



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 12:33 AM EDT

PDB ID : 6VVO
EMDB ID : EMD-21405
Title : Structure of the human clamp loader (Replication Factor C, RFC) bound to the sliding clamp (Proliferating Cell Nuclear Antigen, PCNA)
Authors : Gaubitz, C.; Liu, X.; Stone, N.P.; Kelch, B.A.
Deposited on : 2020-02-18
Resolution : 3.40 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

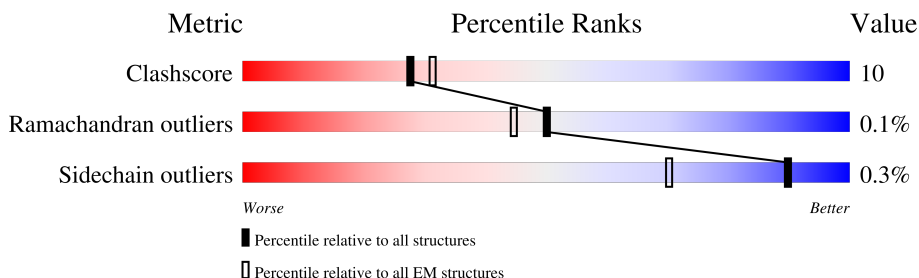
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	595	
2	B	354	
3	C	340	
4	D	363	
5	E	356	
6	F	261	
6	G	261	
6	H	261	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19668 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 Replication factor C subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	448	Total	C	N	O	S	0	0
			3500	2218	608	649	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	554	MET	-	expression tag	UNP P35251
A	555	ASP	-	expression tag	UNP P35251

- Molecule 2 is a protein called Replication factor C subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	316	Total	C	N	O	S	0	0
			2492	1583	432	459	18		

- Molecule 3 is a protein called Replication factor C subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	312	Total	C	N	O	S	0	0
			2486	1585	424	464	13		

- Molecule 4 is a protein called Replication factor C subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	304	Total	C	N	O	S	0	0
			2361	1495	401	455	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	71	GLU	LEU	conflict	UNP P35249

- Molecule 5 is a protein called Replication factor C subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	346	Total	C	N	O	S	0	0
			2759	1738	493	505	23		

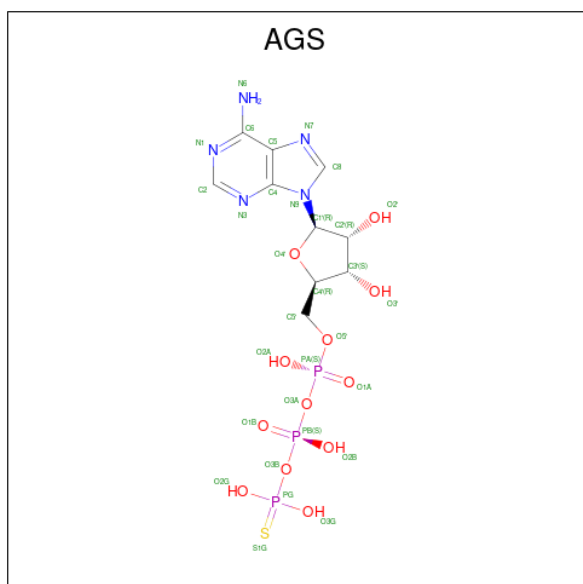
- Molecule 6 is a protein called Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	254	Total	C	N	O	S	1	0
			1960	1231	320	393	16		
6	G	257	Total	C	N	O	S	0	0
			1980	1242	324	398	16		
6	H	256	Total	C	N	O	S	1	0
			1975	1240	323	396	16		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

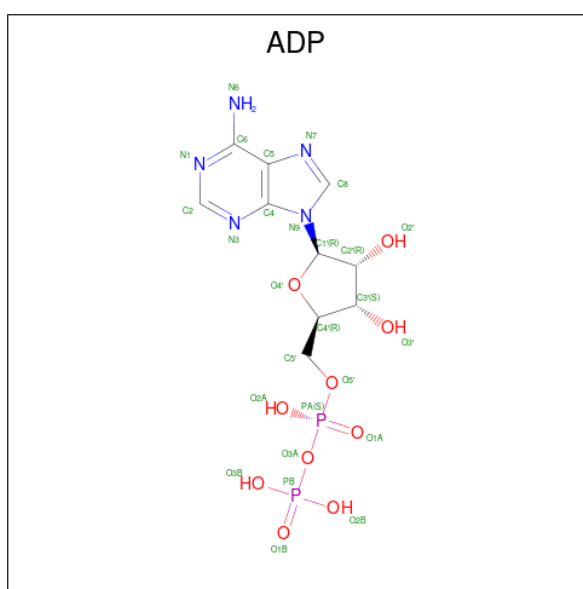
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	C	1	Total	Mg	0
			1	1	
7	D	1	Total	Mg	0
			1	1	

- Molecule 8 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).

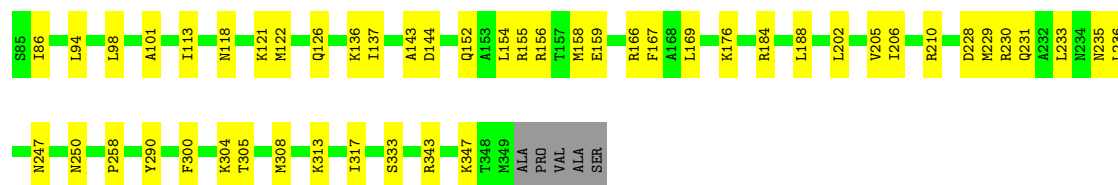


Mol	Chain	Residues	Atoms					AltConf	
8	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
8	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
8	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
8	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



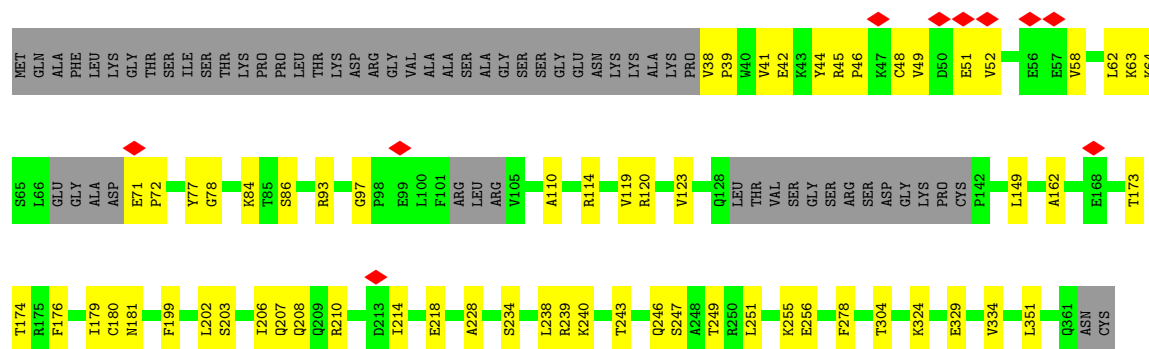
Mol	Chain	Residues	Atoms					AltConf
9	E	1	Total	C	N	O	P	0
			27	10	5	10	2	



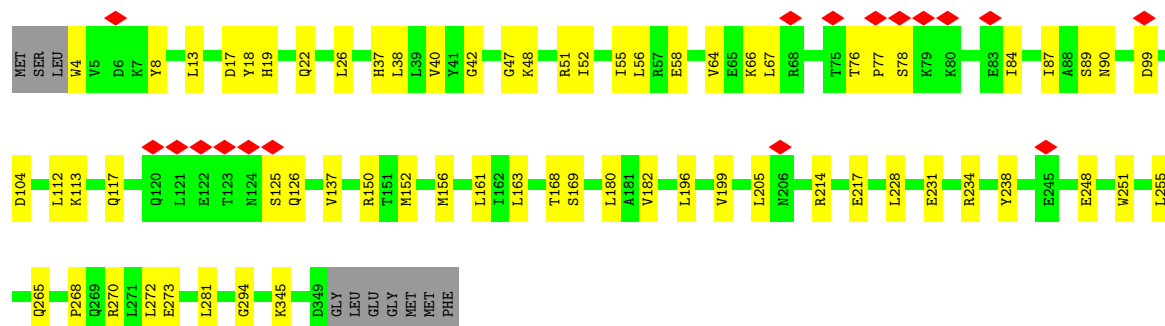
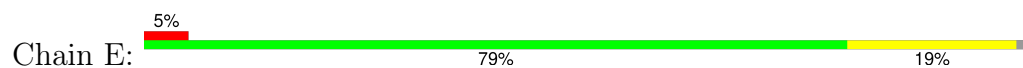
• Molecule 3: Replication factor C subunit 5



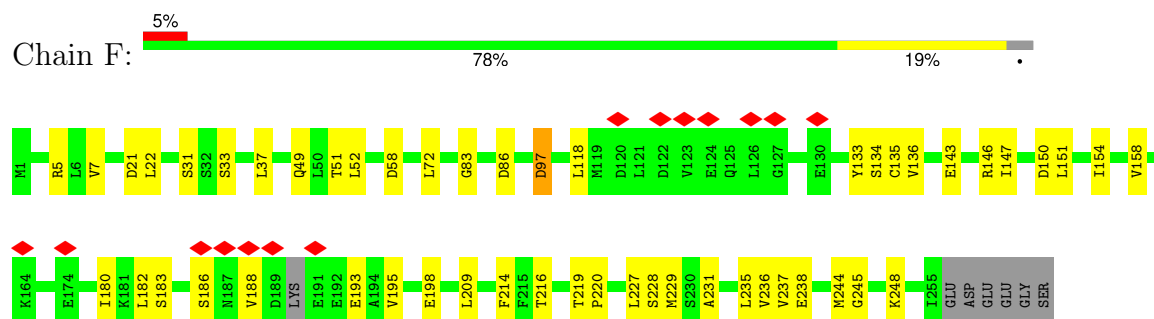
• Molecule 4: Replication factor C subunit 4



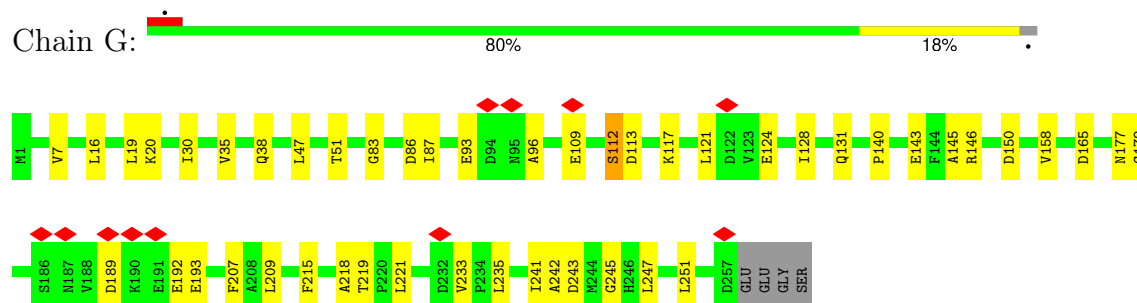
• Molecule 5: Replication factor C subunit 3



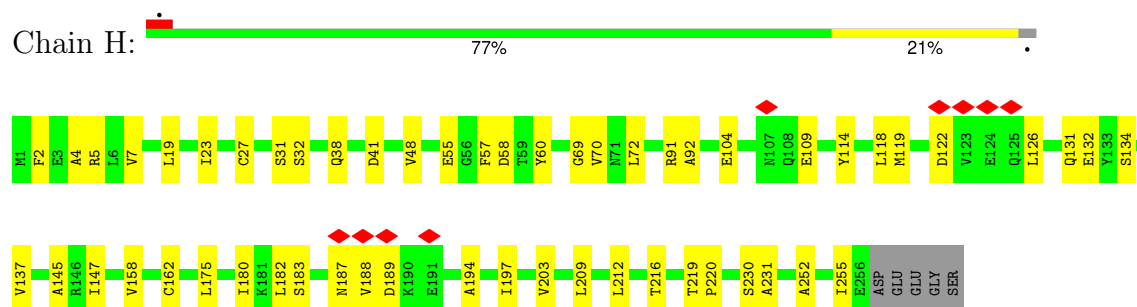
- Molecule 6: Proliferating cell nuclear antigen



