



Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 06:59 AM EDT

PDB ID : 8G1E
EMDB ID : EMD-29668
Title : Structure of ACLY-D1026A-products-async
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2023-02-02
Resolution : 2.80 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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

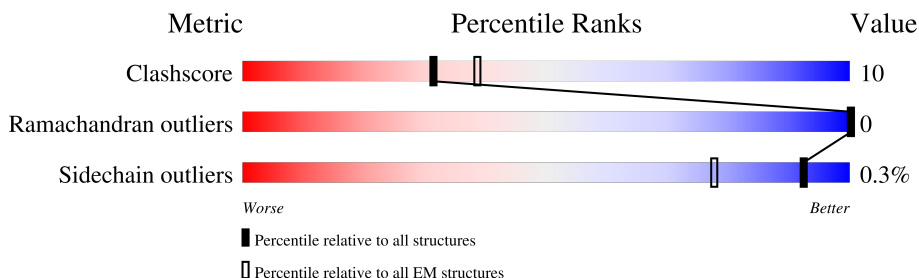
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1101	<div> <div>57%</div> <div>69%</div> <div>25%</div> <div>6%</div> </div>
1	B	1101	<div> <div>70%</div> <div>24%</div> <div>6%</div> </div>
1	C	1101	<div> <div>74%</div> <div>20%</div> <div>6%</div> </div>
1	D	1101	<div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNL	B	2301	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 32649 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.

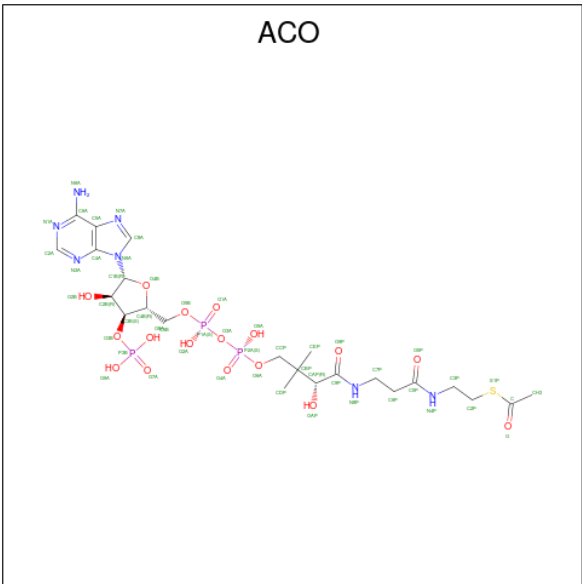
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	B	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	C	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		
1	D	1037	Total	C	N	O	S	2	0
			8017	5133	1360	1478	46		

There are 4 discrepancies between the modelled and reference sequences:

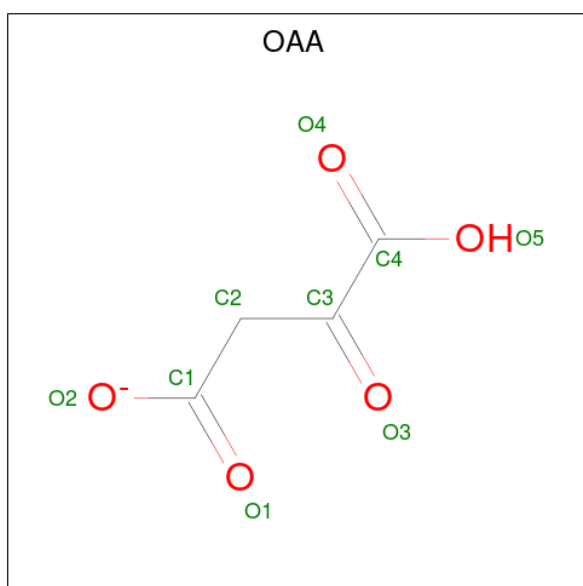
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	B	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	C	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	
2	D	1	Total	C	N	O	P	S	0
			51	23	7	17	3	1	

- Molecule 3 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	4	5	
3	A	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

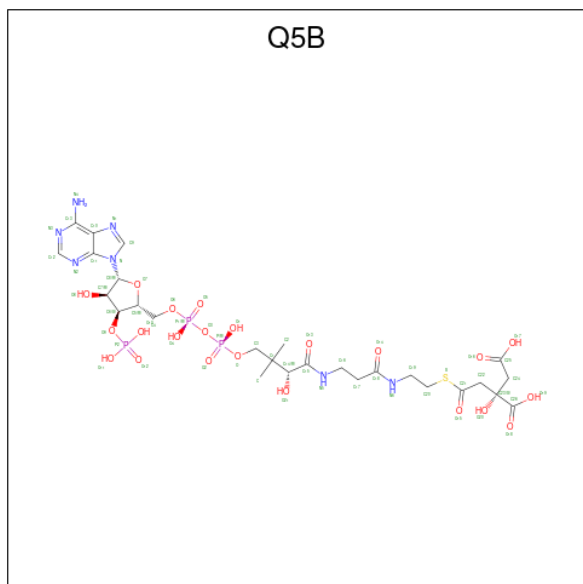
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	C	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total	C	0
			1	1	

- Molecule 5 is (3S)-citryl-Coenzyme A (three-letter code: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$).



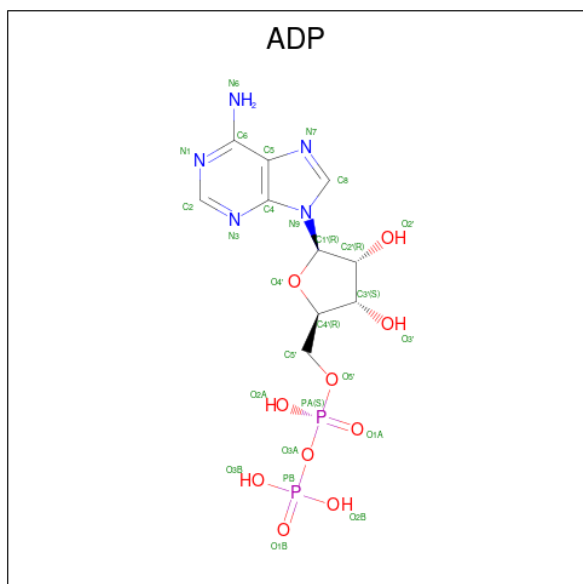
Mol	Chain	Residues	Atoms						AltConf
5	B	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	C	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	
5	D	1	Total	C	N	O	P	S	0
			60	27	7	22	3	1	

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			AltConf
6	B	1	Total	O	P	0
			5	4	1	
6	C	1	Total	O	P	0
			5	4	1	
6	D	1	Total	O	P	0
			5	4	1	

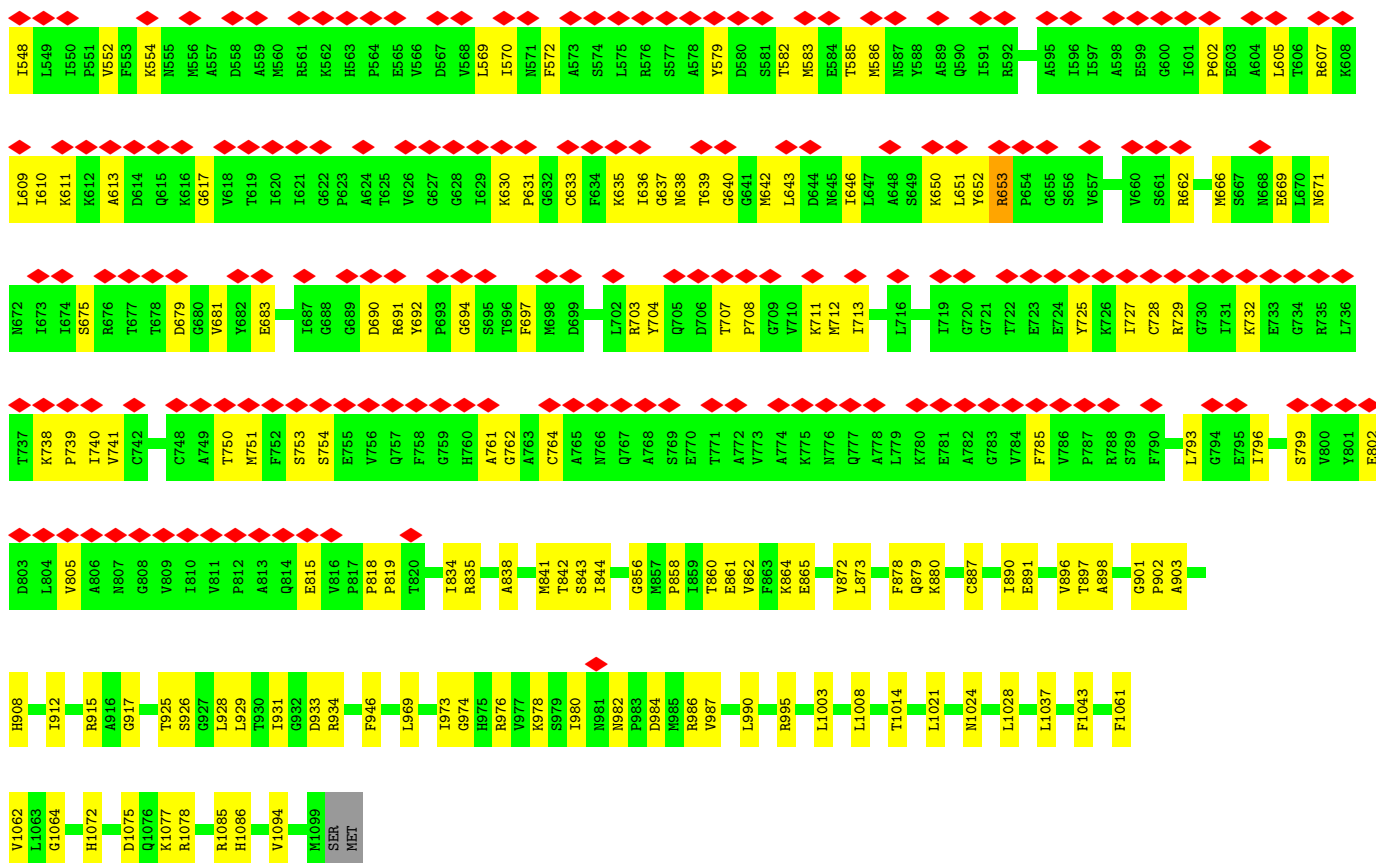
- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



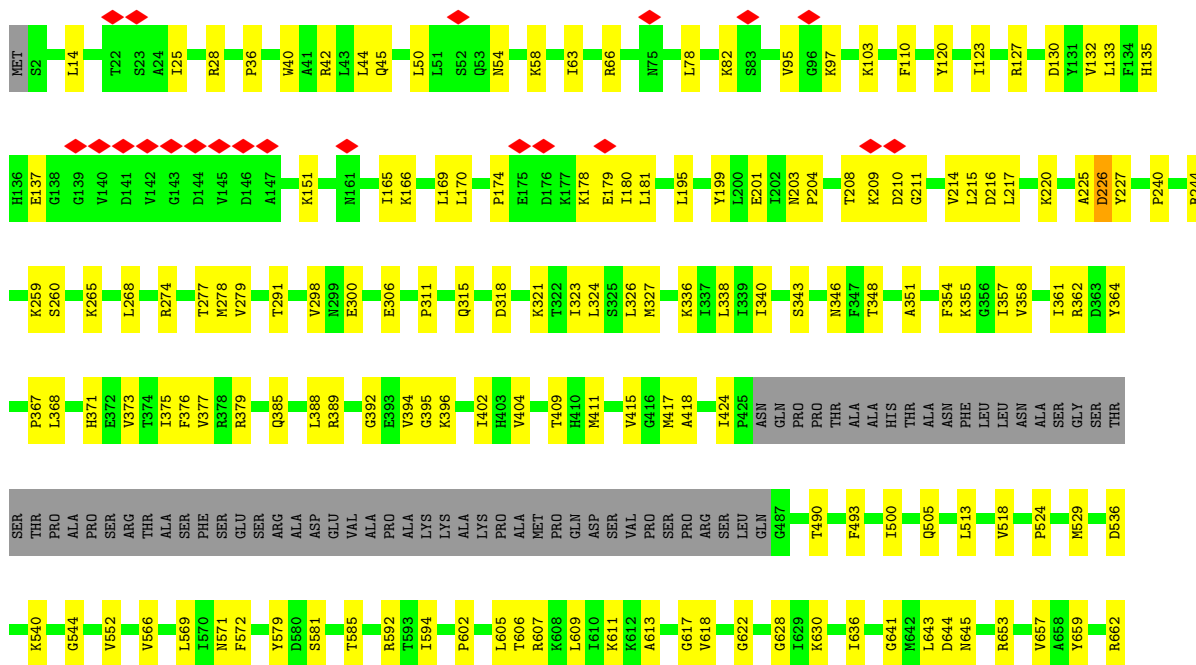
Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
7	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	A	23	Total	O	0
			23	23	
8	B	18	Total	O	0
			18	18	
8	C	29	Total	O	0
			29	29	
8	D	20	Total	O	0
			20	20	

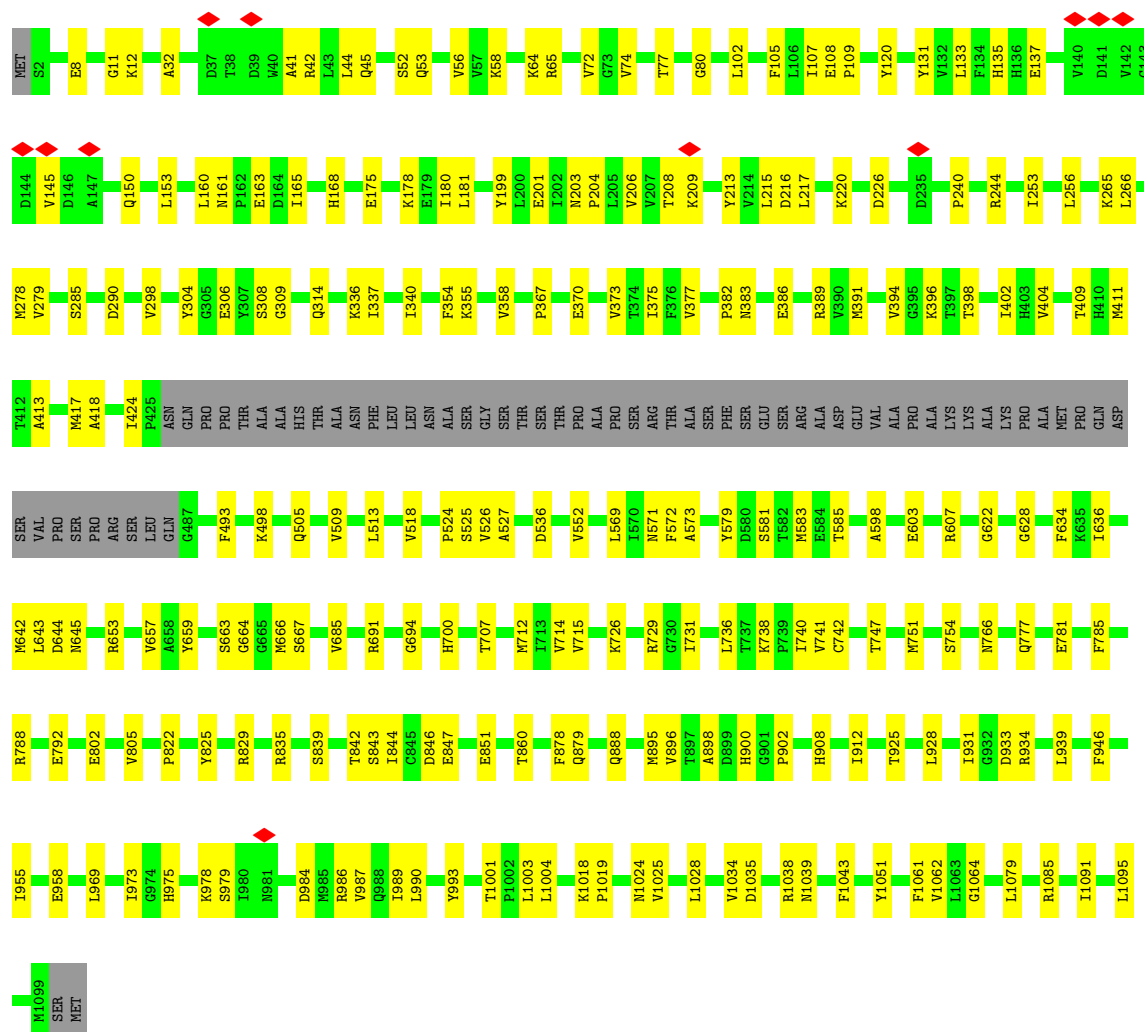


• Molecule 1: ATP-citrate synthase

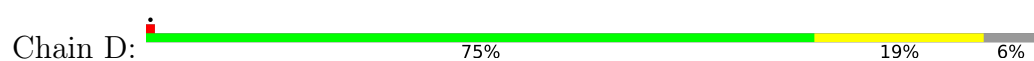




• Molecule 1: ATP-citrate synthase



• Molecule 1: ATP-citrate synthase



L1028	Q888	H700	F493	PRO	L264	H135	MET
V1034	E891	T707	Q505	PRO	K265	G139	S2
D1035		P708	T506	THR	L268	V140	Q9
R1038	M895	K711	R507	ALA		D141	E13
N1039	V896	M712	L513	ALA	T277	V142	L14
	T897	V714	V518	THR	M278	G143	I25
F1043	A898		P524	ASN	V279	D144	Q26
V1062	P902	E718	S525	PHE	C293	V145	N27
L1063		C728	F553	LEU	D294	D146	R28
G1064	H908		K562	ASN	L295	A147	F29
		I731		ALA	N303	L153	K30
H1072	I912	K732	K567	SER	E306	V156	Y31
D1075	R915	R735	D567	GLY			A32
Q1076	A916	L736	V668	SER	I323	I165	R33
K1077	G917	T737	L669	THR	S324	K166	V34
	T925	K738	L569	SER	S325	K167	L44
I1091	L928	V741	F572	THR	L326	H168	Q53
V1094			T585	ALA	M327	L169	N54
	F946	M751	M886	SER	L338	L170	L55
H1098		F752	E599	ARG	I339	P174	K58
M1099	M963	S754	K611	THR	I340	K178	P59
SER	1970	H760	K612	ALA	S343	E179	R66
MET	N971		K628	PHE	F354	D194	V72
	G974	F785	F634	GLU	V358	Y199	N75
	H975	R788	K635	SER	P367	N203	L78
	R976		I636	PHE	L368	L205	D79
	V977	E792	L643	GLU	H371	V206	L89
	K978	L793	D644	VAL	I375	V207	G90
	P983	I797	N645	ALA	F376	T208	Q91
	D984	P822	R653	LYS	V377	K209	K97
	M985	R835	V657	ALA	R378	Y213	F101
	R986	T842	A658	LYS	R379	V214	L102
	V987	S843	Y659	PRO	R389	L215	K103
	Q988	I844	R662	ALA	V390	K220	N104
	T989	E851	S663	PRO	M391	D226	F105
	L990	P858	M666	GLN	G392	Y227	L106
	Y993	I859	V685	ASP	F393	K232	I107
	L1003	T860	V891	SER	V394	P240	E108
	S1016	K864	R691	VAL	V415	R244	P109
	P1019	V872	Y692	PRO	G416		F110
	N1020	F878	S695	SER	R422		Y120
	L1021	Q879		ARG	P425		Y131
	N1024			SER	ASN		L133
	V1025			LEU	GLN		F134
	A1026			G487			
	G1027						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183036	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.00	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.003	Depositor
Minimum map value	-1.655	Depositor
Average map value	0.015	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	182.59999, 182.59999, 182.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: UNL, Q5B, OAA, ADP, ACO, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/8198	0.48	0/11098
1	B	0.26	0/8198	0.49	0/11098
1	C	0.25	0/8198	0.48	0/11098
1	D	0.25	0/8198	0.48	0/11098
All	All	0.25	0/32792	0.48	0/44392

