



Full wwPDB EM Validation Report ⓘ

May 7, 2026 – 04:31 PM JST

PDB ID : 9W1G / pdb_00009w1g
EMDB ID : EMD-65536
Title : The type III CRISPR-associated deaminase in complex cA6 and ATP, State 3
Authors : Li, Z.X.; Kong, J.P.; Wu, W.Q.
Deposited on : 2025-07-25
Resolution : 2.89 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:

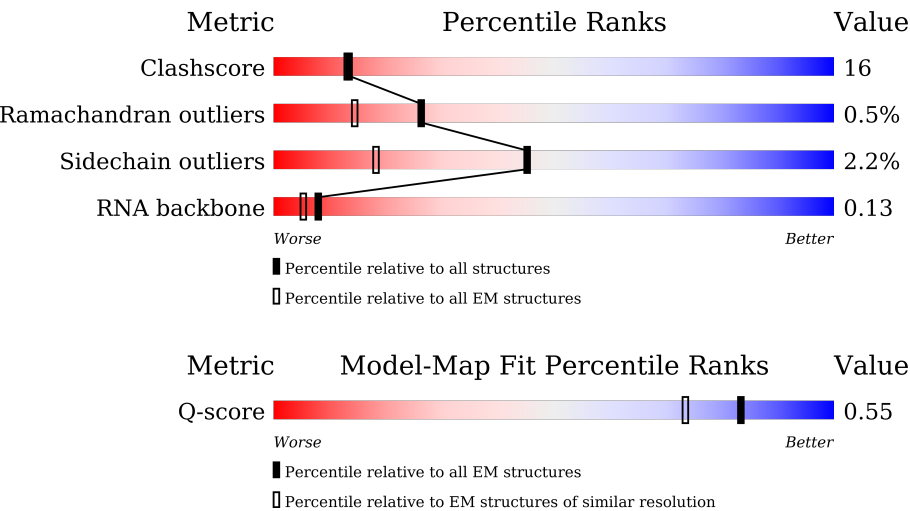
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.89 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	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 (2.39 - 3.39)

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	631	
1	B	631	
1	C	631	

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Mol	Chain	Length	Quality of chain
1	D	631	<div><div><div></div><div></div><div></div></div><div><div>42%</div><div>20%</div><div>38%</div></div></div>
1	E	631	<div><div><div></div><div></div><div></div></div><div><div>38%</div><div>23%</div><div>39%</div></div></div>
1	F	631	<div><div><div></div><div></div><div></div></div><div><div>37%</div><div>24%</div><div>38%</div></div></div>
2	J	6	<div><div><div></div><div></div></div><div><div>50%</div><div>50%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21788 atoms, of which 72 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 adenosine deaminase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	599	Total	C	N	O	S	0	0
			4690	2971	854	845	20		
1	B	589	Total	C	N	O	S	0	0
			4610	2925	841	824	20		
1	C	390	Total	C	N	O	S	0	0
			3027	1913	555	548	11		
1	D	391	Total	C	N	O	S	0	0
			3034	1917	556	550	11		
1	E	385	Total	C	N	O	S	0	0
			2995	1892	550	542	11		
1	F	390	Total	C	N	O	S	0	0
			3030	1915	555	549	11		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	626	HIS	-	expression tag	UNP A0A062XY19
A	627	HIS	-	expression tag	UNP A0A062XY19
A	628	HIS	-	expression tag	UNP A0A062XY19
A	629	HIS	-	expression tag	UNP A0A062XY19
A	630	HIS	-	expression tag	UNP A0A062XY19
A	631	HIS	-	expression tag	UNP A0A062XY19
B	626	HIS	-	expression tag	UNP A0A062XY19
B	627	HIS	-	expression tag	UNP A0A062XY19
B	628	HIS	-	expression tag	UNP A0A062XY19
B	629	HIS	-	expression tag	UNP A0A062XY19
B	630	HIS	-	expression tag	UNP A0A062XY19
B	631	HIS	-	expression tag	UNP A0A062XY19
C	626	HIS	-	expression tag	UNP A0A062XY19
C	627	HIS	-	expression tag	UNP A0A062XY19
C	628	HIS	-	expression tag	UNP A0A062XY19
C	629	HIS	-	expression tag	UNP A0A062XY19
C	630	HIS	-	expression tag	UNP A0A062XY19
C	631	HIS	-	expression tag	UNP A0A062XY19

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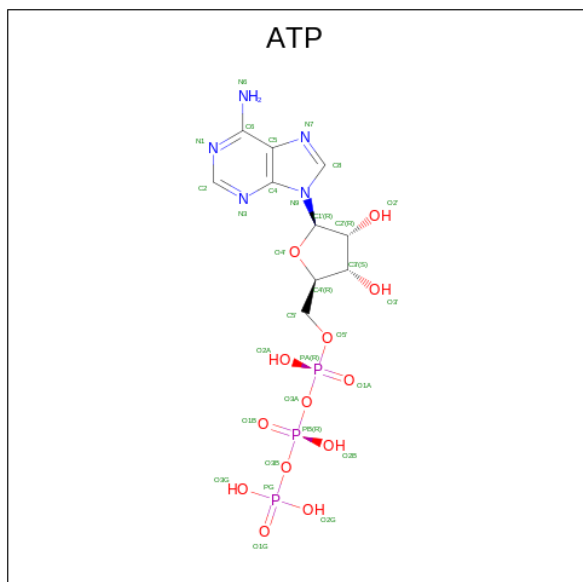
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Chain	Residue	Modelled	Actual	Comment	Reference
D	626	HIS	-	expression tag	UNP A0A062XY19
D	627	HIS	-	expression tag	UNP A0A062XY19
D	628	HIS	-	expression tag	UNP A0A062XY19
D	629	HIS	-	expression tag	UNP A0A062XY19
D	630	HIS	-	expression tag	UNP A0A062XY19
D	631	HIS	-	expression tag	UNP A0A062XY19
E	626	HIS	-	expression tag	UNP A0A062XY19
E	627	HIS	-	expression tag	UNP A0A062XY19
E	628	HIS	-	expression tag	UNP A0A062XY19
E	629	HIS	-	expression tag	UNP A0A062XY19
E	630	HIS	-	expression tag	UNP A0A062XY19
E	631	HIS	-	expression tag	UNP A0A062XY19
F	626	HIS	-	expression tag	UNP A0A062XY19
F	627	HIS	-	expression tag	UNP A0A062XY19
F	628	HIS	-	expression tag	UNP A0A062XY19
F	629	HIS	-	expression tag	UNP A0A062XY19
F	630	HIS	-	expression tag	UNP A0A062XY19
F	631	HIS	-	expression tag	UNP A0A062XY19

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms				AltConf	Trace
2	J	6	Total	C	N	O	P	
			132	60	30	36	6	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	C	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
3	F	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

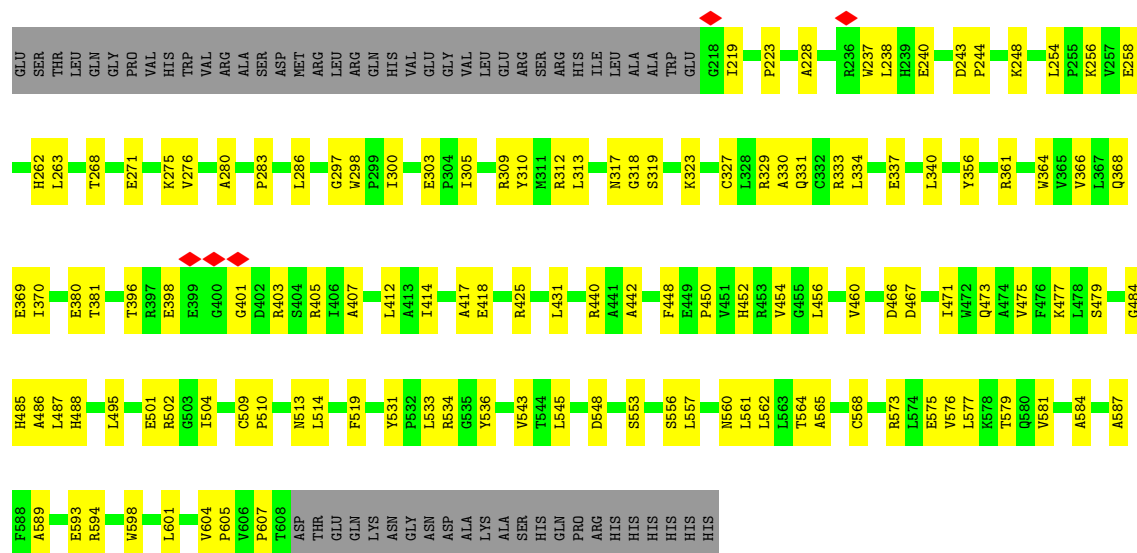
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

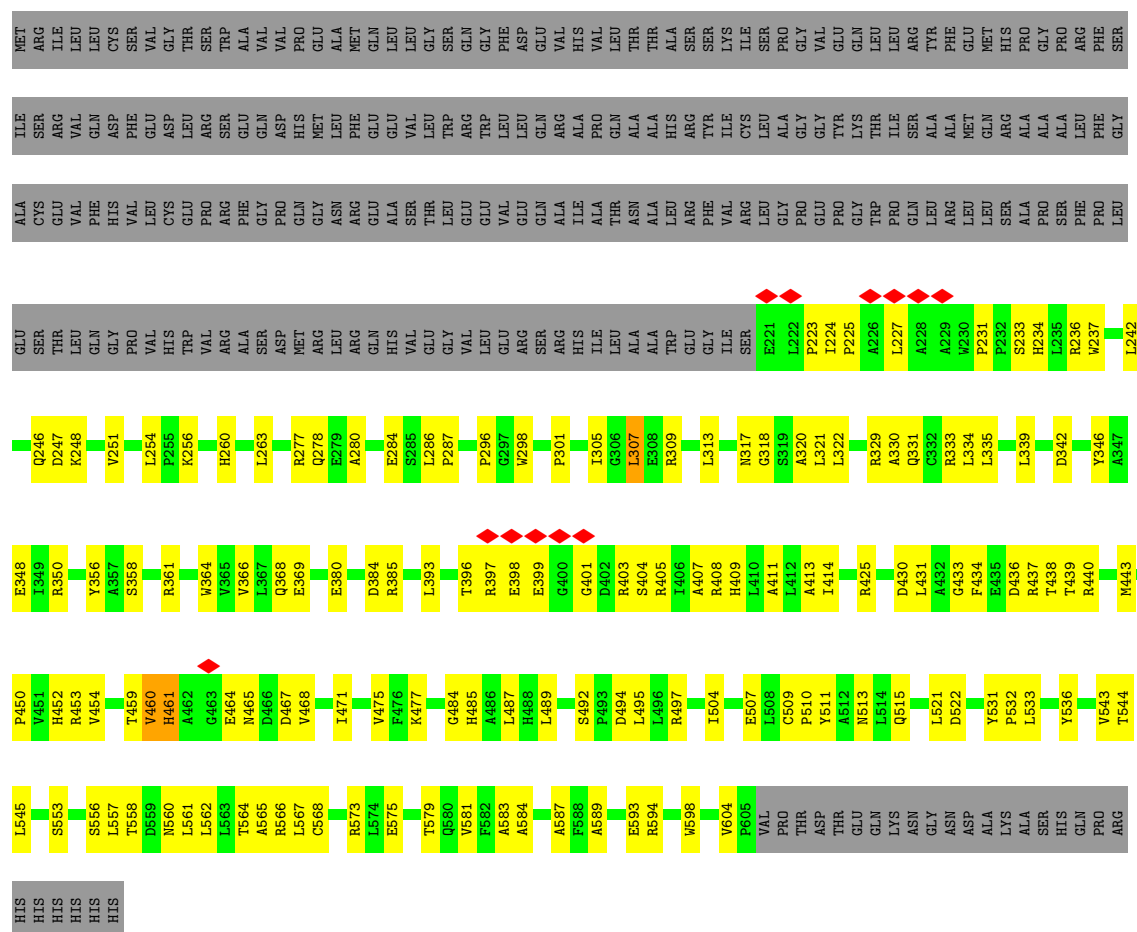
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Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	F	1	1	1	0

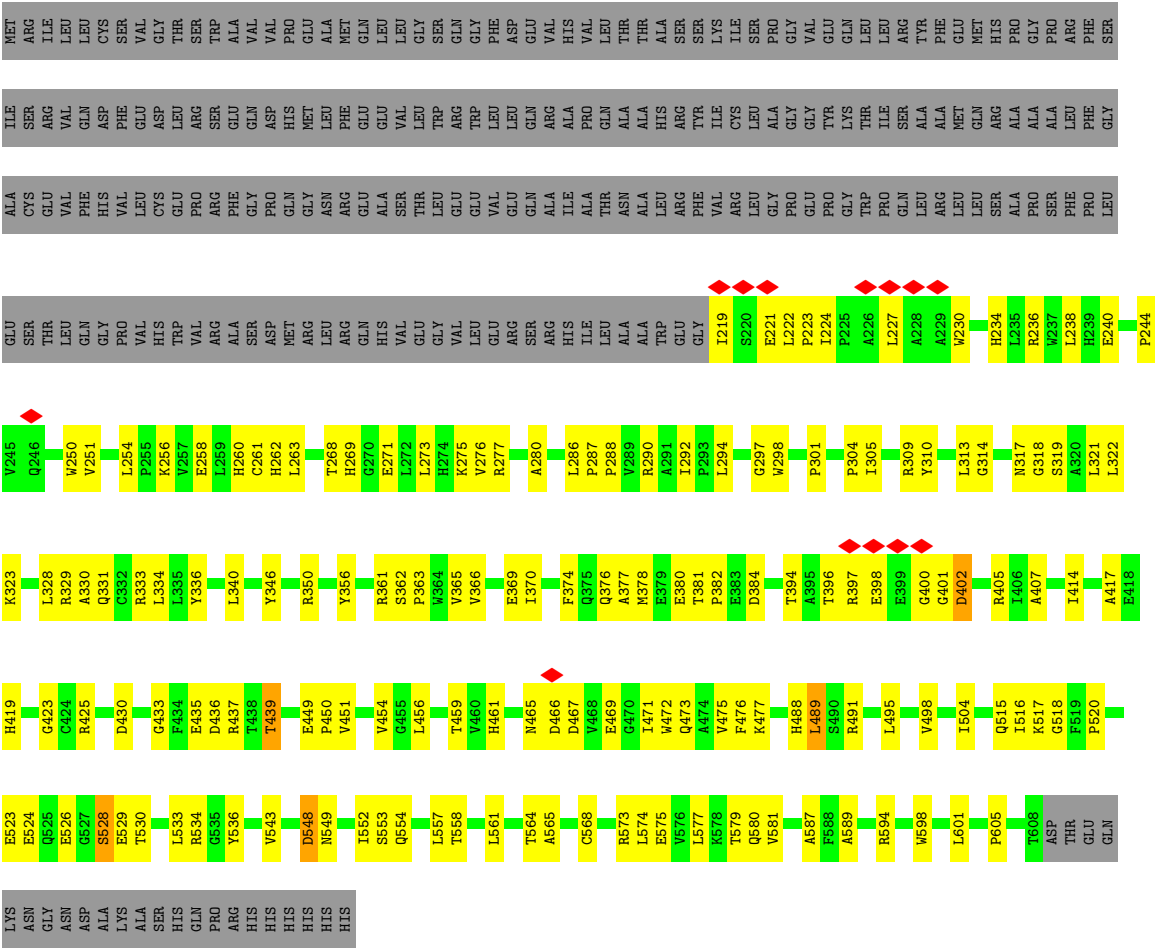


• Molecule 1: adenosine deaminase



• Molecule 1: adenosine deaminase





● Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*AP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105113	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.979	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	357.888, 357.888, 357.888	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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: ATP, 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	0.22	0/4808	0.36	1/6550 (0.0%)
1	B	0.24	0/4726	0.39	0/6439
1	C	0.24	0/3101	0.34	0/4231
1	D	0.23	0/3108	0.32	0/4241
1	E	0.21	0/3068	0.32	1/4185 (0.0%)
1	F	0.27	0/3104	0.37	0/4236
2	J	0.26	0/149	0.52	0/230
All	All	0.24	0/22064	0.35	2/30112 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	296	PRO	CB-CA-C	-6.46	104.52	111.56
1	A	219	ILE	N-CA-C	-6.12	106.26	113.42

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	4690	0	4655	155	0
1	B	4610	0	4593	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3027	0	3015	96	0
1	D	3034	0	3022	102	0
1	E	2995	0	2980	105	0
1	F	3030	0	3019	133	0
2	J	132	0	67	10	0
3	A	31	12	12	0	0
3	B	31	12	12	1	0
3	C	31	12	12	2	0
3	D	31	12	12	3	0
3	E	31	12	12	1	0
3	F	31	12	12	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	21716	72	21423	695	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 16.