- Molecule 6: Proliferating cell nuclear antigen



- Molecule 6: Proliferating cell nuclear antigen



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	193934	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.3, 45	Depositor
Minimum defocus (nm)	Not provided, Not provided	Depositor
Maximum defocus (nm)	Not provided, Not provided	Depositor
Magnification	Not provided, Not provided	Depositor
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.239	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.044	Depositor
Map size (Å)	254.4, 254.4, 254.4	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AGS, 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	0.39	0/3570	0.52	0/4814
2	B	0.42	0/2533	0.49	0/3421
3	C	0.39	0/2529	0.50	0/3422
4	D	0.36	0/2389	0.46	0/3219
5	E	0.39	0/2807	0.50	0/3790
6	F	0.40	0/1988	0.58	0/2686
6	G	0.48	0/2006	0.55	0/2710
6	H	0.47	0/2004	0.54	0/2707
All	All	0.41	0/19826	0.52	0/26769

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3500	0	3521	105	0
2	B	2492	0	2553	44	0
3	C	2486	0	2544	54	0
4	D	2361	0	2433	48	0
5	E	2759	0	2828	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1960	0	1965	38	0
6	G	1980	0	1981	29	0
6	H	1975	0	1982	38	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	31	0	12	2	0
8	B	31	0	12	3	0
8	C	31	0	12	2	0
8	D	31	0	12	6	0
9	E	27	0	12	1	0
All	All	19668	0	19867	377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (377) 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)
3:C:66:LYS:HG2	3:C:174:PHE:HD2	1.45	0.80
5:E:17:ASP:H	9:E:2000:ADP:HN62	1.29	0.78
4:D:239:ARG:HB2	8:D:402:AGS:H5'1	1.64	0.77
2:B:230:ARG:HD3	8:B:402:AGS:H5'1	1.67	0.77
1:A:1024:LEU:HA	1:A:1027:THR:HG22	1.68	0.73
1:A:752:CYS:SG	1:A:753:ASN:N	2.63	0.71
4:D:48:CYS:HB3	4:D:51:GLU:HB2	1.73	0.71
5:E:4:TRP:N	5:E:231:GLU:OE2	2.24	0.70
1:A:1021:VAL:HG11	1:A:1062:PHE:HE1	1.55	0.70
6:G:146:ARG:NH1	6:G:150:ASP:OD1	2.25	0.70
1:A:989:SER:O	1:A:995:ASN:ND2	2.25	0.70
4:D:78:GLY:O	4:D:181:ASN:ND2	2.23	0.69
1:A:1027:THR:HG23	1:A:1028:TYR:CD1	2.28	0.69
3:C:109:ALA:HB1	3:C:149:THR:HG21	1.74	0.69
6:G:93:GLU:HB2	6:G:96:ALA:HB2	1.73	0.69
2:B:71:ASN:HD22	2:B:167:PHE:H	1.39	0.69
4:D:110:ALA:HB2	4:D:149:LEU:HD12	1.75	0.68
1:A:601:GLN:HB2	1:A:606:SER:HB2	1.76	0.68
1:A:775:PRO:HG2	1:A:811:ILE:HD11	1.76	0.67
6:H:134:SER:H	6:H:230:SER:HB2	1.58	0.67
3:C:158:LEU:HD11	3:C:171:ARG:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:LEU:HD12	3:C:21:PRO:HD2	1.76	0.66
6:H:162:CYS:HB2	6:H:203:VAL:HG22	1.77	0.65
1:A:652:PRO:HG2	1:A:655:VAL:HG11	1.78	0.65
5:E:205:LEU:HG	5:E:238:TYR:HE1	1.60	0.65
2:B:63:PHE:HB3	2:B:69:VAL:HG12	1.77	0.65
3:C:179:PRO:O	3:C:183:VAL:HG23	1.97	0.64
6:F:7:VAL:HG23	6:F:58:ASP:HB2	1.79	0.64
5:E:265:GLN:HB2	5:E:270:ARG:HE	1.63	0.63
5:E:37:HIS:HE1	5:E:156:MET:HG2	1.63	0.63
3:C:219:ILE:O	3:C:223:THR:HG22	1.99	0.63
5:E:112:LEU:HD11	5:E:161:LEU:HD11	1.82	0.61
1:A:975:ILE:O	1:A:979:LEU:HD23	2.00	0.61
5:E:18:TYR:O	5:E:51:ARG:NH2	2.34	0.60
4:D:93:ARG:NH2	4:D:97:GLY:O	2.34	0.60
6:F:182:LEU:HD21	6:F:195:VAL:HG21	1.82	0.60
1:A:596:LYS:O	1:A:602:GLN:NE2	2.33	0.60
6:G:83:GLY:N	6:G:86:ASP:OD2	2.34	0.60
1:A:1032:LYS:HE2	1:A:1063:THR:HA	1.84	0.60
8:D:402:AGS:O2B	8:D:402:AGS:O3G	2.19	0.60
1:A:678:SER:O	2:B:121:LYS:NZ	2.32	0.60
6:F:228:SER:HB2	6:F:236:VAL:HG12	1.83	0.60
3:C:214:ARG:NH2	8:C:402:AGS:O2G	2.30	0.60
6:G:30:ILE:HG13	6:G:35:VAL:HG22	1.83	0.60
1:A:793:LEU:HD22	1:A:822:CYS:HB2	1.82	0.60
5:E:13:LEU:HD12	5:E:58:GLU:HG3	1.84	0.59
1:A:891:HIS:HE1	5:E:272:LEU:HD11	1.66	0.59
3:C:55:HIS:HD2	3:C:151:PHE:H	1.50	0.59
1:A:710:SER:OG	1:A:711:VAL:N	2.36	0.59
3:C:112:ARG:HE	6:H:255:ILE:HG22	1.67	0.59
5:E:89:SER:OG	5:E:90:ASN:N	2.36	0.59
1:A:893:LYS:O	1:A:951:GLY:HA3	2.03	0.58
4:D:84:LYS:HG2	4:D:199:PHE:HD2	1.67	0.58
4:D:207:GLN:HE22	4:D:238:LEU:HB2	1.68	0.58
6:H:187:ASN:ND2	6:H:189:ASP:OD2	2.35	0.58
6:G:165:ASP:OD1	6:G:165:ASP:N	2.37	0.58
1:A:586:TRP:CZ2	1:A:791:GLU:HG2	2.38	0.58
1:A:956:PHE:CD1	1:A:957:PRO:HD2	2.39	0.57
6:F:227:LEU:HG	6:F:237:VAL:HG12	1.87	0.57
6:H:2:PHE:HB3	6:H:92:ALA:HB3	1.85	0.57
3:C:39:ASP:OD1	3:C:39:ASP:N	2.34	0.57
3:C:214:ARG:HB2	8:C:402:AGS:H5'1	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:VAL:O	2:B:166:ARG:NH1	2.31	0.57
2:B:228:ASP:HB2	2:B:231:GLN:HB3	1.86	0.57
1:A:729:GLU:HG3	2:B:113:ILE:HB	1.86	0.57
4:D:173:THR:HG23	4:D:174:THR:HG23	1.86	0.57
6:H:5:ARG:NH2	6:H:104:GLU:OE1	2.38	0.56
1:A:1021:VAL:HG11	1:A:1062:PHE:CE1	2.40	0.56
6:H:38:GLN:HE21	6:H:126:LEU:HD23	1.71	0.56
6:H:131:GLN:NE2	6:H:132:GLU:O	2.38	0.56
6:F:136:VAL:HB	6:F:198:GLU:HB2	1.87	0.56
1:A:1025:MET:HG3	1:A:1030:LEU:O	2.05	0.56
4:D:234:SER:O	4:D:234:SER:OG	2.24	0.56
6:F:52:LEU:HD22	6:F:244:MET:HE2	1.87	0.56
6:G:51:THR:O	6:G:245:GLY:HA3	2.05	0.56
5:E:76:THR:HB	5:E:77:PRO:HD2	1.87	0.56
6:H:70:VAL:HG12	6:H:118:LEU:HD22	1.88	0.56
3:C:179:PRO:HB3	3:C:206:VAL:HG11	1.87	0.56
6:F:147:ILE:HD12	6:F:180:ILE:HG21	1.86	0.56
1:A:657:LYS:NZ	8:A:1202:AGS:S1G	2.66	0.56
1:A:959:PHE:CG	1:A:960:PRO:HD2	2.41	0.56
3:C:66:LYS:HG2	3:C:174:PHE:CD2	2.34	0.56
4:D:71:GLU:N	4:D:72:PRO:HD3	2.21	0.56
6:G:177:ASN:OD1	6:G:178:GLY:N	2.39	0.56
1:A:676:ASN:O	1:A:681:ARG:NH1	2.39	0.55
5:E:76:THR:C	5:E:78:SER:H	2.08	0.55
4:D:52:VAL:HG13	8:D:402:AGS:H2	1.88	0.55
2:B:118:ASN:O	2:B:122:MET:HG2	2.06	0.55
4:D:334:VAL:HG21	4:D:351:LEU:HB2	1.88	0.55
1:A:1044:TRP:HZ3	5:E:281:LEU:HD23	1.72	0.55
3:C:197:ILE:HA	3:C:230:VAL:HG23	1.88	0.55
1:A:675:LEU:O	1:A:681:ARG:NH1	2.39	0.55
1:A:908:LEU:HD11	5:E:268:PRO:HG3	1.89	0.55
1:A:1008:GLN:HA	1:A:1011:THR:HG22	1.89	0.55
4:D:304:THR:HG23	5:E:169:SER:HB2	1.89	0.55
3:C:21:PRO:HA	3:C:221:GLN:HE22	1.72	0.54
1:A:884:PHE:O	1:A:888:ASN:ND2	2.41	0.54
2:B:44:PRO:HG2	2:B:84:THR:HG21	1.90	0.54
2:B:94:LEU:HD13	2:B:101:ALA:HB3	1.89	0.54
1:A:988:TYR:CZ	1:A:990:SER:HA	2.41	0.54
3:C:114:ILE:HA	6:H:252:ALA:HB2	1.88	0.54
3:C:311:ARG:HD2	3:C:321:GLN:HE22	1.73	0.54
5:E:19:HIS:HB2	5:E:51:ARG:HH21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:GLN:O	1:A:1011:THR:HG22	2.08	0.54
2:B:343:ARG:O	2:B:347:LYS:HG2	2.08	0.54
4:D:203:SER:OG	4:D:206:ILE:HG12	2.08	0.54
4:D:41:VAL:O	8:D:402:AGS:O3'	2.25	0.54
5:E:38:LEU:HD23	5:E:180:LEU:HB3	1.90	0.53
4:D:119:VAL:O	4:D:123:VAL:HG23	2.09	0.53
5:E:125:SER:OG	5:E:126:GLN:N	2.42	0.53
5:E:205:LEU:HD21	5:E:234:ARG:HD2	1.89	0.53
2:B:247:ASN:OD1	2:B:250:ASN:HB2	2.08	0.53
1:A:977:GLN:HB2	1:A:991:LYS:HG2	1.89	0.53
4:D:77:TYR:HA	4:D:180:CYS:O	2.09	0.53
3:C:55:HIS:CD2	3:C:151:PHE:H	2.26	0.53
4:D:58:VAL:HG21	4:D:199:PHE:HE1	1.74	0.53
6:F:5:ARG:NH1	6:F:58:ASP:OD1	2.41	0.53
6:F:183:SER:OG	6:H:109:GLU:OE1	2.21	0.53
1:A:1008:GLN:HB3	1:A:1009:PRO:HD3	1.90	0.52
6:F:22:LEU:HD21	6:F:214:PHE:HB3	1.92	0.52
6:H:175:LEU:HD23	6:H:175:LEU:H	1.74	0.52
3:C:31:LEU:HG	3:C:41:LEU:HD12	1.91	0.52
1:A:894:PRO:HD2	1:A:904:HIS:ND1	2.25	0.52
1:A:676:ASN:CG	2:B:156:ARG:HG2	2.30	0.52
1:A:902:LYS:HD2	5:E:345:LYS:HG3	1.92	0.52
1:A:1006:LEU:O	1:A:1009:PRO:HD2	2.10	0.52
6:F:143:GLU:O	6:F:147:ILE:HG12	2.09	0.52
6:H:122:ASP:OD1	6:H:122:ASP:N	2.40	0.52
1:A:985:LEU:HG	1:A:1029:TYR:HE1	1.74	0.52
1:A:1032:LYS:HD2	1:A:1066:TYR:CD2	2.45	0.52
1:A:612:LEU:HD11	1:A:668:LEU:HD21	1.93	0.51
5:E:270:ARG:NH2	5:E:273:GLU:OE1	2.43	0.51
1:A:1039:MET:CE	1:A:1051:PHE:HB2	2.41	0.51
1:A:601:GLN:HB2	1:A:606:SER:CB	2.38	0.51
1:A:713:THR:HG23	1:A:714:LYS:HG3	1.90	0.51
1:A:676:ASN:ND2	2:B:156:ARG:HG2	2.25	0.51
1:A:721:GLU:HG2	2:B:155:ARG:NH2	2.26	0.51
1:A:754:ASP:OD1	1:A:754:ASP:N	2.43	0.51
4:D:84:LYS:HB2	8:D:402:AGS:O1B	2.10	0.51
2:B:77:PRO:HG2	2:B:80:THR:HG21	1.92	0.51
6:H:7:VAL:HG22	6:H:58:ASP:OD1	2.10	0.51
3:C:317:ASN:O	3:C:321:GLN:HG2	2.11	0.51
5:E:42:GLY:O	5:E:48:LYS:NZ	2.40	0.51
4:D:46:PRO:HB3	4:D:52:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018:VAL:O	1:A:1022:VAL:HG12	2.10	0.50
1:A:601:GLN:HE22	1:A:772:PHE:HE2	1.59	0.50
6:G:112:SER:HB3	6:H:180:ILE:HG12	1.94	0.50
2:B:333:SER:OG	3:C:309:GLU:OE2	2.20	0.50
3:C:258:ASP:HB3	3:C:261:THR:HG22	1.93	0.49
1:A:601:GLN:O	1:A:601:GLN:HG2	2.10	0.49
2:B:39:VAL:HG23	2:B:40:GLU:HG2	1.93	0.49
5:E:255:LEU:HD21	5:E:294:GLY:HA3	1.95	0.49
1:A:870:LYS:NZ	1:A:947:GLU:OE2	2.38	0.49
2:B:71:ASN:HA	2:B:167:PHE:O	2.12	0.49
2:B:78:PRO:HA	8:B:402:AGS:S1G	2.52	0.49
6:F:31:SER:OG	6:F:33:SER:OG	2.28	0.49
6:G:131:GLN:HE22	6:G:233:VAL:HG11	1.77	0.49
3:C:258:ASP:OD1	3:C:259:PHE:N	2.45	0.49
4:D:48:CYS:SG	4:D:49:VAL:N	2.84	0.49
6:F:97:ASP:OD2	6:F:97:ASP:N	2.45	0.49
1:A:613:ARG:O	1:A:617:ASN:ND2	2.45	0.49
6:F:228:SER:HB2	6:F:236:VAL:CG1	2.43	0.49
6:F:83:GLY:N	6:F:86:ASP:OD2	2.45	0.49
1:A:928:LYS:O	1:A:930:ASN:N	2.46	0.48
3:C:193:GLU:C	3:C:194:LYS:HD2	2.33	0.48
6:H:23:ILE:HG13	6:H:72:LEU:HD12	1.95	0.48
5:E:248:GLU:N	5:E:248:GLU:OE1	2.46	0.48
1:A:696:ASN:OD1	1:A:697:THR:N	2.46	0.48
6:F:51:THR:O	6:F:245:GLY:HA3	2.12	0.48
6:F:235:LEU:HD21	6:F:237:VAL:HG13	1.94	0.48
3:C:179:PRO:HA	3:C:182:MET:HG2	1.94	0.48
3:C:181:LEU:O	3:C:184:PRO:HD2	2.14	0.48
4:D:114:ARG:HH21	5:E:150:ARG:CZ	2.26	0.48
6:G:113:ASP:OD1	6:G:113:ASP:N	2.34	0.48
6:G:218:ALA:HB1	6:G:221:LEU:HD12	1.94	0.48
6:H:158:VAL:HG23	6:H:209:LEU:HD11	1.96	0.48
6:H:145:ALA:HB2	6:H:219:THR:HG21	1.95	0.48
1:A:1044:TRP:CH2	5:E:251:TRP:HB3	2.49	0.48
3:C:311:ARG:NH2	4:D:329:GLU:OE2	2.46	0.48
5:E:22:GLN:HE21	5:E:182:VAL:HG13	1.78	0.48
6:F:134:SER:O	6:F:134:SER:OG	2.27	0.48
1:A:600:GLY:H	8:A:1202:AGS:HN62	1.62	0.47
1:A:1002:LEU:O	1:A:1006:LEU:HG	2.14	0.47
6:F:135:CYS:SG	6:F:229:MET:HG2	2.53	0.47
6:F:146:ARG:NH1	6:F:150:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ARG:NE	1:A:769:ASP:OD2	2.41	0.47
6:F:216:THR:O	6:F:219:THR:OG1	2.23	0.47
3:C:59:TYR:HA	3:C:155:CYS:O	2.15	0.47
4:D:84:LYS:HD2	4:D:179:ILE:HG23	1.96	0.47
