063:GLU:HA	1.98	0.46
2:D:657:GLN:HE22	2:D:718:ARG:HG3	1.80	0.46
1:A:2187:TYR:HB2	1:A:2190:ARG:HG3	1.97	0.46
1:B:1080:LEU:HD11	1:B:1123:LEU:HD21	1.98	0.46
1:B:1304:LEU:HB3	1:B:1353:LEU:HB3	1.97	0.46
1:A:587:LEU:HB3	1:A:647:ILE:HG13	1.98	0.46
1:A:770:LEU:HD22	1:A:812:LEU:HD11	1.98	0.46
1:A:810:LEU:HA	1:A:813:MET:HE2	1.98	0.46
1:A:1471:TRP:CD1	1:A:1500:THR:HG21	2.50	0.46
1:B:1215:VAL:O	1:B:1219:LEU:HB2	2.15	0.46
1:B:1788:GLU:HG3	1:B:1809:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:ILE:HD12	1:A:628:TYR:HE1	1.81	0.46
1:A:2457:TYR:OH	1:A:2519:MET:O	2.33	0.45
1:B:869:LEU:O	1:B:873:THR:HG22	2.16	0.45
1:B:2383:THR:HB	1:B:2482:LEU:HB3	1.98	0.45
1:B:826:GLY:O	1:B:829:LYS:NZ	2.37	0.45
1:B:1222:LEU:HA	1:B:1225:ILE:HG22	1.98	0.45
1:B:224:ARG:HE	2:D:612:LEU:HD22	1.82	0.45
1:B:555:GLN:HG3	1:B:557:LEU:H	1.81	0.45
1:B:1289:MET:HG2	1:B:1338:VAL:HG21	1.98	0.45
1:A:930:LYS:NZ	1:A:993:ARG:O	2.43	0.45
1:A:1138:LEU:HD23	1:A:1148:LYS:HG2	1.98	0.45
1:A:2513:PHE:HE1	1:A:2515:LEU:HD22	1.82	0.45
1:B:143:GLY:HA3	2:D:668:VAL:HG13	1.99	0.45
1:B:937:LEU:HD23	1:B:998:LEU:HD21	1.98	0.45
1:B:1053:LEU:HD22	1:B:1064:LEU:HD11	1.98	0.45
1:B:1743:MET:HE3	1:B:1743:MET:HB2	1.75	0.45
2:C:590:LEU:HD12	2:C:590:LEU:HA	1.80	0.45
1:A:2457:TYR:O	1:A:2461:THR:OG1	2.32	0.45
3:A:5001:AGS:O2B	3:A:5001:AGS:O2A	2.35	0.45
1:B:186:MET:HB3	1:B:189:LEU:HD13	1.98	0.45
1:B:323:GLU:OE1	2:C:391:ARG:NH2	2.43	0.45
1:B:401:LYS:O	1:B:405:MET:HG2	2.17	0.45
1:B:1823:LEU:HD21	1:B:1861:GLU:HB2	1.99	0.45
2:C:563:GLN:O	2:C:567:VAL:HG13	2.17	0.45
2:D:654:GLN:O	2:D:658:GLU:HG2	2.16	0.45
1:A:665:GLU:HG3	1:A:668:ARG:HH22	1.81	0.45
1:B:573:LEU:HD23	1:B:590:LEU:HD11	1.97	0.45
1:B:1863:SER:HB2	1:B:1907:LEU:HD13	1.98	0.45
2:D:310:SER:O	2:D:314:ASN:HB2	2.17	0.45
1:B:770:LEU:HB3	1:B:812:LEU:HG	1.98	0.45
2:C:382:ALA:O	2:C:386:LEU:HD12	2.16	0.45
1:A:103:ILE:O	1:A:107:LEU:HG	2.16	0.45
1:A:2589:LYS:HA	1:A:2589:LYS:HD2	1.77	0.45
1:A:111:ALA:HB2	1:A:123:ILE:HG21	1.98	0.45
1:A:224:ARG:NH2	2:C:572:ALA:O	2.45	0.45
1:A:316:VAL:HG11	2:C:314:ASN:HB3	1.98	0.45
1:A:849:ARG:HD2	1:A:849:ARG:HA	1.76	0.45
2:D:566:LYS:HG3	2:D:605:LEU:HD13	1.98	0.45
1:B:117:HIS:HA	1:B:120:HIS:CG	2.52	0.45
1:B:249:ILE:O	1:B:253:THR:HG23	2.17	0.45
1:A:911:ILE:HD12	1:A:981:VAL:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2263:GLN:NE2	1:A:2343:SER:OG	2.48	0.44
1:B:408:ILE:HA	1:B:411:ILE:HG22	1.99	0.44
1:B:966:HIS:CD2	1:B:970:MET:HE3	2.52	0.44
1:B:1787:VAL:HG12	1:B:1809:LEU:HD22	1.99	0.44
1:A:350:LEU:HD13	1:A:375:ILE:HG21	1.99	0.44
1:A:809:LEU:HD23	1:A:812:LEU:HD12	1.99	0.44
1:A:1424:LEU:HD21	1:A:1510:ILE:HG23	1.99	0.44
1:B:721:MET:HE3	1:B:751:HIS:HB2	1.99	0.44
1:B:948:ALA:HB3	1:B:967:GLN:HB3	1.99	0.44
1:A:931:LYS:HB3	1:A:931:LYS:HE3	1.74	0.44
1:A:1270:GLU:O	1:A:1273:LYS:HB2	2.16	0.44
1:B:2088:PRO:HB3	1:B:2556:THR:HG21	1.99	0.44
1:A:249:ILE:HG23	1:A:298:LEU:HD22	1.98	0.44
1:A:252:LEU:HA	1:A:255:LEU:HB2	2.00	0.44
1:A:621:SER:O	1:A:625:SER:N	2.48	0.44
1:A:764:LYS:HB3	1:A:764:LYS:HE2	1.82	0.44
1:B:2520:VAL:HG13	1:B:2528:THR:HG23	1.99	0.44
2:D:386:LEU:HA	2:D:389:VAL:HG22	1.98	0.44
1:A:1696:ARG:HH12	1:A:1704:GLU:HB3	1.82	0.44
1:B:1356:GLU:HG3	1:B:1827:ARG:HD2	1.98	0.44
1:A:45:LEU:HG	1:A:68:LEU:HD23	1.99	0.44
1:A:1453:ILE:HD13	1:A:1453:ILE:HA	1.90	0.44
1:A:2338:LEU:HD11	1:A:2471:LEU:HD13	1.99	0.44
1:B:1212:LEU:O	1:B:1216:ILE:HG12	2.17	0.44
1:B:1289:MET:O	1:B:1293:GLN:NE2	2.43	0.44
1:A:105:THR:HG23	1:A:194:LEU:HB2	1.99	0.44
1:A:407:ILE:CD1	1:A:456:MET:SD	3.06	0.44
1:A:2335:ASP:N	1:A:2335:ASP:OD1	2.51	0.44
1:B:26:TYR:OH	1:B:81:LEU:O	2.35	0.44
1:B:1266:ALA:HA	1:B:1269:GLN:HB2	2.00	0.44
1:B:1476:LYS:HE3	1:B:1476:LYS:HB2	1.89	0.44
1:A:893:LEU:HD11	1:A:933:ILE:HG12	2.00	0.44
1:A:1077:ASN:HB3	1:A:1133:PHE:CG	2.52	0.44
1:A:1219:LEU:HD22	1:A:1222:LEU:HD12	1.99	0.44
1:A:2169:LEU:HD11	1:A:2204:MET:HB2	2.00	0.44
1:B:2175:ALA:O	1:B:2179:MET:HG3	2.17	0.44
1:B:2554:LEU:HD13	1:B:2595:ILE:HD13	2.00	0.44
1:A:274:LEU:HG	1:A:324:LYS:HG2	2.00	0.44
1:A:770:LEU:HD21	1:A:782:PHE:CG	2.53	0.44
1:A:2219:THR:HG23	1:A:2370:LEU:HD22	1.99	0.44
1:B:213:LEU:O	1:B:217:ILE:HB	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:966:HIS:O	1:B:970:MET:HG2	2.18	0.44
1:B:824:PHE:O	1:B:828:ILE:HB	2.17	0.43
1:B:2108:GLY:HA2	1:B:2112:ARG:HD3	2.00	0.43
1:A:1992:GLU:HB2	1:A:1995:ASN:HB2	2.00	0.43
1:B:284:ASP:OD1	1:B:287:GLN:CD	2.60	0.43
1:B:1364:ILE:HB	1:B:1369:LEU:HD11	2.00	0.43
1:A:84:VAL:HG22	1:A:134:PHE:CE1	2.53	0.43
1:A:461:ILE:H	1:A:461:ILE:HG13	1.67	0.43
1:B:1424:LEU:HD23	1:B:1510:ILE:HD11	2.00	0.43
1:B:2169:LEU:HD11	1:B:2204:MET:HB2	2.00	0.43
1:A:2356:ARG:HA	1:A:2356:ARG:HD2	1.79	0.43
1:B:2335:ASP:OD1	1:B:2335:ASP:N	2.52	0.43
2:D:711:ASP:HA	2:D:714:ARG:HG2	2.00	0.43
1:A:335:MET:SD	1:A:382:VAL:HG12	2.58	0.43
1:A:555:GLN:NE2	1:A:558:ASP:OD2	2.51	0.43
1:A:824:PHE:CE2	1:A:828:ILE:HD11	2.53	0.43
1:A:893:LEU:HB3	1:A:936:PHE:CE2	2.54	0.43
1:B:1769:GLU:O	1:B:1772:THR:HG22	2.19	0.43
2:D:420:LEU:HD22	2:D:538:LEU:CD1	2.48	0.43
2:D:697:GLN:O	2:D:700:THR:OG1	2.29	0.43
1:A:116:CYS:O	1:A:120:HIS:N	2.50	0.43
1:A:1080:LEU:HD23	1:A:1080:LEU:HA	1.88	0.43
1:B:1094:LEU:HB3	1:B:1119:MET:HE2	2.01	0.43
1:A:206:GLU:O	1:A:210:LEU:HB2	2.19	0.43
1:A:483:LYS:HA	1:A:483:LYS:HD3	1.94	0.43
1:A:987:LEU:HG	1:A:991:LEU:HD11	2.01	0.43
1:A:1776:GLU:HA	1:A:1779:TRP:CD1	2.53	0.43
1:A:2554:LEU:HA	1:A:2554:LEU:HD23	1.84	0.43
1:B:144:VAL:O	1:B:148:GLU:HG3	2.18	0.43
1:B:478:GLU:OE2	1:B:546:SER:OG	2.31	0.43
1:A:228:LEU:O	1:A:232:ILE:HG13	2.19	0.43
1:A:1345:ASP:O	1:A:1351:ARG:NH2	2.52	0.43
1:A:1588:LEU:HD22	1:A:1629:VAL:HG13	2.01	0.43
1:B:485:PRO:HB2	1:B:487:ILE:HD12	2.00	0.43
1:B:490:LEU:HD23	1:B:490:LEU:HA	1.87	0.43
2:D:319:GLN:HA	2:D:320:PRO:HA	1.91	0.43
2:D:680:CYS:O	2:D:683:ASN:ND2	2.52	0.43
1:A:1175:MET:HB3	1:A:1175:MET:HE3	1.79	0.43
1:B:1480:LEU:HD23	1:B:1480:LEU:HA	1.93	0.43
2:D:381:LEU:HD23	2:D:381:LEU:HA	1.82	0.43
1:A:75:ILE:O	1:A:79:SER:N	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:VAL:HB	1:A:1028:ILE:HD11	2.01	0.43
1:A:1238:ILE:HD13	1:A:1268:LEU:HD21	1.99	0.43
1:A:1757:ASN:O	1:A:1760:HIS:ND1	2.47	0.43
1:B:828:ILE:HA	1:B:831:ILE:HB	2.00	0.43
1:A:335:MET:CE	1:A:385:ILE:HD13	2.48	0.42
1:A:2422:LYS:HB3	1:A:2422:LYS:HE3	1.80	0.42
1:B:206:GLU:O	1:B:210:LEU:CB	2.49	0.42
1:B:278:LYS:HE3	1:B:278:LYS:HB3	1.72	0.42
1:B:1083:ILE:HD12	1:B:1087:TYR:HA	2.01	0.42
2:C:487:CYS:HB2	2:C:570:LYS:HE2	2.00	0.42
1:B:277:LEU:HB3	1:B:324:LYS:HZ2	1.83	0.42
2:D:481:ILE:O	2:D:485:LEU:HG	2.18	0.42
1:A:710:ILE:HD12	1:A:710:ILE:HA	1.92	0.42
1:B:1285:LEU:HD11	1:B:1318:LEU:HD21	2.02	0.42
1:B:1715:LEU:HD23	1:B:1716:ARG:HD2	2.00	0.42
1:B:2226:CYS:SG	1:B:2326:CYS:HB3	2.59	0.42
1:A:372:VAL:HA	1:A:375:ILE:HD12	2.01	0.42
1:A:923:GLN:NE2	1:A:983:ASP:O	2.53	0.42
1:B:1530:PRO:O	1:B:1534:VAL:HG13	2.20	0.42
1:B:1706:ILE:HD11	1:B:1725:ALA:HB2	2.00	0.42
1:A:1905:ARG:HH12	1:A:1927:SER:HG	1.64	0.42