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	8017	0	8057	193	0
1	B	8017	0	8057	179	0
1	C	8017	0	8057	146	0
1	D	8017	0	8057	143	0
2	A	51	0	34	9	0
2	B	51	0	34	8	0
2	C	51	0	34	5	0
2	D	51	0	34	17	0
3	A	18	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	2	0	0
3	D	9	0	2	1	0
4	B	1	0	0	2	0
4	C	1	0	0	0	0
5	B	60	0	0	0	0
5	C	60	0	0	1	0
5	D	60	0	0	3	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	1	0
7	C	27	0	12	0	0
7	D	27	0	12	0	0
8	A	23	0	0	2	0
8	B	18	0	0	0	0
8	C	29	0	0	0	0
8	D	20	0	0	0	0
All	All	32649	0	32396	625	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 (625) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:976:ARG:HD2	2:D:3301:ACO:H2B	1.37	1.06
1:A:1085:ARG:HH11	2:B:2303:ACO:H62A	1.10	0.96
1:B:925:THR:HG23	1:D:925:THR:HG23	1.60	0.83
1:A:1085:ARG:NH1	2:B:2303:ACO:H62A	1.81	0.78
1:A:925:THR:HG23	1:C:925:THR:HG23	1.66	0.77
1:B:1026:ALA:HB2	2:B:2303:ACO:HH32	1.68	0.75
1:A:97:LYS:HE3	1:A:753:SER:HA	1.71	0.73
1:D:976:ARG:HG3	2:D:3301:ACO:O1A	1.89	0.73
1:A:391:MET:HA	1:A:394:VAL:HG12	1.72	0.71
1:D:663:SER:HB2	1:D:666:MET:HB2	1.72	0.71
1:C:58:LYS:HB3	1:C:72:VAL:HG23	1.71	0.70
1:B:165:ILE:HG23	1:B:169:LEU:HD23	1.72	0.70
1:A:987:VAL:HG13	1:A:1028:LEU:HD22	1.72	0.70
1:A:536:ASP:HA	1:A:552:VAL:O	1.90	0.70
1:D:167:LYS:HE3	1:D:168:HIS:CE1	2.28	0.69
1:B:974:GLY:O	1:B:1024:ASN:ND2	2.23	0.69
1:A:713:ILE:HB	1:A:740:ILE:HG12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:PRO:O	1:D:371:HIS:ND1	2.22	0.68
1:A:653:ARG:NH2	1:A:679:ASP:O	2.27	0.68
1:B:278:MET:HB2	1:B:340:ILE:HA	1.76	0.68
1:C:939:LEU:HD22	1:C:1061:PHE:HB2	1.76	0.68
1:B:123:ILE:HG13	1:B:132:VAL:HG22	1.76	0.68
1:C:1085:ARG:HG2	2:D:3301:ACO:N6A	2.09	0.68
1:A:327:MET:O	1:A:336:LYS:NZ	2.27	0.67
1:A:338:LEU:HB3	1:A:375:ILE:HG12	1.77	0.67
1:D:206:VAL:HG23	1:D:213:TYR:HB2	1.76	0.67
1:B:971:MET:HA	2:B:2303:ACO:H62	1.76	0.67
1:A:277:THR:HG22	1:A:339:ILE:HB	1.77	0.67
1:B:367:PRO:O	1:B:371:HIS:ND1	2.23	0.67
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.76	0.66
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.78	0.66
1:B:976:ARG:HD2	2:B:2303:ACO:H2B	1.77	0.66
1:C:120:TYR:HD1	1:C:203:ASN:HD22	1.44	0.66
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.77	0.66
1:A:934:ARG:NH1	1:B:915:ARG:O	2.29	0.66
2:A:1201:ACO:H62A	1:B:1085:ARG:NH1	1.95	0.65
1:D:27:ASN:HA	1:D:30:LYS:HD3	1.77	0.65
1:C:120:TYR:HB3	1:C:135:HIS:HB3	1.79	0.65
1:A:206:VAL:HG23	1:A:213:TYR:HB2	1.77	0.64
1:A:838:ALA:O	1:B:540:LYS:NZ	2.26	0.64
1:A:343:SER:O	1:A:379:ARG:NH1	2.30	0.64
1:C:336:LYS:HB2	1:C:373:VAL:HG22	1.80	0.64
1:D:156:VAL:HB	1:D:611:LYS:HD2	1.79	0.64
1:D:793:LEU:O	1:D:797:ILE:HG13	1.98	0.64
1:A:509:VAL:HG23	1:A:526:VAL:HG21	1.80	0.64
1:C:835:ARG:HG3	1:D:822:PRO:HB2	1.80	0.63
1:D:513:LEU:HD22	1:D:524:PRO:HB3	1.80	0.63
1:B:58:LYS:NZ	1:B:215:LEU:O	2.30	0.63
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.80	0.63
1:A:1037:LEU:HD22	1:A:1043:PHE:HE2	1.61	0.63
1:B:120:TYR:HB3	1:B:135:HIS:HB3	1.81	0.63
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.81	0.63
1:D:338:LEU:HB3	1:D:375:ILE:HG12	1.81	0.62
1:D:691:ARG:HH11	1:D:692:TYR:HE1	1.45	0.62
1:A:802:GLU:HA	1:A:805:VAL:HG12	1.80	0.62
1:B:741:VAL:HG22	1:B:785:PHE:HB2	1.80	0.62
1:C:513:LEU:HD22	1:C:524:PRO:HB3	1.81	0.62
1:A:510:GLN:OE1	1:B:835:ARG:NH1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:GLN:NE2	1:C:168:HIS:O	2.32	0.62
1:C:979:SER:HB3	1:C:1019:PRO:HB2	1.81	0.62
1:D:1024:ASN:HD22	2:D:3301:ACO:H21	1.64	0.62
1:A:498:LYS:HD2	1:A:527:ALA:HB2	1.82	0.62
1:A:946:PHE:HB3	1:A:1003:LEU:HD11	1.81	0.62
1:A:976:ARG:HB2	2:A:1201:ACO:H3B	1.81	0.62
1:B:170:LEU:O	1:B:178:LYS:NZ	2.32	0.62
1:B:987:VAL:HG13	1:B:1028:LEU:HD22	1.81	0.62
1:C:265:LYS:HB2	1:C:306:GLU:HG3	1.82	0.62
1:C:340:ILE:HB	1:C:377:VAL:HG22	1.82	0.61
1:A:976:ARG:HD2	2:A:1201:ACO:H2B	1.81	0.61
1:B:513:LEU:HD22	1:B:524:PRO:HB3	1.82	0.61
1:A:378:ARG:HB2	1:A:414:ILE:HG21	1.83	0.61
1:C:337:ILE:HG21	1:C:418:ALA:HB1	1.83	0.61
1:D:278:MET:HB2	1:D:340:ILE:HA	1.83	0.61
1:D:987:VAL:HG13	1:D:1028:LEU:HD22	1.81	0.61
1:A:691:ARG:NH1	1:A:764:CYS:O	2.32	0.61
1:A:505:GLN:HB3	1:A:508:ALA:HB3	1.83	0.61
1:C:58:LYS:NZ	1:C:216:ASP:OD1	2.30	0.60
1:D:133:LEU:HD23	1:D:145:VAL:HG22	1.83	0.60
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.83	0.60
1:C:691:ARG:NH2	1:C:766:ASN:OD1	2.34	0.60
1:C:902:PRO:HG2	1:D:1091:ILE:HD13	1.82	0.60
1:B:662:ARG:HG3	1:B:718:GLU:HG2	1.83	0.60
1:C:628:GLY:H	1:C:636:ILE:HB	1.66	0.60
1:B:689:GLY:HA3	1:B:760:HIS:HD1	1.66	0.60
1:B:628:GLY:H	1:B:636:ILE:HB	1.66	0.60
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.83	0.60
1:A:662:ARG:HH22	1:A:762:GLY:HA3	1.67	0.59
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.84	0.59
1:B:338:LEU:HB3	1:B:375:ILE:HG12	1.82	0.59
1:C:32:ALA:HB3	1:C:107:ILE:HB	1.85	0.59
1:B:376:PHE:HE2	1:B:418:ALA:HA	1.68	0.59
1:A:66:ARG:NH2	1:A:216:ASP:OD2	2.36	0.59
1:A:860:THR:HG22	1:C:989:ILE:HD11	1.83	0.59
1:D:295:LEU:HD12	1:D:415:VAL:HG12	1.83	0.59
1:B:518:VAL:HG11	1:B:643:LEU:HD11	1.83	0.59
1:A:707:THR:O	1:A:738:LYS:NZ	2.35	0.59
1:B:44:LEU:HD11	1:B:78:LEU:HD11	1.83	0.59
1:D:928:LEU:HD22	1:D:1062:VAL:HG13	1.84	0.59
1:A:974:GLY:HA2	1:A:1021:LEU:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:LEU:O	1:D:178:LYS:NZ	2.35	0.58
1:D:277:THR:HB	1:D:279:VAL:HG23	1.84	0.58
1:B:721:GLY:N	1:B:770:GLU:OE1	2.36	0.58
1:A:903:ALA:HB2	1:B:1091:ILE:HD11	1.86	0.58
1:B:36:PRO:HG2	1:B:103:LYS:HG3	1.85	0.58
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.38	0.58
1:B:327:MET:O	1:B:336:LYS:NZ	2.31	0.58
1:D:844:ILE:HG22	1:D:879:GLN:NE2	2.19	0.58
1:B:592:ARG:NH2	1:B:617:GLY:O	2.36	0.58
1:D:974:GLY:O	2:D:3301:ACO:H143	2.02	0.58
1:A:741:VAL:HG22	1:A:785:PHE:HB2	1.85	0.58
1:B:340:ILE:HB	1:B:377:VAL:HG22	1.86	0.58
1:D:166:LYS:HE3	1:D:178:LYS:HB3	1.86	0.58
1:A:156:VAL:O	1:A:611:LYS:NZ	2.25	0.58
1:B:602:PRO:HB2	1:B:605:LEU:HD23	1.86	0.58
1:A:569:LEU:HD22	1:A:585:THR:HG21	1.86	0.57
1:C:934:ARG:NH1	1:D:915:ARG:O	2.37	0.57
1:D:97:LYS:HE3	1:D:753:SER:HA	1.85	0.57
1:C:1085:ARG:HG2	2:D:3301:ACO:H62A	1.69	0.57
1:D:976:ARG:HH11	2:D:3301:ACO:H8A	1.68	0.57
1:A:127:ARG:HG3	1:A:692:TYR:CE1	2.40	0.57
1:C:12:LYS:NZ	1:C:108:GLU:OE1	2.38	0.57
1:D:204:PRO:HD2	1:D:215:LEU:HB2	1.87	0.57
1:D:628:GLY:H	1:D:636:ILE:HB	1.69	0.57
1:C:498:LYS:HD2	1:C:527:ALA:HB2	1.86	0.57
1:B:933:ASP:OD1	1:B:934:ARG:N	2.37	0.57
1:B:1078:ARG:NH2	1:D:879:GLN:OE1	2.38	0.57
1:D:167:LYS:HE3	1:D:168:HIS:HE1	1.67	0.57
1:D:340:ILE:HB	1:D:377:VAL:HG22	1.87	0.57
1:D:358:VAL:HG11	1:D:390:VAL:HG12	1.86	0.57
1:D:976:ARG:HD2	2:D:3301:ACO:H8A	1.86	0.57
1:A:974:GLY:O	2:A:1201:ACO:H143	2.05	0.56
1:D:788:ARG:NH2	1:D:792:GLU:OE2	2.38	0.56
1:A:253:ILE:HG13	1:A:266:LEU:HD23	1.87	0.56
1:A:872:VAL:HG21	1:C:895:MET:HG2	1.86	0.56
1:B:260:SER:HB3	1:D:1019:PRO:HD3	1.87	0.56
1:B:1088:TRP:NE1	1:C:847:GLU:OE2	2.30	0.56
1:C:42:ARG:HD2	1:C:45:GLN:HE22	1.70	0.56
1:C:685:VAL:HG11	1:C:700:HIS:CE1	2.41	0.56
1:C:825:TYR:OH	1:C:829:ARG:NH2	2.38	0.56
1:B:343:SER:HB2	1:B:669:GLU:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HA	1:A:391:MET:SD	2.46	0.56
1:B:714:VAL:HG21	1:B:797:ILE:HD12	1.85	0.56
1:B:802:GLU:HA	1:B:805:VAL:HG12	1.87	0.56
1:B:375:ILE:HB	1:B:402:ILE:HG12	1.87	0.56
1:B:750:THR:HG21	1:B:771:THR:HB	1.88	0.56
1:B:1005:ASP:O	1:B:1009:GLU:HG2	2.05	0.56
1:A:54:ASN:HD21	1:A:75:ASN:HA	1.71	0.56
1:B:66:ARG:NH2	1:B:216:ASP:OD2	2.38	0.56
1:A:799:SER:O	1:A:802:GLU:HG3	2.06	0.56
1:C:383:ASN:H	1:C:642:MET:HE1	1.69	0.56
2:A:1201:ACO:HH33	3:A:1202:OAA:H22	1.88	0.56
1:C:822:PRO:HB2	1:D:835:ARG:HB2	1.88	0.56
1:C:1091:ILE:HD13	1:D:902:PRO:HG2	1.87	0.56
1:D:518:VAL:HG11	1:D:643:LEU:HD11	1.87	0.56
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.88	0.55
1:A:324:LEU:HA	1:A:327:MET:HG3	1.89	0.55
1:A:570:ILE:HD13	1:A:637:GLY:H	1.69	0.55
1:B:1094:VAL:HG23	1:C:843:SER:HB3	1.88	0.55
1:A:878:PHE:HB3	1:A:1043:PHE:HZ	1.71	0.55
1:B:844:ILE:HG22	1:B:879:GLN:NE2	2.22	0.55
1:C:53:GLN:HE21	1:C:109:PRO:HG3	1.71	0.55
1:A:216:ASP:OD1	1:A:217:LEU:N	2.39	0.55
1:D:644:ASP:OD1	1:D:645:ASN:N	2.39	0.55
1:A:605:LEU:O	1:A:609:LEU:HG	2.06	0.55
1:B:336:LYS:HB2	1:B:373:VAL:HG22	1.88	0.55
1:B:657:VAL:HG13	1:B:712:MET:HG3	1.89	0.55
1:B:707:THR:O	1:B:738:LYS:NZ	2.40	0.55
1:B:208:THR:HG22	1:B:209:LYS:H	1.71	0.55
1:C:908:HIS:O	1:C:912:ILE:HG12	2.07	0.55
1:A:336:LYS:HB2	1:A:373:VAL:HG22	1.89	0.54
1:C:42:ARG:HD2	1:C:45:GLN:NE2	2.22	0.54
1:D:975:HIS:CG	1:D:976:ARG:H	2.25	0.54
1:A:521:ARG:NH1	1:A:633:CYS:O	2.40	0.54
1:C:644:ASP:OD1	1:C:645:ASN:N	2.41	0.54
2:C:3301:ACO:HN8	2:C:3301:ACO:H62A	1.56	0.54
1:A:834:ILE:HD11	1:B:825:TYR:HA	1.89	0.54
1:C:788:ARG:NH2	1:C:792:GLU:OE2	2.41	0.54
1:B:291:THR:HG23	1:B:415:VAL:HG11	1.88	0.54
1:A:340:ILE:HB	1:A:377:VAL:HG22	1.89	0.54
1:A:199:TYR:HB3	1:A:220:LYS:HB2	1.89	0.54
1:D:860:THR:O	1:D:864:LYS:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:963:MET:HG3	1:D:970:ILE:HG12	1.90	0.54
1:A:159:LYS:NZ	1:A:193:GLU:OE2	2.40	0.54
1:A:1037:LEU:HD22	1:A:1043:PHE:CE2	2.41	0.54
1:B:265:LYS:HB2	1:B:306:GLU:HG3	1.88	0.54
1:A:928:LEU:HD22	1:A:1062:VAL:HG13	1.90	0.53
1:B:199:TYR:OH	1:B:201:GLU:OE1	2.26	0.53
1:B:388:LEU:HD22	1:B:404:VAL:HB	1.90	0.53
1:B:644:ASP:OD1	1:B:645:ASN:N	2.40	0.53
1:D:324:LEU:HA	1:D:327:MET:HG2	1.90	0.53
1:A:543:TRP:HB2	1:A:548:ILE:HG23	1.89	0.53
1:B:343:SER:O	1:B:379:ARG:NH1	2.41	0.53
1:B:606:THR:HA	1:B:609:LEU:HD12	1.89	0.53
1:C:518:VAL:HG11	1:C:643:LEU:HD11	1.90	0.53
1:A:908:HIS:O	1:A:912:ILE:HG12	2.08	0.53
1:C:77:THR:HG23	1:C:80:GLY:H	1.74	0.53
1:A:750:THR:OG1	1:A:751:MET:SD	2.65	0.53
1:D:976:ARG:HD3	2:D:3301:ACO:O2A	2.09	0.53
1:B:216:ASP:OD1	1:B:217:LEU:N	2.42	0.53
1:B:691:ARG:NH2	1:B:766:ASN:OD1	2.42	0.53
1:B:955:ILE:HG13	1:B:958:GLU:H	1.73	0.53
1:B:989:ILE:HD11	1:D:860:THR:HG22	1.90	0.53
1:D:946:PHE:HB3	1:D:1003:LEU:HD11	1.91	0.53
1:A:324:LEU:HD22	1:A:368:LEU:HD21	1.89	0.52
1:C:726:LYS:HG2	1:C:729:ARG:NH2	2.24	0.52
1:A:535:GLY:HA2	1:A:554:LYS:HE2	1.92	0.52
1:A:514:ASP:HA	1:A:517:TYR:HD2	1.73	0.52
1:C:741:VAL:HG22	1:C:785:PHE:HB2	1.91	0.52
1:C:973:ILE:O	2:C:3301:ACO:N6A	2.41	0.52
1:A:887:CYS:O	1:A:891:GLU:HG3	2.09	0.52
1:C:131:TYR:CE1	1:C:153:LEU:HD13	2.45	0.52
1:C:987:VAL:HG13	1:C:1028:LEU:HD22	1.91	0.52
1:D:44:LEU:HD11	1:D:78:LEU:HD11	1.91	0.52
1:D:657:VAL:HG13	1:D:712:MET:HG3	1.92	0.52
1:B:940:ASP:OD2	1:B:944:LYS:NZ	2.38	0.52
1:C:946:PHE:HB3	1:C:1003:LEU:HD11	1.91	0.52
1:D:54:ASN:HD21	1:D:75:ASN:HA	1.75	0.52
1:A:375:ILE:HB	1:A:402:ILE:HG12	1.90	0.52
1:A:902:PRO:HG2	1:B:1091:ILE:HD13	1.92	0.52
1:C:569:LEU:HD22	1:C:585:THR:HG21	1.91	0.52
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.44	0.52
1:A:841:MET:HE3	1:C:1079:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:TYR:HB3	1:B:220:LYS:HB2	1.91	0.52
1:A:683:GLU:HB3	1:A:704:TYR:HE1	1.74	0.52
1:A:690:ASP:HA	1:A:761:ALA:HB3	1.91	0.52
1:D:569:LEU:HD22	1:D:585:THR:HG21	1.92	0.52
2:D:3301:ACO:HH33	3:D:3302:OAA:H22	1.91	0.52
1:A:897:THR:HG21	1:A:1061:PHE:HA	1.92	0.52
1:B:622:GLY:HA2	1:B:694:GLY:H	1.75	0.51
1:C:1024:ASN:HD22	2:C:3301:ACO:H21	1.74	0.51
1:A:377:VAL:HB	1:A:404:VAL:HG12	1.93	0.51
1:B:277:THR:HB	1:B:279:VAL:HG13	1.92	0.51
1:D:31:TYR:HB2	1:D:106:LEU:HD11	1.91	0.51
1:A:32:ALA:HB3	1:A:107:ILE:HB	1.92	0.51
1:A:264:LEU:HD22	1:A:319:TYR:HE2	1.76	0.51
1:A:518:VAL:HG22	1:A:652:TYR:HB3	1.92	0.51
1:D:324:LEU:HD22	1:D:368:LEU:HD21	1.90	0.51
1:D:1026:ALA:HB2	2:D:3301:ACO:HH32	1.92	0.51
1:A:835:ARG:HB2	1:B:822:PRO:HB2	1.92	0.51
1:B:351:ALA:O	1:B:355:LYS:HG2	2.11	0.51
1:D:244:ARG:HH21	1:D:754:SER:HB3	1.76	0.51
1:D:268:LEU:HD13	1:D:303:ASN:HB3	1.92	0.51
1:B:908:HIS:O	1:B:912:ILE:HG12	2.10	0.51
1:C:386:GLU:HA	1:C:389:ARG:HG2	1.92	0.51
1:C:657:VAL:HG13	1:C:712:MET:HG3	1.93	0.51
1:D:971:MET:HA	2:D:3301:ACO:H61	1.92	0.51
1:A:933:ASP:OD1	1:A:934:ARG:N	2.43	0.51
2:A:1201:ACO:N6A	1:B:1085:ARG:NH1	2.59	0.51
1:B:663:SER:HB2	1:B:666:MET:HB2	1.92	0.51
1:C:505:GLN:HG3	1:C:572:PHE:CG	2.45	0.51
1:D:58:LYS:HB3	1:D:72:VAL:HG12	1.91	0.51
1:D:131:TYR:CE1	1:D:153:LEU:HD13	2.46	0.51
1:D:741:VAL:HG22	1:D:785:PHE:HB2	1.93	0.51
1:C:298:VAL:HG21	1:C:751:MET:HB3	1.92	0.51
1:A:166:LYS:HZ1	1:A:179:GLU:HG3	1.76	0.51
1:C:278:MET:HB2	1:C:340:ILE:HA	1.92	0.51
1:A:1094:VAL:HG23	1:D:843:SER:HB3	1.92	0.50
1:C:53:GLN:HG3	1:C:109:PRO:HB3	1.93	0.50
1:C:928:LEU:HD22	1:C:1062:VAL:HG13	1.93	0.50
1:B:1001:THR:HB	1:B:1004:LEU:HB3	1.93	0.50
1:D:53:GLN:HE21	1:D:109:PRO:HB3	1.76	0.50
1:C:201:GLU:O	1:C:217:LEU:HA	2.10	0.50
1:C:955:ILE:HG13	1:C:958:GLU:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:PHE:HZ	1:A:631:PRO:HA	1.76	0.50
1:A:662:ARG:NH2	1:A:690:ASP:O	2.44	0.50
1:B:274:ARG:HG2	1:B:300:GLU:HB3	1.94	0.50
1:B:357:ILE:O	1:B:361:ILE:HG12	2.11	0.50
1:C:290:ASP:OD2	1:C:747:THR:N	2.45	0.50
1:D:851:GLU:OE1	1:D:858:PRO:HB3	2.12	0.50
1:D:59:PRO:O	1:D:66:ARG:NH1	2.40	0.50
1:B:928:LEU:HD22	1:B:1062:VAL:HG13	1.94	0.50
1:C:375:ILE:HB	1:C:402:ILE:HG12	1.94	0.50
1:C:707:THR:O	1:C:738:LYS:NZ	2.44	0.50
1:D:685:VAL:HG11	1:D:700:HIS:CE1	2.46	0.50
1:A:330:GLU:O	1:A:371:HIS:NE2	2.43	0.50
1:A:607:ARG:HA	1:A:692:TYR:HE2	1.75	0.50
1:A:332:HIS:CE1	1:A:334:ASP:HB2	2.46	0.49
1:B:54:ASN:HB3	1:B:110:PHE:HB3	1.92	0.49
1:C:377:VAL:HG21	1:C:391:MET:HE2	1.93	0.49
1:C:1018:LYS:HE3	2:C:3301:ACO:H52A	1.94	0.49
1:D:908:HIS:O	1:D:912:ILE:HG12	2.12	0.49
1:A:130:ASP:OD1	1:A:607:ARG:NH1	2.44	0.49
1:A:529:MET:HB3	1:A:552:VAL:HG22	1.93	0.49
1:B:278:MET:HB2	1:B:340:ILE:HG12	1.93	0.49
1:B:311:PRO:HD2	1:B:348:THR:HG23	1.94	0.49
1:B:613:ALA:HB1	1:B:618:VAL:O	2.13	0.49
1:C:1001:THR:HB	1:C:1004:LEU:HB3	1.93	0.49
1:D:278:MET:HB2	1:D:340:ILE:HG12	1.94	0.49
1:A:253:ILE:HG21	1:A:266:LEU:HB3	1.94	0.49
1:A:328:THR:HG21	1:A:367:PRO:HB2	1.93	0.49
1:C:409:THR:HG22	1:C:411:MET:H	1.77	0.49
1:B:278:MET:SD	1:B:323:ILE:HD11	2.53	0.49
1:D:728:CYS:O	1:D:732:LYS:HG2	2.13	0.49
1:B:728:CYS:O	1:B:732:LYS:HG2	2.12	0.49
1:D:54:ASN:HB3	1:D:110:PHE:HB3	1.95	0.49
1:D:760:HIS:NE2	6:D:3305:PO4:O4	2.42	0.49
1:A:697:PHE:HB3	1:A:727:ILE:HD11	1.94	0.49
1:D:199:TYR:HB3	1:D:220:LYS:HB2	1.95	0.49
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.95	0.49
1:C:64:LYS:HG3	1:C:65:ARG:HG3	1.95	0.49
1:D:567:ASP:N	1:D:567:ASP:OD1	2.44	0.49
1:D:976:ARG:NH1	2:D:3301:ACO:H8A	2.28	0.49
1:A:860:THR:O	1:A:864:LYS:HG2	2.12	0.48
1:A:128:GLU:OE2	1:A:131:TYR:OH	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:TYR:OH	1:A:543:TRP:HA	2.13	0.48
1:A:582:THR:HG21	1:A:609:LEU:HD22	1.95	0.48
1:C:175:GLU:HA	1:C:178:LYS:HG2	1.95	0.48