4:D:208:GLN:HE21	4:D:228:ALA:HA	1.79	0.47
6:F:238:GLU:HG3	6:F:248:LYS:HE2	1.96	0.47
1:A:985:LEU:H	1:A:985:LEU:HD12	1.80	0.47
6:F:154:ILE:HD11	6:H:114:TYR:CD2	2.49	0.47
6:H:31:SER:OG	6:H:32:SER:N	2.47	0.47
6:H:147:ILE:HD11	6:H:182:LEU:HD11	1.97	0.47
6:F:188:VAL:HG23	6:F:188:VAL:O	2.15	0.47
6:G:7:VAL:HA	6:G:87:ILE:HG23	1.97	0.47
6:G:38:GLN:HG3	6:G:47:LEU:HD11	1.97	0.47
3:C:105:ILE:HD11	3:C:124:LEU:HD21	1.96	0.46
3:C:113:THR:HG21	3:C:116:LYS:HE2	1.97	0.46
6:G:16:LEU:O	6:G:20:LYS:HB3	2.14	0.46
6:H:230:SER:OG	6:H:231:ALA:N	2.48	0.46
3:C:98:ILE:HG13	3:C:102:ARG:HH21	1.80	0.46
3:C:180:GLU:HG2	3:C:181:LEU:N	2.30	0.46
5:E:56:LEU:HB3	5:E:64:VAL:HG21	1.97	0.46
1:A:639:ASP:OD1	1:A:641:GLY:N	2.27	0.46
4:D:247:SER:O	4:D:251:LEU:HD23	2.14	0.46
6:H:2:PHE:HE1	6:H:60:TYR:HE1	1.62	0.46
1:A:922:ASP:O	1:A:926:ARG:HG2	2.16	0.46
6:H:55:GLU:OE1	6:H:55:GLU:N	2.47	0.46
2:B:229:MET:HG2	8:B:402:AGS:C4	2.45	0.46
6:F:97:ASP:HA	6:F:118:LEU:HD12	1.97	0.46
2:B:144:ASP:HB2	2:B:176:LYS:HB2	1.96	0.46
2:B:231:GLN:NE2	2:B:235:ASN:HD21	2.14	0.46
5:E:205:LEU:HG	5:E:238:TYR:CE1	2.46	0.46
1:A:999:LEU:HD21	1:A:1041:ILE:HG21	1.98	0.46
1:A:904:HIS:HE2	5:E:268:PRO:HG2	1.81	0.46
3:C:253:TRP:O	3:C:257:GLN:HB2	2.15	0.46
1:A:1047:LYS:HD3	1:A:1047:LYS:HA	1.69	0.45
2:B:152:GLN:OE1	2:B:155:ARG:NH1	2.45	0.45
3:C:37:HIS:HB2	3:C:41:LEU:HD23	1.98	0.45
6:F:37:LEU:O	6:F:49:GLN:HA	2.16	0.45
1:A:672:TYR:HA	1:A:716:ALA:O	2.15	0.45
5:E:196:LEU:HA	5:E:196:LEU:HD23	1.78	0.45
6:G:241:ILE:O	6:G:243:ASP:N	2.49	0.45
1:A:1052:SER:HA	1:A:1059:LYS:HZ3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:178:THR:OG1	3:C:180:GLU:OE1	2.21	0.45
4:D:84:LYS:HA	4:D:199:PHE:CE2	2.51	0.45
6:H:4:ALA:HB1	6:H:57:PHE:CD2	2.52	0.45
1:A:901:MET:HG3	1:A:905:LEU:HD23	1.98	0.45
2:B:54:GLU:O	2:B:58:SER:HB3	2.16	0.45
2:B:74:ILE:HD12	2:B:86:ILE:HG13	1.98	0.45
5:E:47:GLY:O	5:E:51:ARG:HD3	2.16	0.45
1:A:959:PHE:CD1	1:A:960:PRO:HD2	2.52	0.45
3:C:285:HIS:CE1	3:C:289:HIS:HD2	2.35	0.45
1:A:944:LEU:HB3	1:A:945:PRO:HD3	1.97	0.45
1:A:1056:PRO:N	1:A:1059:LYS:HE3	2.32	0.45
2:B:347:LYS:HA	2:B:347:LYS:HD2	1.83	0.45
2:B:126:GLN:O	2:B:136:LYS:NZ	2.46	0.45
1:A:973:ASP:OD1	1:A:991:LYS:HD3	2.17	0.45
3:C:279:ASP:O	3:C:283:GLU:HG2	2.16	0.45
4:D:63:LYS:HB2	4:D:64:LYS:NZ	2.32	0.45
1:A:914:SER:OG	1:A:940:TYR:O	2.33	0.45
2:B:202:LEU:HD22	2:B:236:LEU:HD22	1.99	0.45
4:D:46:PRO:HD2	4:D:86:SER:HB2	1.98	0.45
2:B:313:LYS:O	2:B:317:ILE:HG12	2.17	0.44
4:D:240:LYS:O	4:D:243:THR:HG22	2.17	0.44
6:H:2:PHE:O	6:H:91:ARG:HA	2.16	0.44
3:C:260:THR:OG1	4:D:324:LYS:NZ	2.37	0.44
6:G:192:GLU:HG3	6:G:193:GLU:CD	2.38	0.44
6:H:212:LEU:O	6:H:216:THR:HG23	2.17	0.44
3:C:53:LEU:HD11	3:C:56:LEU:HD11	1.99	0.44
6:F:135:CYS:HB3	6:F:229:MET:H	1.83	0.44
6:F:158:VAL:HB	6:F:209:LEU:HD21	1.99	0.44
6:G:109:GLU:HB3	6:H:183:SER:HB2	1.99	0.44
1:A:715:HIS:NE2	1:A:746:ILE:HG21	2.32	0.44
1:A:856:PHE:HE1	1:A:949:MET:HB2	1.81	0.44
1:A:1018:VAL:HA	1:A:1021:VAL:HG12	1.99	0.44
5:E:113:LYS:O	5:E:117:GLN:HG2	2.17	0.44
1:A:755:ARG:NH2	1:A:764:VAL:HG11	2.33	0.44
3:C:30:THR:HG23	3:C:33:ASP:H	1.83	0.44
6:F:193:GLU:OE1	6:F:193:GLU:HA	2.18	0.44
5:E:37:HIS:CD2	5:E:152:MET:HG3	2.53	0.44
6:G:145:ALA:HB2	6:G:219:THR:HG21	2.00	0.44
6:G:207:PHE:CZ	6:G:235:LEU:HB2	2.52	0.44
6:G:241:ILE:HG22	6:G:242:ALA:H	1.82	0.44
6:H:19:LEU:HD22	6:H:48:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001:LEU:HD13	5:E:228:LEU:HD22	1.99	0.44
1:A:811:ILE:HA	1:A:814:VAL:HG22	2.00	0.43
1:A:904:HIS:NE2	5:E:268:PRO:HG2	2.33	0.43
4:D:84:LYS:HG2	4:D:199:PHE:CD2	2.52	0.43
6:G:124:GLU:OE1	6:G:124:GLU:N	2.49	0.43
2:B:154:LEU:O	2:B:158:MET:HG3	2.17	0.43
3:C:71:LEU:HD23	3:C:71:LEU:HA	1.82	0.43
4:D:246:GLN:O	4:D:249:THR:HG22	2.19	0.43
2:B:94:LEU:HD12	2:B:98:LEU:HD12	2.00	0.43
2:B:258:PRO:HD3	2:B:290:TYR:CD1	2.52	0.43
3:C:26:TYR:CD2	3:C:189:VAL:HG22	2.54	0.43
3:C:204:ALA:HB2	3:C:232:GLU:HG2	2.00	0.43
6:H:7:VAL:HG22	6:H:58:ASP:CG	2.39	0.43
1:A:649:LEU:HD23	1:A:772:PHE:CE1	2.53	0.43
1:A:776:ARG:NE	1:A:778:GLU:OE2	2.46	0.43
2:B:205:VAL:HG21	2:B:233:LEU:HD21	2.01	0.43
4:D:71:GLU:N	4:D:71:GLU:OE1	2.52	0.43
1:A:797:PRO:N	1:A:798:PRO:HD2	2.33	0.43
4:D:63:LYS:HB2	4:D:64:LYS:HZ2	1.84	0.43
2:B:166:ARG:HA	2:B:166:ARG:HD3	1.65	0.43
4:D:38:VAL:HG22	4:D:39:PRO:HD2	1.99	0.43
4:D:238:LEU:HD23	8:D:402:AGS:C8	2.49	0.43
6:F:186:SER:O	6:F:188:VAL:HG13	2.19	0.43
6:H:216:THR:O	6:H:219:THR:HG23	2.18	0.43
1:A:1018:VAL:O	1:A:1021:VAL:HG12	2.19	0.42
4:D:202:LEU:HB2	4:D:207:GLN:OE1	2.19	0.42
5:E:37:HIS:CE1	5:E:156:MET:HG2	2.48	0.42
1:A:1053:LYS:HD2	1:A:1053:LYS:HA	1.76	0.42
6:G:19:LEU:HD21	6:G:247:LEU:HD11	2.00	0.42
3:C:205:LEU:HD21	3:C:220:LEU:HB2	2.01	0.42
5:E:104:ASP:OD2	5:E:104:ASP:N	2.42	0.42
6:F:133:TYR:CB	6:F:228:SER:HB3	2.49	0.42
1:A:1003:ARG:NH2	1:A:1004:ASP:OD1	2.50	0.42
4:D:62:LEU:HD23	4:D:62:LEU:HA	1.86	0.42
6:H:209:LEU:HD23	6:H:209:LEU:HA	1.71	0.42
6:H:23:ILE:HG22	6:H:41:ASP:HA	2.01	0.42
6:H:188:VAL:CG2	6:H:194:ALA:HB2	2.50	0.42
1:A:1031:MET:H	1:A:1034:ASP:HB2	1.85	0.42
2:B:126:GLN:NE2	6:G:117:LYS:HD3	2.35	0.42
6:H:137:VAL:HG22	6:H:197:ILE:HG12	2.01	0.42
1:A:914:SER:OG	1:A:944:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:MET:HE3	2:B:308:MET:HB2	1.93	0.42
3:C:26:TYR:O	3:C:185:ARG:NH2	2.31	0.42
5:E:40:VAL:HG11	5:E:52:ILE:HD11	2.02	0.42
1:A:1021:VAL:O	1:A:1025:MET:HB2	2.20	0.42
1:A:1044:TRP:CZ2	5:E:251:TRP:HB3	2.55	0.42
2:B:56:THR:HG23	2:B:188:LEU:HD13	2.01	0.42
6:G:140:PRO:HG2	6:G:143:GLU:HB2	2.02	0.42
1:A:755:ARG:NE	1:A:771:ARG:HH11	2.18	0.42
1:A:930:ASN:OD1	1:A:932:SER:OG	2.28	0.42
2:B:137:ILE:HA	2:B:166:ARG:O	2.19	0.42
3:C:48:ILE:HD13	3:C:48:ILE:HA	1.86	0.42
4:D:255:LYS:HG3	4:D:256:GLU:H	1.84	0.42
4:D:255:LYS:HG3	4:D:256:GLU:N	2.35	0.42
4:D:278:PHE:HD1	4:D:278:PHE:HA	1.70	0.42
5:E:66:LYS:H	5:E:66:LYS:HG2	1.68	0.42
3:C:55:HIS:HB2	3:C:169:CYS:HB3	2.00	0.42
3:C:223:THR:HG23	3:C:230:VAL:HG12	2.01	0.42
6:F:21:ASP:HB2	6:F:214:PHE:HE1	1.84	0.42
1:A:862:THR:HG23	1:A:863:ALA:H	1.85	0.41
1:A:1025:MET:HA	1:A:1030:LEU:HB2	2.02	0.41
6:F:21:ASP:N	6:F:21:ASP:OD1	2.42	0.41
6:F:72:LEU:HD23	6:F:72:LEU:HA	1.93	0.41
6:G:158:VAL:HG23	6:G:209:LEU:HD11	2.02	0.41
6:H:219:THR:N	6:H:220:PRO:HD2	2.34	0.41
1:A:1027:THR:HG23	1:A:1028:TYR:HD1	1.84	0.41
1:A:1037:ASN:O	1:A:1041:ILE:HB	2.19	0.41
5:E:67:LEU:HD13	5:E:87:ILE:HG23	2.02	0.41
5:E:137:VAL:HG21	5:E:163:LEU:HB3	2.01	0.41
3:C:127:ALA:HB1	3:C:153:LEU:HD23	2.03	0.41
6:H:69:GLY:O	6:H:119:MET:HG3	2.20	0.41
6:H:27:CYS:HA	6:H:69:GLY:HA2	2.02	0.41
2:B:159:GLU:OE1	2:B:184:ARG:NH2	2.54	0.41
6:G:215:PHE:CE2	6:G:251:LEU:HB2	2.56	0.41
3:C:163:PRO:HA	3:C:166:GLN:HG2	2.02	0.41
4:D:44:TYR:OH	4:D:218:GLU:OE2	2.37	0.41
2:B:143:ALA:HB1	2:B:169:LEU:HD23	2.03	0.41
2:B:305:THR:O	2:B:305:THR:OG1	2.37	0.41
1:A:1035:PHE:O	1:A:1039:MET:HG2	2.20	0.41
1:A:1049:SER:C	1:A:1051:PHE:H	2.25	0.41
2:B:300:PHE:HE1	2:B:304:LYS:HD3	1.84	0.41
4:D:38:VAL:CG2	4:D:39:PRO:HD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:LEU:HD13	5:E:55:ILE:HD11	2.02	0.41
6:F:151:LEU:HD23	6:F:151:LEU:HA	1.90	0.41
6:F:219:THR:N	6:F:220:PRO:HD2	2.36	0.41
1:A:760:ILE:O	1:A:764:VAL:HG23	2.21	0.41
4:D:123:VAL:HG11	4:D:176:PHE:HZ	1.86	0.41
5:E:84:ILE:HG22	5:E:99:ASP:OD2	2.20	0.41
1:A:877:ASP:O	1:A:879:SER:N	2.55	0.40
4:D:42:GLU:HA	4:D:45:ARG:HG3	2.04	0.40
4:D:210:ARG:O	4:D:214:ILE:HG12	2.22	0.40
1:A:1039:MET:HE2	1:A:1051:PHE:HB2	2.03	0.40
3:C:114:ILE:HG23	3:C:115:PHE:N	2.36	0.40
4:D:120:ARG:NH1	4:D:162:ALA:HB1	2.36	0.40
1:A:649:LEU:HD23	1:A:772:PHE:HE1	1.85	0.40
1:A:911:ALA:O	1:A:915:ILE:HG13	2.21	0.40
5:E:8:TYR:CD2	5:E:199:VAL:HG13	2.56	0.40
5:E:214:ARG:HA	5:E:217:GLU:HG3	2.03	0.40
6:G:121:LEU:HA	6:G:121:LEU:HD23	1.90	0.40
1:A:683:LYS:HG3	1:A:736:GLU:HB2	2.04	0.40
1:A:703:TYR:CG	6:G:128:ILE:HG22	2.56	0.40
1:A:1044:TRP:CZ3	5:E:281:LEU:HD23	2.53	0.40
1:A:681:ARG:HE	1:A:725:MET:HG2	1.87	0.40
2:B:206:ILE:O	2:B:210:ARG:N	2.47	0.40
3:C:88:LEU:HD23	3:C:122:VAL:HG13	2.04	0.40
3:C:198:SER:OG	3:C:199:GLU:N	2.55	0.40
3:C:209:SER:O	3:C:210:SER:OG	2.34	0.40
6:F:133:TYR:CG	6:F:228:SER:HB3	2.56	0.40
6:F:147:ILE:CD1	6:F:180:ILE:HG21	2.51	0.40
6:G:16:LEU:HD13	6:G:16:LEU:HA	1.88	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	438/595 (74%)	402 (92%)	36 (8%)	0	100	100
2	B	314/354 (89%)	301 (96%)	13 (4%)	0	100	100
3	C	308/340 (91%)	296 (96%)	12 (4%)	0	100	100
4	D	296/363 (82%)	286 (97%)	10 (3%)	0	100	100
5	E	344/356 (97%)	328 (95%)	15 (4%)	1 (0%)	37	66
6	F	251/261 (96%)	238 (95%)	12 (5%)	1 (0%)	30	60
6	G	255/261 (98%)	245 (96%)	9 (4%)	1 (0%)	30	60
6	H	255/261 (98%)	246 (96%)	9 (4%)	0	100	100
All	All	2461/2791 (88%)	2342 (95%)	116 (5%)	3 (0%)	50	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	231	ALA
6	G	189	ASP
5	E	168	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/512 (75%)	382 (99%)	4 (1%)	73	83
2	B	272/296 (92%)	272 (100%)	0	100	100
3	C	281/303 (93%)	281 (100%)	0	100	100
4	D	263/309 (85%)	263 (100%)	0	100	100
5	E	308/316 (98%)	308 (100%)	0	100	100
6	F	223/228 (98%)	222 (100%)	1 (0%)	89	93
6	G	225/228 (99%)	224 (100%)	1 (0%)	89	93
6	H	225/228 (99%)	225 (100%)	0	100	100
All	All	2183/2420 (90%)	2177 (100%)	6 (0%)	90	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	715	HIS
1	A	862	THR
1	A	979	LEU
1	A	1013	GLN
6	F	97	ASP
6	G	112	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	601	GLN
1	A	602	GLN
1	A	617	ASN
1	A	676	ASN
1	A	773	GLN
1	A	816	HIS
1	A	891	HIS
1	A	937	GLN
2	B	71	ASN
2	B	231	GLN
2	B	250	ASN
2	B	336	GLN
3	C	37	HIS
3	C	45	GLN
3	C	55	HIS
3	C	76	GLN
3	C	289	HIS
3	C	300	HIS
3	C	321	GLN
4	D	309	GLN
4	D	347	GLN
5	E	22	GLN
5	E	37	HIS
5	E	284	HIS
5	E	302	ASN
5	E	320	HIS
6	G	184	GLN
6	G	187	ASN
6	G	204	GLN
6	G	246	HIS
6	H	44	HIS