1:A:2368:ILE:HB	1:A:2376:ILE:HG13	2.02	0.42
2:C:482:LEU:HD11	2:C:538:LEU:HD11	2.01	0.42
1:A:149:LEU:HD21	1:A:209:LEU:HD22	2.01	0.42
1:A:803:LYS:HZ2	1:A:845:LEU:HD13	1.85	0.42
1:A:1269:GLN:HA	1:A:1272:ARG:HB2	2.02	0.42
2:C:639:ILE:HG12	2:C:693:MET:HE1	2.02	0.42
2:C:720:LEU:O	2:C:724:VAL:HG12	2.20	0.42
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.94	0.42
1:B:463:TRP:CH2	1:B:500:THR:HG22	2.53	0.42
2:C:416:ALA:HB1	2:C:485:LEU:HD12	2.01	0.42
2:D:601:PRO:O	2:D:605:LEU:HG	2.18	0.42
2:D:614:ALA:HB2	2:D:623:LEU:HD11	2.00	0.42
1:A:770:LEU:HD13	1:A:812:LEU:HD11	2.02	0.42
1:A:821:ARG:NH1	1:A:865:LEU:HD13	2.35	0.42
1:A:1424:LEU:HD23	1:A:1424:LEU:HA	1.83	0.42
1:A:2608:ARG:NE	1:B:2016:PHE:O	2.48	0.42
1:B:67:MET:HE2	1:B:67:MET:HB3	1.97	0.42
1:B:210:LEU:HA	1:B:213:LEU:HG	2.02	0.42
1:B:562:THR:O	1:B:566:VAL:HG23	2.20	0.42
1:B:609:LYS:HA	1:B:614:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:VAL:HG13	1:B:886:PRO:HD3	2.00	0.42
1:B:992:THR:HA	1:B:995:LEU:HD23	2.02	0.42
1:B:1665:LYS:HE2	1:B:1665:LYS:HB3	1.88	0.42
1:B:2135:PRO:HG3	1:B:2166:LYS:HE3	2.00	0.42
2:C:386:LEU:HA	2:C:389:VAL:HG12	2.02	0.42
2:C:603:VAL:HG21	2:C:638:TYR:CZ	2.55	0.42
2:D:329:LEU:O	2:D:333:LEU:N	2.50	0.42
1:A:76:MET:HE1	1:A:130:LEU:HA	2.01	0.42
1:A:351:GLN:HB2	1:A:395:PRO:HG3	2.02	0.42
1:B:1641:LEU:O	1:B:1645:SER:OG	2.30	0.42
1:B:2329:LYS:HA	1:B:2329:LYS:HD3	1.79	0.42
1:A:599:ILE:HG23	1:A:608:LEU:HD21	2.02	0.42
1:A:2335:ASP:O	1:A:2339:MET:HG2	2.19	0.42
1:B:1162:MET:HE2	1:B:1166:HIS:HB3	2.00	0.42
1:B:1253:TYR:HA	1:B:1272:ARG:HH11	1.85	0.42
1:B:1828:ALA:O	1:B:1832:VAL:HG12	2.20	0.42
1:B:2142:PHE:HA	1:B:2145:LEU:HD12	2.01	0.42
2:D:581:PRO:O	2:D:584:GLN:HB2	2.20	0.42
2:D:690:LEU:HD22	2:D:723:THR:HG23	2.02	0.42
1:A:1511:PHE:O	1:A:1515:SER:HB3	2.20	0.41
1:B:1659:GLU:OE1	1:B:2454:ARG:NH1	2.51	0.41
1:B:2318:ASP:OD1	1:B:2318:ASP:N	2.50	0.41
1:B:2510:ILE:HD12	1:B:2632:LEU:HD22	2.02	0.41
2:D:312:LEU:O	2:D:316:LEU:HD12	2.20	0.41
1:B:810:LEU:HD23	1:B:810:LEU:HA	1.79	0.41
1:A:490:LEU:HD12	1:A:490:LEU:HA	1.95	0.41
1:B:135:LYS:HD2	1:B:135:LYS:HA	1.85	0.41
1:B:1733:ILE:HG12	1:B:1737:HIS:HD2	1.85	0.41
2:D:552:ALA:HB3	2:D:556:LEU:HD23	2.01	0.41
1:A:466:LEU:HD12	1:A:496:VAL:HG22	2.02	0.41
1:A:2200:LYS:O	1:A:2204:MET:HG3	2.21	0.41
1:A:2515:LEU:HD12	1:A:2515:LEU:HA	1.84	0.41
1:B:1785:ASP:OD1	1:B:1785:ASP:N	2.52	0.41
2:C:636:TYR:HB2	2:C:685:GLU:HG3	2.03	0.41
1:A:490:LEU:HD23	1:A:565:LYS:HB2	2.01	0.41
1:A:1034:LYS:HA	1:A:1075:LEU:HD12	2.03	0.41
1:A:1235:HIS:CE1	1:A:1239:ILE:HD12	2.55	0.41
1:A:1258:HIS:HB3	1:A:1261:LEU:HD12	2.01	0.41
1:B:1887:LEU:O	1:B:1890:THR:OG1	2.30	0.41
1:A:11:MET:CG	1:A:71:PHE:CZ	2.72	0.41
1:A:213:LEU:HD13	1:A:213:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1405:LEU:HD21	1:A:1453:ILE:HG13	2.03	0.41
1:A:1695:ILE:HD12	1:A:2529:GLU:HG3	2.01	0.41
1:A:1744:LEU:HG	1:A:1752:VAL:HG21	2.02	0.41
1:B:1212:LEU:HG	1:B:1252:ILE:HD11	2.01	0.41
2:D:420:LEU:HB3	2:D:538:LEU:HD11	2.02	0.41
2:D:710:THR:HB	2:D:713:GLN:HB3	2.01	0.41
1:A:26:TYR:OH	1:A:84:VAL:O	2.38	0.41
1:B:1903:LEU:O	1:B:1907:LEU:HG	2.21	0.41
1:A:137:LYS:HD3	1:A:137:LYS:HA	1.84	0.41
1:A:712:GLY:H	1:A:785:ASN:ND2	2.19	0.41
1:A:1865:LYS:HB2	1:A:1865:LYS:HE3	1.85	0.41
1:B:202:LEU:HA	1:B:205:ILE:HG22	2.03	0.41
1:B:2554:LEU:HD23	1:B:2554:LEU:HA	1.86	0.41
2:C:636:TYR:HA	2:C:639:ILE:HG21	2.00	0.41
1:A:71:PHE:CZ	1:A:75:ILE:HD11	2.55	0.41
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.85	0.41
1:A:603:SER:HA	1:A:608:LEU:HD23	2.03	0.41
1:A:845:LEU:HD12	1:A:845:LEU:HA	1.98	0.41
1:A:1080:LEU:HD11	1:A:1123:LEU:HD13	2.03	0.41
1:A:1297:VAL:O	1:A:1301:ILE:HG12	2.21	0.41
1:A:1425:LEU:HD21	1:A:1454:LEU:HD13	2.02	0.41
1:B:41:ILE:O	1:B:45:LEU:N	2.52	0.41
1:B:780:LEU:HA	1:B:783:ILE:HG22	2.03	0.41
1:B:1256:PRO:HB3	1:B:1302:HIS:HE1	1.85	0.41
1:B:2023:LYS:NZ	1:B:2027:ASP:OD2	2.50	0.41
1:B:2335:ASP:HB2	1:B:2367:VAL:HG11	2.02	0.41
1:B:2470:ILE:HD13	1:B:2470:ILE:HA	1.90	0.41
2:D:487:CYS:HA	2:D:574:ASN:HD21	1.85	0.41
1:A:470:ALA:HB2	1:A:496:VAL:HG11	2.03	0.41
1:A:1595:LYS:HD2	1:A:1622:ASP:HB3	2.03	0.41
1:A:2329:LYS:N	1:A:2373:GLU:O	2.54	0.41
1:A:2567:LYS:HD2	1:A:2568:PRO:HD2	2.03	0.41
1:B:1748:GLN:O	1:B:1752:VAL:HG23	2.20	0.41
1:B:2147:SER:HB3	1:B:2333:ARG:HH21	1.87	0.41
2:D:583:PHE:O	2:D:586:VAL:HB	2.21	0.41
1:A:153:PHE:CE1	1:A:206:GLU:HA	2.56	0.40
1:A:241:SER:O	1:A:245:LYS:N	2.45	0.40
1:A:456:MET:HG2	1:A:532:ILE:CG1	2.51	0.40
1:A:899:LYS:HA	1:A:899:LYS:HD3	1.88	0.40
1:A:1212:LEU:O	1:A:1216:ILE:HG12	2.22	0.40
1:B:470:ALA:HB2	1:B:496:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1714:LEU:HD23	1:B:1714:LEU:HA	1.91	0.40
1:B:2338:LEU:HD11	1:B:2471:LEU:HD13	2.02	0.40
2:C:496:LEU:HD21	2:C:538:LEU:HD23	2.04	0.40
2:C:725:LEU:HD13	2:C:725:LEU:HA	1.88	0.40
1:A:213:LEU:HA	1:A:216:ILE:HG12	2.03	0.40
1:A:1504:HIS:HB3	1:A:1507:ALA:HB3	2.03	0.40
1:B:222:PHE:HZ	2:D:668:VAL:HG21	1.85	0.40
1:B:723:TYR:HD1	1:B:750:GLN:HG2	1.87	0.40
2:C:483:GLN:HG3	2:C:566:LYS:HG3	2.02	0.40
1:A:123:ILE:HD13	1:A:123:ILE:HA	1.89	0.40
1:A:334:LEU:HG	1:A:382:VAL:HG11	2.03	0.40
1:A:350:LEU:HD12	1:A:354:LEU:HD23	2.04	0.40
1:A:713:GLN:H	1:A:713:GLN:HG3	1.66	0.40
1:A:786:LEU:HD21	1:A:831:ILE:HD11	2.03	0.40
1:A:826:GLY:HA3	2:C:703:ARG:HH22	1.84	0.40
1:A:1188:PHE:HD2	1:A:1191:LEU:HB3	1.85	0.40
1:B:2052:MET:H	1:B:2052:MET:HG2	1.75	0.40
1:B:2297:ASP:HB3	1:B:2313:SER:HB2	2.03	0.40
2:C:552:ALA:HB3	2:C:556:LEU:HD23	2.04	0.40
1:A:27:ASN:OD1	1:A:28:THR:N	2.53	0.40
1:A:637:VAL:O	1:A:641:THR:HG23	2.21	0.40
1:A:830:HIS:HA	1:A:833:GLU:HG2	2.04	0.40
1:A:995:LEU:HD12	1:A:995:LEU:HA	1.87	0.40
1:A:1162:MET:O	1:A:1166:HIS:ND1	2.54	0.40
1:A:1327:THR:HG22	1:A:2350:ARG:HH21	1.86	0.40
1:A:1361:LEU:HD12	1:A:1361:LEU:HA	1.91	0.40
1:B:210:LEU:HG	1:B:251:PHE:CZ	2.56	0.40
1:B:850:MET:CE	1:B:869:LEU:CD1	2.98	0.40
1:B:1328:VAL:HG13	1:B:1368:ARG:HB3	2.03	0.40
1:B:1706:ILE:O	1:B:1710:GLU:HG3	2.20	0.40
1:B:2021:ILE:H	1:B:2021:ILE:HG13	1.74	0.40
1:B:2356:ARG:HA	1:B:2356:ARG:HD2	1.88	0.40
1:B:2368:ILE:HB	1:B:2376:ILE:HG13	2.04	0.40
1:B:2431:ARG:HA	1:B:2431:ARG:HD2	1.81	0.40
2:C:623:LEU:HB3	2:C:632:LEU:HD11	2.03	0.40
1:A:644:PRO:O	1:A:652:ARG:NH2	2.54	0.40
1:A:1999:HIS:O	1:A:2003:MET:HG3	2.22	0.40
1:A:2013:THR:O	1:B:2608:ARG:NH2	2.54	0.40
1:B:253:THR:HG22	1:B:298:LEU:HA	2.04	0.40
1:B:605:ASP:OD2	1:B:608:LEU:N	2.53	0.40
1:B:852:GLU:O	1:B:856:HIS:ND1	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1961:LYS:HG3	1:B:2005:LEU:HD21	2.03	0.40
2:D:431:CYS:HB2	2:D:545:LEU:HD21	2.03	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	2468/2644 (93%)	2392 (97%)	75 (3%)	1 (0%)	100	100
1	B	2452/2644 (93%)	2391 (98%)	61 (2%)	0	100	100
2	C	349/791 (44%)	326 (93%)	23 (7%)	0	100	100
2	D	349/791 (44%)	337 (97%)	12 (3%)	0	100	100
All	All	5618/6870 (82%)	5446 (97%)	171 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2565	TRP