1:D:293:CYS:HB3	1:D:751:MET:SD	2.53	0.48
1:D:659:TYR:HA	1:D:714:VAL:O	2.13	0.48
1:A:652:TYR:OH	1:A:815:GLU:OE1	2.21	0.48
1:D:265:LYS:HB2	1:D:306:GLU:HG3	1.95	0.48
1:A:708:PRO:O	1:A:711:LYS:NZ	2.47	0.48
1:B:358:VAL:O	1:B:362:ARG:HG3	2.13	0.48
1:B:976:ARG:HG3	2:B:2303:ACO:O1A	2.14	0.48
1:C:663:SER:HB3	1:C:666:MET:HB3	1.95	0.48
1:A:123:ILE:HG23	1:A:132:VAL:HG22	1.94	0.48
1:A:490:THR:HA	1:A:703:ARG:HG2	1.96	0.48
1:A:901:GLY:HA3	1:C:847:GLU:HB3	1.94	0.48
1:A:1078:ARG:NH1	1:C:1051:TYR:OH	2.46	0.48
1:D:208:THR:HG22	1:D:209:LYS:H	1.77	0.48
1:A:691:ARG:HA	1:A:762:GLY:HA2	1.95	0.48
1:B:823:MET:HE3	4:B:2301:UNL:C	2.44	0.48
1:C:844:ILE:HG22	1:C:879:GLN:OE1	2.12	0.48
2:A:1201:ACO:H141	2:A:1201:ACO:H32	1.96	0.48
1:D:888:GLN:HB3	1:D:993:TYR:OH	2.13	0.48
1:A:582:THR:O	1:A:586:MET:HG2	2.14	0.48
1:B:324:LEU:HA	1:B:327:MET:HG2	1.96	0.48
1:B:931:ILE:HD12	1:B:1061:PHE:HE2	1.78	0.48
1:C:203:ASN:O	1:C:216:ASP:HB2	2.14	0.48
1:C:253:ILE:HG13	1:C:266:LEU:HD23	1.96	0.48
1:C:571:ASN:HD21	1:C:581:SER:HB2	1.79	0.48
1:D:9:GLN:OE1	1:D:33:ARG:NH2	2.47	0.48
1:A:671:ASN:HD22	1:A:681:VAL:HG21	1.79	0.48
1:A:1085:ARG:NH2	3:A:1203:OAA:O5	2.37	0.48
1:A:1085:ARG:HD3	2:B:2303:ACO:N7A	2.29	0.48
1:A:345:ALA:HB3	1:A:381:GLY:HA3	1.95	0.48
1:B:42:ARG:HA	1:B:45:GLN:HG3	1.96	0.48
1:B:860:THR:HG22	1:D:989:ILE:HD11	1.96	0.48
1:A:844:ILE:HG22	1:A:879:GLN:NE2	2.28	0.47
1:B:569:LEU:HD22	1:B:585:THR:HG21	1.96	0.47
1:A:712:MET:SD	1:A:739:PRO:HB2	2.54	0.47
1:B:569:LEU:HD23	1:B:594:ILE:HG23	1.96	0.47
1:B:823:MET:CE	4:B:2301:UNL:C	2.92	0.47
1:C:12:LYS:HG2	1:C:217:LEU:HD21	1.96	0.47
1:A:120:TYR:HB3	1:A:135:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ILE:HD11	1:A:694:GLY:HA2	1.96	0.47
1:B:828:ALA:O	1:B:832:GLY:N	2.47	0.47
1:D:1035:ASP:O	1:D:1039:ASN:CB	2.62	0.47
1:A:266:LEU:HD11	1:A:303:ASN:HD22	1.79	0.47
1:A:995:ARG:HH21	1:A:1008:LEU:HD13	1.79	0.47
1:B:244:ARG:HH21	1:B:754:SER:HB3	1.79	0.47
1:C:715:VAL:O	1:C:742:CYS:HA	2.14	0.47
1:D:707:THR:O	1:D:738:LYS:NZ	2.48	0.47
1:A:793:LEU:O	1:A:796:ILE:HG22	2.15	0.47
1:B:240:PRO:HB2	1:B:244:ARG:HB3	1.96	0.47
1:A:531:TYR:CE2	1:A:533:PHE:HB2	2.49	0.47
1:A:986:ARG:NH1	8:A:2405:HOH:O	2.43	0.47
1:B:847:GLU:OE1	1:C:1085:ARG:NH2	2.48	0.47
1:C:8:GLU:HG2	1:C:12:LYS:HE3	1.96	0.47
1:C:664:GLY:O	1:C:667:SER:OG	2.20	0.47
1:A:166:LYS:HZ1	1:A:179:GLU:HA	1.79	0.47
1:A:295:LEU:HD12	1:A:415:VAL:HG12	1.96	0.47
1:B:298:VAL:HG23	1:B:752:PHE:HE1	1.80	0.47
1:B:708:PRO:O	1:B:711:LYS:NZ	2.48	0.47
1:B:1035:ASP:O	1:B:1039:ASN:CB	2.63	0.47
1:C:622:GLY:HA2	1:C:694:GLY:H	1.79	0.47
1:C:986:ARG:CZ	1:C:1025:VAL:HG21	2.45	0.47
1:A:346:ASN:OD1	1:A:640:GLY:N	2.48	0.47
1:A:666:MET:HA	1:A:669:GLU:HB2	1.95	0.47
1:B:1034:VAL:O	1:B:1038:ARG:HG2	2.14	0.47
1:C:898:ALA:HA	1:C:1064:GLY:O	2.15	0.47
1:A:642:MET:CE	1:A:643:LEU:H	2.28	0.47
1:B:794:GLY:O	1:B:797:ILE:HG22	2.15	0.47
1:A:835:ARG:NH1	1:B:544:GLY:O	2.40	0.46
1:A:873:LEU:HD22	1:A:890:ILE:HD13	1.97	0.46
1:C:204:PRO:HB2	1:C:215:LEU:HD22	1.97	0.46
1:A:207:VAL:HG12	1:A:212:VAL:HG12	1.96	0.46
1:A:244:ARG:HH21	1:A:754:SER:HB3	1.80	0.46
1:B:659:TYR:HA	1:B:714:VAL:O	2.15	0.46
1:C:208:THR:HG22	1:C:209:LYS:H	1.79	0.46
1:A:58:LYS:HB3	1:A:72:VAL:HG12	1.97	0.46
1:A:546:LYS:HG2	1:A:547:GLU:H	1.80	0.46
1:B:225:ALA:HB2	1:B:602:PRO:HB3	1.97	0.46
1:B:789:SER:OG	1:B:792:GLU:OE1	2.30	0.46
1:B:846:ASP:HB2	1:C:1095:LEU:HD22	1.96	0.46
1:C:278:MET:HB2	1:C:340:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:PRO:HB2	1:D:244:ARG:HB3	1.97	0.46
1:D:898:ALA:HA	1:D:1064:GLY:O	2.16	0.46
1:B:493:PHE:HB2	1:B:630:LYS:HD3	1.98	0.46
1:C:244:ARG:HH21	1:C:754:SER:HB3	1.79	0.46
1:A:21:THR:HG21	1:A:184:PHE:HA	1.98	0.46
1:A:131:TYR:CE1	1:A:153:LEU:HD13	2.51	0.46
1:A:386:GLU:O	1:A:390:VAL:HG13	2.16	0.46
1:B:259:LYS:HD3	1:D:1016:SER:HA	1.97	0.46
1:B:986:ARG:CZ	1:B:1025:VAL:HG21	2.46	0.46
1:C:240:PRO:HB2	1:C:244:ARG:HB3	1.97	0.46
1:D:493:PHE:CZ	1:D:636:ILE:HD11	2.51	0.46
1:D:735:ARG:HG3	1:D:735:ARG:HH11	1.79	0.46
2:D:3301:ACO:O1A	2:D:3301:ACO:H3B	2.16	0.46
1:B:97:LYS:HE3	1:B:753:SER:HA	1.97	0.46
1:C:931:ILE:HD12	1:C:1061:PHE:HE2	1.81	0.46
1:D:9:GLN:HB3	1:D:33:ARG:HH21	1.81	0.46
1:C:358:VAL:HG12	1:C:394:VAL:HG11	1.98	0.46
1:A:898:ALA:HA	1:A:1064:GLY:O	2.15	0.45
1:A:980:ILE:O	1:C:314:GLN:HG2	2.16	0.45
1:C:354:PHE:O	1:C:358:VAL:HG13	2.16	0.45
1:A:57:VAL:HG21	1:A:85:LEU:HD21	1.97	0.45
1:B:174:PRO:O	1:B:178:LYS:HG3	2.16	0.45
1:B:130:ASP:OD1	1:B:607:ARG:NH1	2.40	0.45
1:B:195:LEU:O	1:B:195:LEU:HD23	2.15	0.45
1:A:54:ASN:OD1	1:A:55:LEU:N	2.44	0.45
1:A:891:GLU:OE1	8:A:2401:HOH:O	2.21	0.45
1:B:324:LEU:HD22	1:B:368:LEU:HD21	1.98	0.45
1:C:536:ASP:HA	1:C:552:VAL:O	2.17	0.45
1:D:55:LEU:HD13	1:D:107:ILE:HG21	1.97	0.45
1:A:650:LYS:HE2	1:A:675:SER:HB2	1.97	0.45
1:B:794:GLY:HA2	1:B:797:ILE:HG22	1.98	0.45
1:C:731:ILE:HG12	1:C:736:LEU:HB2	1.99	0.45
1:C:888:GLN:HB3	1:C:993:TYR:OH	2.15	0.45
1:D:358:VAL:HG12	1:D:394:VAL:HG11	1.98	0.45
1:A:225:ALA:HB2	1:A:602:PRO:HB3	1.99	0.45
1:B:376:PHE:CE2	1:B:418:ALA:HA	2.50	0.45
1:B:1097:GLU:HG3	1:B:1098:HIS:N	2.32	0.45
1:C:11:GLY:HA3	1:C:217:LEU:HD11	1.98	0.45
1:D:101:PHE:HB2	1:D:103:LYS:NZ	2.32	0.45
1:B:579:TYR:CG	1:B:605:LEU:HD12	2.52	0.45
1:A:2:SER:OG	1:A:3:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASN:HD21	1:A:640:GLY:H	1.65	0.45
1:B:14:LEU:HD21	1:B:195:LEU:HD21	1.99	0.45
1:C:394:VAL:O	1:C:398:THR:OG1	2.28	0.45
1:C:659:TYR:HA	1:C:714:VAL:O	2.17	0.45
1:D:976:ARG:NH1	2:D:3301:ACO:C8A	2.80	0.45
1:A:298:VAL:HG21	1:A:751:MET:HB3	1.98	0.45
1:B:25:ILE:HG23	1:B:28:ARG:HH21	1.81	0.45
1:C:279:VAL:HG21	1:C:285:SER:HA	1.99	0.45
1:C:573:ALA:O	1:C:598:ALA:HB2	2.17	0.45
1:A:203:ASN:HA	1:A:204:PRO:HA	1.72	0.45
1:A:856:GLY:HA3	1:D:1098:HIS:HA	1.99	0.45
1:B:389:ARG:O	1:B:392:GLY:N	2.50	0.45
1:B:843:SER:OG	1:D:1075:ASP:OD1	2.34	0.45
1:A:635:LYS:HD2	1:A:639:THR:O	2.17	0.44
1:A:978:LYS:HE2	1:A:982:ASN:O	2.16	0.44
1:C:969:LEU:HD22	2:C:3301:ACO:C4A	2.47	0.44
1:D:194:ASP:O	1:D:232:LYS:NZ	2.34	0.44
1:D:1026:ALA:HB2	2:D:3301:ACO:CH3	2.47	0.44
1:B:571:ASN:HD21	1:B:581:SER:HB2	1.83	0.44
1:C:1035:ASP:O	1:C:1039:ASN:CB	2.65	0.44
1:A:725:TYR:HB3	1:A:729:ARG:HH12	1.82	0.44
1:B:354:PHE:O	1:B:358:VAL:HG13	2.17	0.44
1:A:279:VAL:HB	1:A:285:SER:OG	2.18	0.44
1:A:976:ARG:NH1	2:A:1201:ACO:O2B	2.50	0.44
1:D:662:ARG:HG3	1:D:718:GLU:HG2	1.99	0.44
1:D:983:PRO:O	1:D:985:MET:HG2	2.17	0.44
1:A:274:ARG:HD2	1:A:332:HIS:CE1	2.52	0.44
1:A:274:ARG:HG2	1:A:300:GLU:OE2	2.16	0.44
1:B:888:GLN:HB3	1:B:993:TYR:OH	2.17	0.44
1:A:843:SER:HB3	1:D:1094:VAL:HG23	1.99	0.44
1:A:858:PRO:O	1:A:862:VAL:HG23	2.18	0.44
1:B:602:PRO:O	1:B:606:THR:HG23	2.18	0.44
1:B:685:VAL:HG11	1:B:700:HIS:CE1	2.53	0.44
1:B:917:GLY:HA2	1:B:1077:LYS:NZ	2.32	0.44
1:C:1034:VAL:O	1:C:1038:ARG:HG2	2.17	0.44
1:A:278:MET:SD	1:A:340:ILE:HG12	2.58	0.44
1:C:52:SER:HB2	1:C:53:GLN:OE1	2.18	0.44
1:C:285:SER:HB3	1:C:304:TYR:CE1	2.52	0.44
1:B:984:ASP:HB3	1:B:987:VAL:H	1.83	0.44
1:C:377:VAL:HB	1:C:404:VAL:HG12	2.00	0.44
1:D:257:ASP:OD1	1:D:264:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ALA:O	1:A:617:GLY:N	2.51	0.44
1:A:728:CYS:O	1:A:732:LYS:HG2	2.18	0.44
1:A:926:SER:HA	1:A:929:LEU:HD12	2.00	0.44
1:B:536:ASP:HA	1:B:552:VAL:O	2.18	0.44
1:D:323:ILE:HA	1:D:326:LEU:HB2	1.98	0.44
1:D:1034:VAL:O	1:D:1038:ARG:HG2	2.17	0.44
1:A:878:PHE:HB3	1:A:1043:PHE:CZ	2.50	0.43
1:B:946:PHE:HB3	1:B:1003:LEU:HD11	1.99	0.43
1:C:509:VAL:HG13	1:C:526:VAL:HG21	1.99	0.43
1:D:343:SER:O	1:D:379:ARG:NH1	2.51	0.43
1:A:973:ILE:HG21	1:A:1014:THR:HG21	2.00	0.43
1:B:135:HIS:NE2	1:B:137:GLU:OE1	2.51	0.43
1:B:500:ILE:HG13	1:B:566:VAL:HG21	1.98	0.43
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.99	0.43
1:D:389:ARG:O	1:D:392:GLY:N	2.51	0.43
1:A:493:PHE:O	1:A:630:LYS:NZ	2.39	0.43
1:C:135:HIS:NE2	1:C:137:GLU:OE1	2.52	0.43
1:D:586:MET:HB3	1:D:612:LYS:HE2	2.01	0.43
1:A:543:TRP:CD1	1:A:546:LYS:HE2	2.54	0.43
1:A:969:LEU:HD22	5:C:3305:Q5B:C10	2.48	0.43
1:B:409:THR:HG22	1:B:411:MET:H	1.83	0.43
1:B:991:LYS:O	1:B:995:ARG:HG2	2.19	0.43
1:C:391:MET:HA	1:C:394:VAL:HG12	2.00	0.43
1:D:13:GLU:OE1	1:D:14:LEU:HD22	2.19	0.43
1:A:52:SER:HB2	1:A:53:GLN:OE1	2.19	0.43
1:A:880:LYS:HG3	1:A:1043:PHE:HE1	1.83	0.43
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.36	0.43
1:B:203:ASN:O	1:B:216:ASP:HB3	2.18	0.43
1:B:210:ASP:OD1	1:B:211:GLY:N	2.51	0.43
1:C:417:MET:HB3	1:C:424:ILE:HG12	2.00	0.43
1:D:917:GLY:HA2	1:D:1077:LYS:NZ	2.33	0.43
1:B:358:VAL:HG12	1:B:394:VAL:HG11	1.99	0.43
1:D:255:ASP:O	1:D:259:LYS:HG2	2.18	0.43
1:D:354:PHE:O	1:D:358:VAL:HG13	2.18	0.43
1:B:729:ARG:HG3	1:B:729:ARG:HH11	1.83	0.43
1:C:308:SER:OG	1:C:309:GLY:N	2.52	0.43
1:C:355:LYS:HA	1:C:358:VAL:HG22	2.01	0.43
1:C:900:HIS:O	1:C:900:HIS:ND1	2.51	0.43
1:C:933:ASP:OD1	1:C:933:ASP:N	2.51	0.43
1:D:416:GLY:HA3	1:D:422:ARG:HE	1.82	0.43
1:A:318:ASP:HA	1:A:321:LYS:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:HIS:HE1	1:A:334:ASP:HB2	1.82	0.43
1:A:917:GLY:HA2	1:A:1077:LYS:NZ	2.33	0.43
1:D:203:ASN:HA	1:D:204:PRO:HA	1.73	0.42
2:A:1201:ACO:H62A	1:B:1085:ARG:HG3	1.84	0.42
1:B:490:THR:HA	1:B:703:ARG:HG2	2.01	0.42
1:C:102:LEU:HD23	1:C:105:PHE:CZ	2.54	0.42
1:C:206:VAL:HG23	1:C:213:TYR:HB2	2.02	0.42
1:D:599:GLU:HB2	5:D:3303:Q5B:C17	2.49	0.42
1:D:695:SER:OG	1:D:700:HIS:NE2	2.50	0.42
1:A:635:LYS:NZ	1:A:638:ASN:HA	2.34	0.42
1:B:1095:LEU:HD22	1:C:846:ASP:HB2	2.02	0.42
1:C:851:GLU:OE2	1:C:860:THR:OG1	2.31	0.42
1:D:278:MET:SD	1:D:323:ILE:HD11	2.59	0.42
1:A:515:PHE:HA	1:A:518:VAL:HG12	2.00	0.42
1:B:203:ASN:HA	1:B:204:PRO:HA	1.71	0.42
1:B:226[B]:ASP:OD1	1:B:227:TYR:N	2.53	0.42
1:A:210:ASP:OD1	1:A:211:GLY:N	2.53	0.42
1:B:878:PHE:HB3	1:B:1043:PHE:CE2	2.54	0.42
1:C:367:PRO:HA	1:C:370:GLU:HG3	2.00	0.42
1:A:204:PRO:HD2	1:A:215:LEU:HB2	2.01	0.42
1:C:199:TYR:HB3	1:C:220:LYS:HB2	2.01	0.42
1:C:603:GLU:O	1:C:607:ARG:HG3	2.20	0.42
1:D:174:PRO:O	1:D:178:LYS:HG3	2.19	0.42
1:D:902:PRO:HB3	1:D:1072:HIS:CE1	2.55	0.42
1:D:975:HIS:CG	1:D:976:ARG:N	2.84	0.42
1:B:983:PRO:HG2	1:B:985:MET:CE	2.49	0.42
1:C:180:ILE:HG13	1:C:181:LEU:N	2.34	0.42
1:C:382:PRO:HA	1:C:642:MET:CE	2.50	0.42
1:A:517:TYR:OH	1:A:542:TYR:O	2.21	0.42
1:A:818:PRO:HA	1:A:819:PRO:HD3	1.95	0.42
1:A:915:ARG:NH1	1:C:839:SER:O	2.40	0.42
1:B:40:TRP:CE2	1:B:82:LYS:HE3	2.55	0.42
1:B:385:GLN:O	1:B:389:ARG:HG2	2.20	0.42
1:D:553:PHE:CE1	1:D:562:LYS:HD2	2.54	0.42
1:A:175:GLU:HA	1:A:178:LYS:HG3	2.02	0.42
1:A:284:ALA:O	1:A:287:VAL:HG12	2.20	0.42
1:C:133:LEU:HD13	1:C:145:VAL:HG22	2.02	0.42
1:C:493:PHE:CZ	1:C:636:ILE:HD11	2.55	0.42
1:A:386:GLU:O	1:A:389:ARG:HG2	2.19	0.42
1:A:505:GLN:HG3	1:A:572:PHE:CD2	2.55	0.42
1:B:133:LEU:HD11	1:B:151:LYS:HE2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLY:HA3	1:B:402:ILE:HD12	2.02	0.42
1:B:729:ARG:HG3	1:B:729:ARG:NH1	2.35	0.42
1:B:898:ALA:HA	1:B:1064:GLY:O	2.20	0.42
1:D:226[B]:ASP:OD1	1:D:227:TYR:N	2.53	0.42
1:A:902:PRO:HB3	1:A:1072:HIS:CE1	2.55	0.41
1:C:409:THR:HG23	1:C:413:ALA:HB3	2.02	0.41
1:C:777:GLN:O	1:C:781:GLU:OE1	2.37	0.41
1:C:975:HIS:CE1	1:C:978:LYS:HE2	2.55	0.41
1:D:25:ILE:HG23	1:D:28:ARG:HD2	2.02	0.41
1:D:34:VAL:CG2	1:D:105:PHE:HB2	2.50	0.41
1:D:27:ASN:ND2	1:D:109:PRO:HG2	2.35	0.41
1:A:337:ILE:HG21	1:A:418:ALA:HB1	2.01	0.41
1:A:531:TYR:HD2	1:A:534:THR:HG22	1.85	0.41
1:C:161:ASN:ND2	1:C:163:GLU:OE2	2.53	0.41
1:C:525:SER:HB2	1:C:634:PHE:CE1	2.55	0.41
1:C:878:PHE:HB3	1:C:1043:PHE:CE2	2.55	0.41
1:D:708:PRO:O	1:D:711:LYS:NZ	2.52	0.41
1:D:731:ILE:HG12	1:D:736:LEU:HB2	2.02	0.41
1:A:931:ILE:HD12	1:A:1061:PHE:HE2	1.85	0.41
1:B:180:ILE:HG13	1:B:181:LEU:N	2.36	0.41
1:B:214:VAL:HG11	1:B:217:LEU:HD23	2.02	0.41
1:B:895:MET:HG2	1:D:872:VAL:HG21	2.01	0.41
1:C:56:VAL:HG23	1:C:74:VAL:HA	2.01	0.41
1:C:396:LYS:HB2	1:C:396:LYS:HE2	1.91	0.41
1:D:977:VAL:HG23	1:D:978:LYS:HG3	2.02	0.41
1:A:54:ASN:HB3	1:A:110:PHE:HB3	2.02	0.41
1:A:493:PHE:CE2	1:A:636:ILE:HD11	2.54	0.41
1:A:579:TYR:O	1:A:583:MET:HG2	2.19	0.41
1:A:646:ILE:HG23	1:A:651:LEU:HB2	2.03	0.41
1:B:712:MET:HE1	1:B:797:ILE:HG13	2.02	0.41
1:B:969:LEU:HD22	5:D:3303:Q5B:C10	2.50	0.41
1:B:44:LEU:HD13	1:B:50:LEU:HD12	2.03	0.41
1:B:689:GLY:HA3	1:B:760:HIS:ND1	2.34	0.41
1:D:323:ILE:HA	1:D:326:LEU:HD12	2.03	0.41
1:A:974:GLY:O	1:A:1024:ASN:ND2	2.52	0.41
1:B:260:SER:OG	1:B:315:GLN:OE1	2.30	0.41
1:D:89:LEU:O	1:D:91:GLN:NE2	2.39	0.41
1:D:525:SER:HB2	1:D:634:PHE:CE1	2.56	0.41
1:A:40:TRP:CE2	1:A:82:LYS:HE3	2.56	0.41
1:B:417:MET:SD	1:B:424:ILE:HA	2.60	0.41
1:C:579:TYR:O	1:C:583:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:978:LYS:HD2	1:C:984:ASP:HA	2.03	0.41
1:D:166:LYS:HD2	1:D:170:LEU:HD12	2.03	0.41
1:D:878:PHE:HB3	1:D:1043:PHE:CE2	2.56	0.41
1:A:150:GLN:NE2	1:A:168:HIS:O	2.53	0.41
1:B:166:LYS:NZ	1:B:179:GLU:HA	2.36	0.41
1:B:204:PRO:HG2	1:B:215:LEU:HD12	2.03	0.41
1:B:396:LYS:HB2	1:B:396:LYS:HE2	1.91	0.41
1:C:160:LEU:HG	1:C:165:ILE:HD11	2.02	0.41
1:C:731:ILE:HD11	1:C:740:ILE:HD12	2.03	0.41
1:C:802:GLU:HA	1:C:805:VAL:HG12	2.03	0.41
1:D:976:ARG:HH11	2:D:3301:ACO:C8A	2.34	0.41
1:A:378:ARG:NH1	1:A:411:MET:SD	2.95	0.40
1:B:127:ARG:O	1:B:611:LYS:NZ	2.52	0.40
1:B:529:MET:HB3	1:B:529:MET:HE2	1.89	0.40
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.40
1:C:878:PHE:HB3	1:C:1043:PHE:HE2	1.86	0.40
1:D:891:GLU:O	1:D:895:MET:HG3	2.20	0.40
1:A:346:ASN:ND2	1:A:640:GLY:H	2.19	0.40
1:A:861:GLU:O	1:A:865:GLU:HG2	2.21	0.40
1:B:63:ILE:HG21	1:B:95:VAL:HG21	2.03	0.40
1:A:984:ASP:HB3	1:A:987:VAL:H	1.86	0.40
1:C:41:ALA:O	1:C:44:LEU:N	2.44	0.40
1:D:735:ARG:HG3	1:D:735:ARG:NH1	2.36	0.40
5:D:3303:Q5B:O15	5:D:3303:Q5B:O20	2.38	0.40
1:A:1086:HIS:O	2:B:2303:ACO:N6A	2.47	0.40
1:B:318:ASP:HA	1:B:321:LYS:HG2	2.03	0.40
1:B:321:LYS:HB2	1:B:364:TYR:HE2	1.87	0.40
1:B:878:PHE:HB3	1:B:1043:PHE:HE2	1.85	0.40
1:D:165:ILE:O	1:D:169:LEU:HB2	2.20	0.40
1:A:170:LEU:O	1:A:178:LYS:NZ	2.55	0.40
1:B:268:LEU:HD21	1:B:326:LEU:HD13	2.04	0.40
1:B:346:ASN:O	1:B:641:GLY:HA2	2.22	0.40
1:B:713:ILE:O	1:B:740:ILE:HA	2.21	0.40
1:B:984:ASP:O	1:B:985:MET:HB2	2.22	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	1035/1101 (94%)	992 (96%)	43 (4%)	0	100	100
1	B	1035/1101 (94%)	999 (96%)	36 (4%)	0	100	100
1	C	1035/1101 (94%)	1003 (97%)	32 (3%)	0	100	100
1	D	1035/1101 (94%)	1007 (97%)	28 (3%)	0	100	100
All	All	4140/4404 (94%)	4001 (97%)	139 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	852/908 (94%)	849 (100%)	3 (0%)	91	97
1	B	852/908 (94%)	849 (100%)	3 (0%)	91	97
1	C	852/908 (94%)	849 (100%)	3 (0%)	91	97
1	D	852/908 (94%)	848 (100%)	4 (0%)	88	96
All	All	3408/3632 (94%)	3395 (100%)	13 (0%)	92	97