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Mol	Chain	Res	Type
6	H	187	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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$
8	AGS	A	1202	7	28,33,33	1.18	3 (10%)	31,52,52	1.03	2 (6%)
8	AGS	C	402	7	28,33,33	0.92	1 (3%)	31,52,52	1.10	2 (6%)
8	AGS	D	402	7	28,33,33	0.89	1 (3%)	31,52,52	1.20	3 (9%)
8	AGS	B	402	7	28,33,33	1.13	3 (10%)	31,52,52	1.06	2 (6%)
9	ADP	E	2000	-	24,29,29	0.87	0	29,45,45	1.42	3 (10%)

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
8	AGS	A	1202	7	-	4/17/38/38	0/3/3/3
8	AGS	C	402	7	-	2/17/38/38	0/3/3/3
8	AGS	D	402	7	-	1/17/38/38	0/3/3/3
8	AGS	B	402	7	-	6/17/38/38	0/3/3/3
9	ADP	E	2000	-	-	4/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1202	AGS	PB-O3A	-2.91	1.56	1.59
8	A	1202	AGS	PA-O3A	-2.80	1.56	1.59
8	B	402	AGS	PB-O3A	-2.66	1.56	1.59
8	B	402	AGS	PB-O3B	-2.59	1.56	1.59
8	A	1202	AGS	PB-O3B	-2.25	1.57	1.59
8	B	402	AGS	PA-O3A	-2.21	1.57	1.59
8	C	402	AGS	PB-O3B	-2.08	1.57	1.59
8	D	402	AGS	PG-S1G	2.00	1.95	1.90