All (695) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:LEU:HD23	1:C:565:ALA:HB2	1.43	1.00
1:E:307:LEU:HD12	1:E:464:GLU:HG3	1.44	0.98
1:A:3:ILE:HG23	1:A:29:GLU:HB3	1.46	0.96
1:A:469:GLU:HB2	1:E:401:GLY:HA3	1.48	0.96
1:C:414:ILE:HG23	1:C:454:VAL:HG21	1.47	0.94
1:D:414:ILE:HG23	1:D:454:VAL:HG21	1.51	0.93
1:A:200:GLN:HA	1:A:203:GLU:HB2	1.53	0.91
1:F:268:THR:HG22	1:F:317:ASN:HB3	1.52	0.90
1:C:533:LEU:CD2	1:C:564:THR:CG2	2.52	0.88
1:C:533:LEU:HD23	1:C:564:THR:CG2	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ALA:HB1	1:E:450:PRO:HB3	1.56	0.86
1:A:101:LEU:HD21	1:A:113:GLN:HB2	1.56	0.85
1:C:533:LEU:HD23	1:C:564:THR:HG23	1.59	0.84
1:C:219:ILE:HD11	1:C:228:ALA:HA	1.60	0.83
1:C:407:ALA:HB1	1:F:450:PRO:HB3	1.62	0.82
1:A:407:ALA:HB1	1:D:450:PRO:HB3	1.62	0.82
1:C:533:LEU:CD2	1:C:564:THR:HG21	2.11	0.80
1:A:242:LEU:HD23	1:A:565:ALA:HB2	1.64	0.79
1:B:99:ILE:HD12	1:B:116:ALA:HB2	1.65	0.79
1:C:417:ALA:HB2	1:C:456:LEU:HD21	1.65	0.78
1:B:469:GLU:HB2	1:D:401:GLY:HA3	1.64	0.77
1:E:544:THR:HG23	1:E:583:ALA:HB2	1.67	0.76
1:F:414:ILE:HG23	1:F:454:VAL:HG21	1.65	0.76
1:F:251:VAL:HG12	1:F:558:THR:HG23	1.69	0.74
1:A:432:ALA:HA	1:A:461:HIS:HB3	1.70	0.73
1:C:254:LEU:HD23	1:C:255:PRO:HD2	1.70	0.73
1:B:85:ARG:NH1	1:B:179:PRO:O	2.22	0.73
1:E:584:ALA:O	1:E:594:ARG:NH1	2.23	0.71
1:A:466:ASP:HB2	1:A:491:ARG:HH21	1.55	0.71
1:A:544:THR:HG23	1:A:583:ALA:HB2	1.72	0.71
1:B:106:LYS:HE2	2:J:2:A:H5"	1.71	0.71
1:B:2:ARG:NH1	1:B:26:GLY:O	2.23	0.71
1:A:397:ARG:HA	1:A:406:ILE:HD11	1.73	0.70
1:B:395:ALA:HB1	1:B:406:ILE:HG23	1.71	0.70
1:F:262:HIS:CD2	1:F:548:ASP:OD1	2.43	0.70
1:A:547:THR:HG23	1:A:557:LEU:HD13	1.74	0.69
1:F:361:ARG:NH2	1:F:369:GLU:OE1	2.25	0.69
1:B:450:PRO:HB3	1:E:407:ALA:HB1	1.73	0.69
1:B:34:THR:HG23	1:B:63:ARG:HG3	1.74	0.69
1:E:437:ARG:HH22	1:E:465:ASN:HB3	1.57	0.69
1:A:199:ARG:O	1:A:203:GLU:N	2.25	0.69
1:E:434:PHE:O	1:E:440:ARG:NH1	2.26	0.69
1:F:471:ILE:HB	1:F:495:LEU:HD21	1.74	0.69
1:F:298:TRP:CH2	1:F:305:ILE:HD13	2.28	0.68
1:B:39:LYS:HE3	2:J:4:A:H62	1.58	0.68
1:C:375:GLN:HE21	1:C:423:GLY:HA3	1.59	0.68
1:F:260:HIS:CD2	1:F:548:ASP:OD1	2.46	0.68
1:E:494:ASP:OD1	1:E:497:ARG:NH2	2.26	0.68
1:C:294:LEU:HD23	1:C:313:LEU:HD22	1.76	0.68
1:F:475:VAL:HG22	1:F:504:ILE:HD13	1.74	0.67
1:D:310:TYR:HH	1:D:553:SER:HG	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:CD2	1:C:564:THR:HG23	2.19	0.67
1:B:5:LEU:HD13	1:B:87:LEU:HD12	1.78	0.66
1:A:228:ALA:HB3	1:B:216:TRP:CH2	2.31	0.66
1:A:237:TRP:O	1:A:573:ARG:NH1	2.29	0.66
1:A:556:SER:O	1:A:560:ASN:ND2	2.28	0.65
1:A:263:LEU:O	1:A:331:GLN:NE2	2.29	0.65
1:A:5:LEU:HD11	1:A:97:ARG:HG3	1.78	0.65
1:C:450:PRO:HB3	1:F:407:ALA:HB1	1.79	0.65
1:D:254:LEU:O	1:D:256:LYS:NZ	2.26	0.65
1:F:244:PRO:HG3	1:F:565:ALA:HB3	1.79	0.65
1:D:466:ASP:OD2	1:D:488:HIS:ND1	2.28	0.65
1:D:244:PRO:HG3	1:D:565:ALA:HB3	1.78	0.64
1:A:251:VAL:HG12	1:A:558:THR:HG23	1.79	0.64
1:C:435:GLU:O	1:C:465:ASN:ND2	2.30	0.64
1:A:64:VAL:HG22	1:A:82:VAL:HG11	1.79	0.64
1:A:561:LEU:O	1:A:564:THR:OG1	2.15	0.64
1:B:587:ALA:O	1:B:594:ARG:NH2	2.31	0.64
1:A:74:GLN:HA	1:A:77:MET:HE2	1.79	0.64
1:B:296:PRO:HB2	1:B:302:GLU:OE2	1.98	0.64
1:A:240:GLU:HB2	1:A:573:ARG:HH12	1.63	0.63
1:A:450:PRO:HB3	1:D:407:ALA:HB1	1.78	0.63
1:E:587:ALA:O	1:E:594:ARG:NH2	2.30	0.63
1:D:333:ARG:NH2	1:D:380:GLU:OE1	2.31	0.63
1:A:174:SER:HB2	1:A:176:PRO:HD2	1.79	0.63
1:D:254:LEU:HD12	1:D:605:PRO:HD2	1.80	0.63
1:F:288:PRO:O	1:F:290:ARG:NH1	2.30	0.63
1:E:361:ARG:NH2	1:E:369:GLU:OE1	2.28	0.63
1:E:561:LEU:O	1:E:564:THR:OG1	2.15	0.62
1:F:322:LEU:HD22	1:F:328:LEU:HA	1.79	0.62
1:F:533:LEU:HD13	1:F:543:VAL:HG11	1.81	0.62
1:C:432:ALA:HA	1:C:461:HIS:HB2	1.80	0.62
1:C:481:ARG:HD3	1:D:502:ARG:HD2	1.82	0.62
1:E:589:ALA:HB1	1:E:593:GLU:HB2	1.81	0.62
1:A:254:LEU:O	1:A:256:LYS:NZ	2.28	0.62
1:B:375:GLN:O	1:B:379:GLU:HG2	2.00	0.62
1:E:277:ARG:NH2	1:E:287:PRO:O	2.30	0.61
1:E:509:CYS:O	1:E:513:ASN:ND2	2.31	0.61
1:A:15:VAL:HB	1:A:16:PRO:HD3	1.82	0.61
1:C:254:LEU:O	1:C:256:LYS:NZ	2.29	0.61
1:C:397:ARG:HB2	1:C:433:GLY:HA2	1.82	0.61
1:A:396:THR:HA	1:A:432:ALA:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:NH2	1:B:369:GLU:OE1	2.27	0.61
1:B:132:ARG:NH2	1:B:155:ALA:HB2	2.15	0.61
1:A:37:SER:HB3	1:A:40:ILE:HG12	1.83	0.61
1:C:262:HIS:CE1	1:C:548:ASP:OD1	2.54	0.61
1:A:1:MET:O	1:A:96:HIS:HB3	2.01	0.61
1:C:365:VAL:HG23	1:F:419:HIS:HE1	1.66	0.61
1:C:533:LEU:HD13	1:C:543:VAL:HG11	1.83	0.61
1:E:254:LEU:O	1:E:256:LYS:NZ	2.28	0.61
1:F:223:PRO:HG2	1:F:224:ILE:HD12	1.82	0.61
1:A:308:GLU:OE1	1:A:312:ARG:NH1	2.34	0.61
1:A:560:ASN:O	1:A:564:THR:HG23	2.01	0.60
1:B:298:TRP:CH2	1:B:305:ILE:HD13	2.35	0.60
1:E:333:ARG:NH2	1:E:380:GLU:OE1	2.33	0.60
1:D:364:TRP:NE1	1:D:368:GLN:OE1	2.34	0.60
1:F:397:ARG:HG3	1:F:400:GLY:N	2.16	0.60
1:F:313:LEU:HB2	1:F:552:ILE:HG23	1.84	0.60
1:D:219:ILE:HD11	1:D:228:ALA:HA	1.83	0.60
1:A:5:LEU:CD1	1:A:87:LEU:HD22	2.32	0.59
1:F:314:GLY:HA3	1:F:552:ILE:CD1	2.32	0.59
1:A:449:GLU:N	1:A:449:GLU:OE1	2.34	0.59
1:C:482:ARG:NE	1:C:507:GLU:OE2	2.34	0.59
1:A:5:LEU:HD13	1:A:87:LEU:HD22	1.84	0.59
1:E:533:LEU:HD13	1:E:543:VAL:HG11	1.84	0.59
1:A:356:TYR:HB2	1:A:366:VAL:HG11	1.84	0.59
1:B:16:PRO:HB2	1:B:147:VAL:HG11	1.84	0.59
1:F:301:PRO:HD3	1:F:515:GLN:HG2	1.84	0.59
1:F:401:GLY:H	1:F:439:THR:HB	1.68	0.59
1:B:482:ARG:NE	1:B:507:GLU:OE2	2.34	0.59
1:C:240:GLU:HB2	1:C:573:ARG:HH12	1.68	0.59
1:E:475:VAL:HG22	1:E:504:ILE:HD13	1.84	0.59
1:B:140:GLU:HB2	2:J:5:A:N6	2.17	0.59
1:D:263:LEU:O	1:D:331:GLN:NE2	2.35	0.59
1:C:556:SER:O	1:C:560:ASN:ND2	2.30	0.58
1:F:374:PHE:O	1:F:378:MET:HG3	2.02	0.58
1:E:256:LYS:HB3	1:E:557:LEU:HD23	1.85	0.58
1:F:309:ARG:O	1:F:313:LEU:HG	2.04	0.58
1:B:386:ARG:O	1:B:600:ARG:NH1	2.31	0.58
1:C:533:LEU:HD21	1:C:564:THR:HG21	1.84	0.58
1:E:364:TRP:NE1	1:E:368:GLN:OE1	2.37	0.58
1:B:87:LEU:HD11	1:B:99:ILE:HD11	1.86	0.58
1:B:254:LEU:HD12	1:B:605:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ARG:O	1:E:333:ARG:HG3	2.03	0.58
1:F:333:ARG:NH2	1:F:380:GLU:OE1	2.32	0.58
1:B:128:LEU:HD22	2:J:6:A:H5'	1.86	0.57
1:B:34:THR:OG1	1:B:40:ILE:HG21	2.05	0.57
1:E:531:TYR:HB3	1:E:568:CYS:SG	2.43	0.57
1:B:135:PRO:HD3	1:B:139:ARG:HH12	1.69	0.57
1:E:398:GLU:OE2	1:E:438:THR:HB	2.04	0.57
1:A:555:ALA:HB1	1:A:559:ASP:HB2	1.86	0.57
1:B:263:LEU:O	1:B:331:GLN:NE2	2.36	0.57
1:A:533:LEU:HB3	1:A:568:CYS:SG	2.45	0.57
1:B:177:SER:O	1:B:179:PRO:HD3	2.04	0.57
1:F:356:TYR:HB2	1:F:366:VAL:HG11	1.86	0.57
1:B:218:GLY:O	1:B:221:GLU:N	2.28	0.57
1:C:238:LEU:HD23	1:C:573:ARG:HB2	1.87	0.57
1:C:418:GLU:OE2	1:F:363:PRO:HD2	2.04	0.56
1:E:251:VAL:O	1:E:256:LYS:NZ	2.38	0.56
1:A:497:ARG:HG2	1:A:501:GLU:OE2	2.05	0.56
1:B:5:LEU:HD11	1:B:91:ALA:CB	2.35	0.56
1:B:374:PHE:O	1:B:378:MET:HG3	2.06	0.56
1:C:262:HIS:HE1	1:C:548:ASP:OD1	1.89	0.56
1:D:533:LEU:HB3	1:D:568:CYS:SG	2.45	0.56
1:B:531:TYR:HB3	1:B:568:CYS:SG	2.45	0.56
1:F:436:ASP:HB3	1:F:439:THR:CG2	2.35	0.56
1:A:432:ALA:HA	1:A:461:HIS:CB	2.35	0.56
1:B:91:ALA:HB1	1:B:97:ARG:HG2	1.86	0.56
1:B:50:TYR:HA	1:B:53:MET:HE2	1.86	0.56
1:B:407:ALA:CB	1:E:450:PRO:HB3	2.33	0.56
1:F:310:TYR:O	1:F:552:ILE:HG21	2.06	0.56
1:E:437:ARG:NH2	1:E:465:ASN:HB3	2.21	0.56
1:F:298:TRP:HZ3	1:F:301:PRO:HB3	1.70	0.56
1:A:6:CYS:O	1:A:32:VAL:HA	2.06	0.56
1:B:53:MET:HE1	1:B:144:LEU:HD22	1.88	0.55
1:C:333:ARG:O	1:C:337:GLU:HG2	2.05	0.55
1:F:516:ILE:HG22	1:F:517:LYS:HD2	1.87	0.55
1:A:93:GLN:HB2	1:A:96:HIS:CE1	2.40	0.55
1:A:29:GLU:HG2	1:A:31:HIS:CE1	2.41	0.55
1:A:31:HIS:CD2	1:A:90:ARG:HB3	2.42	0.55
1:A:471:ILE:HB	1:A:495:LEU:HD21	1.87	0.55
1:E:223:PRO:HB2	1:E:581:VAL:HG21	1.88	0.55
1:B:533:LEU:HD13	1:B:543:VAL:HG11	1.88	0.55
1:D:487:LEU:HD13	1:D:519:PHE:HZ	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:LEU:HD22	1:E:443:MET:HE2	1.88	0.55
1:F:319:SER:O	1:F:323:LYS:HG3	2.05	0.55
1:A:81:GLU:HG2	1:A:85:ARG:HE	1.72	0.55
1:B:101:LEU:HD21	1:B:124:VAL:HG12	1.88	0.55
1:C:418:GLU:OE2	1:F:362:SER:HB2	2.06	0.55
1:B:88:LEU:O	1:B:175:ALA:HB2	2.07	0.55
1:C:255:PRO:HB2	1:C:601:LEU:HD23	1.89	0.55
1:A:6:CYS:SG	1:A:15:VAL:HG22	2.47	0.55
1:A:99:ILE:HD12	1:A:116:ALA:HB2	1.87	0.55
1:B:173:LEU:HD21	1:B:201:HIS:CD2	2.41	0.55
1:A:482:ARG:NE	1:A:507:GLU:OE2	2.34	0.55
1:B:135:PRO:HG2	1:B:136:GLN:HG3	1.89	0.55
1:B:130:GLU:HG2	1:B:155:ALA:O	2.07	0.55
1:D:303:GLU:N	1:D:303:GLU:OE1	2.40	0.55
1:F:553:SER:O	1:F:554:GLN:C	2.50	0.55
1:C:402:ASP:O	1:C:406:ILE:HG22	2.07	0.54
1:A:53:MET:O	1:A:55:PRO:HD3	2.07	0.54
1:A:105:TYR:HD1	2:J:6:A:H5''	1.72	0.54
1:A:565:ALA:HA	1:A:571:ILE:CG2	2.38	0.54
1:E:522:ASP:OD1	1:E:566:ARG:NE	2.27	0.54
1:A:41:SER:HB2	1:A:42:PRO:HD3	1.89	0.54
1:B:41:SER:OG	1:B:63:ARG:NH2	2.36	0.54
1:B:297:GLY:O	1:B:298:TRP:C	2.50	0.54
1:B:477:LYS:HA	1:B:477:LYS:HE2	1.90	0.54
1:F:280:ALA:HB2	1:F:286:LEU:HD21	1.89	0.54
1:A:34:THR:OG1	1:A:35:THR:N	2.40	0.54
1:F:467:ASP:OD1	1:F:467:ASP:N	2.40	0.54
1:B:170:LEU:HD13	1:B:202:VAL:HG13	1.89	0.54
1:A:584:ALA:O	1:A:594:ARG:NH1	2.41	0.54
2:J:5:A:HO2'	2:J:6:A:P	2.30	0.54
1:A:5:LEU:HD11	1:A:97:ARG:CG	2.37	0.54
1:E:356:TYR:HB2	1:E:366:VAL:HG11	1.89	0.54
1:A:545:LEU:HD13	1:A:564:THR:HG21	1.89	0.53
1:B:453:ARG:NH1	1:E:403:ARG:HB2	2.23	0.53
1:C:577:LEU:O	1:C:581:VAL:HG23	2.08	0.53
1:F:489:LEU:HB2	1:F:536:TYR:OH	2.08	0.53
1:F:417:ALA:HB2	1:F:456:LEU:HD21	1.90	0.53
1:C:558:THR:O	1:C:562:LEU:HG	2.08	0.53
1:D:361:ARG:NH2	1:D:369:GLU:OE2	2.41	0.53
1:E:575:GLU:O	1:E:579:THR:HG23	2.09	0.53
1:F:423:GLY:O	1:F:425:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ARG:O	1:C:333:ARG:HG3	2.08	0.53
1:C:430:ASP:HA	1:C:459:THR:HG23	1.90	0.53
1:C:300:ILE:HG23	1:C:514:LEU:HD21	1.90	0.53
1:C:589:ALA:HB1	1:C:593:GLU:HB2	1.91	0.53
1:F:310:TYR:OH	1:F:553:SER:HB2	2.08	0.53
1:F:581:VAL:HG13	1:F:598:TRP:CH2	2.44	0.53
1:F:589:ALA:O	1:F:594:ARG:NH1	2.36	0.53
1:D:396:THR:HB	1:D:405:ARG:HH21	1.73	0.53
1:E:301:PRO:HD3	1:E:515:GLN:HG2	1.91	0.53
1:F:254:LEU:O	1:F:256:LYS:NZ	2.35	0.53
1:F:398:GLU:HB3	1:F:405:ARG:HB2	1.89	0.53
1:A:127:VAL:HG12	1:A:158:PHE:CD2	2.44	0.53
1:B:466:ASP:O	1:B:491:ARG:NH1	2.42	0.53
1:B:533:LEU:HB3	1:B:568:CYS:SG	2.49	0.53
1:D:584:ALA:HB2	1:D:601:LEU:HD11	1.91	0.53
1:E:471:ILE:HG22	1:E:495:LEU:HD11	1.90	0.53
1:A:469:GLU:HB2	1:E:401:GLY:CA	2.31	0.52
1:E:430:ASP:HA	1:E:459:THR:HG23	1.90	0.52
1:F:436:ASP:HB3	1:F:439:THR:HG22	1.89	0.52