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226[A]	ASP
1	A	226[B]	ASP

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Mol	Chain	Res	Type
1	A	653	ARG
1	B	226[A]	ASP
1	B	226[B]	ASP
1	B	653	ARG
1	C	226[A]	ASP
1	C	226[B]	ASP
1	C	653	ARG
1	D	226[A]	ASP
1	D	226[B]	ASP
1	D	507	ARG
1	D	653	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
1	A	1072	HIS
1	D	168	HIS
1	D	1072	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 2 are unknown - leaving 16 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
2	ACO	B	2303	-	45,53,53	0.83	1 (2%)	56,79,79	1.21	5 (8%)
2	ACO	A	1201	-	45,53,53	0.86	1 (2%)	56,79,79	1.09	4 (7%)
6	PO4	D	3305	-	4,4,4	0.91	0	6,6,6	0.42	0
7	ADP	C	3303	-	24,29,29	0.97	1 (4%)	29,45,45	1.47	4 (13%)
7	ADP	D	3304	-	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
5	Q5B	B	2302	-	54,62,62	2.58	18 (33%)	70,93,93	1.56	10 (14%)
5	Q5B	C	3305	-	54,62,62	2.59	16 (29%)	70,93,93	1.55	14 (20%)
3	OAA	C	3302	-	8,8,8	1.31	1 (12%)	9,10,10	1.34	1 (11%)
6	PO4	C	3306	-	4,4,4	0.92	0	6,6,6	0.32	0
3	OAA	A	1203	-	8,8,8	1.33	1 (12%)	9,10,10	1.34	1 (11%)
5	Q5B	D	3303	-	54,62,62	2.62	17 (31%)	70,93,93	1.63	13 (18%)
6	PO4	B	2304	-	4,4,4	0.92	0	6,6,6	0.43	0
2	ACO	D	3301	-	45,53,53	0.82	1 (2%)	56,79,79	1.22	4 (7%)
2	ACO	C	3301	-	45,53,53	0.80	1 (2%)	56,79,79	1.24	4 (7%)
3	OAA	D	3302	-	8,8,8	1.33	1 (12%)	9,10,10	1.38	1 (11%)
3	OAA	A	1202	-	8,8,8	1.31	1 (12%)	9,10,10	1.35	1 (11%)