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	2224/2363 (94%)	2181 (98%)	43 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	2213/2363 (94%)	2178 (98%)	35 (2%)	55	79
2	C	319/678 (47%)	313 (98%)	6 (2%)	50	76
2	D	319/678 (47%)	310 (97%)	9 (3%)	38	70
All	All	5075/6082 (83%)	4982 (98%)	93 (2%)	51	77

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	26	TYR
1	A	66	VAL
1	A	136	SER
1	A	182	LEU
1	A	255	LEU
1	A	258	LEU
1	A	281	VAL
1	A	350	LEU
1	A	482	LEU
1	A	655	VAL
1	A	710	ILE
1	A	740	LEU
1	A	885	VAL
1	A	941	LEU
1	A	944	SER
1	A	1029	LEU
1	A	1118	LEU
1	A	1186	ASP
1	A	1208	LEU
1	A	1243	ASP
1	A	1325	SER
1	A	1441	GLN
1	A	1505	ASP
1	A	1513	CYS
1	A	1538	LEU
1	A	1578	THR
1	A	1639	ASP
1	A	1721	CYS
1	A	1752	VAL
1	A	1760	HIS
1	A	1768	ASP
1	A	1772	THR

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Mol	Chain	Res	Type
1	A	1785	ASP
1	A	1786	LEU
1	A	1884	VAL
1	A	1889	MET
1	A	2022	MET
1	A	2046	TYR
1	A	2052	MET
1	A	2335	ASP
1	A	2374	CYS
1	A	2563	VAL
1	B	247	LEU
1	B	251	PHE
1	B	367	VAL
1	B	454	VAL
1	B	594	LEU
1	B	634	SER
1	B	688	VAL
1	B	691	ILE
1	B	710	ILE
1	B	719	HIS
1	B	738	VAL
1	B	835	LEU
1	B	836	ASP
1	B	841	PHE
1	B	914	LEU
1	B	997	VAL
1	B	1150	MET
1	B	1188	PHE
1	B	1211	LEU
1	B	1319	ILE
1	B	1398	MET
1	B	1524	VAL
1	B	1529	LEU
1	B	1594	HIS
1	B	1636	ILE
1	B	1645	SER
1	B	1683	MET
1	B	1734	ILE
1	B	1832	VAL
1	B	1864	ILE
1	B	2113	VAL
1	B	2225	LEU

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Mol	Chain	Res	Type
1	B	2318	ASP
1	B	2454	ARG
1	B	2609	VAL
2	C	311	ILE
2	C	562	THR
2	C	628	GLU
2	C	631	LEU
2	C	668	VAL
2	C	686	VAL
2	D	423	VAL
2	D	497	LEU
2	D	539	LEU
2	D	540	LYS
2	D	542	LEU
2	D	630	CYS
2	D	662	LEU
2	D	693	MET
2	D	770	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	414	GLN
1	A	468	GLN
1	A	602	HIS
1	A	633	GLN
1	A	657	ASN
1	A	750	GLN
1	A	785	ASN
1	A	811	ASN
1	A	942	HIS
1	A	1076	HIS
1	A	1153	ASN
1	A	1235	HIS
1	A	1459	ASN
1	A	1466	GLN
1	A	1575	GLN
1	A	1579	GLN
1	A	1668	ASN
1	A	1748	GLN
1	A	1783	GLN