1:A:471:ILE:HD13	1:A:489:LEU:HD13	1.90	0.52
1:D:271:GLU:O	1:D:275:LYS:HG3	2.10	0.52
1:D:475:VAL:HG22	1:D:504:ILE:HD13	1.89	0.52
1:F:435:GLU:O	1:F:465:ASN:ND2	2.38	0.52
1:B:549:ASN:O	1:B:553:SER:OG	2.22	0.52
1:A:251:VAL:CG1	1:A:558:THR:HG23	2.39	0.52
1:B:15:VAL:HB	1:B:16:PRO:HD3	1.91	0.52
1:D:560:ASN:O	1:D:564:THR:HG23	2.10	0.52
1:E:487:LEU:HD11	1:E:513:ASN:OD1	2.09	0.52
1:E:531:TYR:CD1	1:E:532:PRO:HD2	2.45	0.52
1:F:317:ASN:OD1	1:F:318:GLY:N	2.42	0.52
1:A:57:PRO:HG2	1:A:59:PHE:CE1	2.44	0.52
1:E:453:ARG:NH2	1:F:469:GLU:OE2	2.39	0.52
1:A:143:THR:O	1:A:147:VAL:HG23	2.10	0.52
1:C:303:GLU:OE1	1:C:303:GLU:N	2.42	0.52
1:C:317:ASN:HA	1:C:321:LEU:HD23	1.92	0.52
1:A:81:GLU:OE1	1:A:196:MET:HA	2.09	0.52
1:A:184:LEU:HD22	1:A:189:HIS:CD2	2.45	0.52
1:A:557:LEU:O	1:A:561:LEU:HD13	2.10	0.52
1:A:589:ALA:HB1	1:A:593:GLU:HB2	1.92	0.52
1:B:5:LEU:HD11	1:B:91:ALA:HB2	1.92	0.52
1:B:101:LEU:HD21	1:B:124:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:GLU:OE2	1:D:403:ARG:HA	2.10	0.52
1:D:589:ALA:HB1	1:D:593:GLU:HB2	1.92	0.52
1:C:564:THR:HG22	1:C:571:ILE:CD1	2.39	0.52
1:D:460:VAL:O	1:D:484:GLY:N	2.40	0.52
1:F:227:LEU:HD11	1:F:577:LEU:HD23	1.92	0.52
1:F:401:GLY:O	1:F:402:ASP:HB2	2.09	0.52
1:D:417:ALA:HB2	1:D:456:LEU:HD21	1.92	0.51
1:F:397:ARG:HB2	1:F:439:THR:HG21	1.90	0.51
1:F:581:VAL:HG13	1:F:598:TRP:HH2	1.74	0.51
1:A:16:PRO:HB2	1:A:147:VAL:HG11	1.93	0.51
1:C:467:ASP:N	1:C:467:ASP:OD1	2.41	0.51
1:A:384:ASP:OD1	1:A:385:ARG:HG2	2.11	0.51
1:C:233:SER:HA	1:C:236:ARG:HG2	1.92	0.51
1:B:119:PHE:O	1:B:171:ARG:HG3	2.10	0.51
1:B:589:ALA:O	1:B:594:ARG:NH1	2.43	0.51
1:D:219:ILE:HD11	1:D:228:ALA:CB	2.40	0.51
1:D:329:ARG:O	1:D:333:ARG:HG2	2.10	0.51
1:F:557:LEU:O	1:F:561:LEU:HD13	2.11	0.51
1:A:5:LEU:HD22	1:A:91:ALA:HB2	1.93	0.51
1:B:133:PHE:HB2	1:B:140:GLU:O	2.11	0.51
1:B:173:LEU:HD21	1:B:201:HIS:HD2	1.76	0.51
1:D:244:PRO:HG3	1:D:565:ALA:CB	2.40	0.51
1:D:318:GLY:HA3	3:D:701:ATP:O1B	2.11	0.51
1:B:254:LEU:O	1:B:256:LYS:NZ	2.34	0.51
1:E:397:ARG:HD3	1:E:436:ASP:OD2	2.10	0.51
1:E:431:LEU:HB3	1:E:443:MET:HE1	1.92	0.51
1:C:547:THR:HG23	1:C:557:LEU:HD13	1.92	0.51
1:D:545:LEU:HD13	1:D:564:THR:HG21	1.93	0.51
1:A:47:LEU:HD22	1:A:51:PHE:CZ	2.46	0.51
1:B:99:ILE:HB	1:B:124:VAL:HG13	1.93	0.51
1:B:471:ILE:CG2	1:B:495:LEU:HD21	2.40	0.51
1:B:469:GLU:O	1:B:473:GLN:HG2	2.11	0.50
1:B:471:ILE:HB	1:B:495:LEU:HD21	1.91	0.50
1:E:545:LEU:HD13	1:E:564:THR:HG21	1.93	0.50
1:D:403:ARG:CD	1:D:442:ALA:HB1	2.41	0.50
1:E:263:LEU:O	1:E:331:GLN:NE2	2.44	0.50
1:F:397:ARG:HG3	1:F:400:GLY:H	1.75	0.50
1:B:307:LEU:HD23	1:B:516:ILE:HD13	1.93	0.50
1:B:537:LEU:HD13	1:B:575:GLU:HG2	1.93	0.50
1:D:248:LYS:HD3	1:D:562:LEU:CD1	2.41	0.50
1:D:475:VAL:HG13	1:D:504:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:556:SER:O	1:D:560:ASN:ND2	2.44	0.50
1:F:297:GLY:O	1:F:298:TRP:C	2.54	0.50
1:F:475:VAL:HG13	1:F:504:ILE:HD11	1.94	0.50
1:A:126:HIS:CE1	1:B:106:LYS:HB2	2.47	0.50
1:D:254:LEU:HD11	1:D:577:LEU:HD21	1.94	0.50
1:A:131:PRO:HA	1:A:139:ARG:O	2.12	0.50
1:A:157:ARG:HH22	2:J:3:A:H62	1.59	0.50
1:A:527:GLY:O	1:A:530:THR:OG1	2.18	0.50
1:D:533:LEU:HD13	1:D:543:VAL:HG11	1.93	0.50
1:A:284:GLU:OE1	1:A:284:GLU:N	2.39	0.50
1:B:170:LEU:HA	1:B:173:LEU:HD13	1.94	0.50
1:E:511:TYR:HB3	1:E:553:SER:OG	2.12	0.49
1:B:521:LEU:HD23	1:B:566:ARG:CZ	2.42	0.49
1:A:85:ARG:HB2	1:A:180:LEU:HD13	1.94	0.49
1:C:475:VAL:HG22	1:C:504:ILE:HD13	1.95	0.49
1:F:301:PRO:HG3	1:F:515:GLN:HA	1.94	0.49
1:A:89:GLN:HG2	1:A:90:ARG:HD2	1.95	0.49
1:B:329:ARG:O	1:B:333:ARG:HG3	2.12	0.49
1:B:447:ASP:OD1	1:B:449:GLU:HG3	2.11	0.49
1:F:240:GLU:HB2	1:F:573:ARG:NH1	2.27	0.49
1:F:396:THR:HG22	3:F:701:ATP:H4'	1.95	0.49
1:A:237:TRP:CH2	1:A:607:PRO:HB3	2.47	0.49
1:D:330:ALA:O	1:D:334:LEU:HG	2.12	0.49
1:E:286:LEU:HD22	1:E:321:LEU:HD12	1.95	0.49
1:B:180:LEU:HD13	1:B:191:VAL:HG12	1.94	0.49
1:C:575:GLU:O	1:C:579:THR:HG23	2.12	0.49
1:C:537:LEU:HD13	1:C:575:GLU:HG2	1.94	0.49
1:C:581:VAL:HG13	1:C:598:TRP:CH2	2.48	0.49
1:D:403:ARG:HD3	1:D:442:ALA:HB1	1.95	0.49
1:D:473:GLN:HG2	1:D:477:LYS:HG3	1.95	0.49
1:F:587:ALA:O	1:F:594:ARG:NH2	2.44	0.49
1:A:308:GLU:O	1:A:312:ARG:HG2	2.13	0.49
1:E:225:PRO:HB2	1:F:219:ILE:O	2.13	0.49
1:E:251:VAL:CG1	1:E:558:THR:HG23	2.43	0.49
1:F:451:VAL:HG13	1:F:456:LEU:HB2	1.95	0.49
1:A:8:VAL:HG12	1:A:34:THR:HB	1.95	0.49
1:A:105:TYR:CD1	2:J:6:A:H5''	2.48	0.49
1:E:330:ALA:O	1:E:334:LEU:HG	2.13	0.49
1:E:531:TYR:CD2	1:E:567:LEU:HD13	2.48	0.49
1:A:89:GLN:HG2	1:A:90:ARG:CD	2.43	0.48
1:E:242:LEU:HD23	1:E:565:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:VAL:HG12	1:E:558:THR:HG23	1.94	0.48
1:B:81:GLU:OE2	1:B:85:ARG:NE	2.44	0.48
1:C:317:ASN:OD1	1:C:318:GLY:N	2.45	0.48
1:E:335:LEU:O	1:E:339:LEU:HG	2.13	0.48
1:E:581:VAL:HG13	1:E:598:TRP:CH2	2.49	0.48
1:A:17:GLU:OE1	1:A:156:LEU:HD22	2.14	0.48
1:A:258:GLU:OE2	1:A:547:THR:OG1	2.32	0.48
1:C:236:ARG:O	1:C:240:GLU:HG2	2.13	0.48
1:E:396:THR:HG22	3:E:701:ATP:H4'	1.95	0.48
1:C:473:GLN:O	1:C:477:LYS:HB2	2.13	0.48
1:D:280:ALA:CB	1:D:286:LEU:HD11	2.44	0.48
1:E:301:PRO:CD	1:E:515:GLN:HG2	2.44	0.48
1:F:394:THR:HA	1:F:430:ASP:HB3	1.94	0.48
1:B:520:PRO:HG2	1:B:529:GLU:O	2.14	0.48
1:D:238:LEU:HD23	1:D:573:ARG:HB2	1.95	0.48
1:F:488:HIS:HB3	1:F:491:ARG:HE	1.79	0.48
1:B:11:SER:O	1:B:14:VAL:HG12	2.14	0.48
1:C:254:LEU:HD23	1:C:255:PRO:CD	2.40	0.48
1:A:472:TRP:CE2	1:A:495:LEU:HD13	2.49	0.48
1:C:396:THR:HG22	3:C:701:ATP:H4'	1.95	0.48
1:E:468:VAL:HG11	1:E:492:SER:HB2	1.94	0.48
1:B:300:ILE:HG23	1:B:514:LEU:HD21	1.96	0.48
1:B:330:ALA:O	1:B:334:LEU:HG	2.14	0.48
1:C:222:LEU:HD13	1:C:227:LEU:HB3	1.96	0.48
1:F:362:SER:O	1:F:366:VAL:HG23	2.13	0.48
1:F:575:GLU:O	1:F:579:THR:HG23	2.14	0.48
1:A:408:ARG:HH11	1:D:454:VAL:HG22	1.79	0.48
1:E:460:VAL:O	1:E:484:GLY:N	2.36	0.48
1:D:340:LEU:HD21	1:D:381:THR:HG21	1.95	0.48
1:E:533:LEU:CD1	1:E:543:VAL:HG11	2.44	0.48
1:F:273:LEU:O	1:F:277:ARG:HG3	2.14	0.48
1:A:200:GLN:HG2	1:A:203:GLU:OE1	2.14	0.47
1:B:30:VAL:HB	1:B:59:PHE:CE1	2.48	0.47
1:D:452:HIS:CE1	1:D:479:SER:HB2	2.49	0.47
1:E:243:ASP:N	1:E:247:ASP:OD2	2.34	0.47
1:F:256:LYS:HB3	1:F:557:LEU:HD23	1.95	0.47
1:F:298:TRP:CZ3	1:F:301:PRO:HB3	2.47	0.47
1:B:574:LEU:O	1:B:578:LYS:HG3	2.13	0.47
1:A:81:GLU:CD	1:A:196:MET:HA	2.39	0.47
1:A:240:GLU:HB2	1:A:573:ARG:NH1	2.29	0.47
1:A:431:LEU:HD21	1:A:448:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:THR:HG23	1:A:557:LEU:CD1	2.43	0.47
1:C:222:LEU:HD13	1:C:227:LEU:CB	2.44	0.47
1:A:237:TRP:CZ3	1:A:607:PRO:HB3	2.50	0.47
1:E:246:GLN:N	1:E:246:GLN:OE1	2.48	0.47
1:F:276:VAL:HG12	1:F:321:LEU:HD21	1.95	0.47
1:C:533:LEU:CD1	1:C:543:VAL:HG11	2.44	0.47
1:E:224:ILE:HB	1:E:227:LEU:HG	1.97	0.47
1:D:268:THR:HG22	1:D:317:ASN:HB3	1.97	0.47
1:A:12:TRP:CH2	1:A:144:LEU:HD12	2.50	0.47
1:B:362:SER:O	1:B:366:VAL:HG23	2.14	0.47
1:D:283:PRO:HA	1:D:286:LEU:HD13	1.95	0.47
1:F:377:ALA:O	1:F:381:THR:HG23	2.15	0.47
1:F:396:THR:O	1:F:397:ARG:HG2	2.14	0.47
1:F:534:ARG:HG2	1:F:568:CYS:HB3	1.97	0.47
1:B:356:TYR:HB2	1:B:366:VAL:HG11	1.97	0.47
1:C:322:LEU:HD22	1:C:328:LEU:HA	1.96	0.47
1:D:431:LEU:HD11	1:D:448:PHE:CZ	2.50	0.47
1:F:304:PRO:HG3	1:F:518:GLY:HA3	1.97	0.47
1:A:471:ILE:HD13	1:A:489:LEU:CD1	2.45	0.47
1:B:265:GLY:HA3	1:B:549:ASN:OD1	2.15	0.47
1:D:486:ALA:O	1:D:536:TYR:OH	2.32	0.47
1:E:318:GLY:O	1:E:322:LEU:HB2	2.15	0.47
1:E:405:ARG:O	1:E:409:HIS:ND1	2.48	0.47
1:A:363:PRO:HD2	1:D:418:GLU:CG	2.45	0.47
1:E:284:GLU:OE1	1:E:284:GLU:N	2.38	0.47
1:C:240:GLU:HB2	1:C:573:ARG:NH1	2.30	0.46
1:D:298:TRP:CH2	1:D:305:ILE:HD13	2.50	0.46
1:D:557:LEU:O	1:D:561:LEU:HD13	2.14	0.46
1:F:276:VAL:CG1	1:F:321:LEU:HD21	2.45	0.46
1:C:228:ALA:HB3	1:D:228:ALA:HB3	1.96	0.46
1:D:561:LEU:O	1:D:564:THR:OG1	2.32	0.46
1:F:398:GLU:HB2	1:F:401:GLY:O	2.14	0.46
1:A:75:ASP:N	1:A:75:ASP:OD1	2.48	0.46
1:B:460:VAL:HG23	1:B:480:ALA:HB2	1.97	0.46
1:E:397:ARG:HD2	1:E:398:GLU:H	1.80	0.46
1:A:558:THR:O	1:A:562:LEU:HG	2.16	0.46
1:B:218:GLY:O	1:B:220:SER:N	2.48	0.46
1:D:248:LYS:HD3	1:D:562:LEU:HD13	1.98	0.46
1:D:364:TRP:HE3	1:D:412:LEU:HD11	1.81	0.46
1:A:434:PHE:HB3	1:A:436:ASP:OD1	2.16	0.46
1:B:30:VAL:HB	1:B:59:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:HIS:HB3	3:D:701:ATP:O2A	2.14	0.46
1:A:37:SER:HB2	1:A:68:GLU:O	2.16	0.46
1:A:472:TRP:CD2	1:A:495:LEU:HD13	2.50	0.46
1:E:358:SER:OG	1:E:361:ARG:HG3	2.15	0.46
1:F:350:ARG:HD3	1:F:430:ASP:OD2	2.15	0.46
1:F:376:GLN:O	1:F:380:GLU:HG3	2.15	0.46
1:C:553:SER:O	1:C:554:GLN:C	2.59	0.46
1:C:564:THR:HG22	1:C:571:ILE:HD13	1.97	0.46
1:D:280:ALA:HB2	1:D:327:CYS:SG	2.56	0.46
1:D:356:TYR:HB2	1:D:366:VAL:HG11	1.98	0.46
1:F:350:ARG:HB3	1:F:394:THR:OG1	2.16	0.46
1:F:430:ASP:HA	1:F:459:THR:HG23	1.97	0.46
1:A:277:ARG:HG2	1:A:321:LEU:HD11	1.98	0.46
1:A:310:TYR:CD2	1:A:516:ILE:HD11	2.51	0.46
1:B:533:LEU:CD1	1:B:543:VAL:HG11	2.46	0.46
1:C:534:ARG:HG3	1:C:568:CYS:HB3	1.98	0.46
1:A:330:ALA:O	1:A:334:LEU:HG	2.16	0.46
1:A:434:PHE:CZ	1:A:474:ALA:HB2	2.51	0.46
1:C:371:ARG:CZ	1:C:375:GLN:HG3	2.46	0.46
1:E:237:TRP:CH2	1:E:573:ARG:HD3	2.50	0.46
1:E:317:ASN:OD1	1:E:318:GLY:N	2.49	0.46
1:F:362:SER:OG	1:F:365:VAL:HG23	2.15	0.46
1:A:58:ARG:HH21	1:A:90:ARG:HH21	1.62	0.45
1:A:251:VAL:O	1:A:256:LYS:NZ	2.49	0.45
1:C:264:GLY:HA3	3:C:701:ATP:O2B	2.16	0.45
1:F:238:LEU:HD23	1:F:574:LEU:HD23	1.97	0.45
1:F:258:GLU:CD	1:F:261:CYS:HB2	2.41	0.45
1:D:305:ILE:O	1:D:309:ARG:HB2	2.16	0.45
1:F:314:GLY:CA	1:F:552:ILE:HG12	2.45	0.45
1:F:526:GLU:HG3	1:F:530:THR:HG21	1.98	0.45
1:D:487:LEU:HD13	1:D:519:PHE:CZ	2.50	0.45
1:D:577:LEU:HD11	1:D:604:VAL:HG11	1.97	0.45
1:E:439:THR:O	1:E:443:MET:HG3	2.16	0.45
1:A:104:GLY:HA2	2:J:1:A:N3	2.31	0.45
1:D:509:CYS:SG	1:D:548:ASP:HB2	2.56	0.45
1:E:471:ILE:CG2	1:E:495:LEU:HD21	2.47	0.45
1:C:242:LEU:HD12	1:C:247:ASP:OD2	2.17	0.45
1:C:531:TYR:CD1	1:C:532:PRO:HD2	2.51	0.45
1:D:256:LYS:HB3	1:D:557:LEU:HD23	1.99	0.45
1:F:436:ASP:OD1	1:F:437:ARG:N	2.49	0.45
1:A:61:ILE:O	1:A:188:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:HD3	1:B:106:LYS:HZ2	1.81	0.45
1:B:467:ASP:OD2	1:B:469:GLU:HB3	2.16	0.45
1:D:237:TRP:HA	1:D:240:GLU:HG3	1.99	0.45
1:E:256:LYS:HB3	1:E:557:LEU:CD2	2.46	0.45
1:F:269:HIS:CE1	1:F:294:LEU:HD21	2.51	0.45
1:F:330:ALA:O	1:F:334:LEU:HG	2.17	0.45
1:A:83:LEU:O	1:A:87:LEU:HG	2.16	0.45
1:B:35:THR:HB	1:B:67:PHE:HD1	1.82	0.45