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
2	ACO	B	2303	-	-	12/47/67/67	0/3/3/3
2	ACO	A	1201	-	-	12/47/67/67	0/3/3/3
7	ADP	C	3303	-	-	4/12/32/32	0/3/3/3
7	ADP	D	3304	-	-	5/12/32/32	0/3/3/3
5	Q5B	B	2302	-	-	11/62/83/83	0/3/3/3
5	Q5B	C	3305	-	-	16/62/83/83	0/3/3/3
3	OAA	C	3302	-	-	6/8/8/8	-
3	OAA	A	1203	-	-	5/8/8/8	-
5	Q5B	D	3303	-	-	20/62/83/83	0/3/3/3
2	ACO	D	3301	-	-	16/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	C	3301	-	-	23/47/67/67	0/3/3/3
3	OAA	D	3302	-	-	6/8/8/8	-
3	OAA	A	1202	-	-	6/8/8/8	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3303	Q5B	C6-C5	-7.89	1.31	1.52
5	B	2302	Q5B	C6-C5	-7.86	1.31	1.52
5	C	3305	Q5B	C6-C5	-7.59	1.32	1.52
5	D	3303	Q5B	C18-N6	7.54	1.50	1.33
5	C	3305	Q5B	C18-N6	7.49	1.50	1.33
5	B	2302	Q5B	C18-N6	7.46	1.50	1.33
5	C	3305	Q5B	C7-C6	7.34	1.69	1.52
5	D	3303	Q5B	C15-N5	7.12	1.49	1.33
5	D	3303	Q5B	C7-C6	7.08	1.68	1.52
5	C	3305	Q5B	C15-N5	7.07	1.49	1.33
5	B	2302	Q5B	C15-N5	6.93	1.48	1.33
5	B	2302	Q5B	C7-C6	6.91	1.68	1.52
5	D	3303	Q5B	O7-C5	3.79	1.53	1.45
5	D	3303	Q5B	C21-S	3.71	1.85	1.76
5	C	3305	Q5B	O7-C5	3.59	1.53	1.45
5	B	2302	Q5B	O7-C5	3.54	1.52	1.45
5	C	3305	Q5B	C21-S	3.46	1.84	1.76
5	C	3305	Q5B	O20-C23	-3.40	1.36	1.43
5	D	3303	Q5B	O20-C23	-3.36	1.36	1.43
5	B	2302	Q5B	C23-C26	-3.32	1.50	1.53
5	B	2302	Q5B	O20-C23	-3.28	1.36	1.43
5	D	3303	Q5B	C22-C23	3.28	1.57	1.53
5	B	2302	Q5B	C21-S	3.26	1.84	1.76
5	D	3303	Q5B	P2-O9	3.00	1.65	1.59
5	C	3305	Q5B	P2-O9	3.00	1.65	1.59
5	C	3305	Q5B	C23-C26	-2.89	1.50	1.53
5	C	3305	Q5B	C22-C23	2.79	1.57	1.53
5	D	3303	Q5B	O13-C15	-2.78	1.17	1.23
5	C	3305	Q5B	O14-C18	-2.77	1.17	1.23
5	B	2302	Q5B	O14-C18	-2.76	1.17	1.23
5	B	2302	Q5B	C-C1	-2.70	1.47	1.53
5	D	3303	Q5B	C23-C26	-2.69	1.50	1.53
5	C	3305	Q5B	O13-C15	-2.65	1.18	1.23
5	D	3303	Q5B	O14-C18	-2.61	1.18	1.23
5	B	2302	Q5B	O13-C15	-2.59	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2302	Q5B	P2-O9	2.58	1.64	1.59
5	B	2302	Q5B	C22-C23	2.51	1.56	1.53
7	C	3303	ADP	C5-C4	2.51	1.47	1.40
7	D	3304	ADP	C5-C4	2.49	1.47	1.40
5	D	3303	Q5B	C-C1	-2.45	1.48	1.53
2	D	3301	ACO	C5A-C4A	2.35	1.47	1.40
5	C	3305	Q5B	C-C1	-2.32	1.48	1.53
5	B	2302	Q5B	C2-C1	2.28	1.58	1.53
2	B	2303	ACO	C5A-C4A	2.27	1.46	1.40
5	D	3303	Q5B	C22-C21	2.26	1.56	1.51
5	C	3305	Q5B	C22-C21	2.24	1.56	1.51
2	A	1201	ACO	C5A-C4A	2.24	1.46	1.40
2	C	3301	ACO	C5A-C4A	2.19	1.46	1.40
5	D	3303	Q5B	O-C3	-2.16	1.36	1.43
5	D	3303	Q5B	C2-C1	2.13	1.58	1.53
3	D	3302	OAA	O3-C3	-2.12	1.18	1.23
5	D	3303	Q5B	P1-O6	2.12	1.67	1.59
5	B	2302	Q5B	C22-C21	2.11	1.55	1.51
3	A	1203	OAA	O3-C3	-2.09	1.18	1.23
3	A	1202	OAA	O3-C3	-2.08	1.18	1.23
3	C	3302	OAA	O3-C3	-2.08	1.18	1.23
5	C	3305	Q5B	C2-C1	2.06	1.58	1.53
5	B	2302	Q5B	C7-C8	-2.05	1.50	1.53
5	B	2302	Q5B	P1-O6	2.05	1.67	1.59
5	C	3305	Q5B	P1-O6	2.04	1.67	1.59
5	B	2302	Q5B	C10-C11	-2.03	1.35	1.40

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2302	Q5B	N2-C12-N3	-5.42	120.20	128.68
5	C	3305	Q5B	N2-C12-N3	-5.17	120.59	128.68
5	C	3305	Q5B	C22-C21-S	5.09	119.92	113.63
5	D	3303	Q5B	C22-C21-S	4.95	119.75	113.63
5	D	3303	Q5B	N2-C12-N3	-4.91	121.00	128.68
2	D	3301	ACO	P2A-O3A-P1A	-4.73	116.60	132.83
5	B	2302	Q5B	C22-C21-S	4.66	119.40	113.63
2	C	3301	ACO	P2A-O3A-P1A	-4.55	117.20	132.83
2	B	2303	ACO	P2A-O3A-P1A	-3.97	119.21	132.83
5	C	3305	Q5B	O19-C26-C23	3.76	119.58	113.05
5	D	3303	Q5B	O19-C26-C23	3.66	119.41	113.05
2	A	1201	ACO	N3A-C2A-N1A	-3.48	123.23	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	3304	ADP	C3'-C2'-C1'	3.47	106.21	100.98
2	C	3301	ACO	N3A-C2A-N1A	-3.44	123.30	128.68
7	C	3303	ADP	C3'-C2'-C1'	3.42	106.12	100.98
7	D	3304	ADP	PA-O3A-PB	-3.37	121.25	132.83
7	C	3303	ADP	PA-O3A-PB	-3.34	121.36	132.83
2	B	2303	ACO	N3A-C2A-N1A	-3.33	123.47	128.68
2	D	3301	ACO	N3A-C2A-N1A	-3.33	123.47	128.68
5	D	3303	Q5B	C14-C15-N5	3.25	123.04	116.58
7	C	3303	ADP	N3-C2-N1	-3.19	123.69	128.68
5	B	2302	Q5B	C8-N-C11	-3.18	121.05	126.64
5	B	2302	Q5B	C17-C18-N6	3.15	121.73	116.42
7	D	3304	ADP	N3-C2-N1	-3.11	123.82	128.68
5	B	2302	Q5B	O19-C26-C23	3.09	118.42	113.05
5	D	3303	Q5B	C16-C17-C18	3.04	117.42	112.36
2	A	1201	ACO	P2A-O3A-P1A	-3.04	122.40	132.83
5	D	3303	Q5B	P1-O3-P	-3.03	122.42	132.83
2	B	2303	ACO	C4A-C5A-N7A	-2.93	106.34	109.40
5	D	3303	Q5B	O7-C8-C7	-2.87	102.73	106.93
5	D	3303	Q5B	O-C3-C1	-2.82	106.02	110.55
5	C	3305	Q5B	P1-O3-P	-2.75	123.40	132.83
5	C	3305	Q5B	C8-N-C11	-2.74	121.83	126.64
2	A	1201	ACO	C4A-C5A-N7A	-2.73	106.56	109.40
7	C	3303	ADP	C4-C5-N7	-2.68	106.60	109.40
5	B	2302	Q5B	C20-S-C21	2.66	110.17	101.87
7	D	3304	ADP	C4-C5-N7	-2.65	106.64	109.40
2	C	3301	ACO	C4A-C5A-N7A	-2.60	106.69	109.40
2	A	1201	ACO	C3B-C2B-C1B	2.56	105.55	99.89
5	D	3303	Q5B	C-C1-C14	2.52	113.19	108.82
5	C	3305	Q5B	C20-S-C21	2.49	109.64	101.87
5	B	2302	Q5B	C11-C10-N1	-2.47	106.82	109.40
2	D	3301	ACO	C4A-C5A-N7A	-2.47	106.83	109.40
5	C	3305	Q5B	C2-C1-C14	2.41	113.00	108.82
5	D	3303	Q5B	O13-C15-N5	-2.38	117.88	122.99
5	C	3305	Q5B	C17-C18-N6	2.33	120.34	116.42
5	C	3305	Q5B	C16-N5-C15	-2.32	118.44	122.59
5	C	3305	Q5B	C11-C10-N1	-2.29	107.01	109.40
5	D	3303	Q5B	C20-S-C21	2.29	109.00	101.87
3	D	3302	OAA	O5-C4-C3	2.26	120.15	113.97
5	B	2302	Q5B	C19-N6-C18	-2.26	118.65	122.84
3	A	1202	OAA	O5-C4-C3	2.24	120.11	113.97
5	D	3303	Q5B	O15-C21-S	-2.24	119.71	122.61
5	C	3305	Q5B	O15-C21-S	-2.23	119.72	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1203	OAA	O5-C4-C3	2.22	120.06	113.97
3	C	3302	OAA	O5-C4-C3	2.22	120.05	113.97
2	D	3301	ACO	C3B-C2B-C1B	2.16	104.67	99.89
5	D	3303	Q5B	C17-C18-N6	2.13	120.01	116.42
2	C	3301	ACO	C3B-C2B-C1B	2.13	104.61	99.89
2	B	2303	ACO	C7P-C6P-C5P	-2.11	108.85	112.36
5	C	3305	Q5B	O15-C21-C22	-2.05	120.35	123.64
5	C	3305	Q5B	C19-N6-C18	-2.05	119.04	122.84
5	C	3305	Q5B	O-C3-C1	-2.04	107.27	110.55
5	B	2302	Q5B	O15-C21-S	-2.01	120.00	122.61
5	B	2302	Q5B	C2-C1-C14	2.01	112.30	108.82
2	B	2303	ACO	C3B-C2B-C1B	2.01	104.33	99.89

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACO	C3B-O3B-P3B-O8A
2	A	1201	ACO	CCP-O6A-P2A-O3A
2	A	1201	ACO	CCP-O6A-P2A-O4A
2	A	1201	ACO	CCP-O6A-P2A-O5A
2	A	1201	ACO	C6P-C5P-N4P-C3P
2	A	1201	ACO	O-C-S1P-C2P
2	A	1201	ACO	CH3-C-S1P-C2P
2	B	2303	ACO	CBP-CCP-O6A-P2A
2	B	2303	ACO	CEP-CBP-CCP-O6A
2	B	2303	ACO	CAP-CBP-CCP-O6A
2	B	2303	ACO	C3P-C2P-S1P-C
2	B	2303	ACO	O-C-S1P-C2P
2	B	2303	ACO	CH3-C-S1P-C2P
2	C	3301	ACO	C5B-O5B-P1A-O1A
2	C	3301	ACO	CCP-O6A-P2A-O3A
2	C	3301	ACO	CAP-CBP-CCP-O6A
2	C	3301	ACO	CAP-C9P-N8P-C7P
2	C	3301	ACO	C6P-C5P-N4P-C3P
2	C	3301	ACO	O5P-C5P-N4P-C3P
2	C	3301	ACO	O-C-S1P-C2P
2	C	3301	ACO	CH3-C-S1P-C2P
2	D	3301	ACO	CBP-CCP-O6A-P2A
2	D	3301	ACO	CDP-CBP-CCP-O6A
2	D	3301	ACO	CEP-CBP-CCP-O6A
2	D	3301	ACO	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	D	3301	ACO	CAP-C9P-N8P-C7P
2	D	3301	ACO	O9P-C9P-N8P-C7P
2	D	3301	ACO	C5P-C6P-C7P-N8P
2	D	3301	ACO	C6P-C5P-N4P-C3P
2	D	3301	ACO	O-C-S1P-C2P
2	D	3301	ACO	CH3-C-S1P-C2P
3	A	1202	OAA	C1-C2-C3-O3
3	A	1202	OAA	C2-C3-C4-O4
3	A	1202	OAA	C2-C3-C4-O5
3	A	1203	OAA	O2-C1-C2-C3
3	A	1203	OAA	C2-C3-C4-O4
3	A	1203	OAA	C2-C3-C4-O5
3	C	3302	OAA	O2-C1-C2-C3
3	C	3302	OAA	O3-C3-C4-O4
3	C	3302	OAA	O3-C3-C4-O5
3	C	3302	OAA	C2-C3-C4-O5
3	D	3302	OAA	O2-C1-C2-C3
3	D	3302	OAA	C2-C3-C4-O4
3	D	3302	OAA	C2-C3-C4-O5
5	B	2302	Q5B	C22-C21-S-C20
5	B	2302	Q5B	O15-C21-S-C20
5	B	2302	Q5B	P-O3-P1-O6
5	B	2302	Q5B	C6-O9-P2-O10
5	C	3305	Q5B	N6-C19-C20-S
5	C	3305	Q5B	C21-C22-C23-C24
5	C	3305	Q5B	C21-C22-C23-C26
5	C	3305	Q5B	C21-C22-C23-O20
5	C	3305	Q5B	O20-C23-C24-C25
5	C	3305	Q5B	C6-O9-P2-O10
5	D	3303	Q5B	C3-O-P-O2
5	D	3303	Q5B	C-C1-C14-O21
5	D	3303	Q5B	C3-C1-C14-O21
5	D	3303	Q5B	C-C1-C3-O
5	D	3303	Q5B	C14-C1-C3-O
5	D	3303	Q5B	C2-C1-C3-O
5	D	3303	Q5B	C14-C15-N5-C16
5	D	3303	Q5B	N5-C16-C17-C18
5	D	3303	Q5B	C21-C22-C23-C24
5	D	3303	Q5B	C21-C22-C23-C26
5	D	3303	Q5B	C21-C22-C23-O20
5	D	3303	Q5B	O6-C4-C5-O7
5	D	3303	Q5B	P-O3-P1-O6

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Mol	Chain	Res	Type	Atoms
7	C	3303	ADP	C5'-O5'-PA-O2A
7	C	3303	ADP	C5'-O5'-PA-O3A
7	C	3303	ADP	C3'-C4'-C5'-O5'
7	D	3304	ADP	C5'-O5'-PA-O1A
7	D	3304	ADP	C5'-O5'-PA-O2A
2	A	1201	ACO	O5P-C5P-N4P-C3P
2	D	3301	ACO	O5P-C5P-N4P-C3P
5	D	3303	Q5B	O13-C15-N5-C16
2	C	3301	ACO	O4B-C4B-C5B-O5B
5	C	3305	Q5B	O6-C4-C5-O7
7	D	3304	ADP	C3'-C4'-C5'-O5'
2	B	2303	ACO	O5P-C5P-N4P-C3P
2	A	1201	ACO	C4B-C3B-O3B-P3B
2	C	3301	ACO	C4B-C3B-O3B-P3B
5	C	3305	Q5B	C22-C23-C24-C25
5	C	3305	Q5B	C26-C23-C24-C25
2	B	2303	ACO	C6P-C5P-N4P-C3P
2	C	3301	ACO	C3B-C4B-C5B-O5B
5	B	2302	Q5B	O6-C4-C5-O7
7	C	3303	ADP	O4'-C4'-C5'-O5'
2	B	2303	ACO	CDP-CBP-CCP-O6A
2	C	3301	ACO	CDP-CBP-CCP-O6A
2	C	3301	ACO	CEP-CBP-CCP-O6A
2	C	3301	ACO	O9P-C9P-N8P-C7P
2	A	1201	ACO	O4B-C4B-C5B-O5B
2	C	3301	ACO	O9P-C9P-CAP-OAP
5	D	3303	Q5B	C2-C1-C14-O21
3	A	1203	OAA	O1-C1-C2-C3
7	D	3304	ADP	O4'-C4'-C5'-O5'
5	B	2302	Q5B	N6-C19-C20-S
2	C	3301	ACO	N8P-C9P-CAP-CBP
5	C	3305	Q5B	O15-C21-S-C20
5	D	3303	Q5B	O15-C21-S-C20
2	B	2303	ACO	P1A-O3A-P2A-O6A
2	D	3301	ACO	P1A-O3A-P2A-O6A
5	C	3305	Q5B	P-O3-P1-O6
5	C	3305	Q5B	O6-C4-C5-C6
3	C	3302	OAA	O1-C1-C2-C3
3	D	3302	OAA	O1-C1-C2-C3
5	C	3305	Q5B	C22-C21-S-C20
5	D	3303	Q5B	C22-C21-S-C20
2	B	2303	ACO	C5P-C6P-C7P-N8P

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Mol	Chain	Res	Type	Atoms
2	C	3301	ACO	C6P-C7P-N8P-C9P
3	A	1202	OAA	O2-C1-C2-C3
3	D	3302	OAA	C1-C2-C3-O3
5	B	2302	Q5B	C4-O6-P1-O3
5	D	3303	Q5B	C6-O9-P2-O10
7	D	3304	ADP	C5'-O5'-PA-O3A
5	B	2302	Q5B	C4-O6-P1-O5
3	A	1202	OAA	O3-C3-C4-O4
3	A	1203	OAA	O3-C3-C4-O4
3	D	3302	OAA	O3-C3-C4-O4
3	C	3302	OAA	C2-C3-C4-O4
3	A	1202	OAA	O1-C1-C2-C3
2	C	3301	ACO	C2B-C3B-O3B-P3B
2	D	3301	ACO	C4B-C5B-O5B-P1A
5	B	2302	Q5B	C5-C4-O6-P1
5	B	2302	Q5B	N5-C16-C17-C18
2	C	3301	ACO	O9P-C9P-CAP-CBP
2	A	1201	ACO	C3P-C2P-S1P-C
2	C	3301	ACO	C3P-C2P-S1P-C
2	D	3301	ACO	C3P-C2P-S1P-C
5	B	2302	Q5B	C19-C20-S-C21
5	C	3305	Q5B	C24-C23-C26-O19
2	C	3301	ACO	C3B-O3B-P3B-O9A
2	C	3301	ACO	C5B-O5B-P1A-O3A
2	D	3301	ACO	CCP-O6A-P2A-O3A
5	C	3305	Q5B	C-C1-C14-O21
5	D	3303	Q5B	C3-O-P-O3
2	A	1201	ACO	C5B-O5B-P1A-O1A
2	C	3301	ACO	CCP-O6A-P2A-O4A
2	D	3301	ACO	CCP-O6A-P2A-O5A
5	D	3303	Q5B	O6-C4-C5-C6
2	B	2303	ACO	C4B-C5B-O5B-P1A
5	C	3305	Q5B	C20-C19-N6-C18

There are no ring outliers.