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Mol	Chain	Res	Type
1	A	1891	GLN
1	A	1970	HIS
1	A	2153	HIS
1	A	2477	HIS
1	A	2597	GLN
1	A	2631	ASN
1	B	417	GLN
1	B	744	ASN
1	B	788	HIS
1	B	811	ASN
1	B	945	GLN
1	B	967	GLN
1	B	1020	GLN
1	B	1135	ASN
1	B	1153	ASN
1	B	1241	ASN
1	B	1286	GLN
1	B	1587	HIS
1	B	1911	ASN
1	B	1946	ASN
1	B	1970	HIS
1	B	1999	HIS
1	B	2227	ASN
1	B	2371	ASN
1	B	2521	ASN
1	B	2621	HIS
2	C	622	GLN
2	C	679	ASN
2	C	683	ASN
2	C	712	GLN
2	C	750	GLN
2	D	308	GLN
2	D	488	HIS
2	D	654	GLN
2	D	669	GLN
2	D	713	GLN

5.3.3 RNA ⓘ

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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	AGS	B	5001	4	29,33,33	0.47	1 (3%)	39,52,52	0.72	1 (2%)
3	AGS	A	5001	4	29,33,33	0.46	1 (3%)	39,52,52	0.68	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	B	5001	4	-	6/21/38/38	0/3/3/3
3	AGS	A	5001	4	-	4/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5001	AGS	PG-S1G	2.12	1.95	1.90
3	A	5001	AGS	PG-S1G	2.09	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5001	AGS	PA-O3A-PB	-3.74	119.98	132.83
3	A	5001	AGS	PA-O3A-PB	-3.15	122.01	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

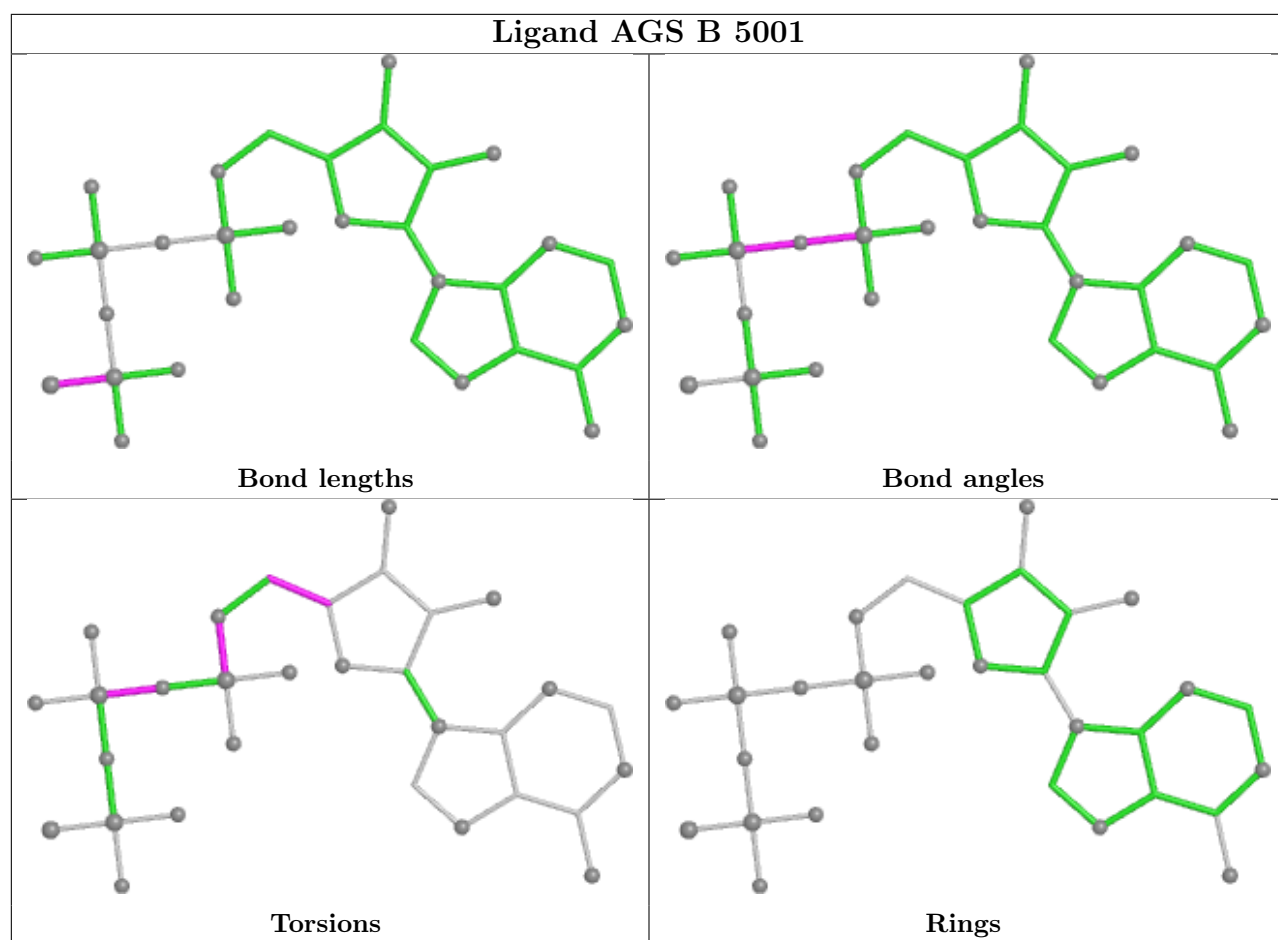
Mol	Chain	Res	Type	Atoms
3	B	5001	AGS	O4'-C4'-C5'-O5'
3	B	5001	AGS	C3'-C4'-C5'-O5'
3	B	5001	AGS	C5'-O5'-PA-O3A
3	B	5001	AGS	C5'-O5'-PA-O1A
3	B	5001	AGS	C5'-O5'-PA-O2A
3	A	5001	AGS	PG-O3B-PB-O1B
3	A	5001	AGS	PA-O3A-PB-O2B
3	A	5001	AGS	C4'-C5'-O5'-PA
3	B	5001	AGS	PA-O3A-PB-O2B
3	A	5001	AGS	PG-O3B-PB-O3A

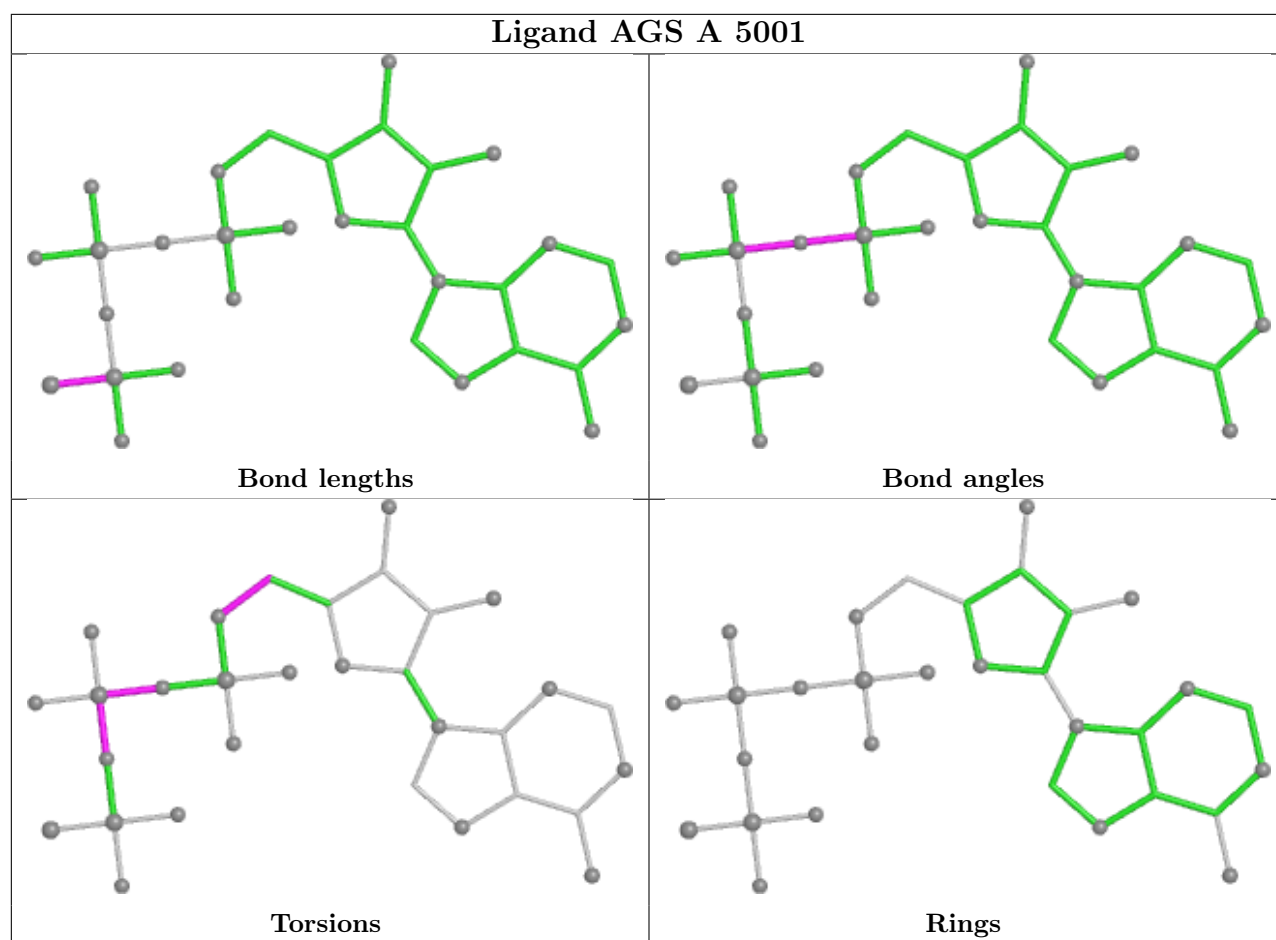
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5001	AGS	1	0
3	A	5001	AGS	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.