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	402	AGS	PB-O3B-PG	-4.24	117.65	133.17
8	D	402	AGS	PB-O3B-PG	-4.13	118.06	133.17
9	E	2000	ADP	N3-C2-N1	-3.78	123.55	128.67
8	B	402	AGS	PB-O3B-PG	-3.62	119.93	133.17
8	A	1202	AGS	PB-O3B-PG	-3.32	121.00	133.17
9	E	2000	ADP	O4'-C1'-N9	3.18	112.96	108.75
9	E	2000	ADP	C4-C5-N7	-2.71	106.47	109.34
8	D	402	AGS	C5-C6-N6	2.32	123.84	120.31
8	C	402	AGS	C5-C6-N6	2.28	123.79	120.31
8	A	1202	AGS	C5-C6-N6	2.26	123.76	120.31
8	B	402	AGS	C5-C6-N6	2.20	123.66	120.31
8	D	402	AGS	C4'-O4'-C1'	2.17	111.91	109.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1202	AGS	PB-O3B-PG-O2G
8	A	1202	AGS	PB-O3B-PG-O3G
8	A	1202	AGS	C5'-O5'-PA-O1A

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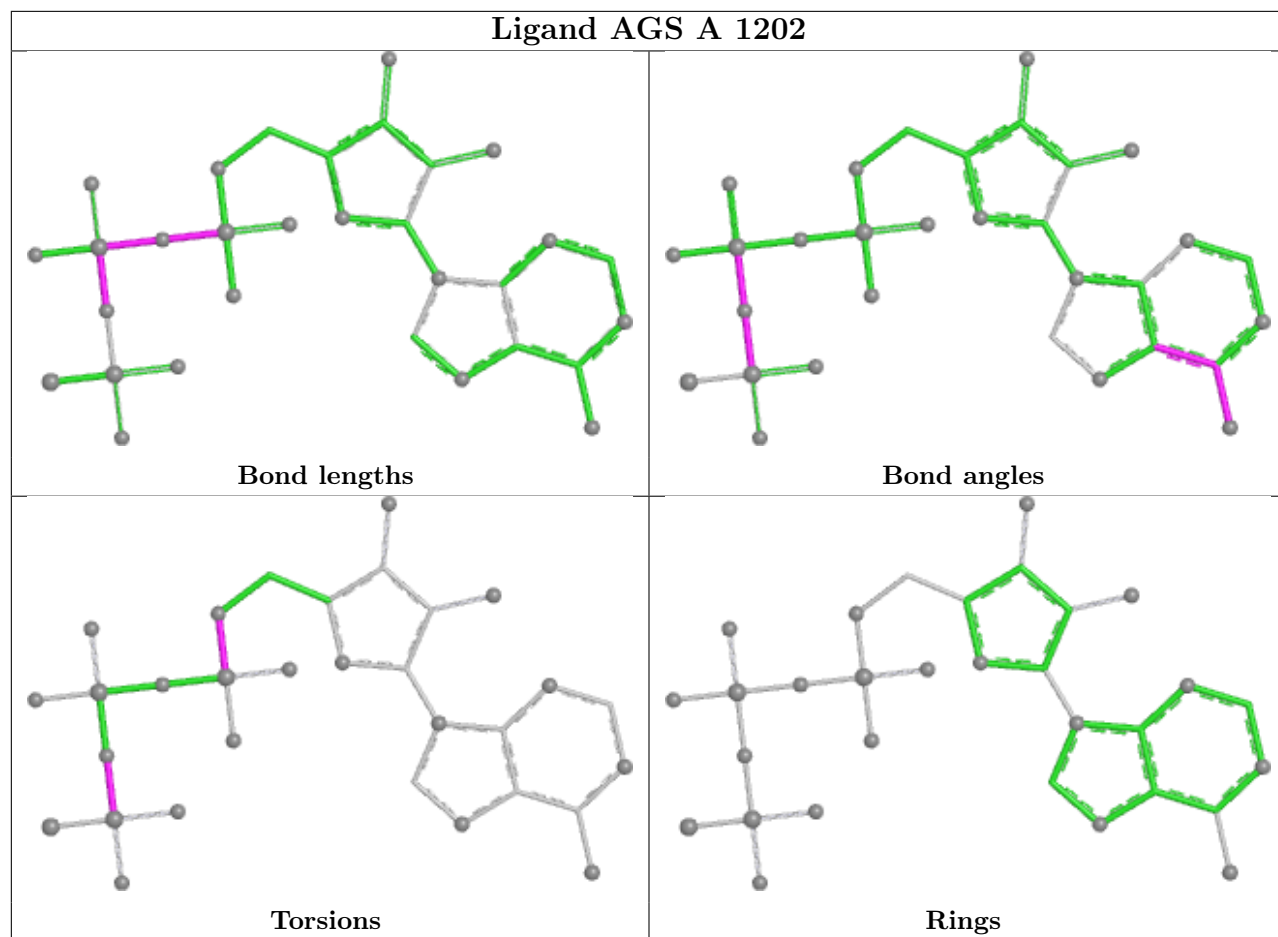
Mol	Chain	Res	Type	Atoms
8	B	402	AGS	C5'-O5'-PA-O1A
8	B	402	AGS	C5'-O5'-PA-O2A
8	B	402	AGS	C5'-O5'-PA-O3A
8	C	402	AGS	C5'-O5'-PA-O1A
9	E	2000	ADP	O4'-C4'-C5'-O5'
9	E	2000	ADP	C3'-C4'-C5'-O5'
8	B	402	AGS	PA-O3A-PB-O1B
9	E	2000	ADP	PB-O3A-PA-O1A
8	A	1202	AGS	C5'-O5'-PA-O3A
8	C	402	AGS	C5'-O5'-PA-O3A
8	B	402	AGS	PB-O3B-PG-O2G
8	B	402	AGS	PB-O3B-PG-O3G
8	D	402	AGS	PB-O3B-PG-O2G
9	E	2000	ADP	PB-O3A-PA-O2A

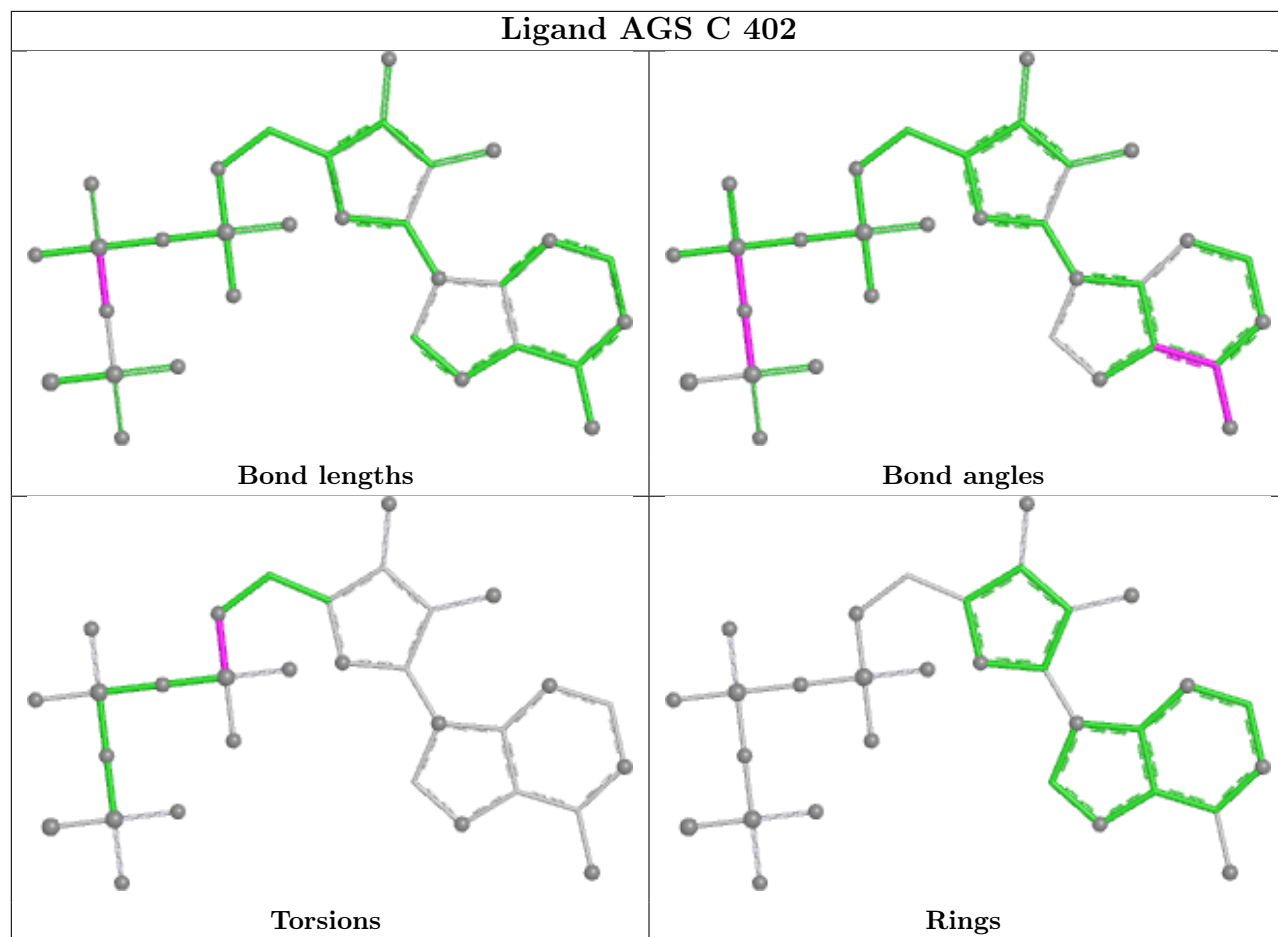
There are no ring outliers.

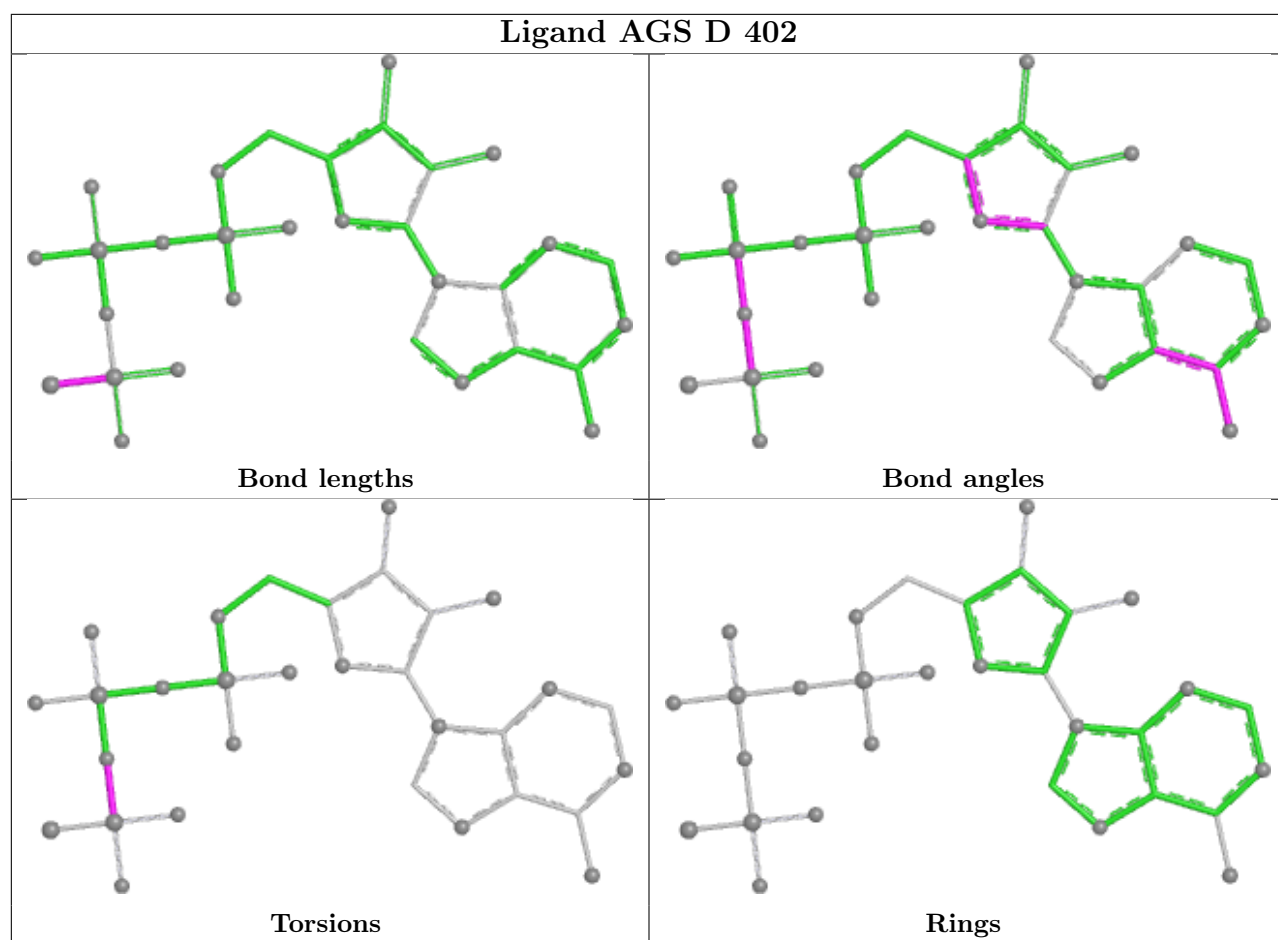
5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1202	AGS	2	0
8	C	402	AGS	2	0
8	D	402	AGS	6	0
8	B	402	AGS	3	0
9	E	2000	ADP	1	0