1:B:301:PRO:HD3	1:B:515:GLN:HG2	1.99	0.45
1:C:237:TRP:CH2	1:C:573:ARG:HD3	2.51	0.45
1:D:581:VAL:HG13	1:D:598:TRP:CH2	2.52	0.45
1:E:467:ASP:OD1	1:E:467:ASP:N	2.48	0.45
1:B:462:ALA:HB3	1:B:484:GLY:O	2.17	0.45
1:B:508:LEU:HD12	1:B:543:VAL:CG1	2.46	0.45
1:B:525:GLN:NE2	1:B:526:GLU:O	2.49	0.45
1:D:300:ILE:HG23	1:D:514:LEU:HD21	1.98	0.45
1:F:340:LEU:HD11	1:F:381:THR:HG21	1.99	0.45
1:F:472:TRP:CH2	1:F:498:VAL:HG21	2.51	0.45
1:D:467:ASP:OD1	1:D:467:ASP:N	2.48	0.45
1:E:489:LEU:HB2	1:E:536:TYR:OH	2.17	0.45
1:F:520:PRO:HG3	1:F:529:GLU:HG3	1.98	0.45
1:C:348:GLU:HA	1:C:390:ASN:O	2.16	0.45
1:D:280:ALA:HB1	1:D:286:LEU:HD11	1.99	0.45
1:D:510:PRO:HD2	1:D:560:ASN:HB3	1.97	0.45
1:E:280:ALA:CB	1:E:286:LEU:HD11	2.47	0.45
1:E:286:LEU:HD22	1:E:321:LEU:CD1	2.46	0.45
1:E:414:ILE:HG23	1:E:454:VAL:HG11	1.99	0.45
1:F:292:ILE:HG21	1:F:313:LEU:HA	1.99	0.45
1:F:366:VAL:O	1:F:370:ILE:HG13	2.17	0.45
1:A:431:LEU:HD21	1:A:448:PHE:CZ	2.52	0.44
1:A:521:LEU:HD13	1:A:566:ARG:NH2	2.32	0.44
1:B:366:VAL:O	1:B:370:ILE:HG13	2.17	0.44
1:A:12:TRP:CZ3	1:A:16:PRO:HG2	2.53	0.44
1:B:65:GLN:HG3	1:B:190:TRP:HE3	1.82	0.44
1:D:587:ALA:O	1:D:594:ARG:NH2	2.50	0.44
1:A:265:GLY:HA3	1:A:549:ASN:OD1	2.16	0.44
1:A:434:PHE:CE2	1:A:460:VAL:HG11	2.52	0.44
1:B:218:GLY:C	1:B:220:SER:N	2.76	0.44
1:E:477:LYS:HE2	1:E:477:LYS:HB2	1.83	0.44
1:E:581:VAL:HG13	1:E:598:TRP:HH2	1.80	0.44
1:C:508:LEU:HD12	1:C:543:VAL:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:ARG:NH2	1:E:507:GLU:OE2	2.51	0.44
1:E:393:LEU:HD22	1:E:413:ALA:HA	1.99	0.44
1:E:431:LEU:HD22	1:E:443:MET:CE	2.46	0.44
1:F:305:ILE:HB	1:F:309:ARG:HD2	2.00	0.44
1:F:528:SER:O	1:F:529:GLU:HG2	2.17	0.44
1:A:132:ARG:NH2	1:A:155:ALA:HB2	2.33	0.44
1:C:472:TRP:CH2	1:C:498:VAL:HG21	2.51	0.44
1:E:399:GLU:H	1:E:403:ARG:HH22	1.64	0.44
1:F:472:TRP:CE2	1:F:495:LEU:HD13	2.53	0.44
1:A:51:PHE:HB3	1:A:59:PHE:CD2	2.53	0.44
1:A:161:LEU:HD22	1:B:76:HIS:CD2	2.53	0.44
1:C:384:ASP:OD1	1:C:385:ARG:N	2.50	0.44
1:D:575:GLU:O	1:D:579:THR:HG23	2.17	0.44
1:E:256:LYS:HD2	1:E:557:LEU:HD23	1.99	0.44
1:F:277:ARG:NH2	1:F:287:PRO:O	2.41	0.44
1:F:526:GLU:OE2	1:F:534:ARG:HB2	2.18	0.44
1:C:356:TYR:HB2	1:C:366:VAL:HG11	2.00	0.44
1:D:576:VAL:O	1:D:579:THR:OG1	2.28	0.44
1:A:32:VAL:HB	1:A:61:ILE:HD12	1.99	0.44
1:A:106:LYS:HD3	1:B:106:LYS:NZ	2.32	0.44
1:C:557:LEU:O	1:C:561:LEU:HD13	2.17	0.44
1:F:251:VAL:O	1:F:256:LYS:NZ	2.50	0.44
1:F:433:GLY:O	1:F:439:THR:HG23	2.17	0.44
1:F:523:GLU:O	1:F:524:GLU:HB3	2.17	0.44
1:B:34:THR:CG2	1:B:63:ARG:HG3	2.46	0.43
1:D:219:ILE:HD11	1:D:228:ALA:CA	2.47	0.43
1:D:533:LEU:CD1	1:D:543:VAL:HG11	2.48	0.43
1:F:262:HIS:HD2	1:F:548:ASP:OD1	1.94	0.43
1:B:41:SER:HB2	1:B:42:PRO:HD3	2.00	0.43
1:B:237:TRP:O	1:B:573:ARG:NH1	2.50	0.43
1:B:254:LEU:HD11	1:B:577:LEU:HD21	2.01	0.43
1:B:271:GLU:OE2	1:B:275:LYS:NZ	2.47	0.43
1:C:423:GLY:O	1:C:425:ARG:HG2	2.18	0.43
1:D:334:LEU:O	1:D:337:GLU:HG2	2.17	0.43
1:D:440:ARG:NH1	1:D:467:ASP:OD1	2.49	0.43
1:E:224:ILE:HD12	1:E:604:VAL:HG21	2.00	0.43
1:E:248:LYS:HG3	1:E:562:LEU:HD11	1.99	0.43
1:E:475:VAL:HG13	1:E:504:ILE:HD11	2.00	0.43
1:F:473:GLN:O	1:F:477:LYS:N	2.45	0.43
1:A:361:ARG:NH2	1:A:369:GLU:OE1	2.51	0.43
1:B:237:TRP:CZ3	1:B:607:PRO:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.75	0.43
1:F:450:PRO:O	1:F:454:VAL:HG23	2.19	0.43
1:A:175:ALA:N	1:A:176:PRO:HD2	2.34	0.43
1:A:14:VAL:HG21	1:A:102:ALA:O	2.17	0.43
1:A:69:ASP:OD1	2:J:1:A:N6	2.52	0.43
1:A:101:LEU:CD2	1:A:113:GLN:HB2	2.39	0.43
1:B:524:GLU:O	1:B:525:GLN:HB3	2.18	0.43
1:C:494:ASP:OD1	1:C:494:ASP:N	2.52	0.43
1:D:471:ILE:CG2	1:D:495:LEU:HD21	2.49	0.43
1:B:575:GLU:O	1:B:579:THR:HG23	2.19	0.43
1:E:556:SER:O	1:E:560:ASN:ND2	2.50	0.43
1:F:466:ASP:OD2	1:F:488:HIS:ND1	2.51	0.43
1:B:218:GLY:O	1:B:219:ILE:C	2.62	0.43
1:F:263:LEU:O	1:F:331:GLN:NE2	2.50	0.43
1:A:57:PRO:HG2	1:A:59:PHE:CZ	2.54	0.43
1:B:12:TRP:CH2	1:B:144:LEU:HD23	2.54	0.43
1:B:178:PHE:CD2	1:B:198:LEU:HD13	2.53	0.43
1:B:329:ARG:HB2	1:B:373:HIS:CE1	2.53	0.43
1:E:433:GLY:O	1:E:439:THR:HB	2.19	0.43
1:F:261:CYS:HA	1:F:548:ASP:O	2.19	0.43
1:F:271:GLU:O	1:F:275:LYS:HG3	2.19	0.43
1:F:313:LEU:HB2	1:F:552:ILE:CG2	2.48	0.43
1:A:110:ALA:HB1	1:B:113:GLN:OE1	2.19	0.43
1:D:319:SER:O	1:D:323:LYS:HG3	2.19	0.43
1:A:109:SER:HB2	1:B:106:LYS:HD3	2.01	0.42
1:A:195:ASP:OD1	1:A:197:ARG:HB2	2.18	0.42
1:A:509:CYS:SG	1:A:548:ASP:HB2	2.59	0.42
1:B:489:LEU:HB2	1:B:536:TYR:OH	2.19	0.42
1:C:466:ASP:OD1	1:C:466:ASP:N	2.39	0.42
1:F:318:GLY:O	1:F:322:LEU:HB2	2.18	0.42
1:F:336:TYR:HE2	1:F:381:THR:HG21	1.84	0.42
1:A:13:ALA:O	1:A:17:GLU:HG3	2.18	0.42
1:A:157:ARG:HH11	1:B:71:ARG:HA	1.84	0.42
1:D:254:LEU:HD21	1:D:577:LEU:CD2	2.49	0.42
1:E:233:SER:HB2	1:E:236:ARG:HH21	1.84	0.42
1:B:272:LEU:HD12	1:B:272:LEU:HA	1.78	0.42
1:B:411:ALA:HB1	1:E:411:ALA:HA	2.01	0.42
1:B:453:ARG:CZ	1:E:403:ARG:HB2	2.50	0.42
1:B:525:GLN:HG2	1:B:526:GLU:H	1.83	0.42
1:C:393:LEU:HB3	1:C:409:HIS:NE2	2.34	0.42
1:D:276:VAL:HG23	1:D:334:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:589:ALA:HB1	1:D:593:GLU:CB	2.49	0.42
1:A:169:GLN:HE21	1:B:213:LEU:HB3	1.84	0.42
1:A:475:VAL:HG13	1:A:504:ILE:CD1	2.49	0.42
1:B:474:ALA:HA	1:B:478:LEU:HB2	2.00	0.42
1:C:272:LEU:HD23	1:C:272:LEU:HA	1.91	0.42
1:D:509:CYS:O	1:D:513:ASN:ND2	2.51	0.42
1:E:346:TYR:CE2	1:E:348:GLU:HG3	2.54	0.42
1:A:533:LEU:HD12	1:A:543:VAL:HG11	2.02	0.42
1:B:81:GLU:HG3	1:B:85:ARG:HD2	2.02	0.42
1:B:346:TYR:CE2	1:B:348:GLU:HG3	2.54	0.42
1:C:552:ILE:HG22	1:C:552:ILE:O	2.20	0.42
1:D:223:PRO:HB2	1:D:581:VAL:HG21	2.01	0.42
1:F:219:ILE:HG23	1:F:222:LEU:HD22	2.01	0.42
1:F:280:ALA:CB	1:F:286:LEU:HD11	2.50	0.42
1:B:5:LEU:HD23	1:B:31:HIS:HB2	2.00	0.42
1:B:180:LEU:HD12	1:B:180:LEU:O	2.19	0.42
1:B:432:ALA:HA	1:B:461:HIS:HB3	2.01	0.42
1:A:243:ASP:O	1:A:247:ASP:HB2	2.20	0.42
1:D:258:GLU:OE1	1:D:557:LEU:HD22	2.20	0.42
1:F:298:TRP:HH2	1:F:305:ILE:HD13	1.78	0.42
1:F:382:PRO:HB2	1:F:384:ASP:OD1	2.20	0.42
1:A:435:GLU:HG3	1:A:448:PHE:CZ	2.55	0.42
1:A:435:GLU:HG3	1:A:448:PHE:HZ	1.84	0.42
1:B:139:ARG:HG2	1:B:140:GLU:H	1.85	0.42
1:C:447:ASP:OD1	1:C:449:GLU:HB2	2.20	0.42
1:D:414:ILE:HD11	1:D:450:PRO:HB2	2.01	0.42
1:E:384:ASP:OD1	1:E:385:ARG:N	2.52	0.42
1:E:404:SER:O	1:E:408:ARG:HG3	2.20	0.42
1:D:398:GLU:OE1	1:D:403:ARG:HG2	2.20	0.42
1:A:565:ALA:HA	1:A:571:ILE:HG21	2.02	0.41
1:B:471:ILE:HD13	1:B:489:LEU:CD1	2.50	0.41
1:D:312:ARG:HA	1:D:312:ARG:HD3	1.68	0.41
1:F:310:TYR:HE2	1:F:549:ASN:HD22	1.68	0.41
1:B:475:VAL:HG13	1:B:504:ILE:CD1	2.50	0.41
1:C:547:THR:HG22	1:C:560:ASN:ND2	2.35	0.41
1:E:260:HIS:HE2	1:E:461:HIS:CE1	2.38	0.41
1:F:236:ARG:O	1:F:240:GLU:HG2	2.19	0.41
1:F:250:TRP:NE1	1:F:605:PRO:HG2	2.36	0.41
1:F:534:ARG:CG	1:F:568:CYS:HB3	2.50	0.41
1:A:15:VAL:HG21	1:A:47:LEU:HD11	2.02	0.41
1:A:317:ASN:OD1	1:A:318:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:TRP:HH2	1:C:498:VAL:HG21	1.85	0.41
1:D:297:GLY:O	1:D:298:TRP:C	2.62	0.41
1:E:233:SER:HB2	1:E:236:ARG:NH2	2.35	0.41
1:F:262:HIS:HB2	1:F:549:ASN:OD1	2.20	0.41
1:A:397:ARG:NH2	1:A:435:GLU:HB3	2.34	0.41
1:A:417:ALA:HB2	1:A:456:LEU:HD21	2.02	0.41
1:D:534:ARG:HG3	1:D:568:CYS:HB3	2.02	0.41
1:E:231:PRO:HD2	1:E:234:HIS:ND1	2.35	0.41
1:F:221:GLU:OE1	1:F:221:GLU:N	2.53	0.41
1:F:548:ASP:HB3	1:F:549:ASN:H	1.76	0.41
1:B:299:PRO:O	1:B:515:GLN:NE2	2.43	0.41
1:E:510:PRO:HD2	1:E:560:ASN:HB3	2.02	0.41
1:F:346:TYR:CE2	1:F:587:ALA:HB1	2.55	0.41
1:F:601:LEU:HD23	1:F:601:LEU:HA	1.87	0.41
1:A:494:ASP:O	1:A:498:VAL:HG23	2.20	0.41
1:D:513:ASN:ND2	1:D:531:TYR:OH	2.43	0.41
1:E:452:HIS:HB3	1:F:476:PHE:CZ	2.56	0.41
1:F:533:LEU:HD23	1:F:564:THR:CG2	2.50	0.41
1:B:36:ALA:HB2	1:B:64:VAL:O	2.20	0.41
1:C:437:ARG:HH11	1:C:465:ASN:HB3	1.85	0.41
1:A:31:HIS:HB3	1:A:86:TRP:CZ2	2.55	0.41
1:C:280:ALA:CB	1:C:286:LEU:HD11	2.50	0.41
1:C:472:TRP:CE2	1:C:495:LEU:HD13	2.55	0.41
1:D:545:LEU:CD1	1:D:564:THR:HG21	2.51	0.41
1:A:9:GLY:O	1:A:40:ILE:HG23	2.21	0.41
1:A:97:ARG:NH1	1:A:119:PHE:O	2.54	0.41
1:A:460:VAL:HG23	1:A:480:ALA:HB2	2.02	0.41
1:A:559:ASP:N	1:A:559:ASP:OD1	2.54	0.41
1:B:237:TRP:CH2	1:B:607:PRO:HB3	2.55	0.41
1:B:262:HIS:HB3	3:B:701:ATP:O2A	2.21	0.41
1:C:243:ASP:O	1:C:247:ASP:HB2	2.20	0.41
1:C:466:ASP:OD2	1:C:488:HIS:ND1	2.49	0.41
1:D:248:LYS:HE2	1:D:248:LYS:HB2	1.91	0.41
1:D:258:GLU:OE1	1:D:557:LEU:HD13	2.20	0.41
1:D:398:GLU:CD	1:D:403:ARG:HA	2.46	0.41
1:D:471:ILE:HG21	1:D:495:LEU:HD21	2.03	0.41
1:E:298:TRP:CH2	1:E:515:GLN:HB3	2.56	0.41
1:F:329:ARG:O	1:F:333:ARG:HG3	2.21	0.41
1:A:39:LYS:H	1:A:39:LYS:HG3	1.68	0.41
1:A:213:LEU:HD11	1:B:209:SER:HB3	2.03	0.41
1:B:13:ALA:O	1:B:17:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ALA:O	1:C:334:LEU:HG	2.21	0.41
1:F:298:TRP:CH2	1:F:515:GLN:HB3	2.56	0.41
1:B:340:LEU:HD23	1:B:340:LEU:HA	1.84	0.40
1:B:523:GLU:O	1:B:524:GLU:HB3	2.21	0.40
1:C:237:TRP:CZ2	1:C:607:PRO:HB3	2.56	0.40
1:D:396:THR:HG23	3:D:701:ATP:O2'	2.20	0.40
1:E:399:GLU:H	1:E:403:ARG:NH2	2.19	0.40
1:F:449:GLU:HB3	1:F:450:PRO:HD3	2.02	0.40
1:B:135:PRO:HD3	1:B:139:ARG:NH1	2.36	0.40
1:C:224:ILE:HG23	1:C:581:VAL:HG21	2.03	0.40
1:D:366:VAL:O	1:D:370:ILE:HG13	2.20	0.40
1:E:560:ASN:O	1:E:564:THR:HG23	2.21	0.40
1:A:44:VAL:HG13	1:A:61:ILE:HG12	2.04	0.40
1:A:196:MET:HE3	1:A:196:MET:HB3	1.73	0.40
1:A:408:ARG:HH12	1:D:454:VAL:HA	1.85	0.40
1:D:237:TRP:CH2	1:D:607:PRO:HB3	2.57	0.40
1:F:414:ILE:CG2	1:F:454:VAL:HG21	2.42	0.40
1:A:280:ALA:HB1	1:A:324:ASP:OD2	2.21	0.40
1:B:74:GLN:HA	1:B:77:MET:CE	2.52	0.40
1:C:269:HIS:NE2	1:C:294:LEU:HD21	2.37	0.40
1:C:287:PRO:HG3	1:C:320:ALA:O	2.22	0.40
1:C:346:TYR:HB2	1:C:597:LEU:HD13	2.03	0.40
1:C:350:ARG:NH1	1:C:430:ASP:OD2	2.54	0.40
1:C:487:LEU:HD23	1:C:508:LEU:HD22	2.04	0.40
1:D:243:ASP:HA	1:D:244:PRO:HD3	1.96	0.40
1:E:256:LYS:HE2	1:E:342:ASP:O	2.22	0.40
1:E:305:ILE:O	1:E:309:ARG:HB2	2.21	0.40
1:F:230:TRP:CE3	1:F:234:HIS:HB3	2.57	0.40
1:F:262:HIS:HB3	3:F:701:ATP:O1A	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	595/631 (94%)	570 (96%)	24 (4%)	1 (0%)	43	72
1	B	583/631 (92%)	548 (94%)	30 (5%)	5 (1%)	14	41
1	C	388/631 (62%)	375 (97%)	13 (3%)	0	100	100
1	D	389/631 (62%)	370 (95%)	18 (5%)	1 (0%)	36	65
1	E	383/631 (61%)	367 (96%)	13 (3%)	3 (1%)	16	44
1	F	388/631 (62%)	370 (95%)	15 (4%)	3 (1%)	16	44
All	All	2726/3786 (72%)	2600 (95%)	113 (4%)	13 (0%)	26	54