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.

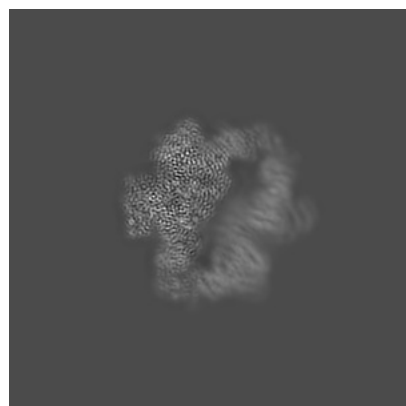
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-68918. These allow visual inspection of the internal detail of the map and identification of artifacts.

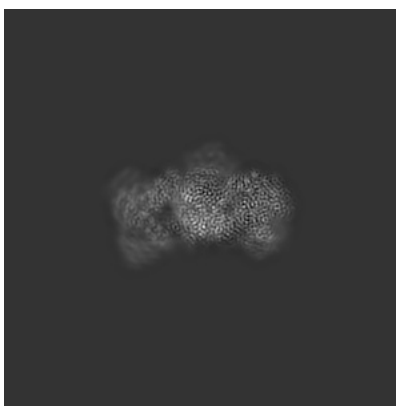
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X

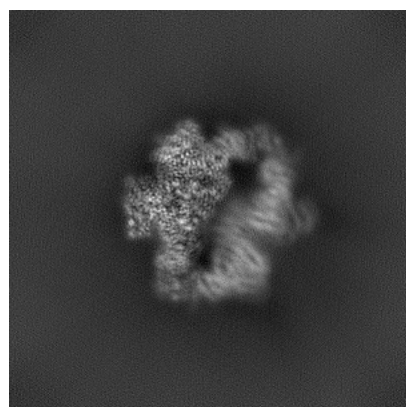


Y

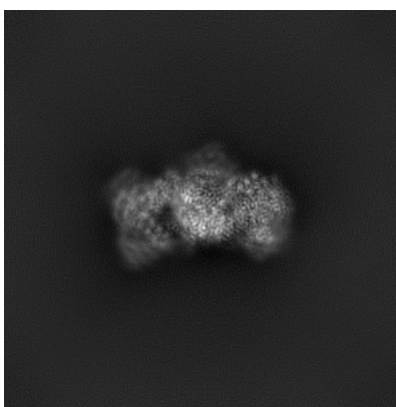


Z

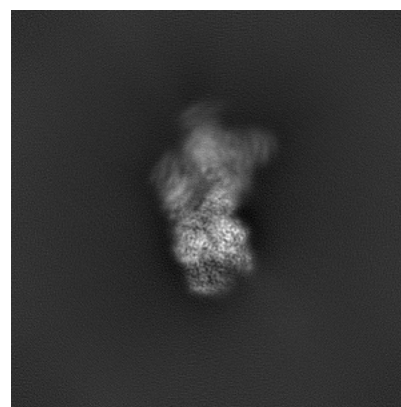
6.1.2 Raw map



X



Y

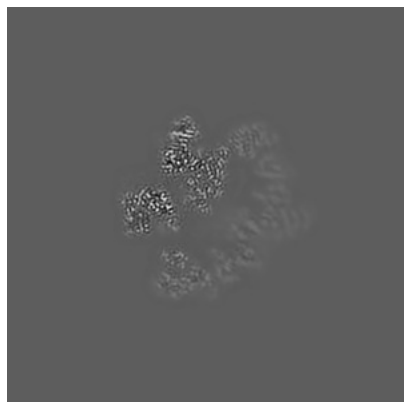


Z

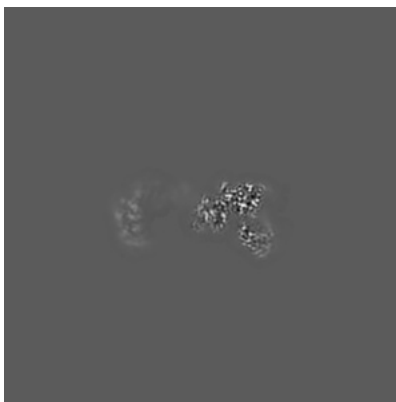
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 216

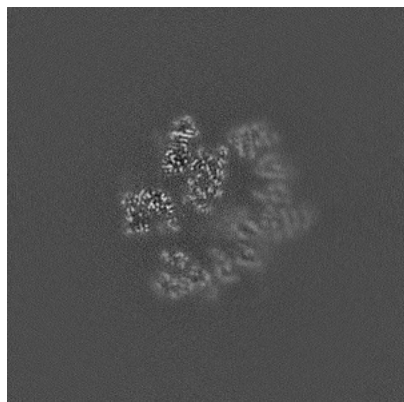


Y Index: 216



Z Index: 216

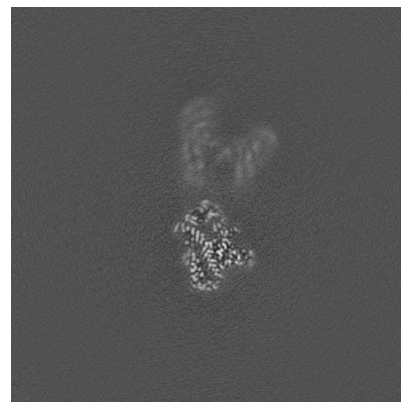
6.2.2 Raw map



X Index: 216



Y Index: 216

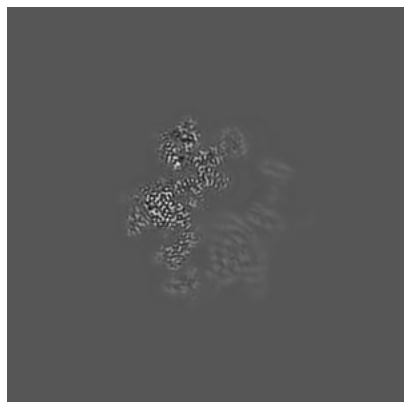


Z Index: 216

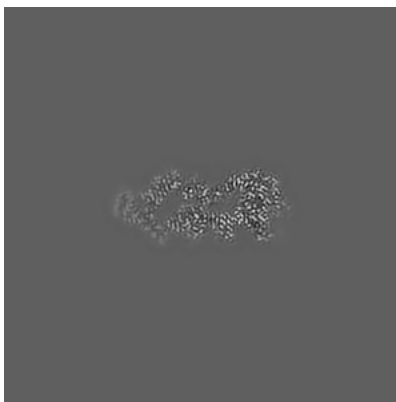
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 228

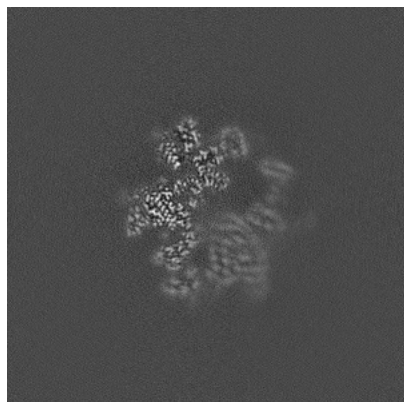


Y Index: 180

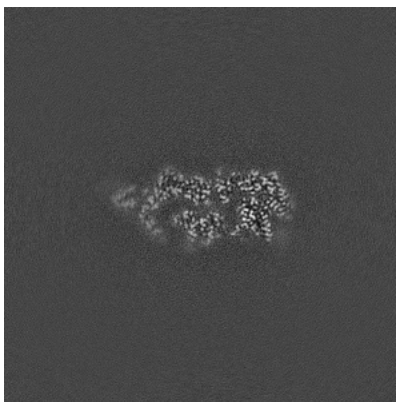


Z Index: 216

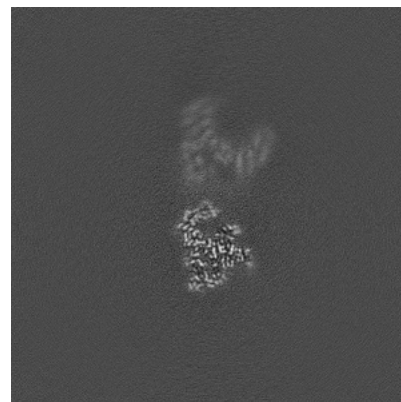
6.3.2 Raw map



X Index: 228



Y Index: 189

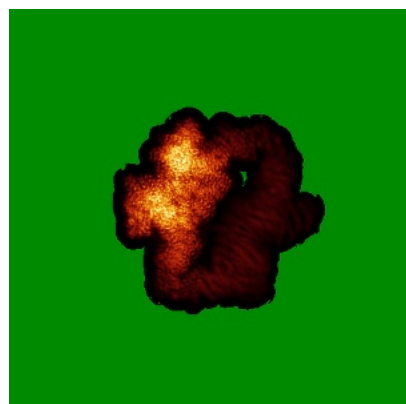


Z Index: 212

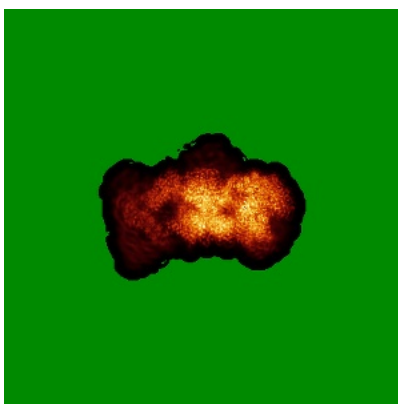
The images above show the largest variance slices of the map in three orthogonal directions.