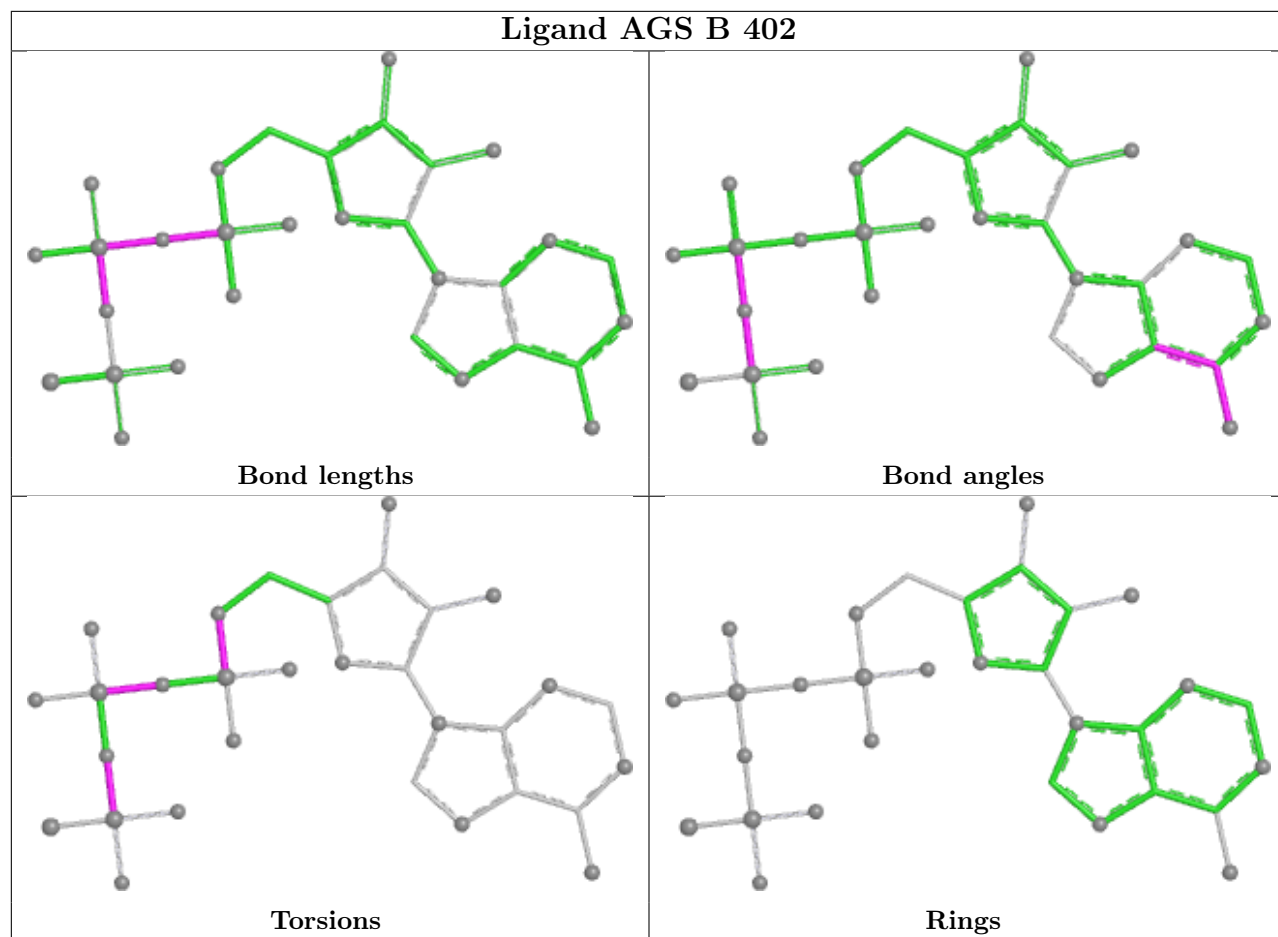
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



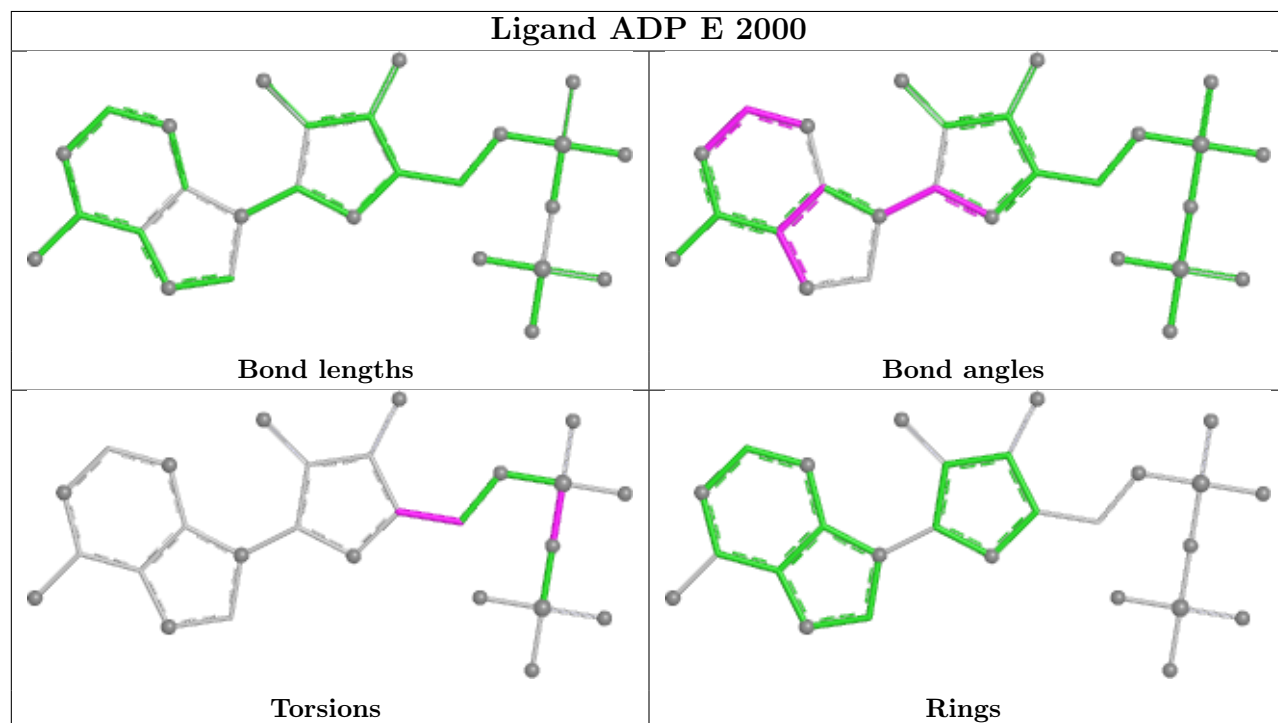




Ligand AGS B 402



Ligand ADP E 2000



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

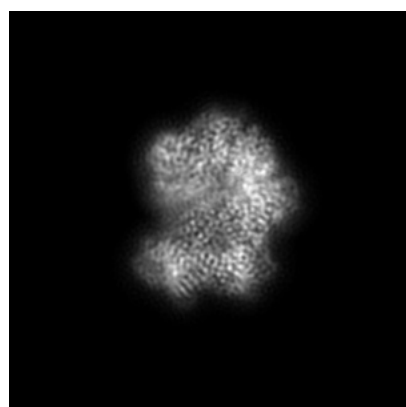
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21405. These allow visual inspection of the internal detail of the map and identification of artifacts.

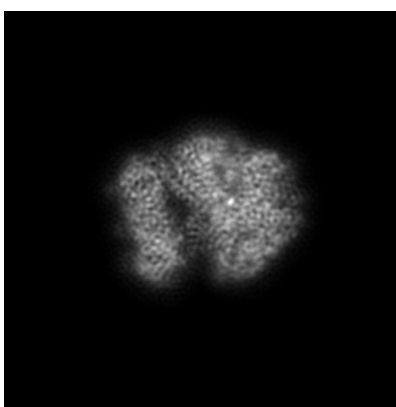
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

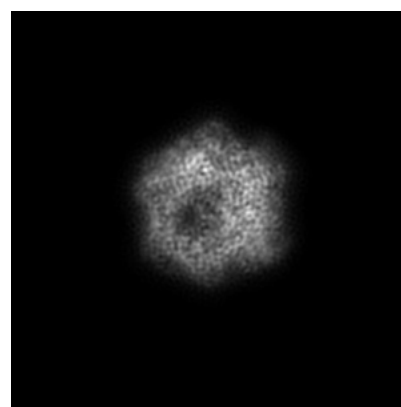
6.1.1 Primary map



X



Y

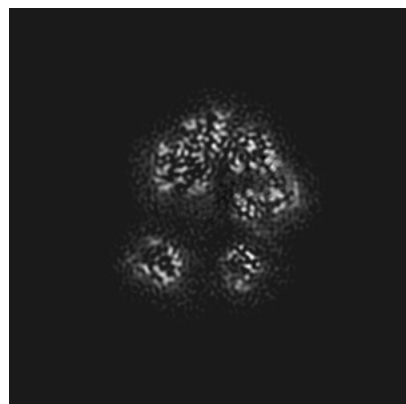


Z

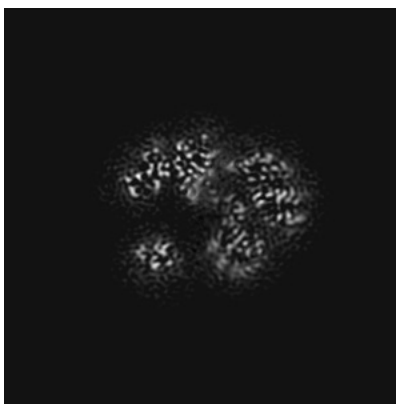
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

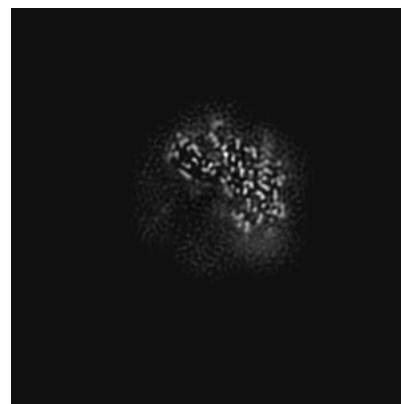
6.2.1 Primary map



X Index: 120



Y Index: 120

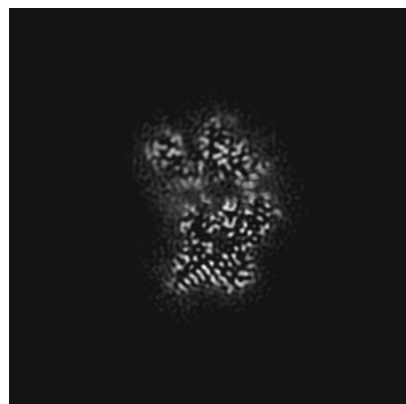


Z Index: 120

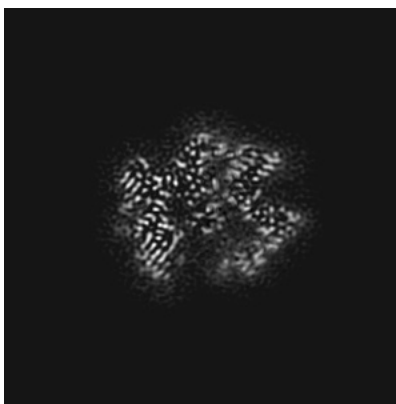
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

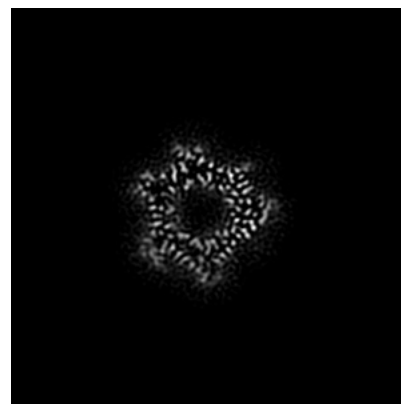
6.3.1 Primary map



X Index: 140



Y Index: 138

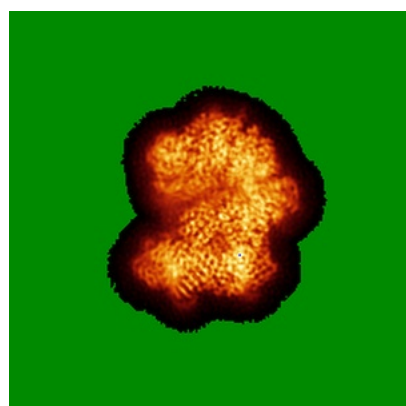


Z Index: 90

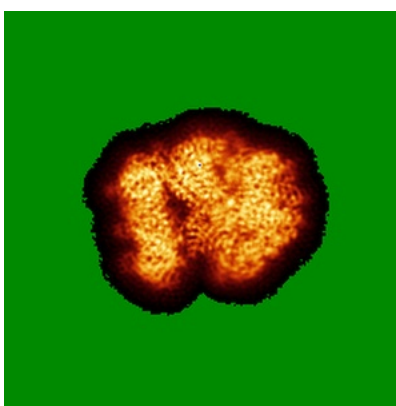
The images above show the largest variance slices of the map in three orthogonal directions.