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	TRP
1	F	402	ASP
1	E	320	ALA
1	B	218	GLY
1	B	524	GLU
1	F	528	SER
1	B	548	ASP
1	D	485	HIS
1	E	485	HIS
1	E	521	LEU
1	F	548	ASP
1	B	219	ILE
1	B	528	SER

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	491/517 (95%)	471 (96%)	20 (4%)	27	61
1	B	483/517 (93%)	473 (98%)	10 (2%)	47	77
1	C	314/517 (61%)	307 (98%)	7 (2%)	45	77
1	D	315/517 (61%)	312 (99%)	3 (1%)	68	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	310/517 (60%)	304 (98%)	6 (2%)	50 79
1	F	315/517 (61%)	311 (99%)	4 (1%)	61 86
All	All	2228/3102 (72%)	2178 (98%)	50 (2%)	45 77

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	CYS
1	A	8	VAL
1	A	25	GLN
1	A	34	THR
1	A	35	THR
1	A	61	ILE
1	A	65	GLN
1	A	70	LEU
1	A	75	ASP
1	A	96	HIS
1	A	107	THR
1	A	144	LEU
1	A	171	ARG
1	A	196	MET
1	A	198	LEU
1	A	217	GLU
1	A	219	ILE
1	A	275	LYS
1	A	279	GLU
1	B	70	LEU
1	B	73	GLU
1	B	101	LEU
1	B	124	VAL
1	B	248	LYS
1	B	272	LEU
1	B	278	GLN
1	B	350	ARG
1	B	384	ASP
1	B	472	TRP
1	C	243	ASP
1	C	246	GLN
1	C	254	LEU
1	C	292	ILE

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Mol	Chain	Res	Type
1	C	418	GLU
1	C	461	HIS
1	C	553	SER
1	D	313	LEU
1	D	425	ARG
1	D	501	GLU
1	E	278	GLN
1	E	307	LEU
1	E	313	LEU
1	E	425	ARG
1	E	460	VAL
1	E	461	HIS
1	F	439	THR
1	F	461	HIS
1	F	489	LEU
1	F	580	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	76	HIS
1	A	93	GLN
1	A	96	HIS
1	A	154	ASN
1	A	169	GLN
1	A	211	HIS
1	A	591	GLN
1	B	31	HIS
1	B	76	HIS
1	B	246	GLN
1	B	546	ASN
1	B	554	GLN
1	C	375	GLN
1	C	390	ASN
1	C	422	ASN
1	D	373	HIS
1	D	485	HIS
1	D	513	ASN
1	E	390	ASN
1	F	316	ASN
1	F	452	HIS

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Mol	Chain	Res	Type
1	F	485	HIS
1	F	513	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	J	5/6 (83%)	3 (60%)	1 (20%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	J	2	A
2	J	5	A
2	J	6	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	J	5	A

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 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	ATP	E	701	4	29,33,33	0.52	0	44,52,52	0.57	0
3	ATP	A	701	-	29,33,33	0.48	0	44,52,52	0.54	0
3	ATP	F	701	4	29,33,33	0.38	0	44,52,52	0.75	1 (2%)
3	ATP	B	701	-	29,33,33	0.49	0	44,52,52	0.58	0
3	ATP	D	701	4	29,33,33	0.38	0	44,52,52	0.84	1 (2%)
3	ATP	C	701	4	29,33,33	0.36	0	44,52,52	0.76	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	ATP	E	701	4	-	4/22/38/38	0/3/3/3
3	ATP	A	701	-	-	0/22/38/38	0/3/3/3
3	ATP	F	701	4	-	5/22/38/38	0/3/3/3
3	ATP	B	701	-	-	3/22/38/38	0/3/3/3
3	ATP	D	701	4	-	4/22/38/38	0/3/3/3
3	ATP	C	701	4	-	3/22/38/38	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	ATP	PB-O3B-PG	2.06	139.90	132.83
3	F	701	ATP	PB-O3B-PG	2.04	139.83	132.83
3	D	701	ATP	PB-O3B-PG	2.01	139.72	132.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	701	ATP	C3'-C4'-C5'-O5'
3	D	701	ATP	C5'-O5'-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O2A
3	F	701	ATP	C5'-O5'-PA-O1A
3	F	701	ATP	C5'-O5'-PA-O2A
3	E	701	ATP	O4'-C4'-C5'-O5'
3	B	701	ATP	O4'-C4'-C5'-O5'

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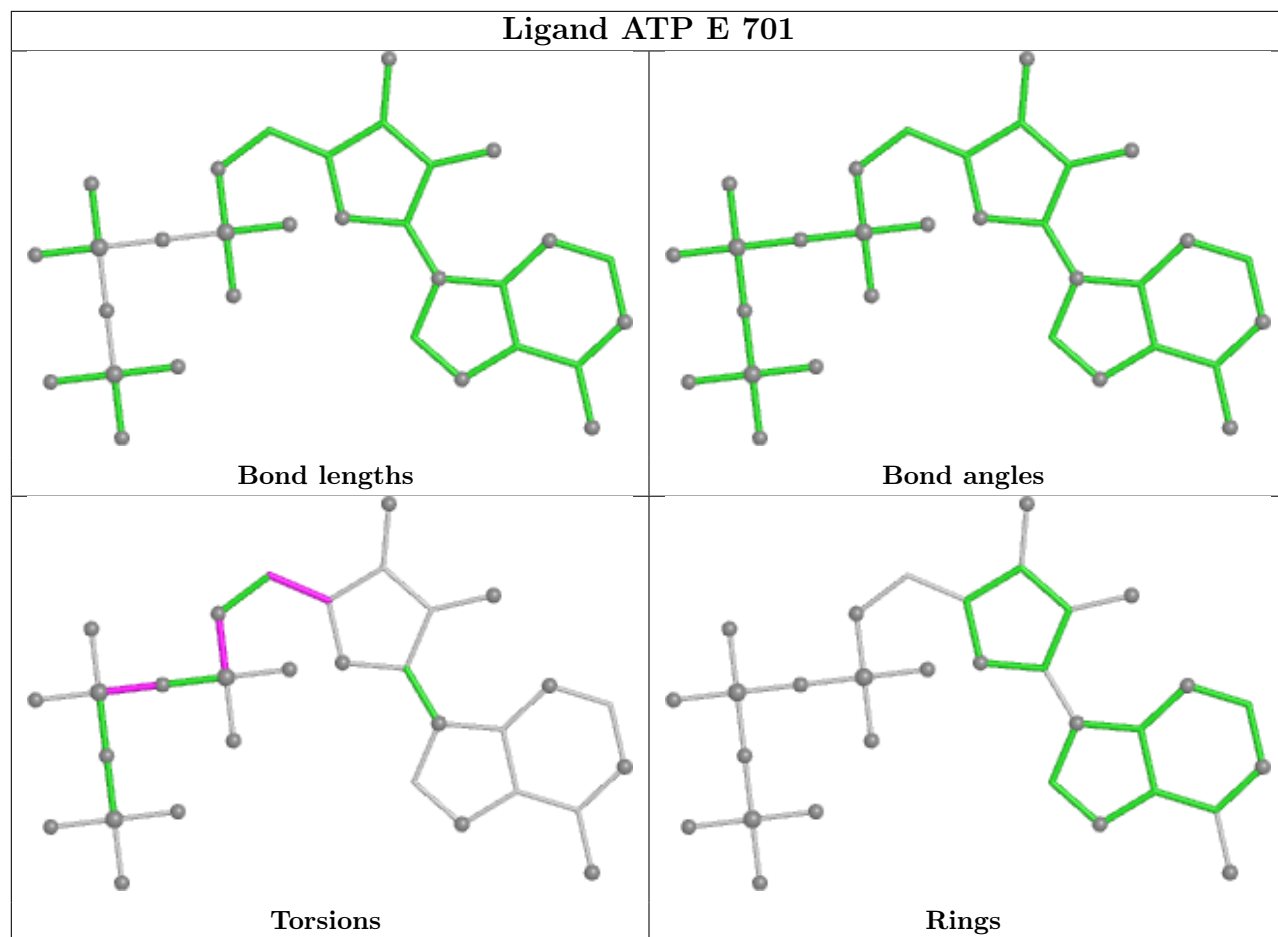
Mol	Chain	Res	Type	Atoms
3	C	701	ATP	PG-O3B-PB-O3A
3	B	701	ATP	PB-O3A-PA-O5'
3	D	701	ATP	PB-O3A-PA-O5'
3	F	701	ATP	PB-O3A-PA-O5'
3	F	701	ATP	C5'-O5'-PA-O3A
3	C	701	ATP	O4'-C4'-C5'-O5'
3	F	701	ATP	PB-O3A-PA-O1A
3	D	701	ATP	C5'-O5'-PA-O3A
3	C	701	ATP	PG-O3B-PB-O1B
3	E	701	ATP	PA-O3A-PB-O1B
3	E	701	ATP	C5'-O5'-PA-O1A
3	E	701	ATP	PA-O3A-PB-O3B