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

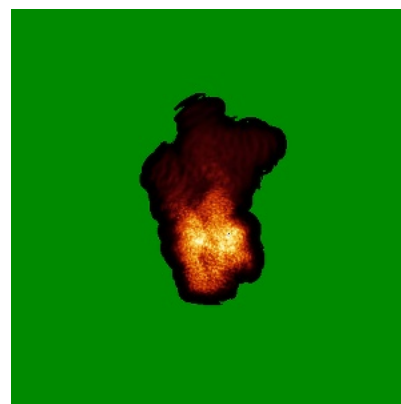
6.4.1 Primary map



X

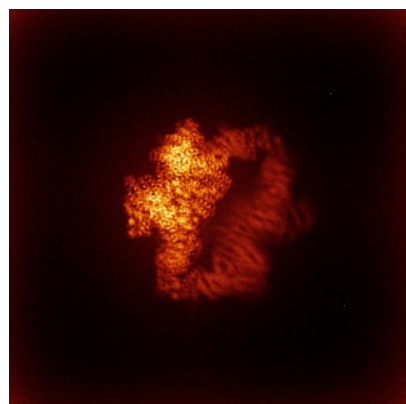


Y

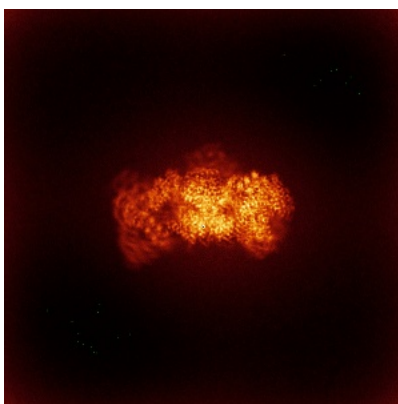


Z

6.4.2 Raw map



X



Y

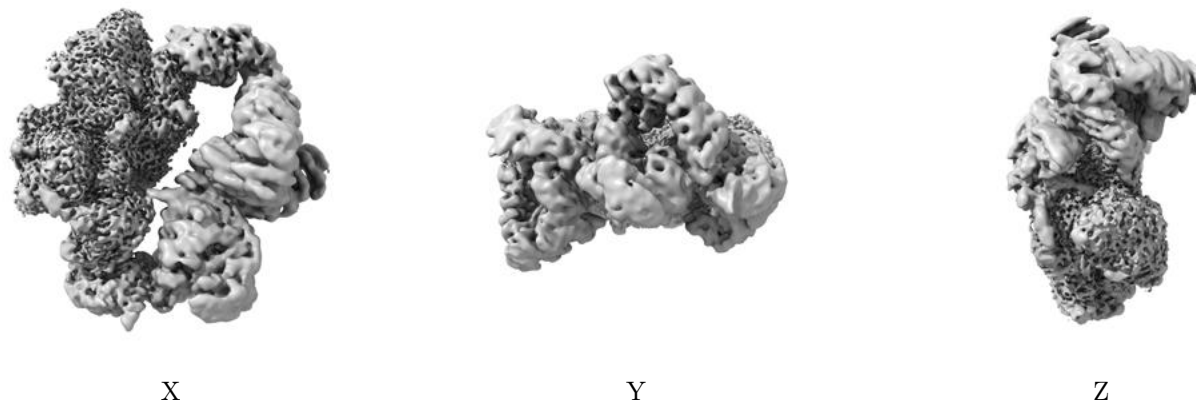


Z

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

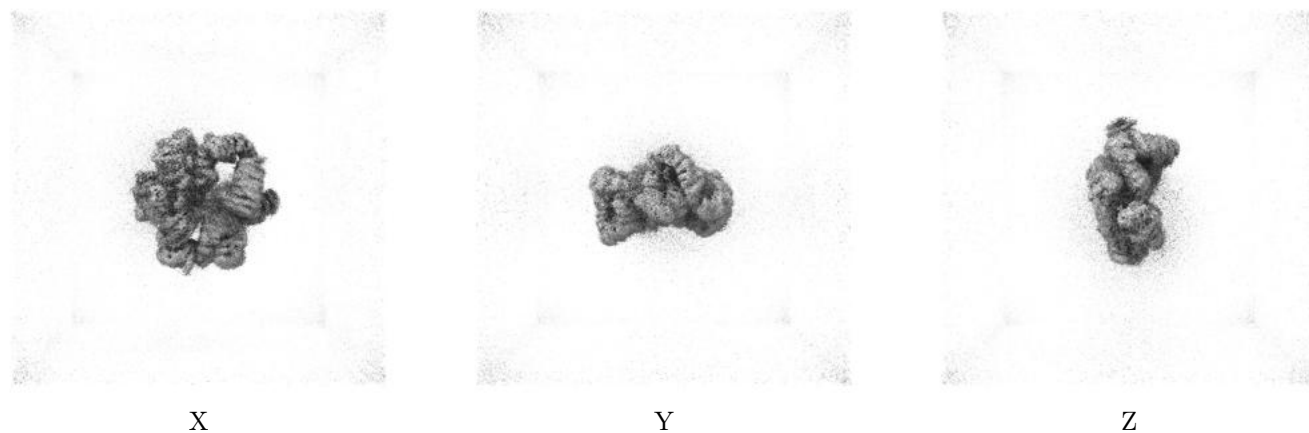
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

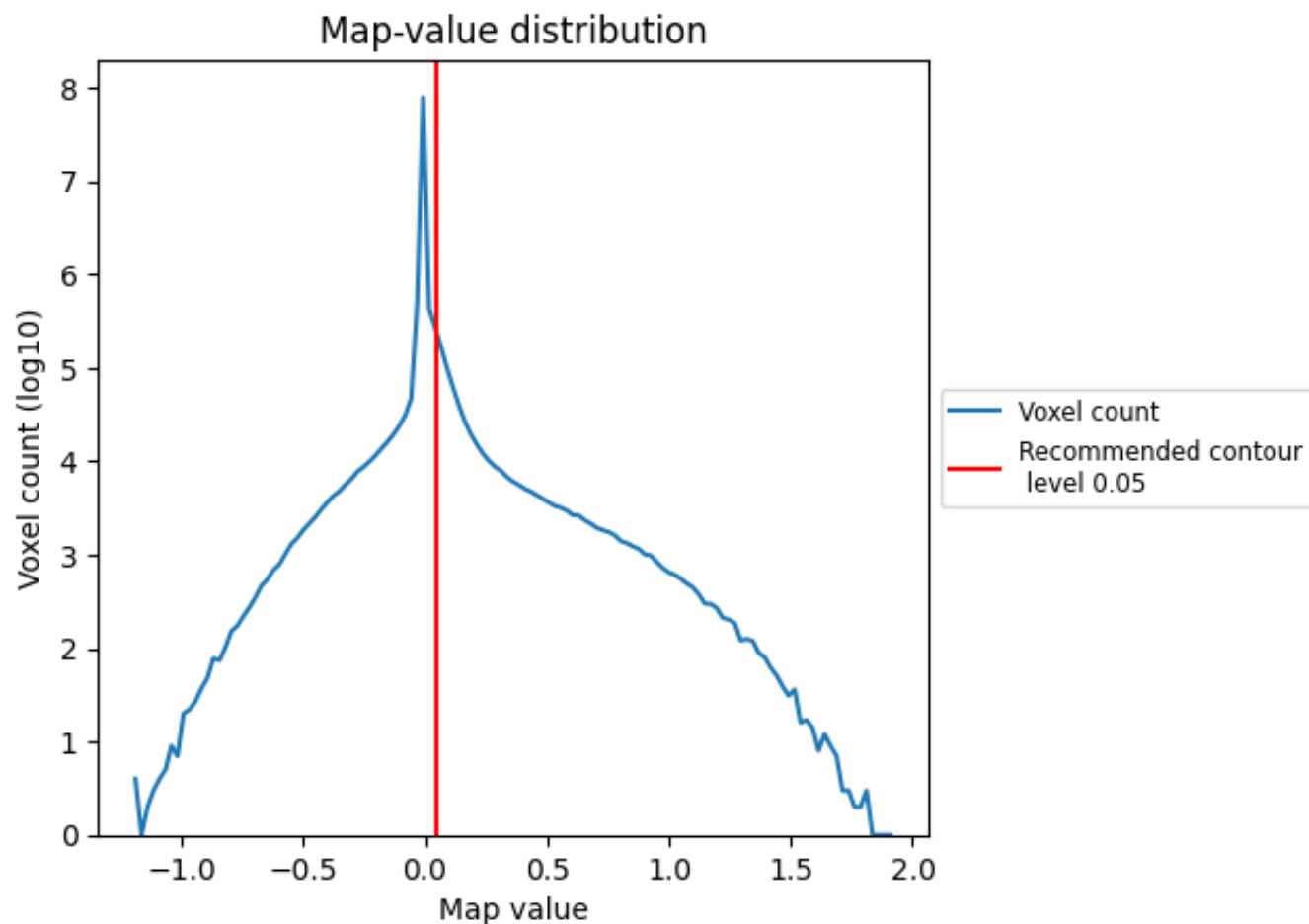
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