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

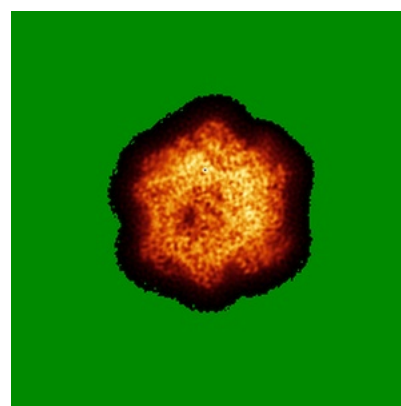
6.4.1 Primary map



X



Y

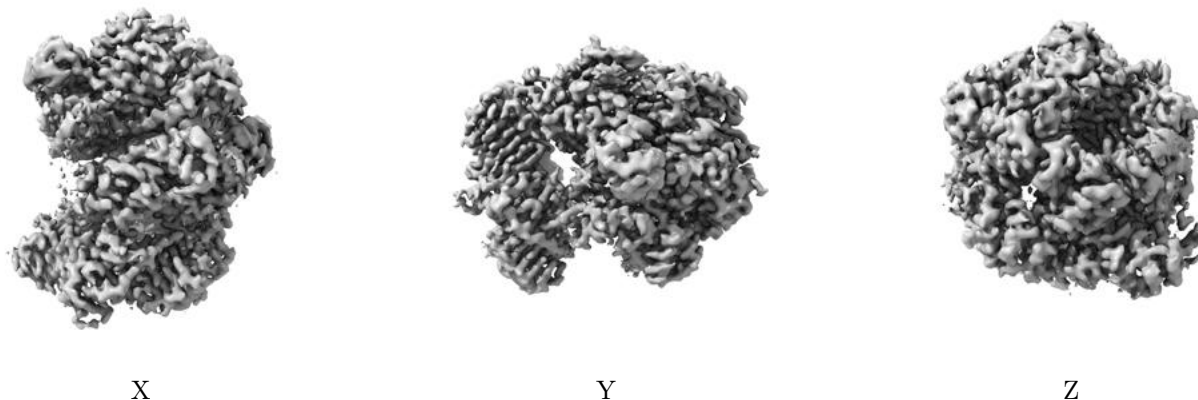


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.044. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

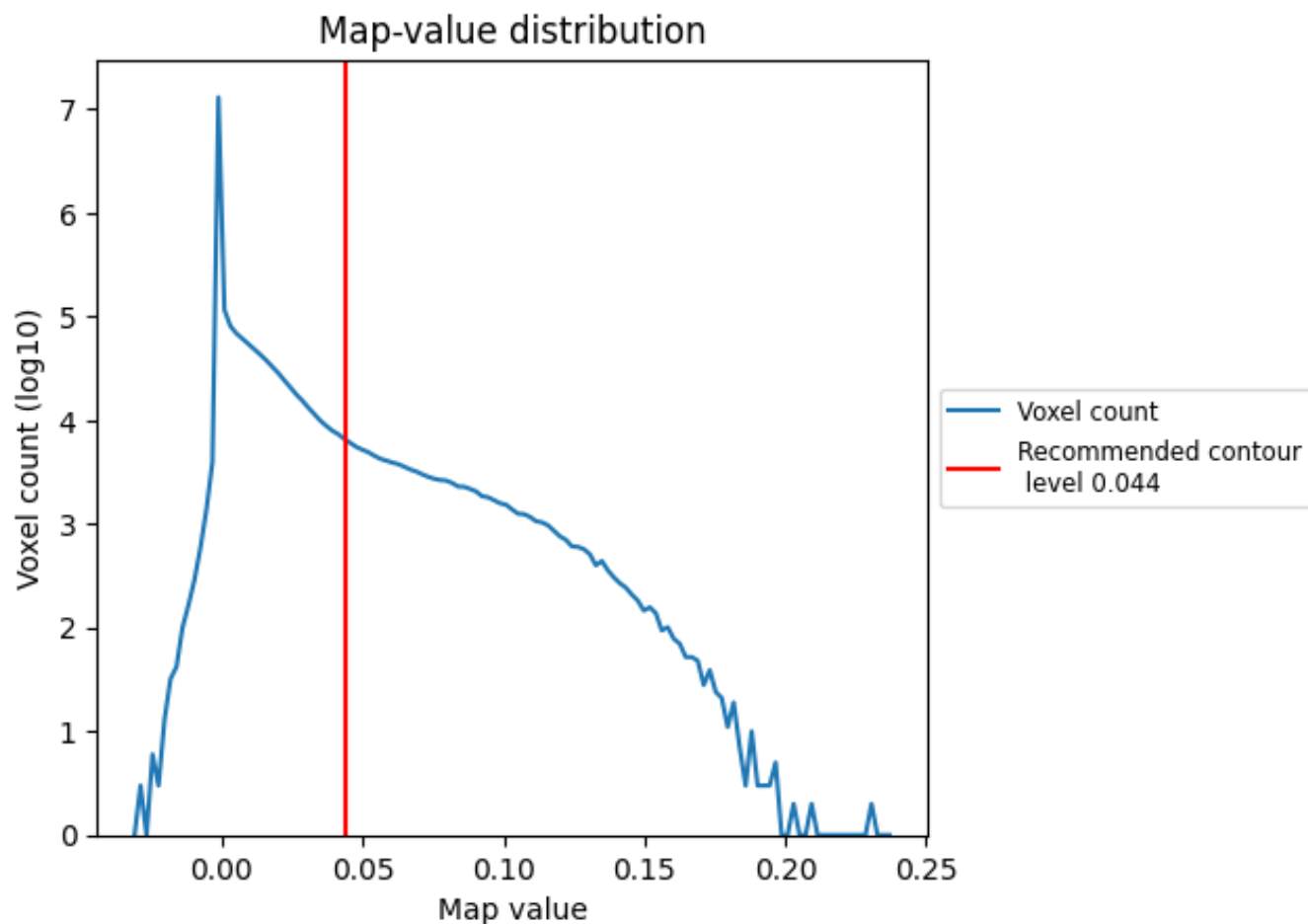
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

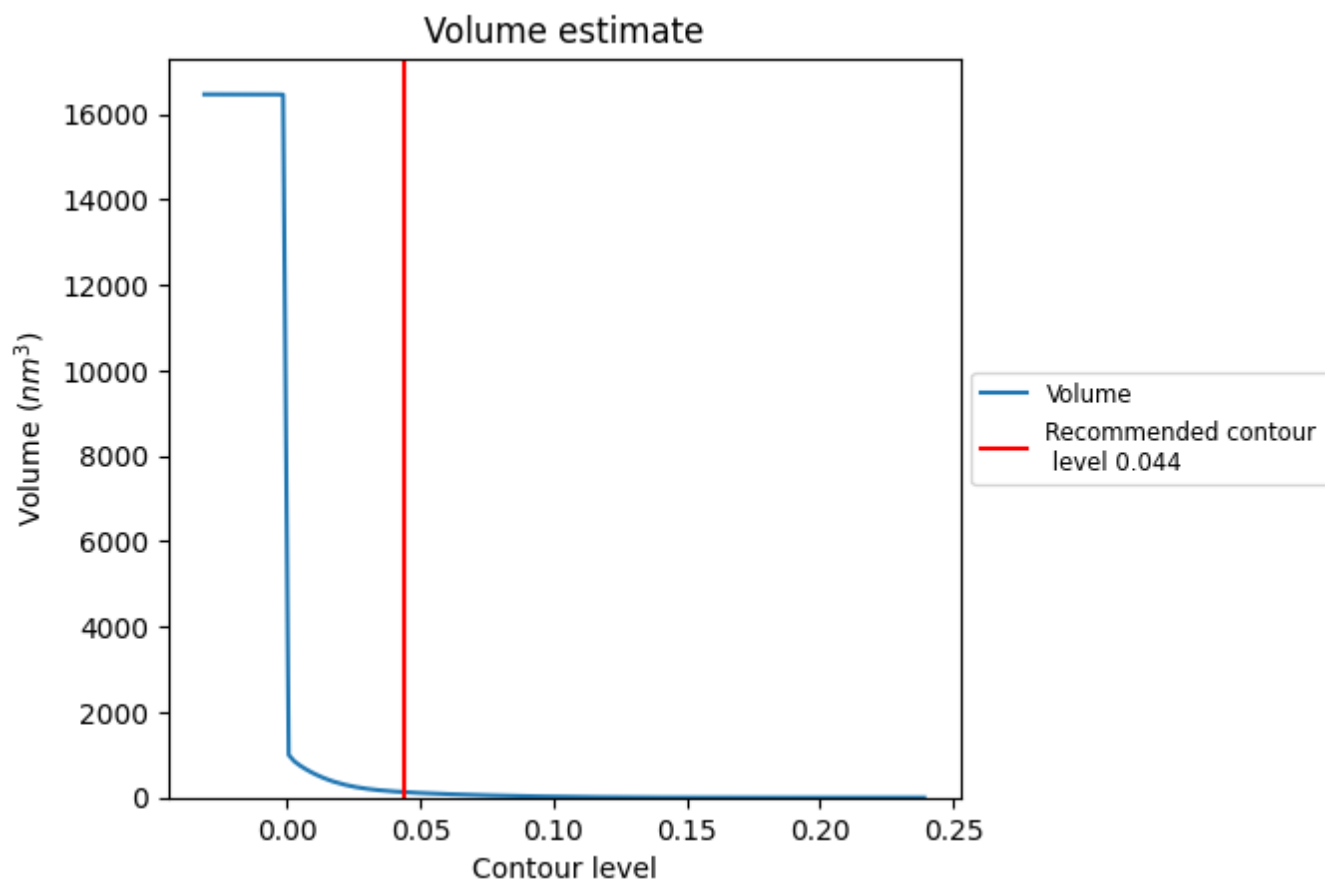
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