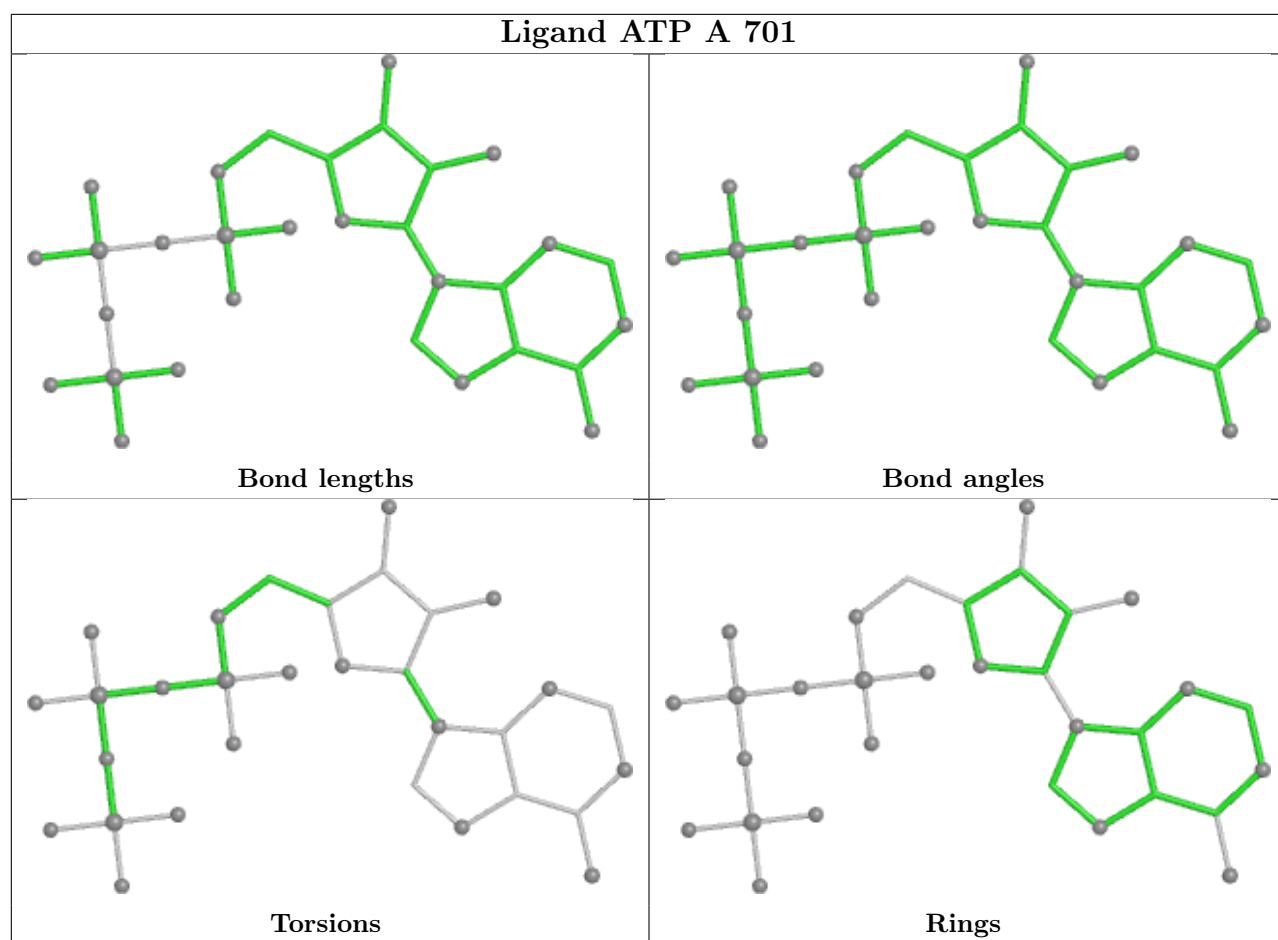
There are no ring outliers.

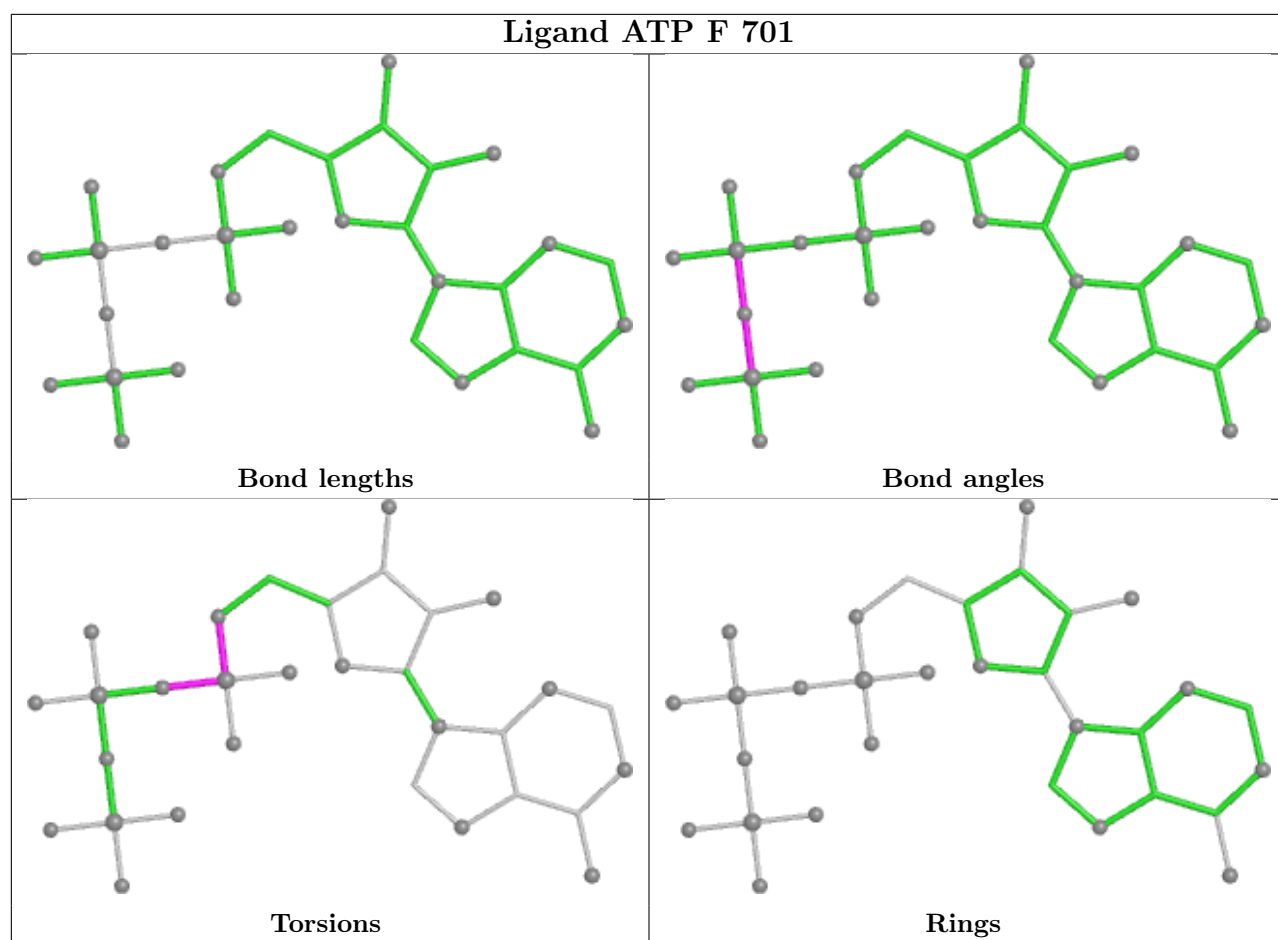
5 monomers are involved in 9 short contacts:

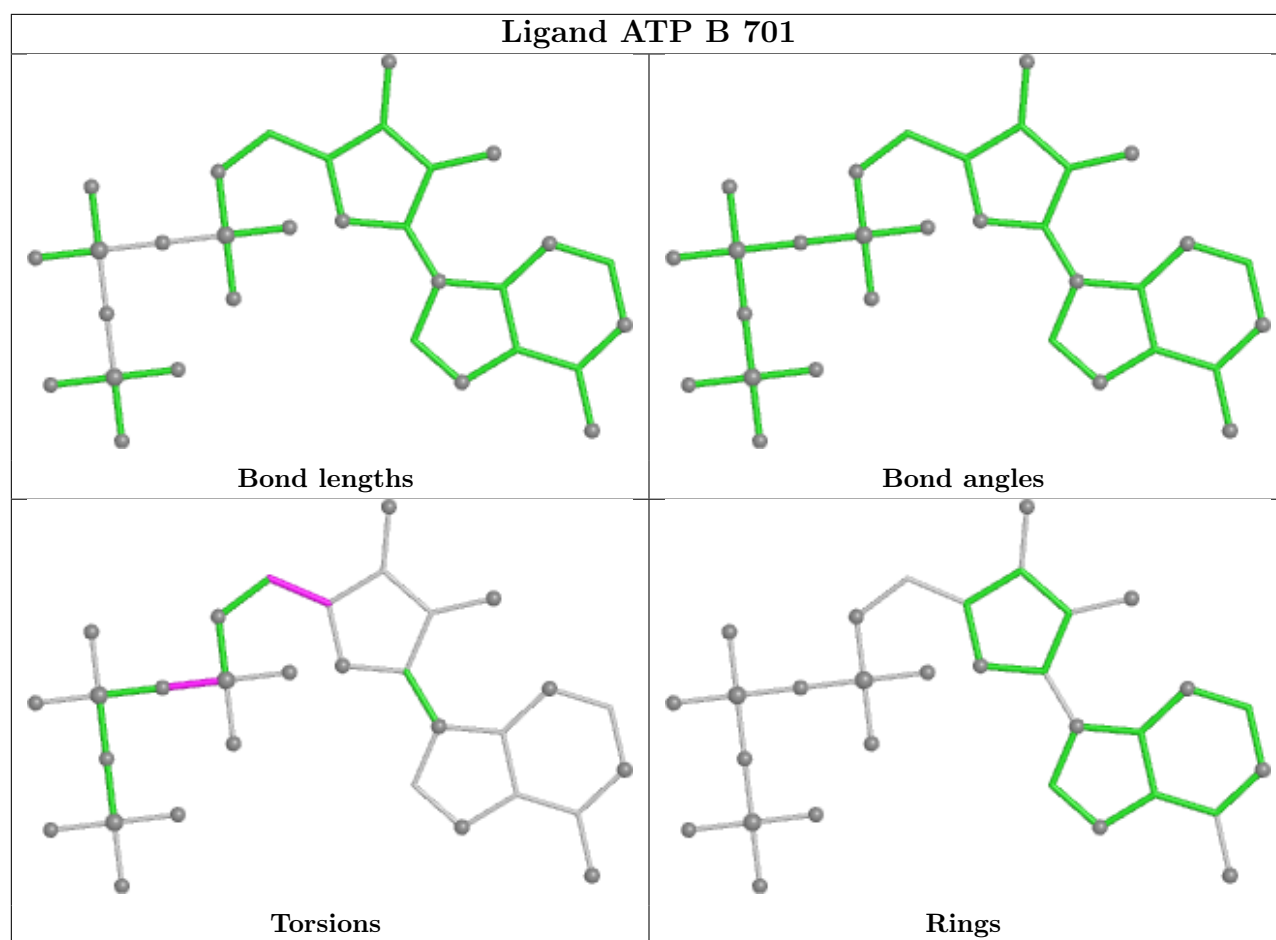
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	701	ATP	1	0
3	F	701	ATP	2	0
3	B	701	ATP	1	0
3	D	701	ATP	3	0
3	C	701	ATP	2	0

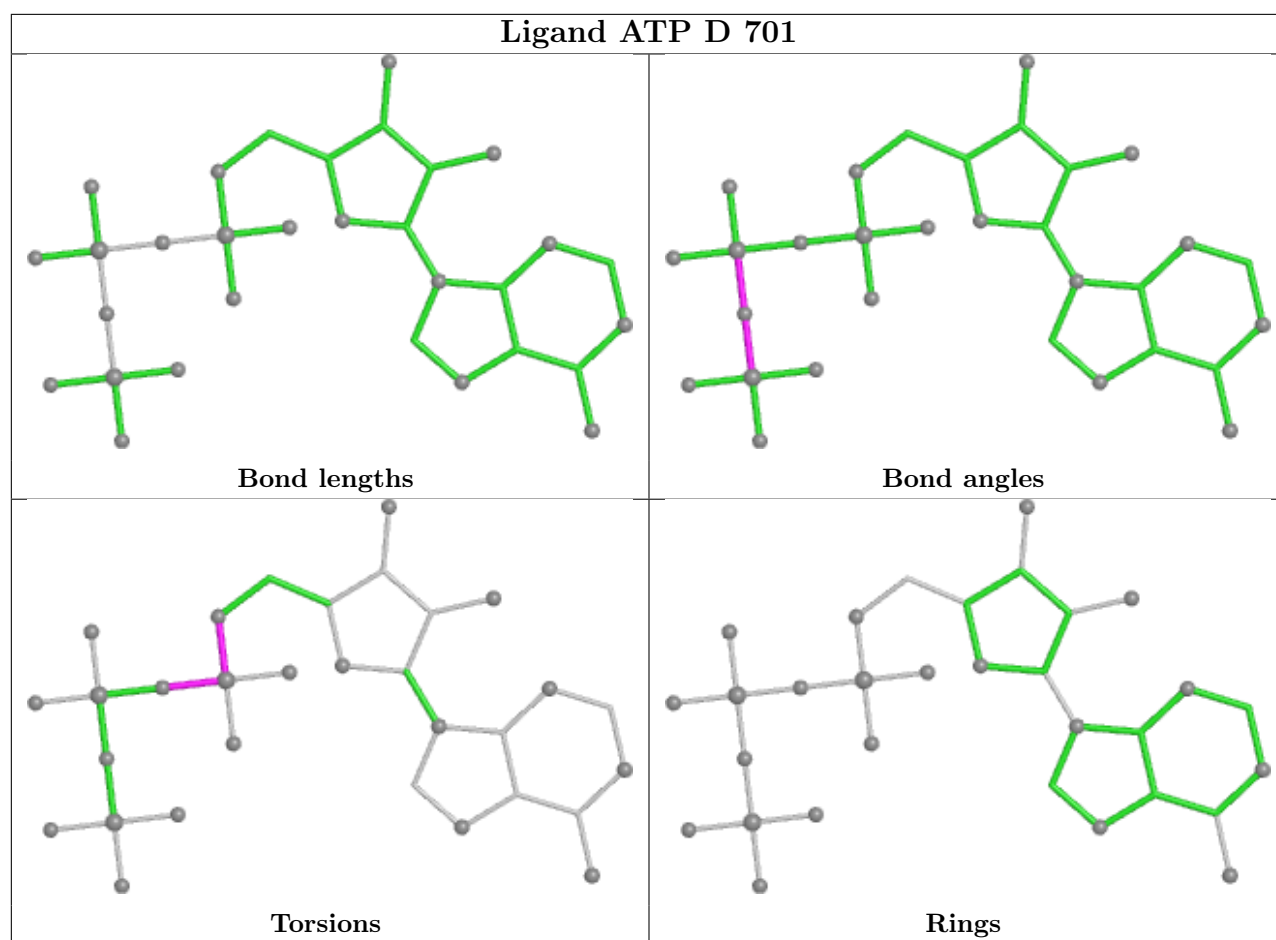
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