10 monomers are involved in 45 short contacts:

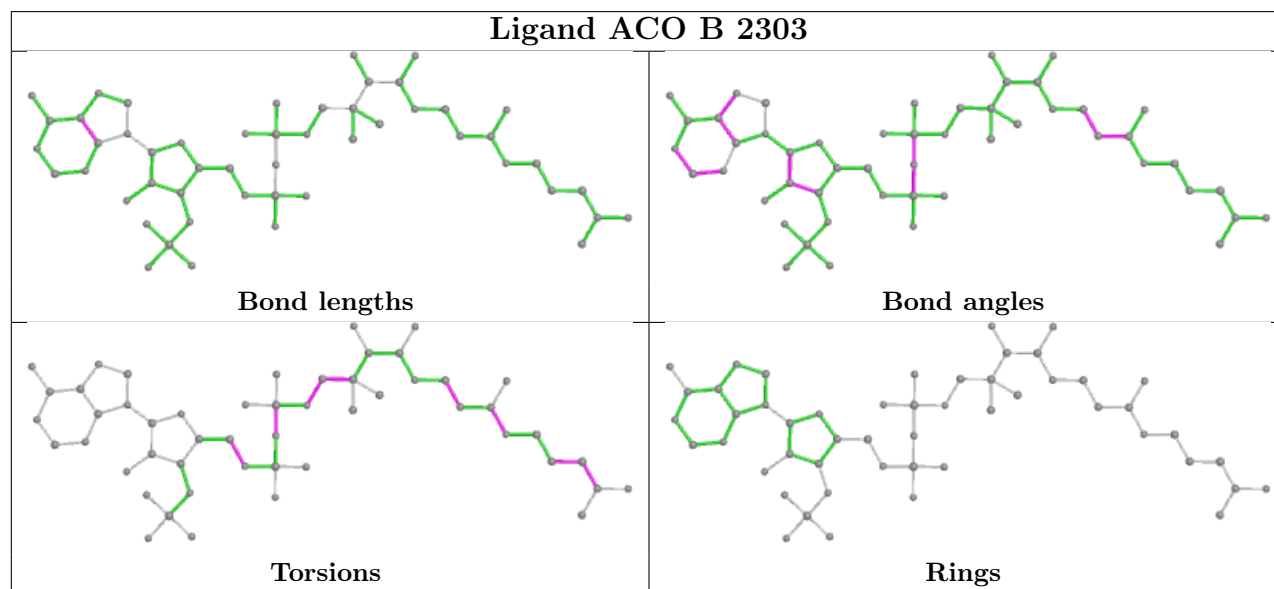
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2303	ACO	8	0
2	A	1201	ACO	9	0
6	D	3305	PO4	1	0
5	C	3305	Q5B	1	0

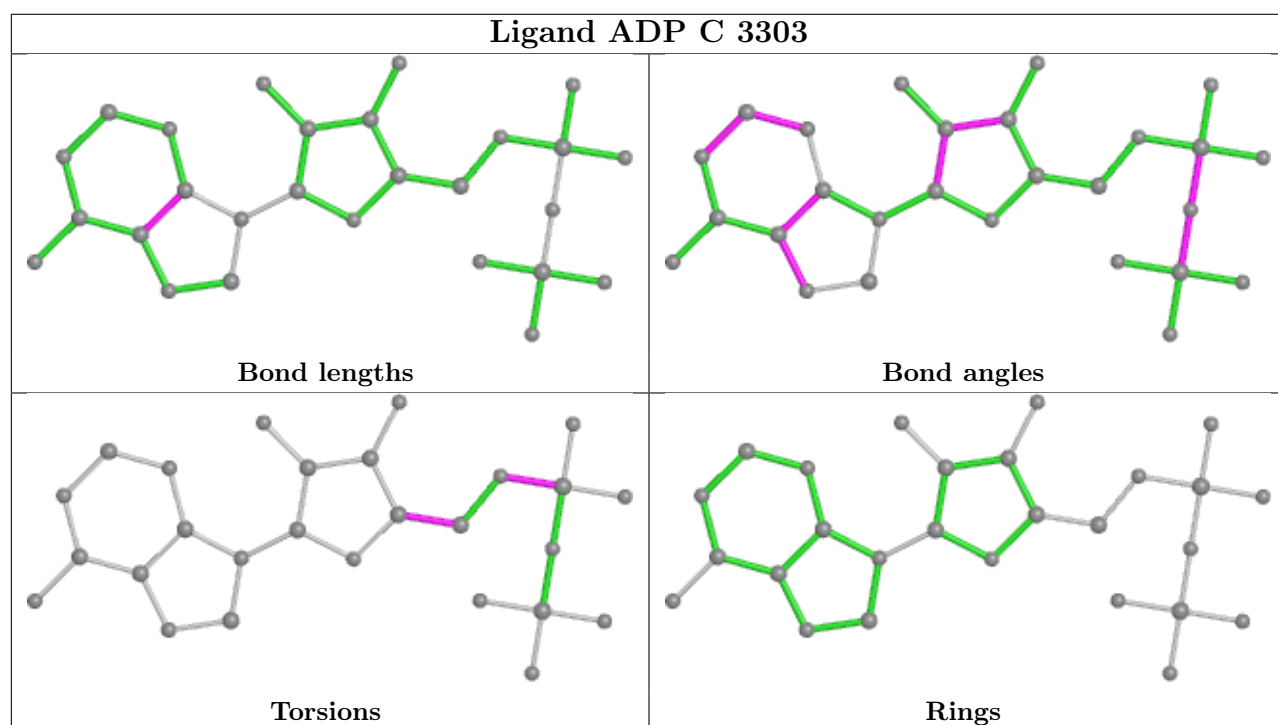
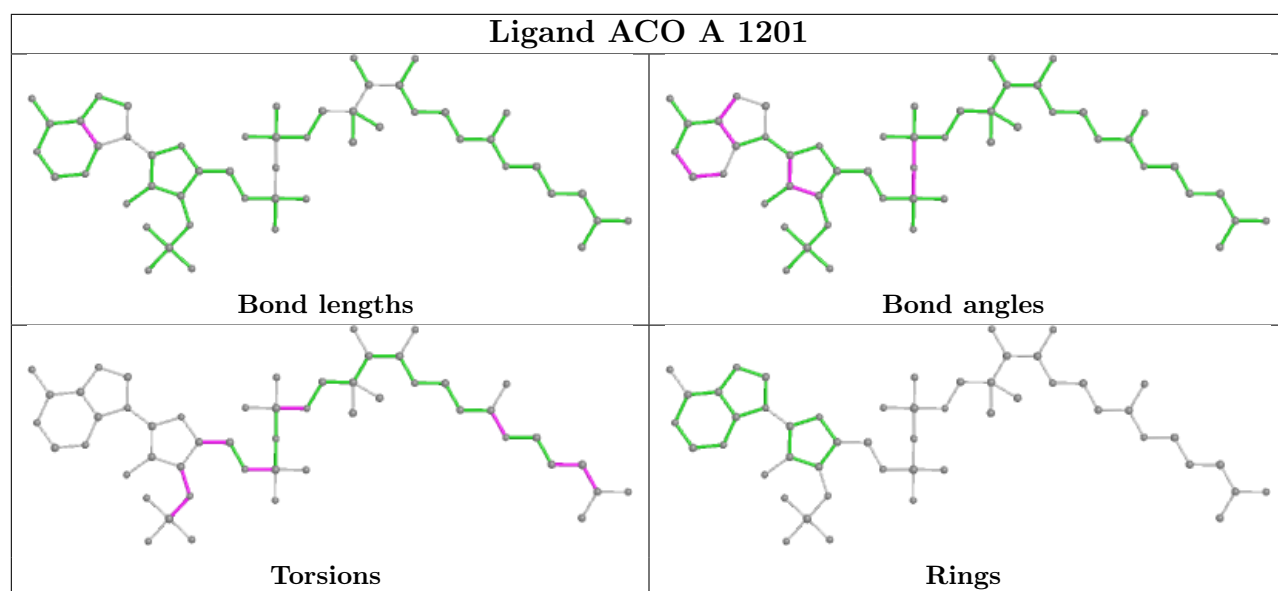
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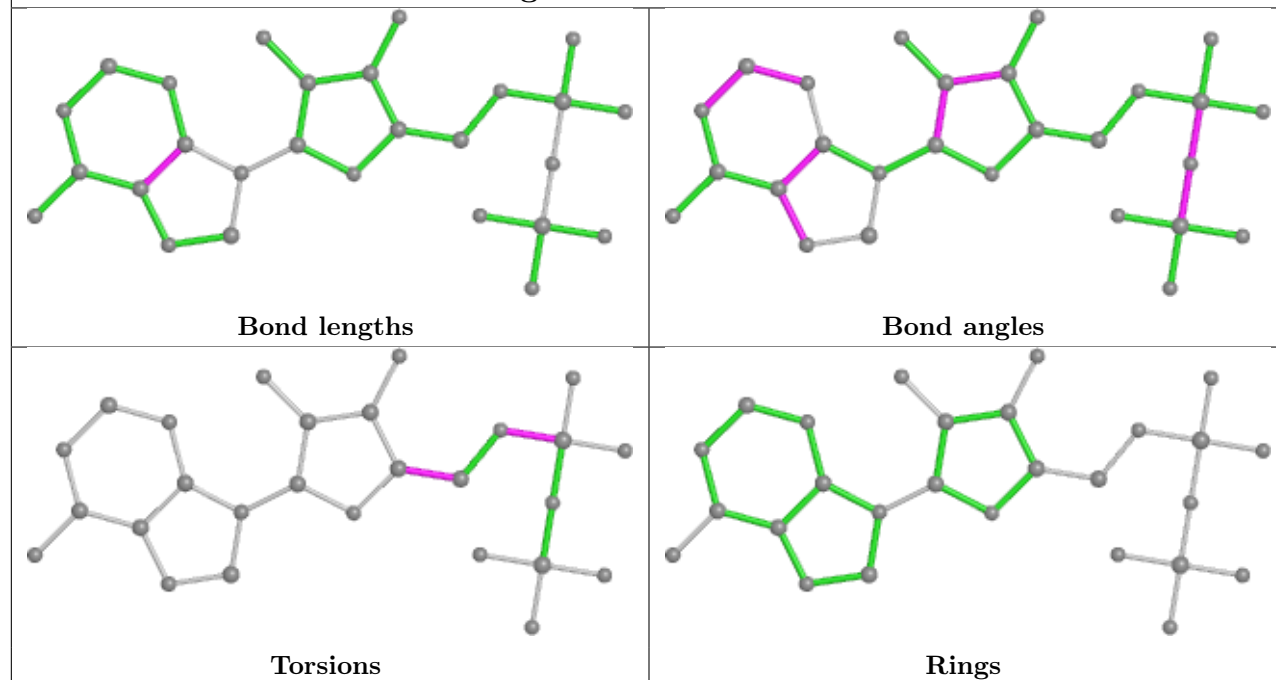
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1203	OAA	1	0
5	D	3303	Q5B	3	0
2	D	3301	ACO	17	0
2	C	3301	ACO	5	0
3	D	3302	OAA	1	0
3	A	1202	OAA	1	0

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.