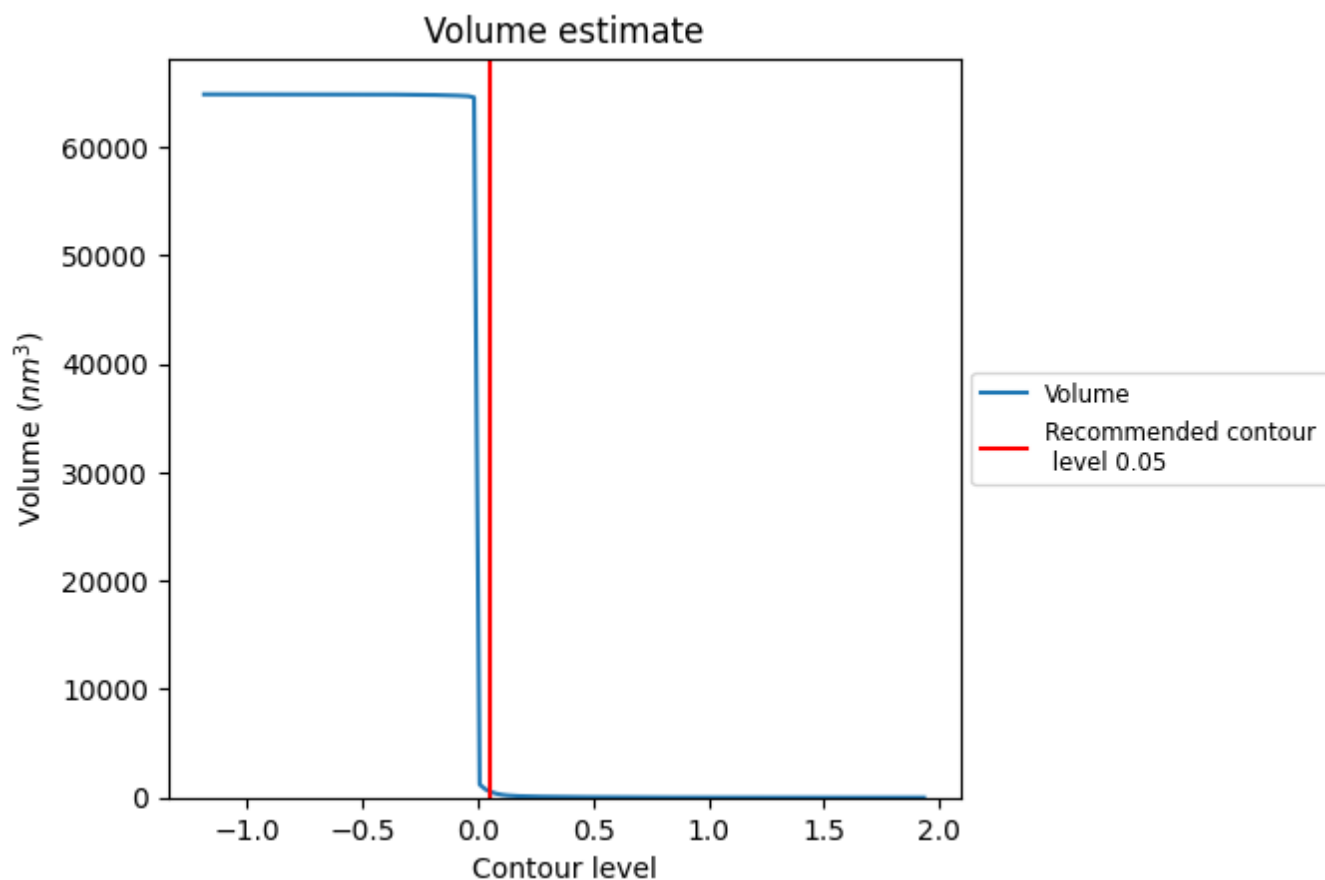
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

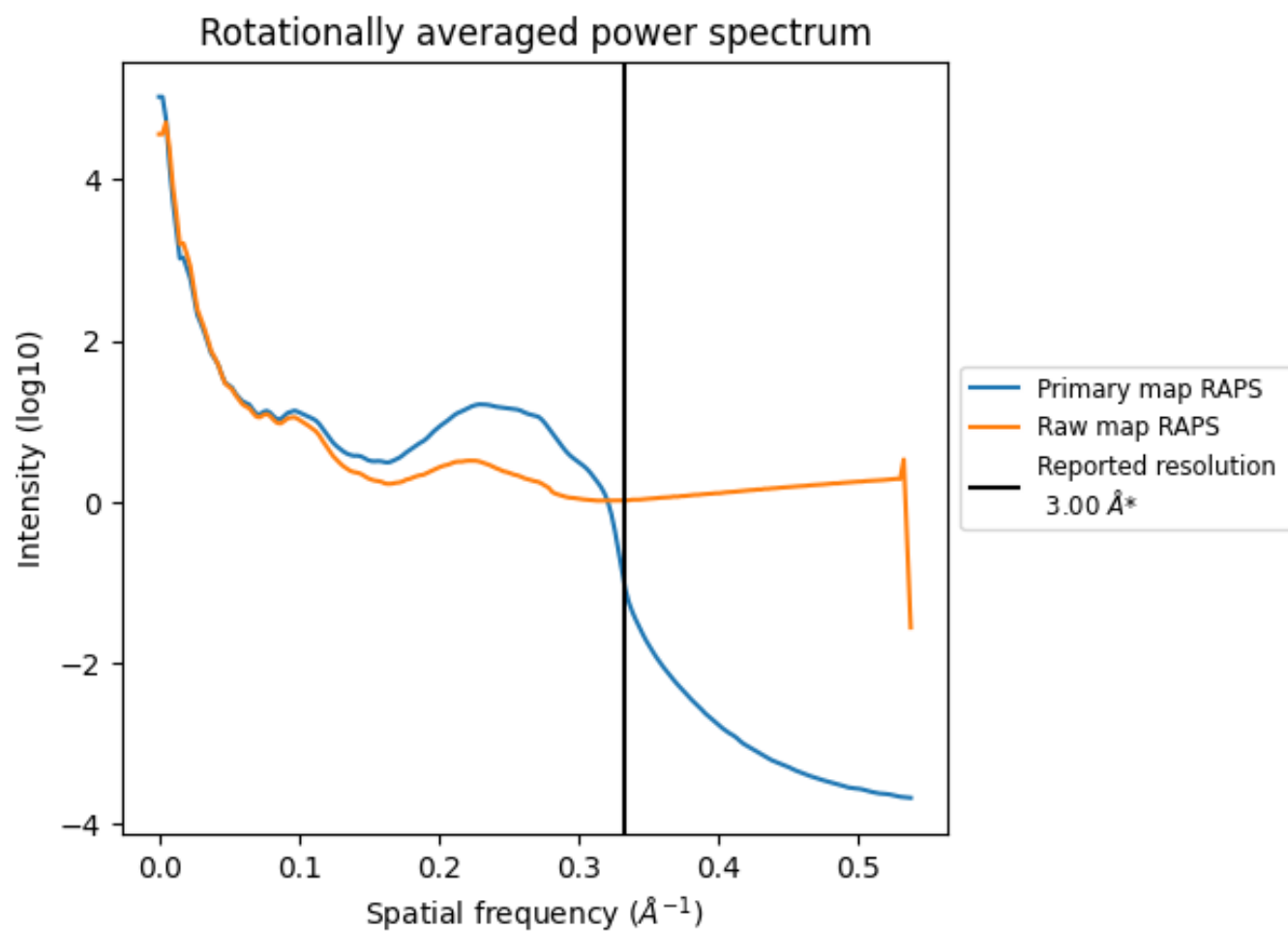
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 581 nm³; this corresponds to an approximate mass of 525 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 ⓘ

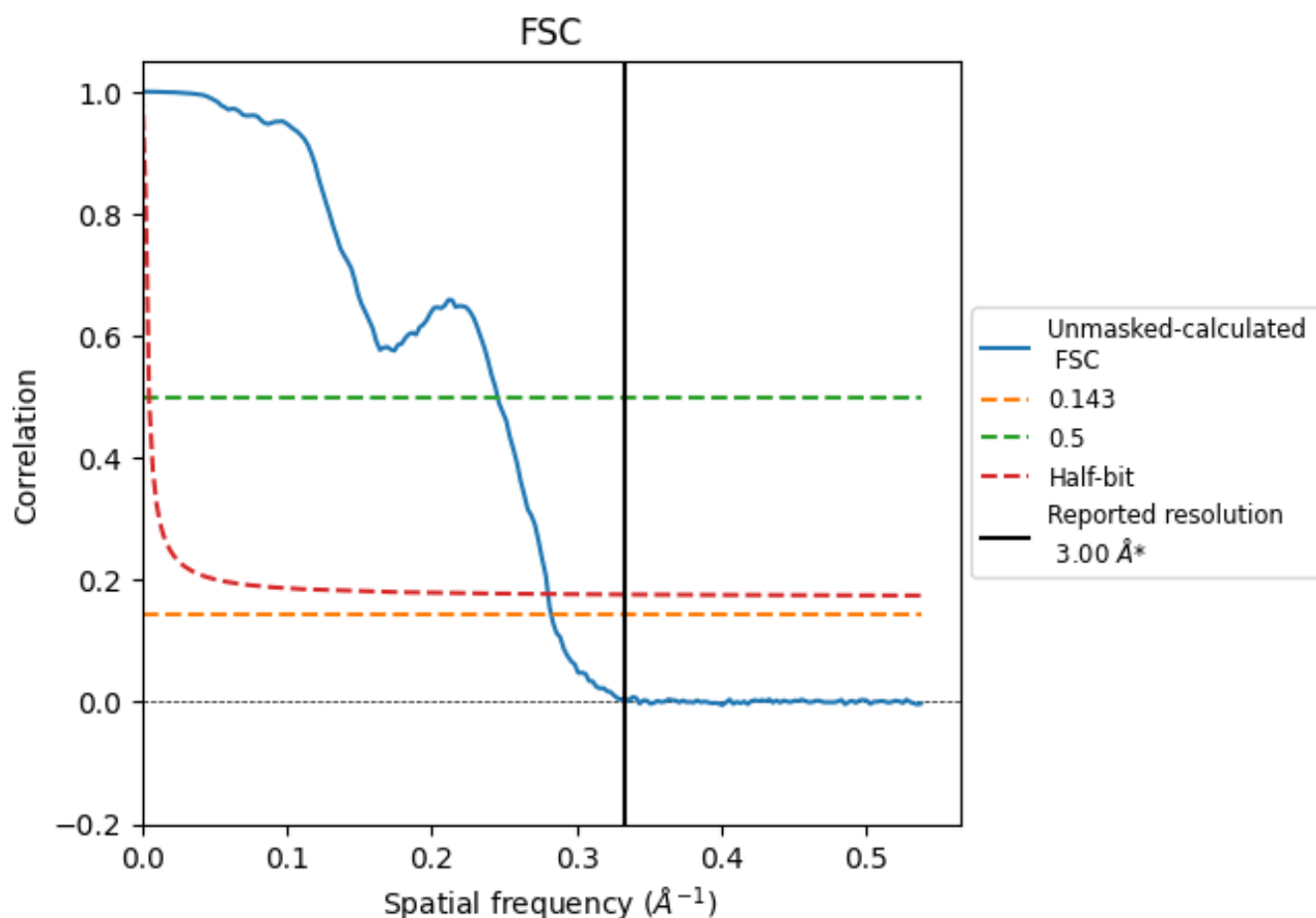


*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.333 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