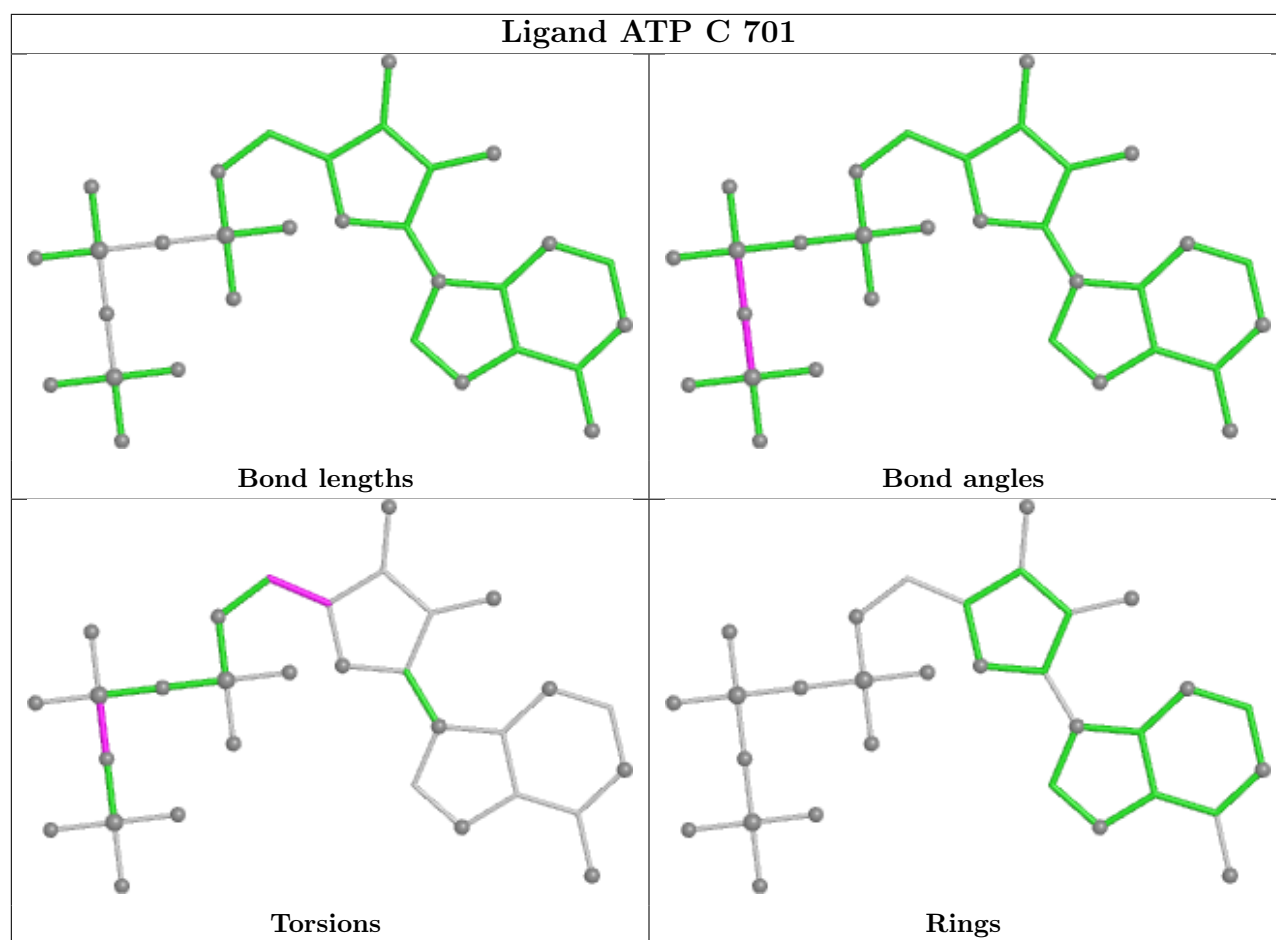












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

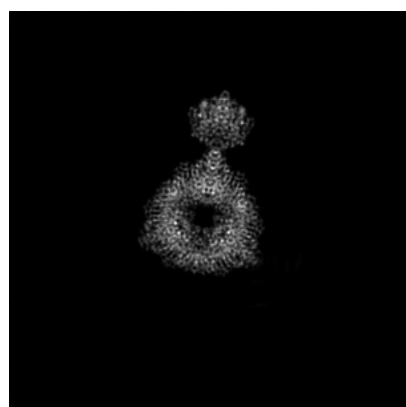
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-65536. These allow visual inspection of the internal detail of the map and identification of artifacts.

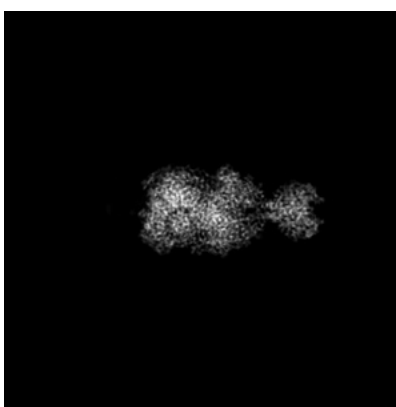
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

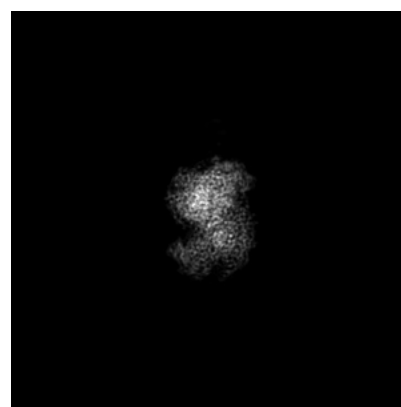
6.1.1 Primary map



X



Y



Z

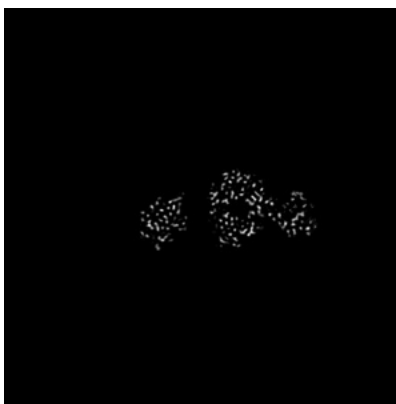
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

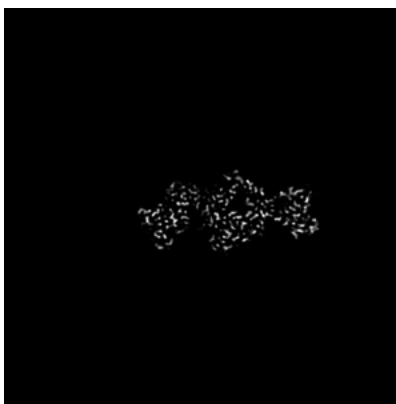
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

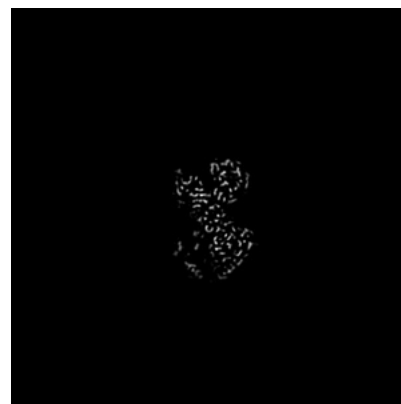
6.3.1 Primary map



X Index: 195



Y Index: 199

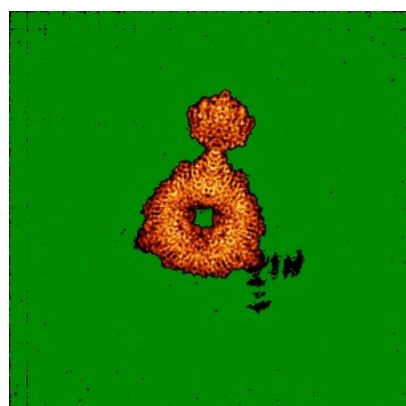


Z Index: 162

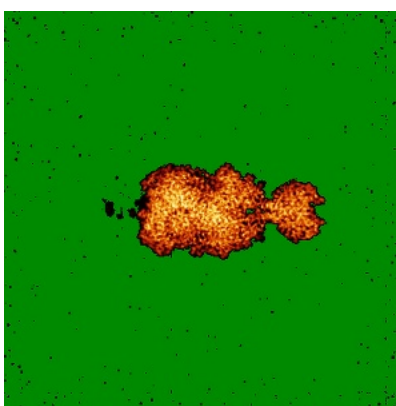
The images above show the largest variance slices of the map in three orthogonal directions.

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

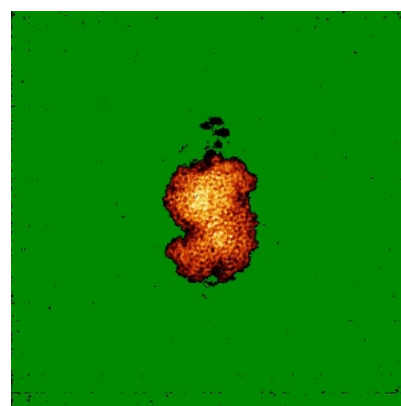
6.4.1 Primary map



X



Y

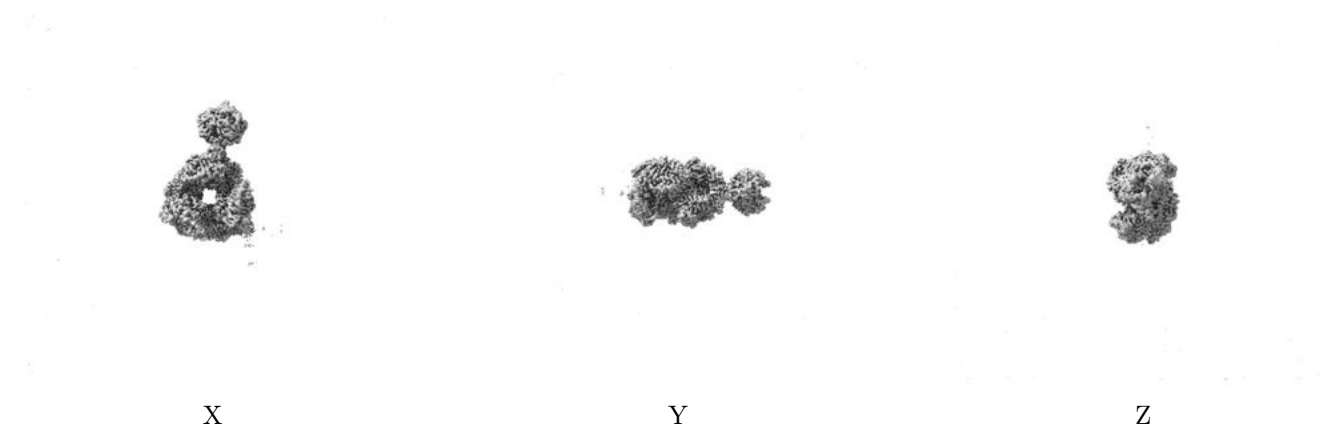


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

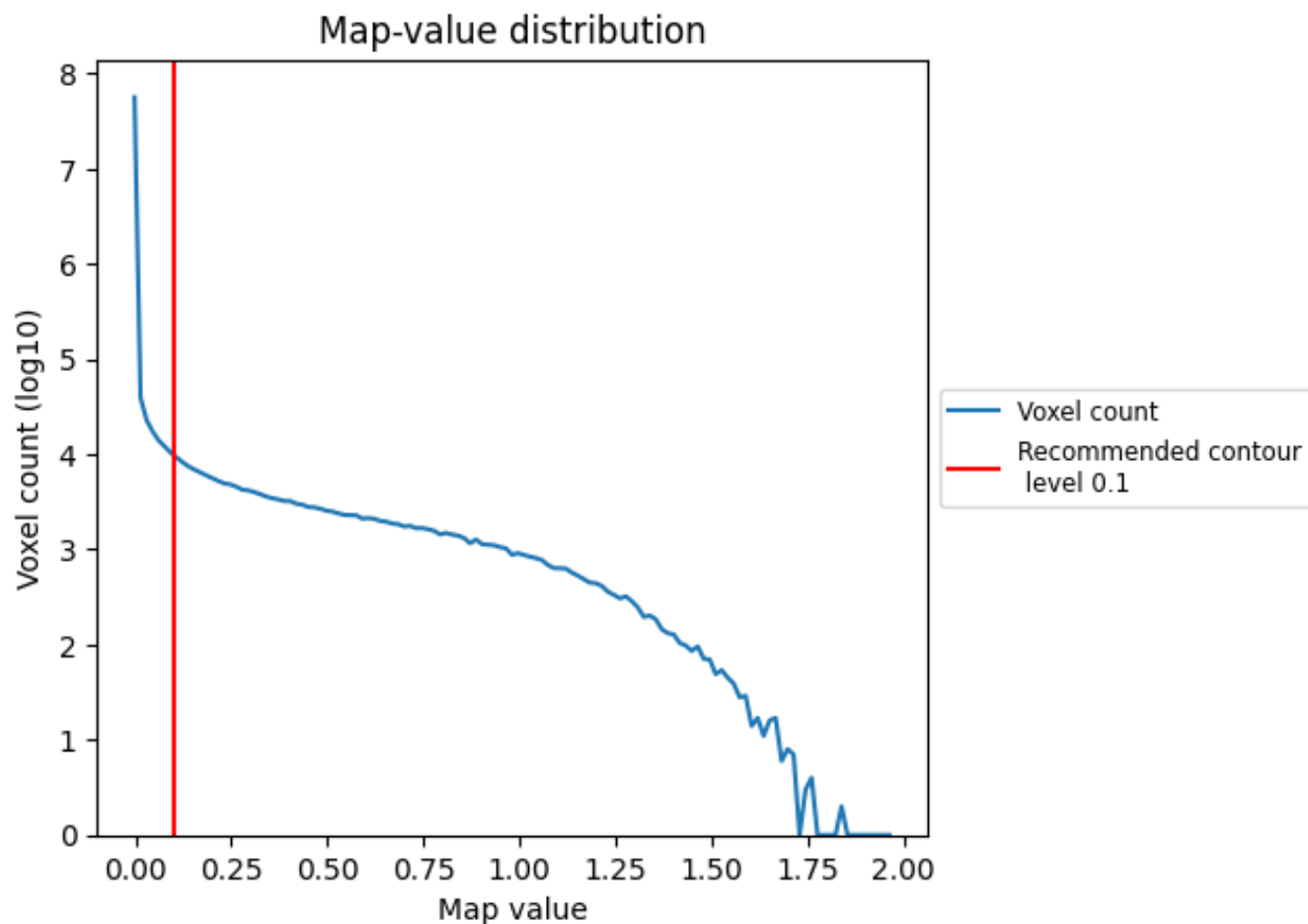
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