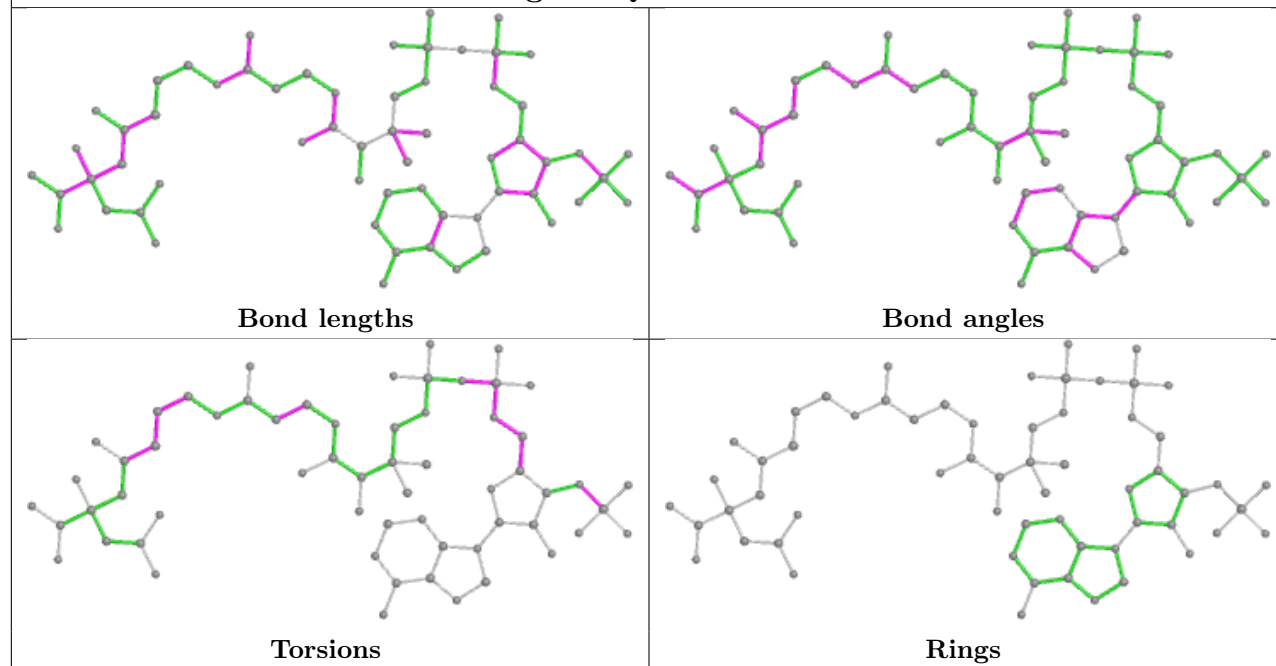




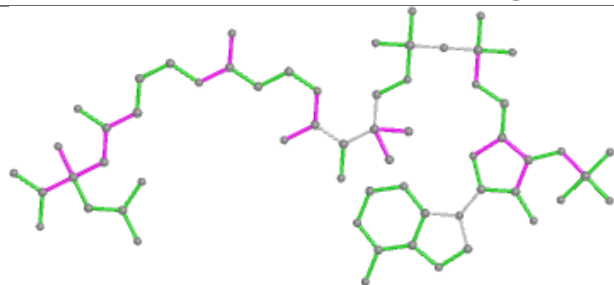
Ligand ADP D 3304



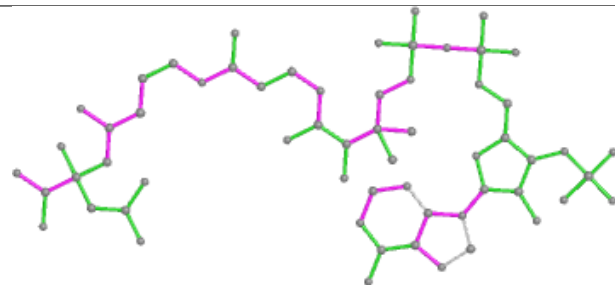
Ligand Q5B B 2302



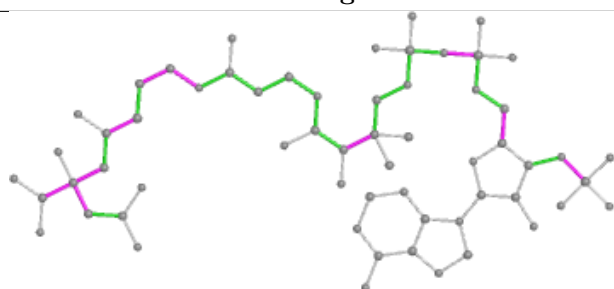
Ligand Q5B C 3305



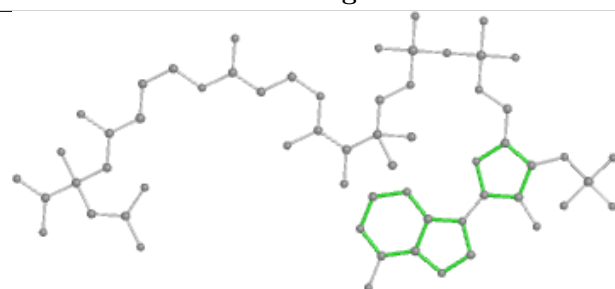
Bond lengths



Bond angles

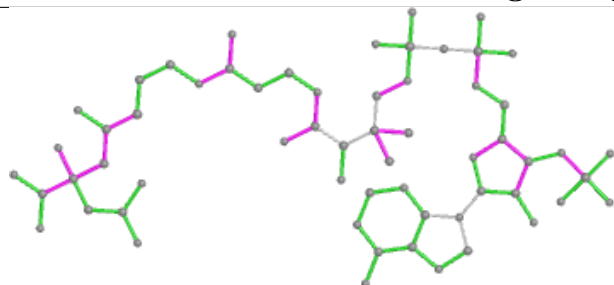


Torsions

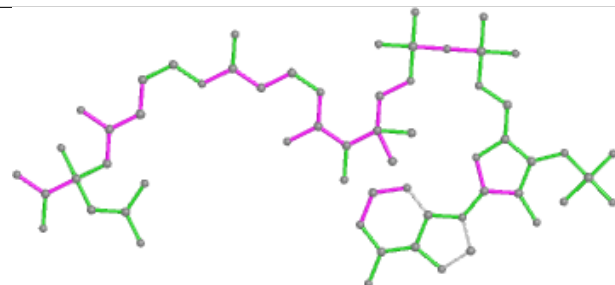


Rings

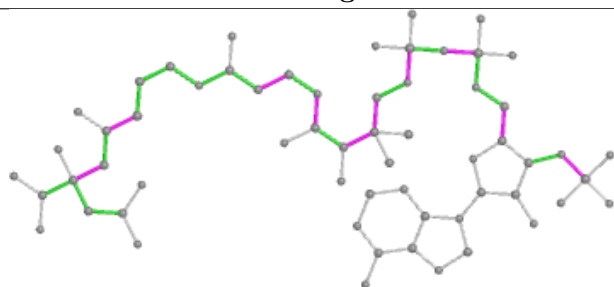
Ligand Q5B D 3303



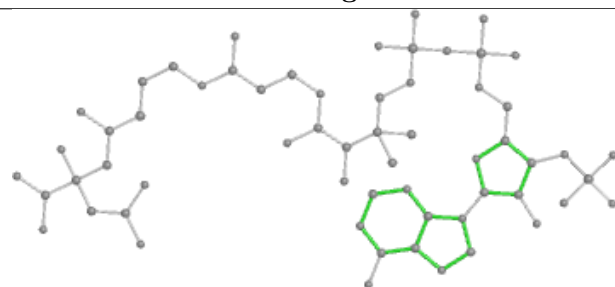
Bond lengths



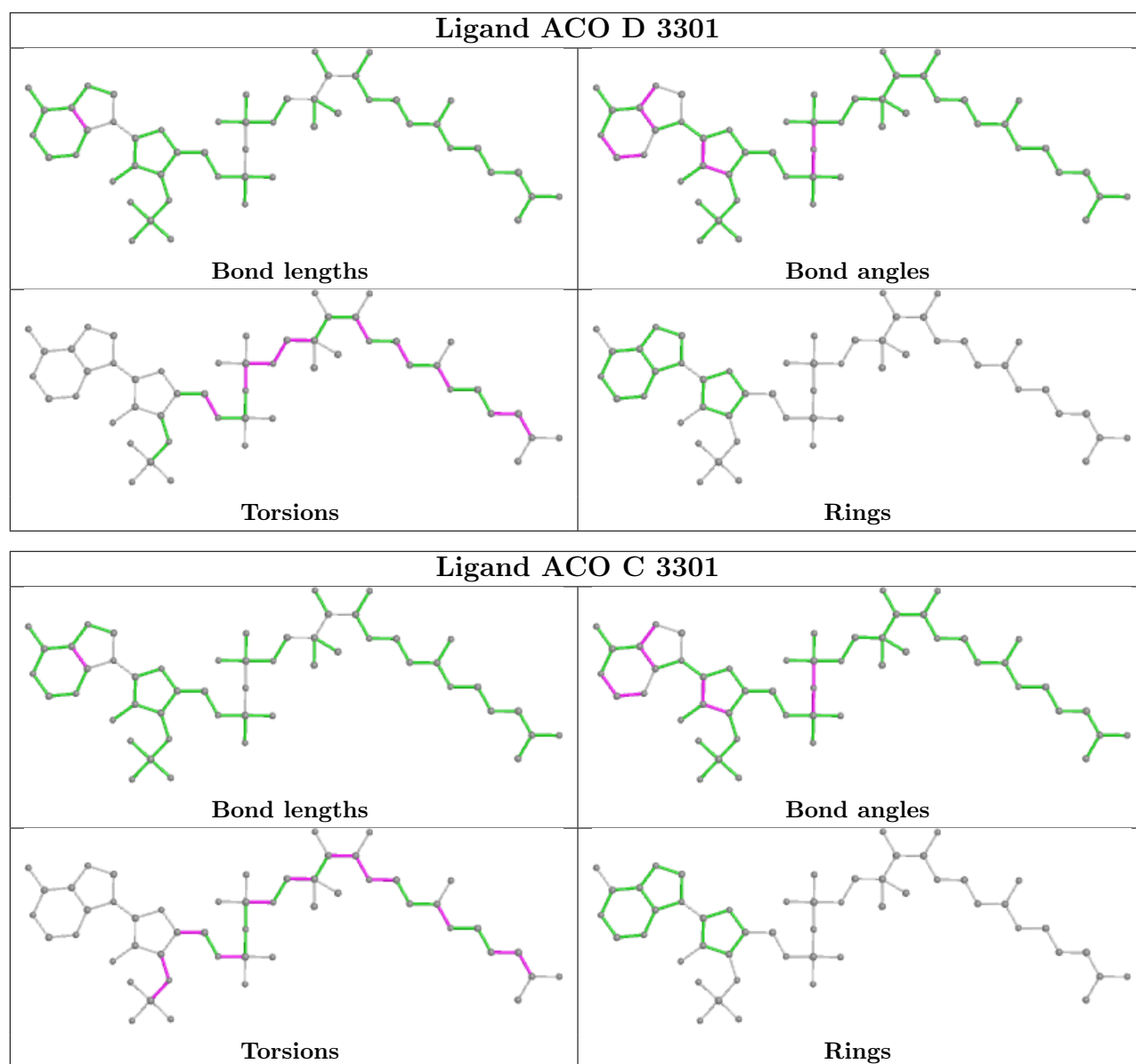
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

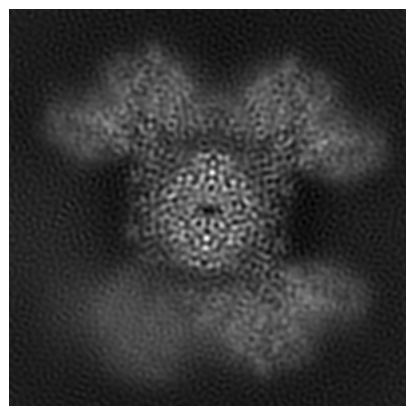
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29668. These allow visual inspection of the internal detail of the map and identification of artifacts.

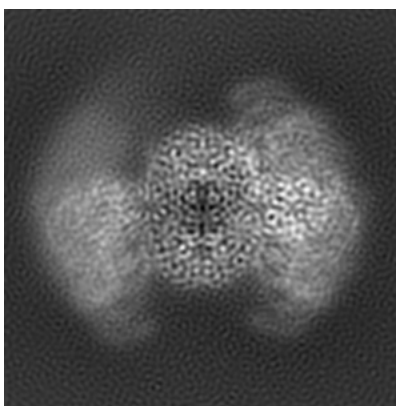
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

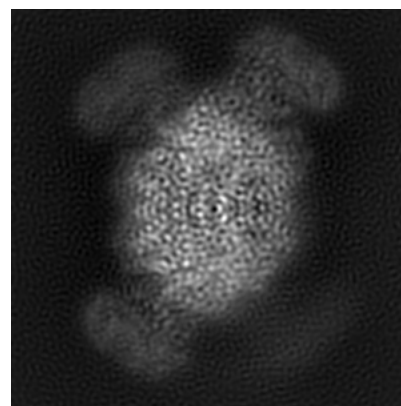
6.1.1 Primary map



X

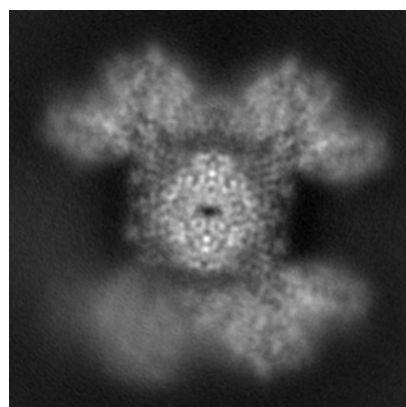


Y

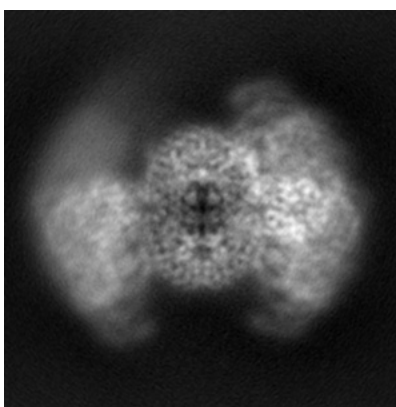


Z

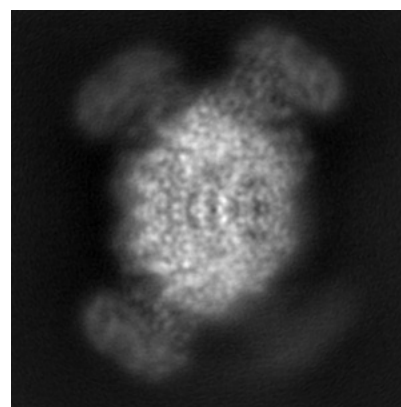
6.1.2 Raw map



X



Y

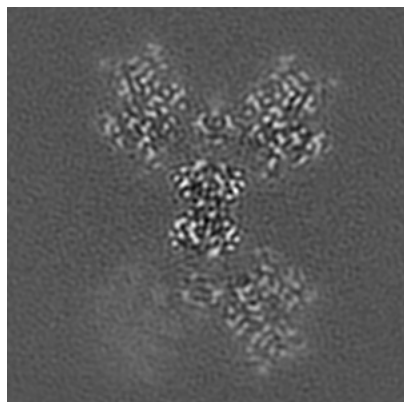


Z

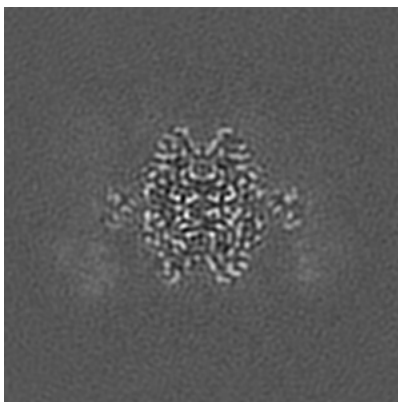
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

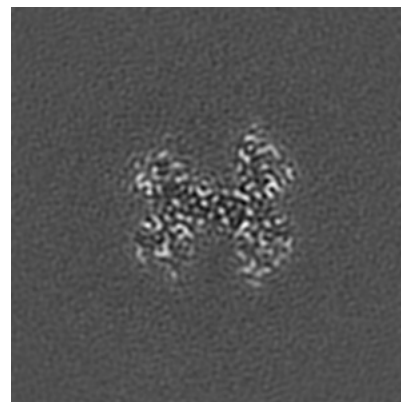
6.2.1 Primary map



X Index: 110

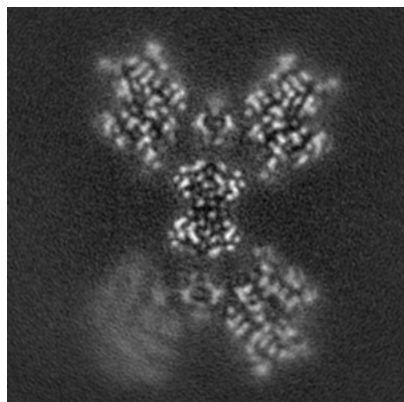


Y Index: 110

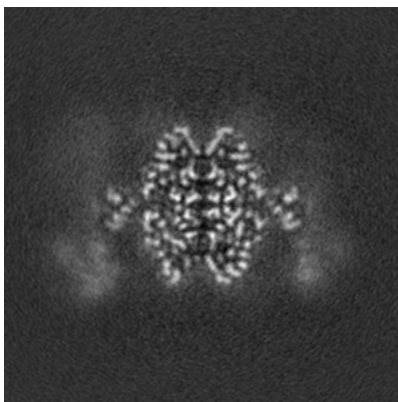


Z Index: 110

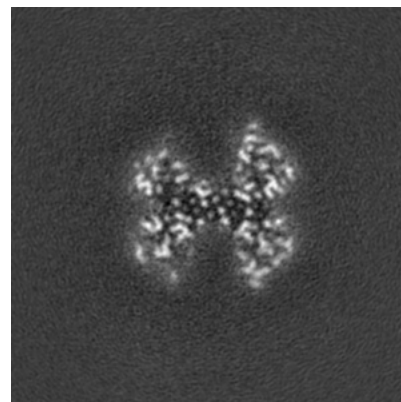
6.2.2 Raw map



X Index: 110



Y Index: 110

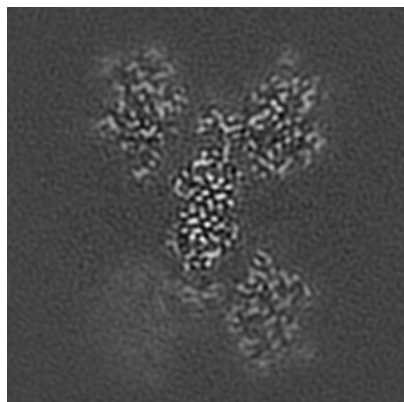


Z Index: 110

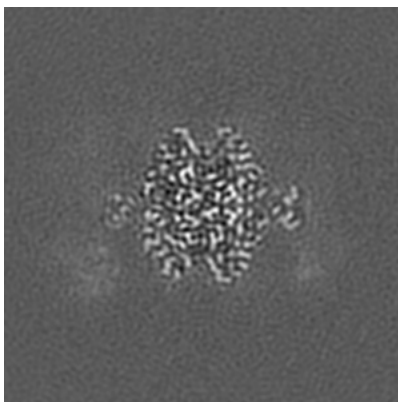
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

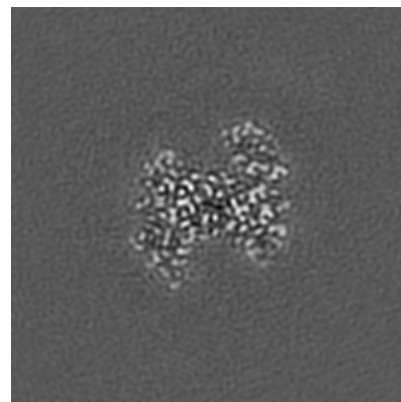
6.3.1 Primary map



X Index: 105

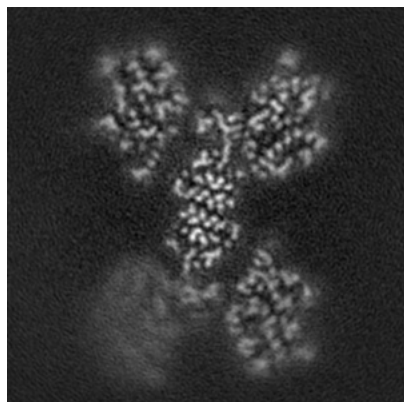


Y Index: 111

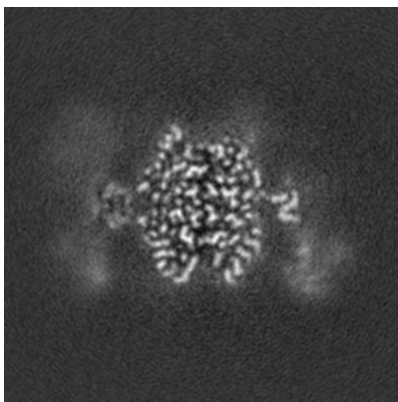


Z Index: 119

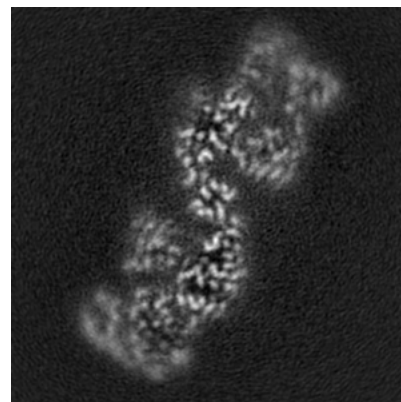
6.3.2 Raw map



X Index: 105



Y Index: 106

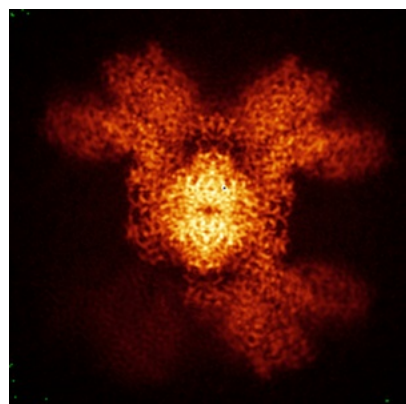


Z Index: 154

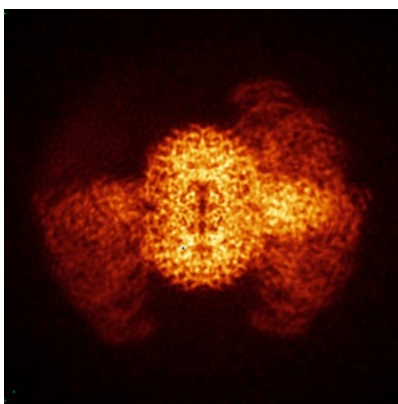
The images above show the largest variance slices of the map in three orthogonal directions.

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

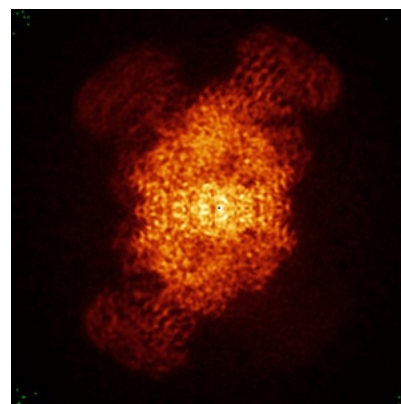
6.4.1 Primary map



X

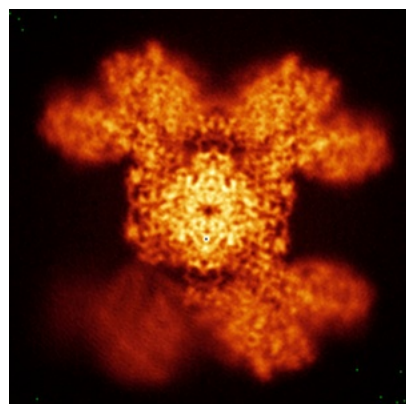


Y

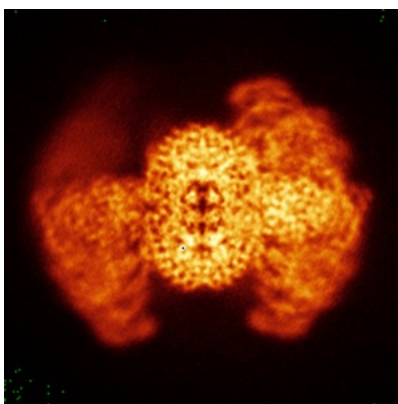


Z

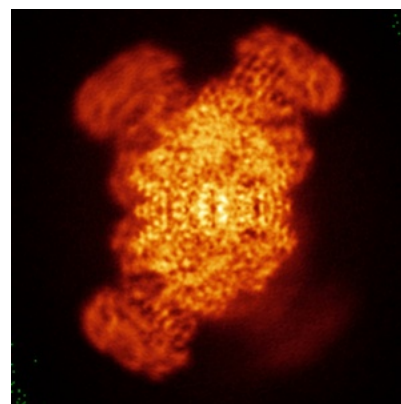
6.4.2 Raw map



X



Y

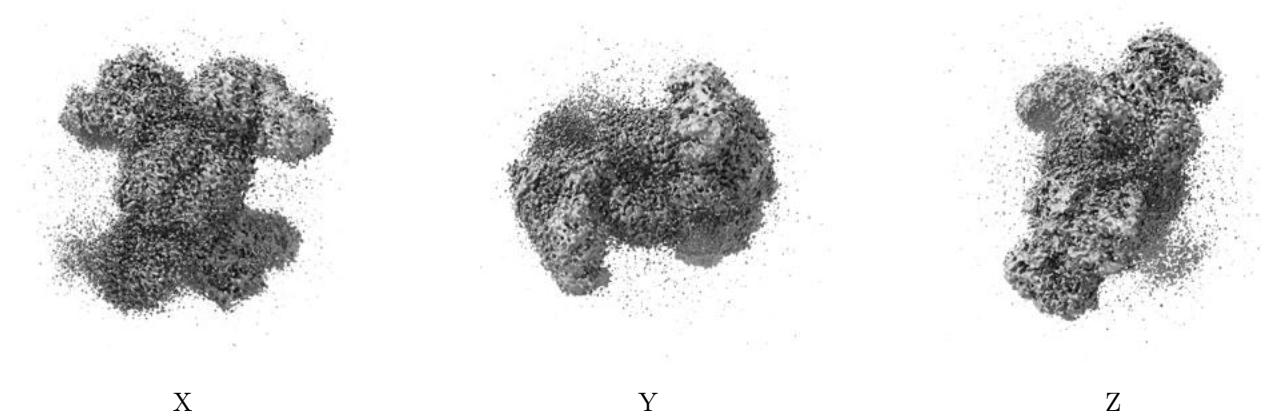


Z

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

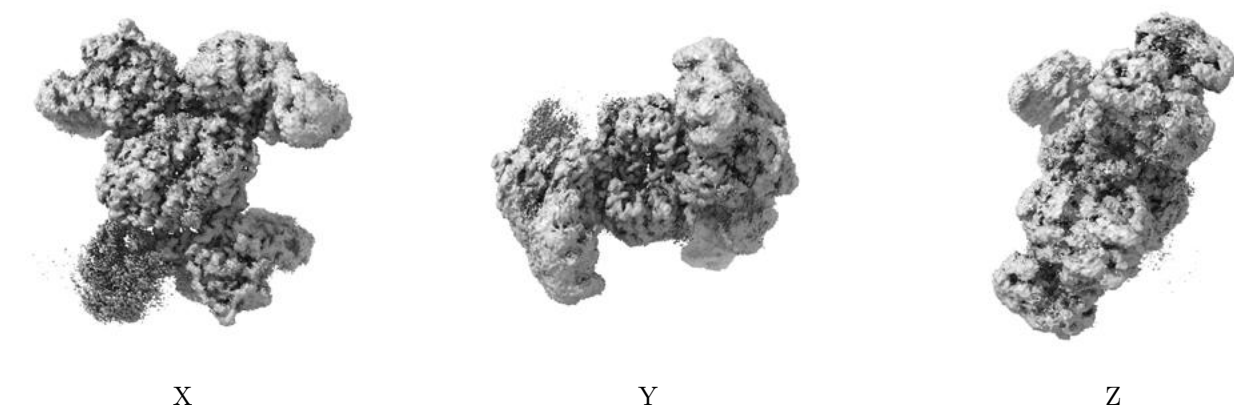
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