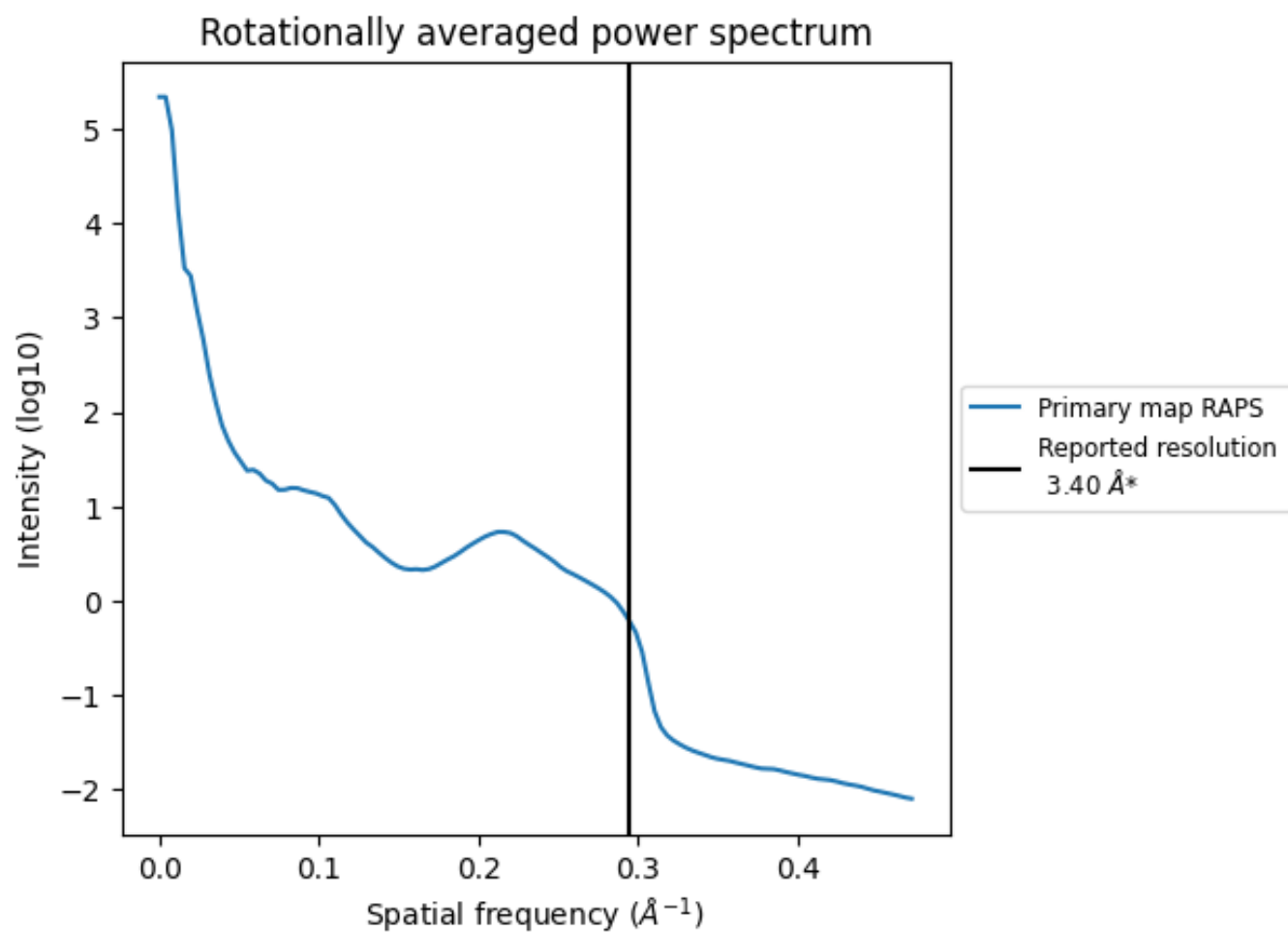
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 128 nm³; this corresponds to an approximate mass of 115 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 0.294 Å⁻¹

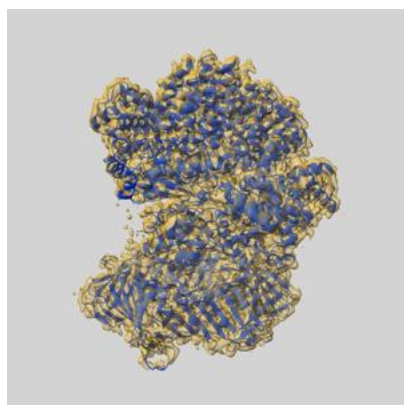
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

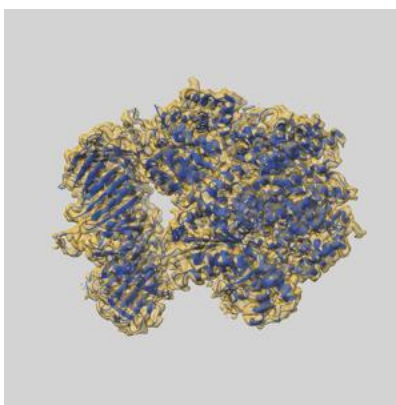
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21405 and PDB model 6VVO. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

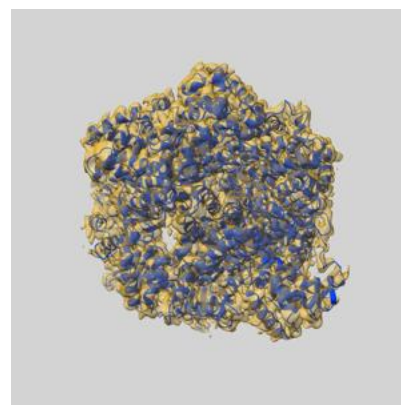
9.1 Map-model overlay [i](#)



X



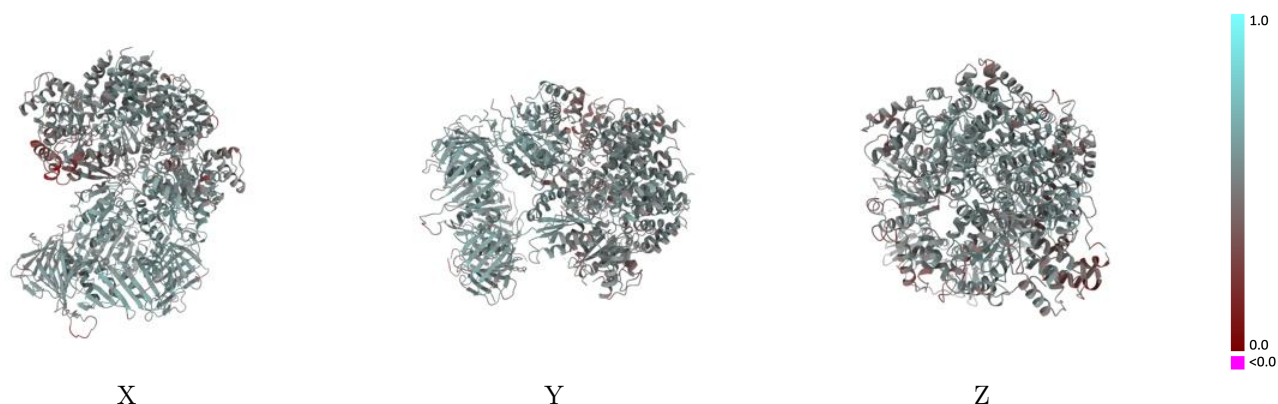
Y



Z

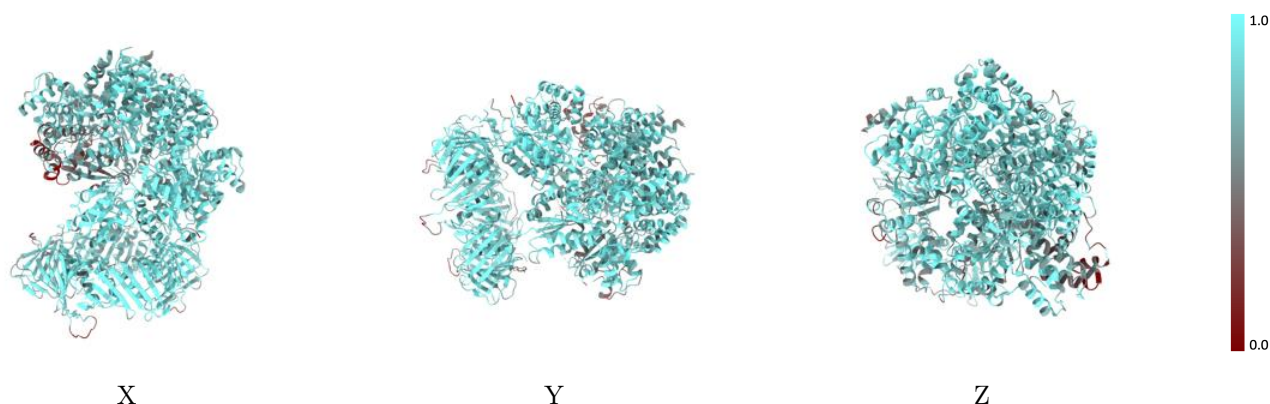
The images above show the 3D surface view of the map at the recommended contour level 0.044 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



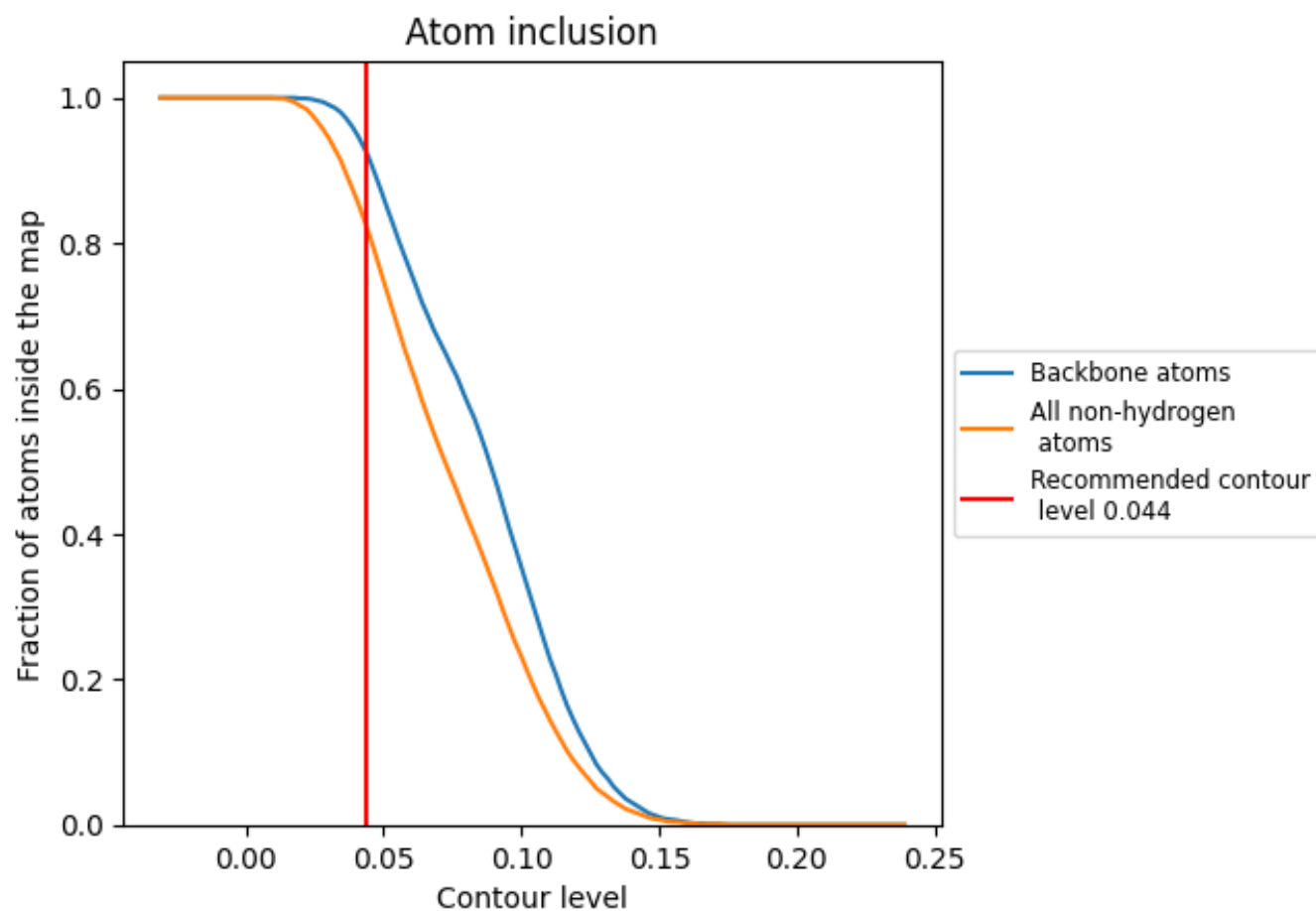
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.044).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.044) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8210	<div></div> 0.5150
A	<div></div> 0.7880	<div></div> 0.4940
B	<div></div> 0.9000	<div></div> 0.5330
C	<div></div> 0.8580	<div></div> 0.5220
D	<div></div> 0.7750	<div></div> 0.4900
E	<div></div> 0.7990	<div></div> 0.5080
F	<div></div> 0.7820	<div></div> 0.5040
G	<div></div> 0.8520	<div></div> 0.5520
H	<div></div> 0.8230	<div></div> 0.5360