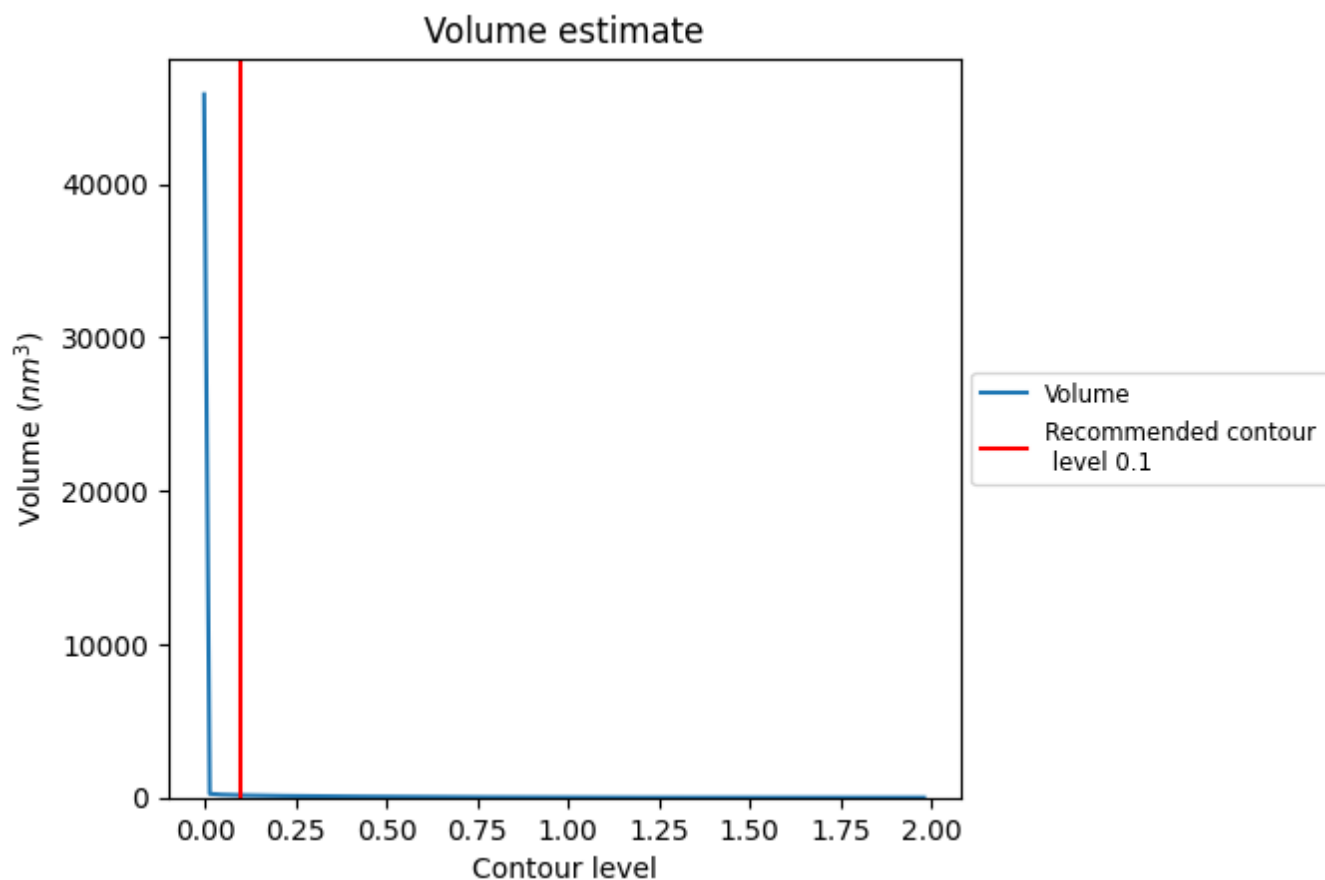
This section contains the results of statistical analysis of the map.

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.

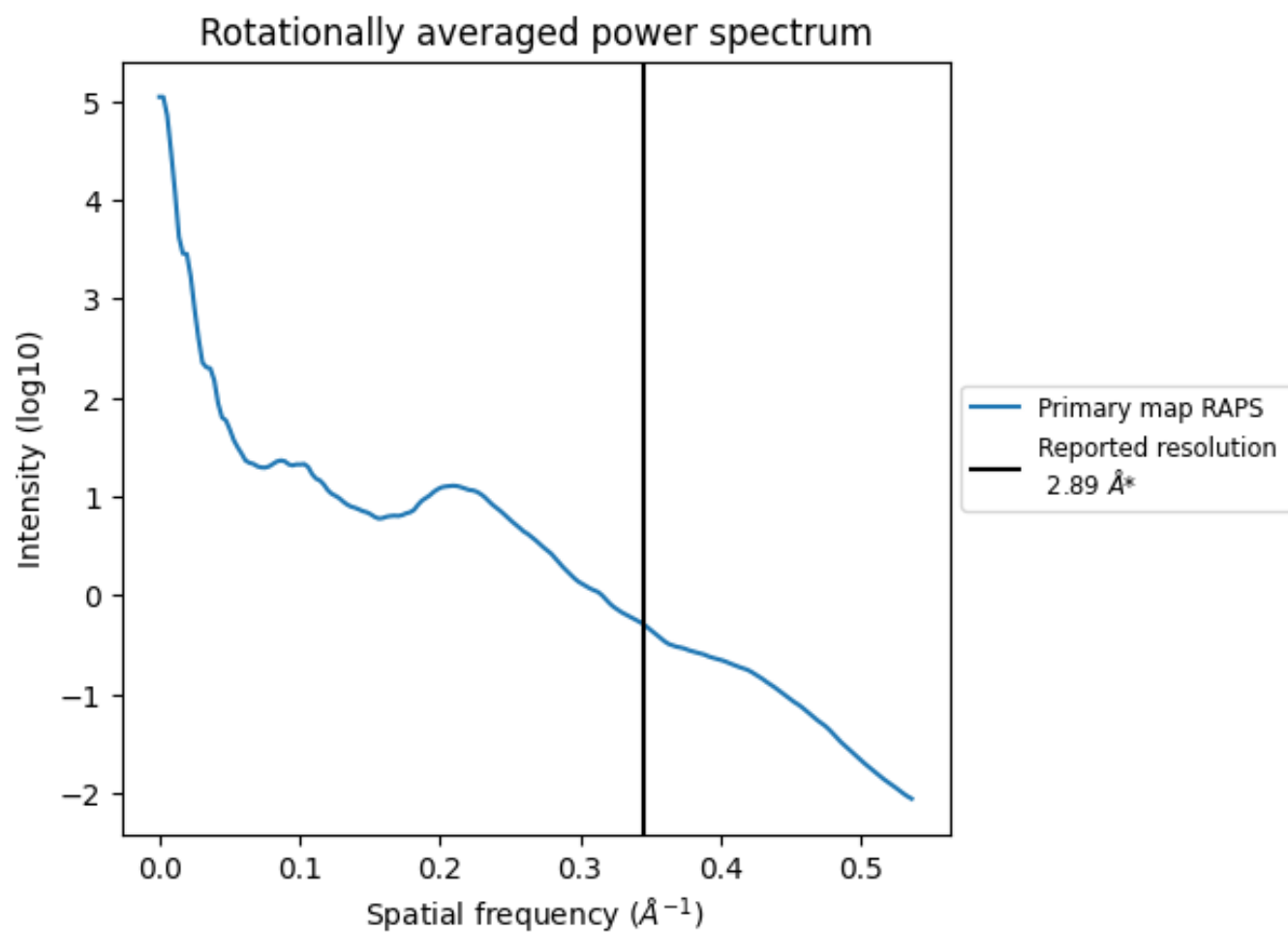
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 153 nm³; this corresponds to an approximate mass of 139 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 0.346 Å⁻¹

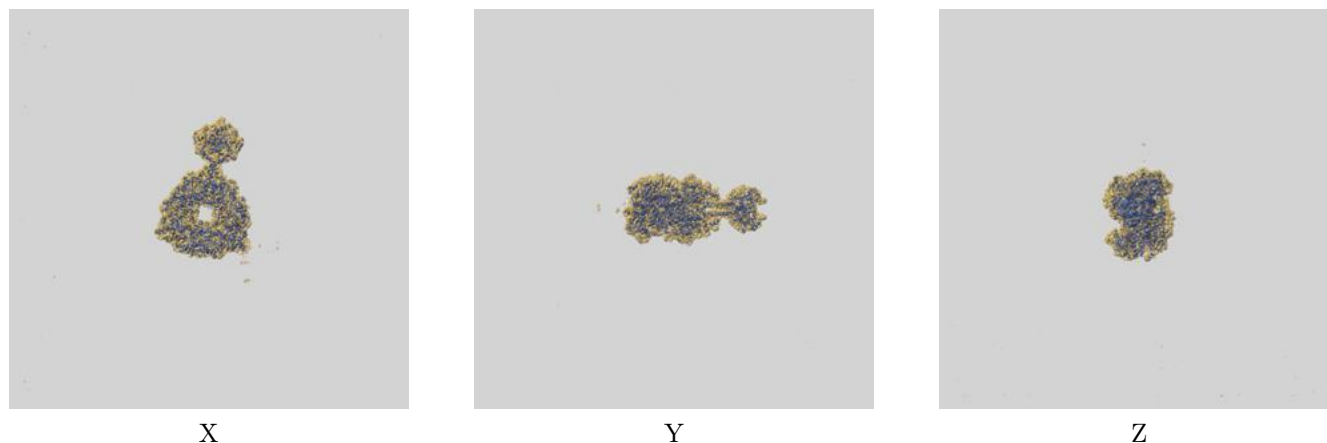
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

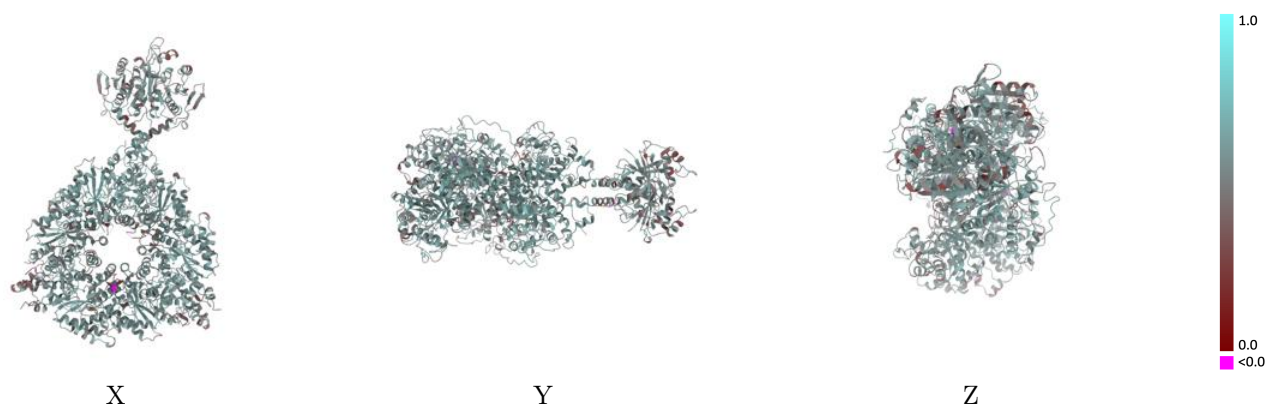
This section contains information regarding the fit between EMDB map EMD-65536 and PDB model 9W1G. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



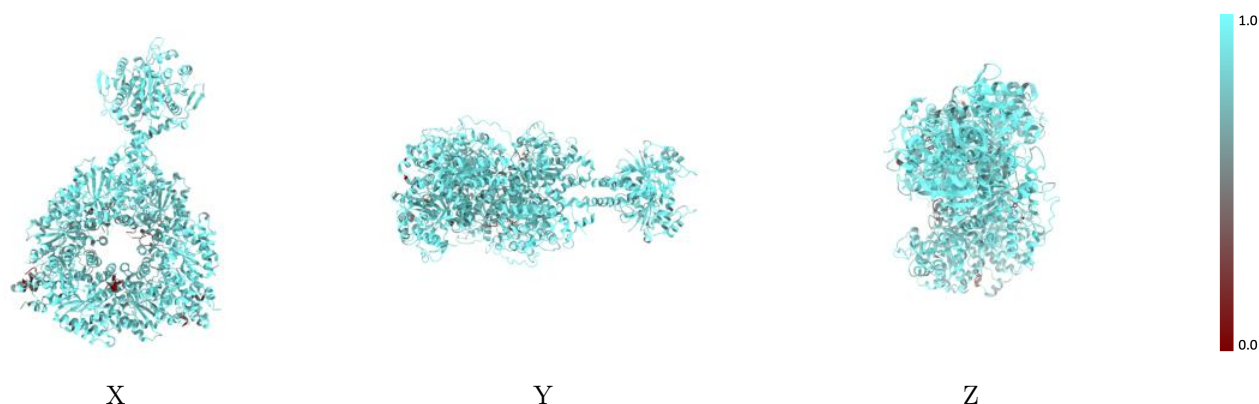
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



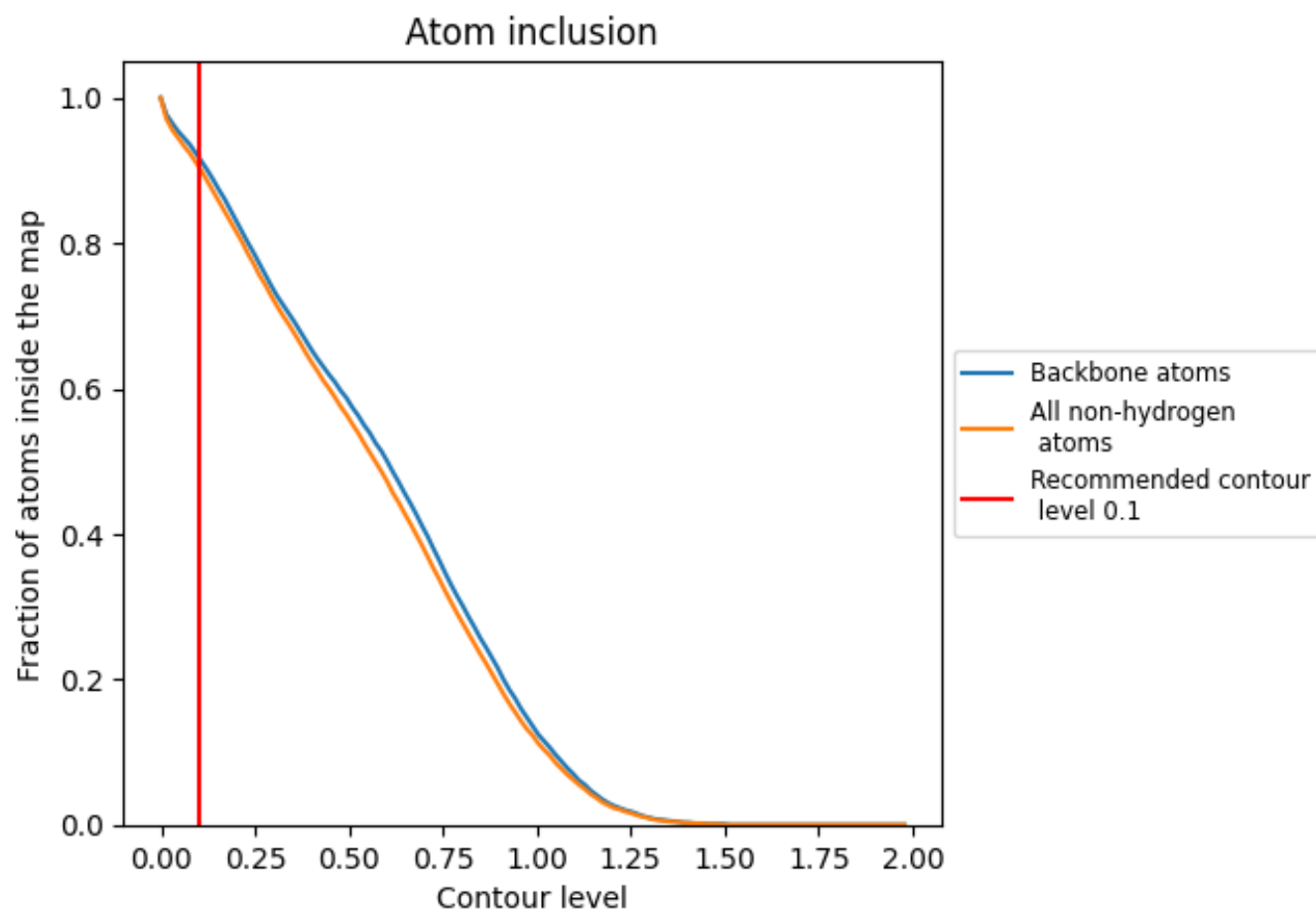
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9050	<div><div></div></div> 0.5500
A	<div><div></div></div> 0.9070	<div><div></div></div> 0.5460
B	<div><div></div></div> 0.9250	<div><div></div></div> 0.5520
C	<div><div></div></div> 0.9230	<div><div></div></div> 0.5620
D	<div><div></div></div> 0.9180	<div><div></div></div> 0.5670
E	<div><div></div></div> 0.8830	<div><div></div></div> 0.5340
F	<div><div></div></div> 0.8910	<div><div></div></div> 0.5430
J	<div><div></div></div> 0.9700	<div><div></div></div> 0.5410

1.0

0.0

<0.0