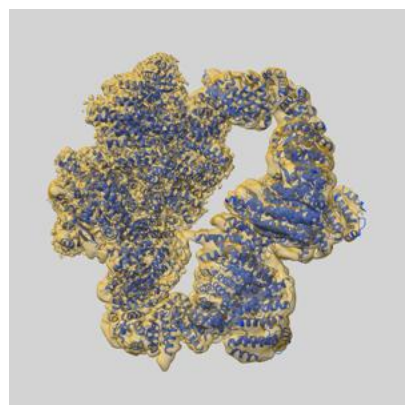
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.54	4.07	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.54 differs from the reported value 3.0 by more than 10 %

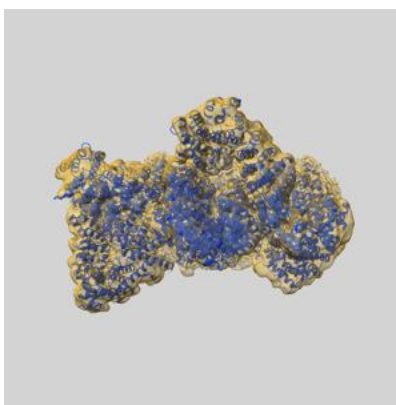
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-68918 and PDB model 23FB. Per-residue inclusion information can be found in section [3](#) on page [5](#).

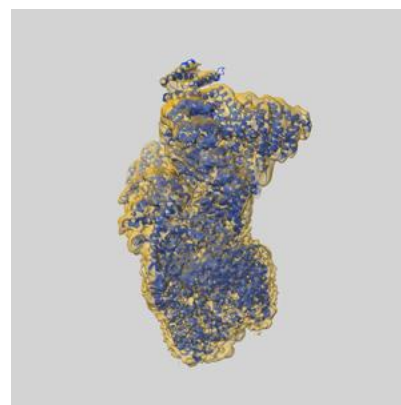
9.1 Map-model overlay [i](#)



X



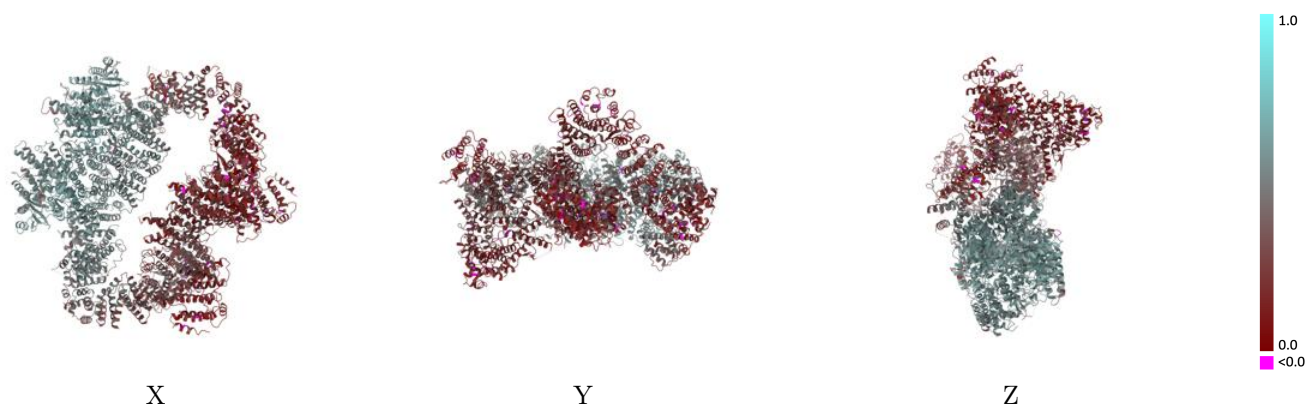
Y



Z

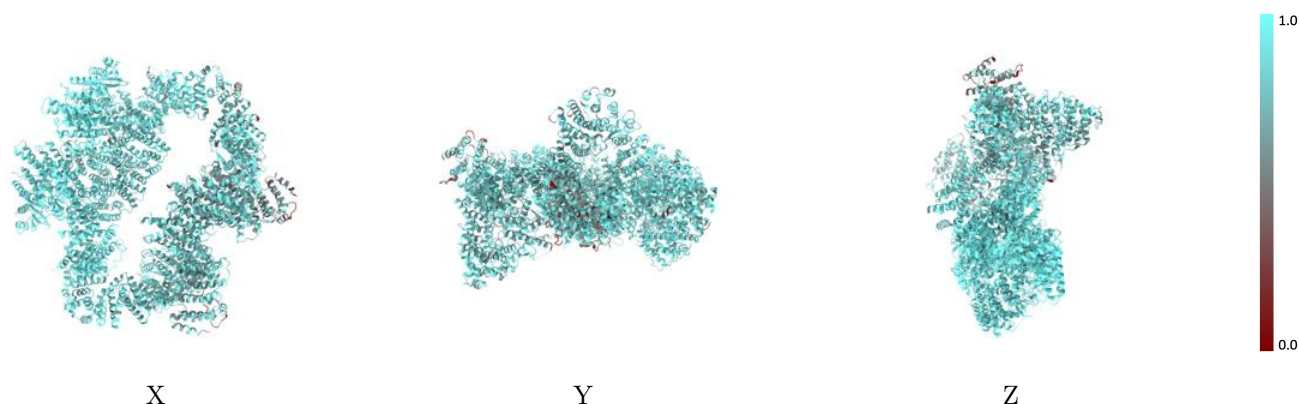
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



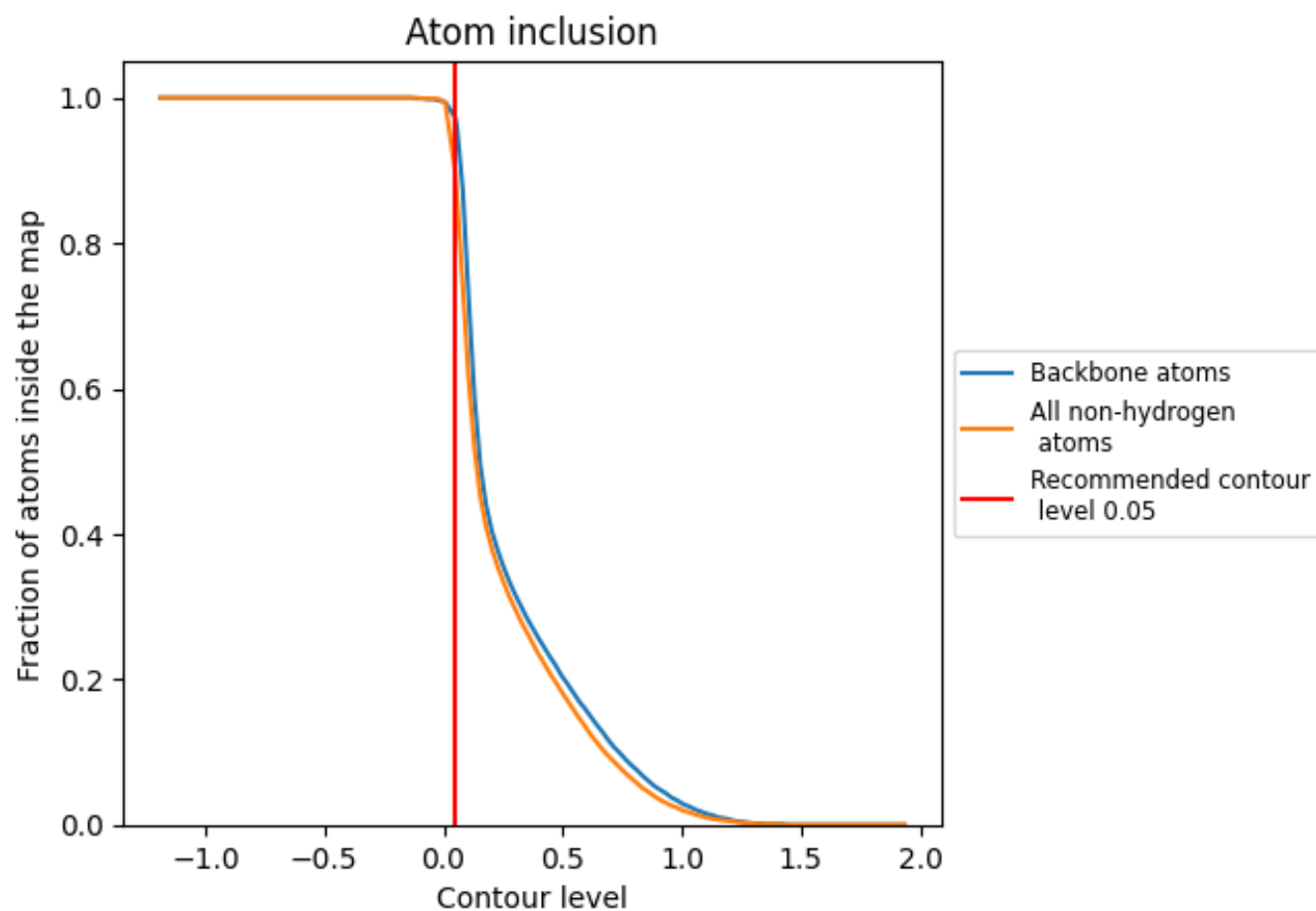
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.3850
A	0.9200	0.4340
B	0.8800	0.3760
C	0.8680	0.2780
D	0.8390	0.2130