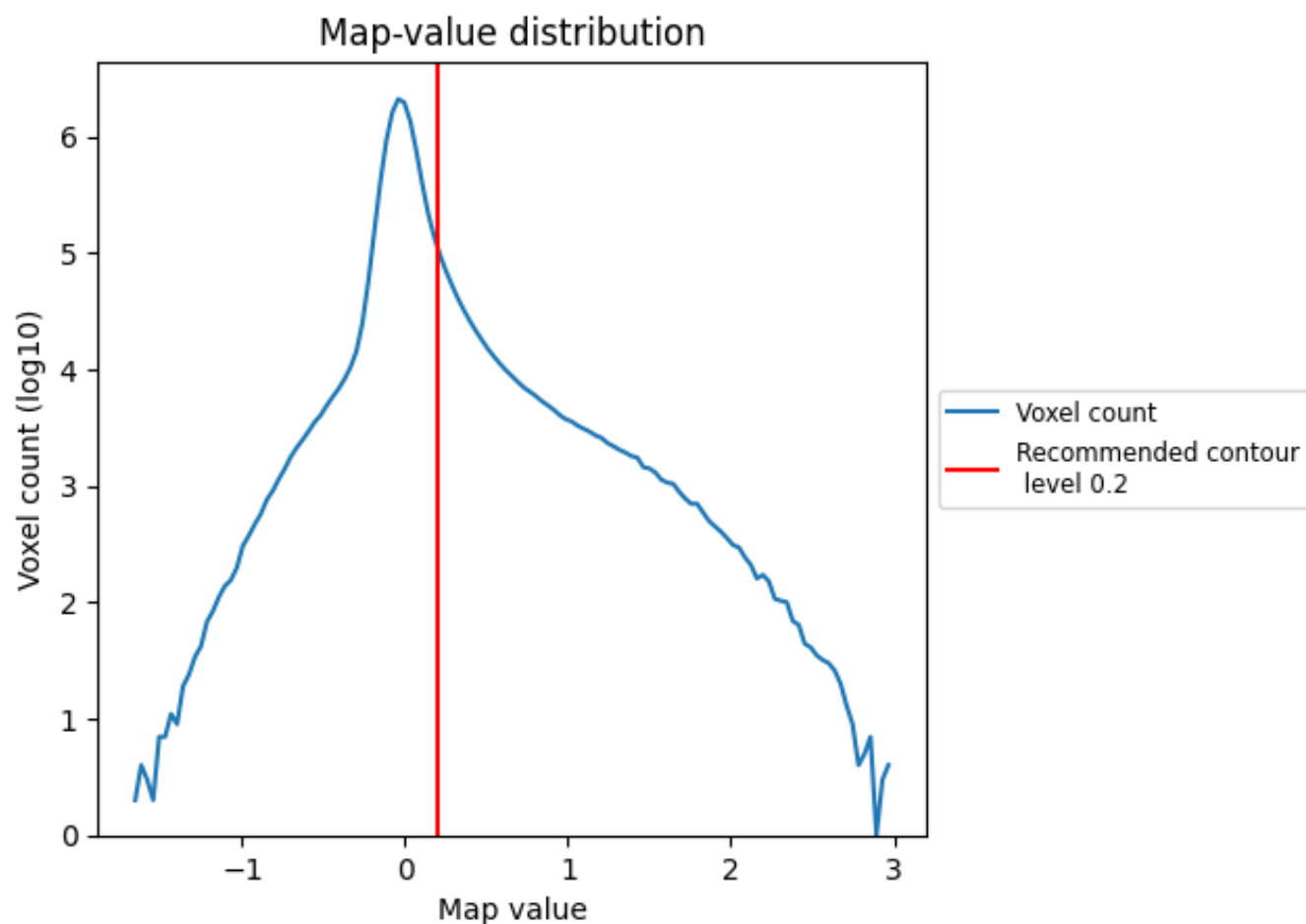
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

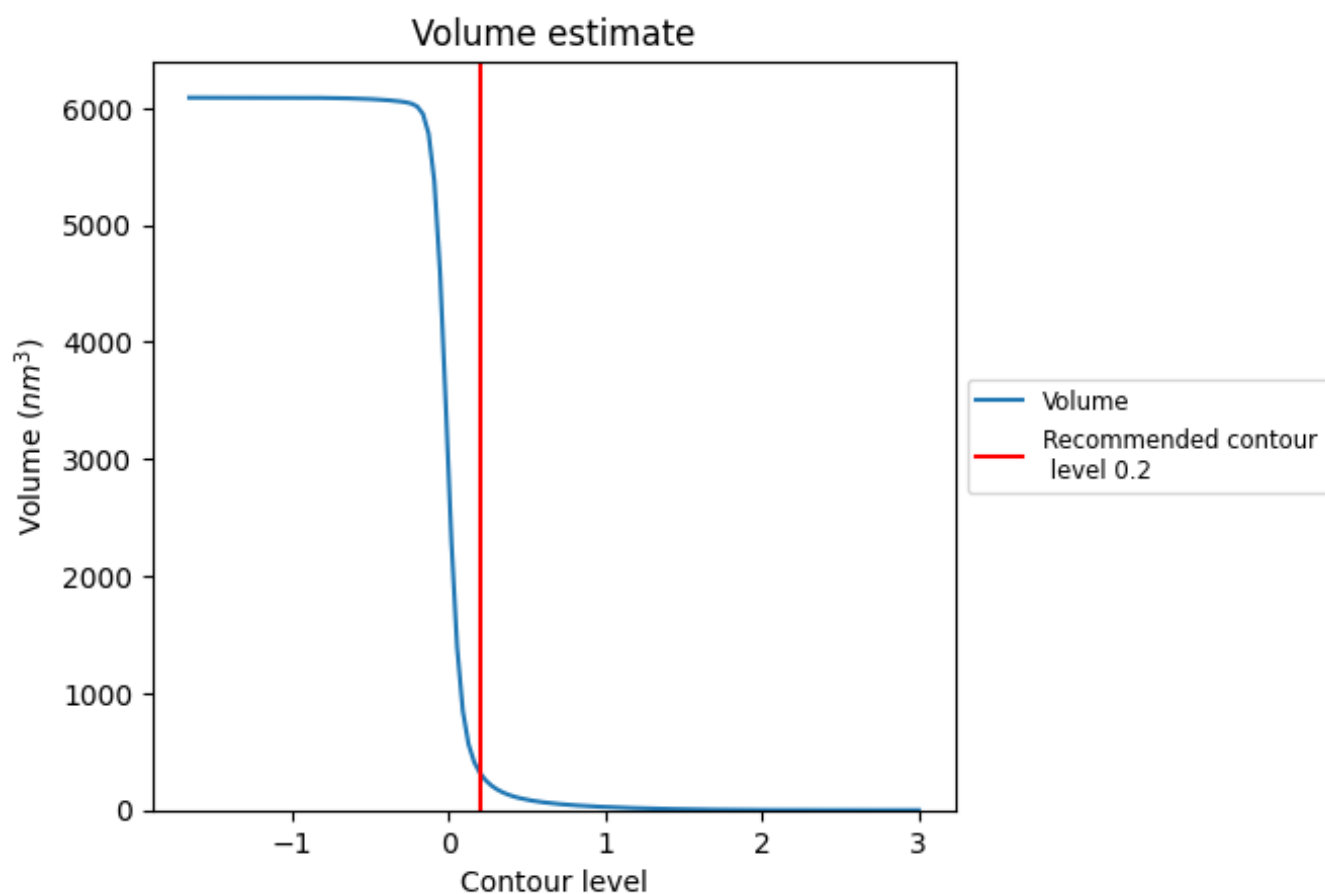
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

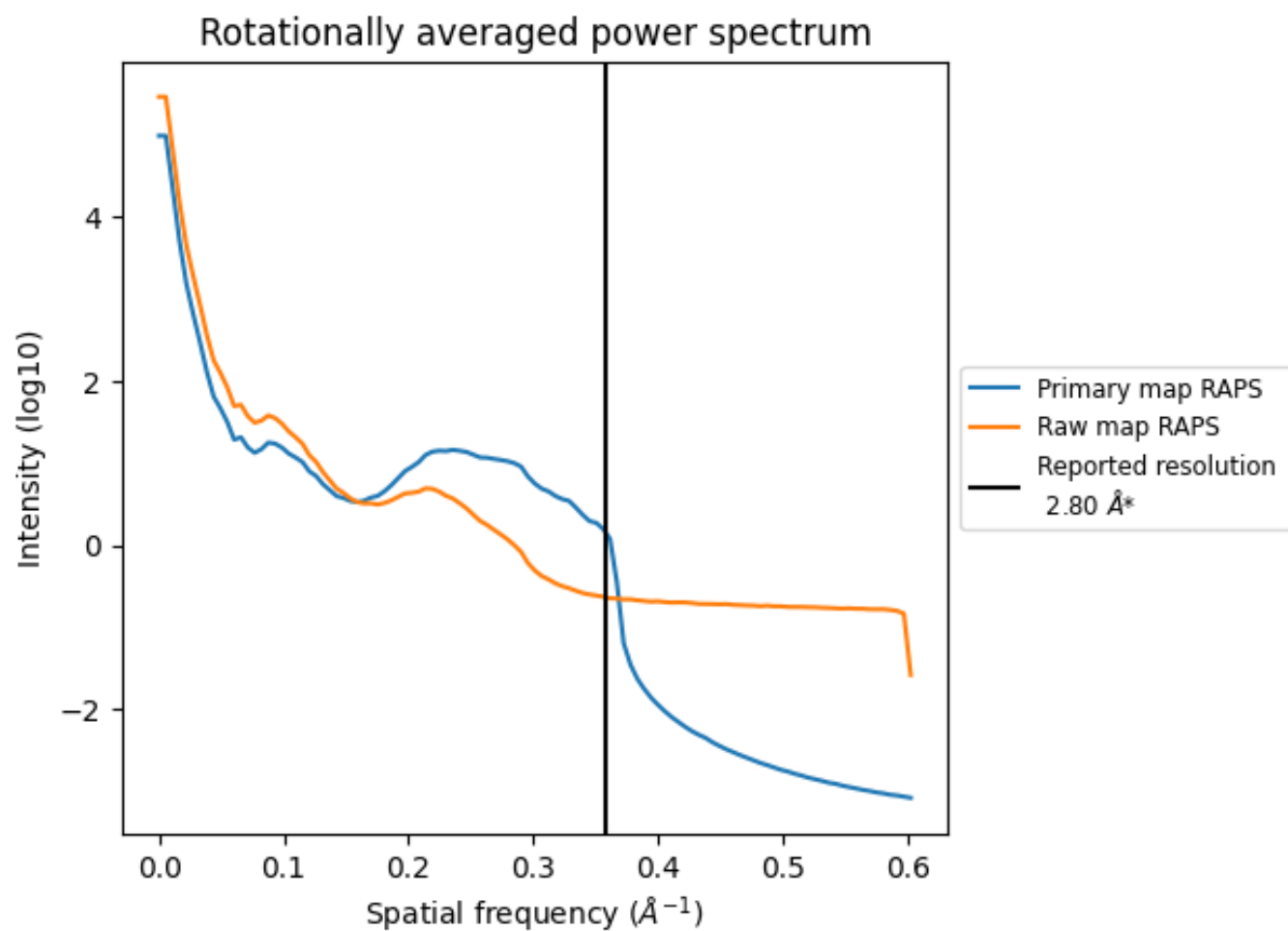
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 320 nm³; this corresponds to an approximate mass of 289 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 ⓘ

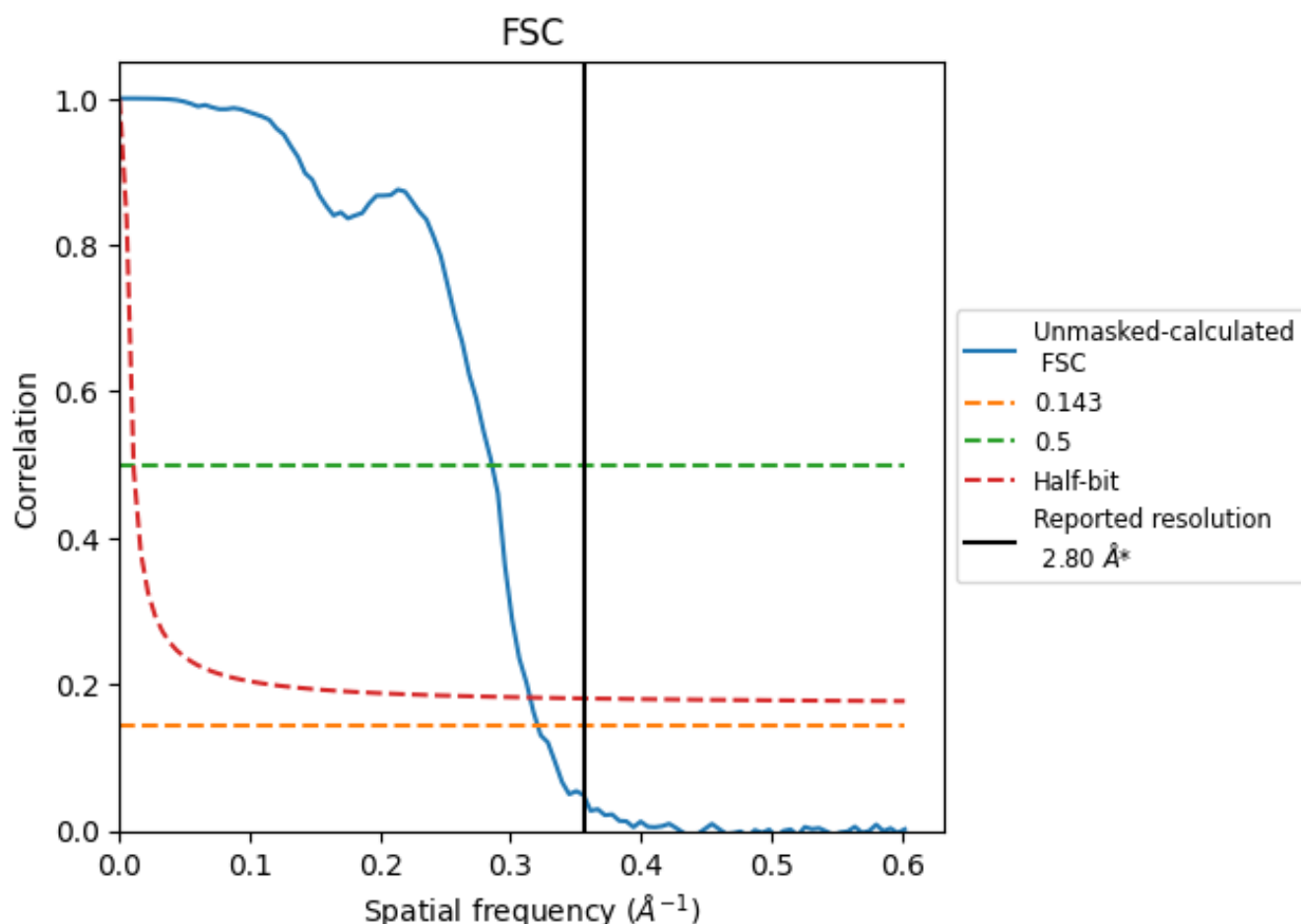


*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 \AA^{-1}

8.2 Resolution estimates [i](#)

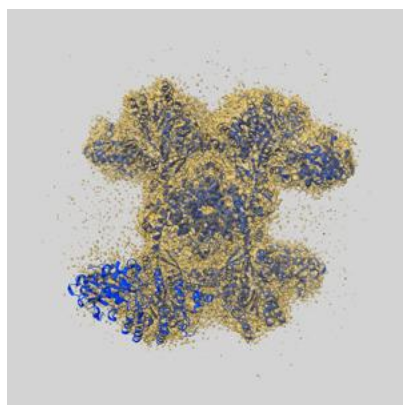
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	3.50	3.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.12 differs from the reported value 2.8 by more than 10 %

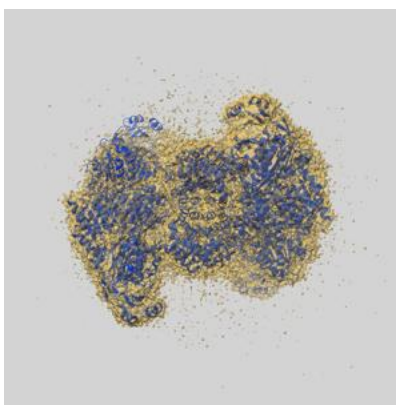
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29668 and PDB model 8G1E. Per-residue inclusion information can be found in section [3](#) on page [8](#).

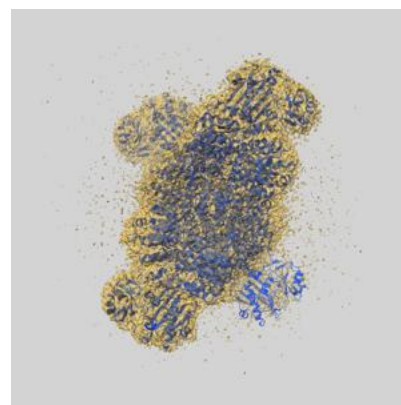
9.1 Map-model overlay [i](#)



X



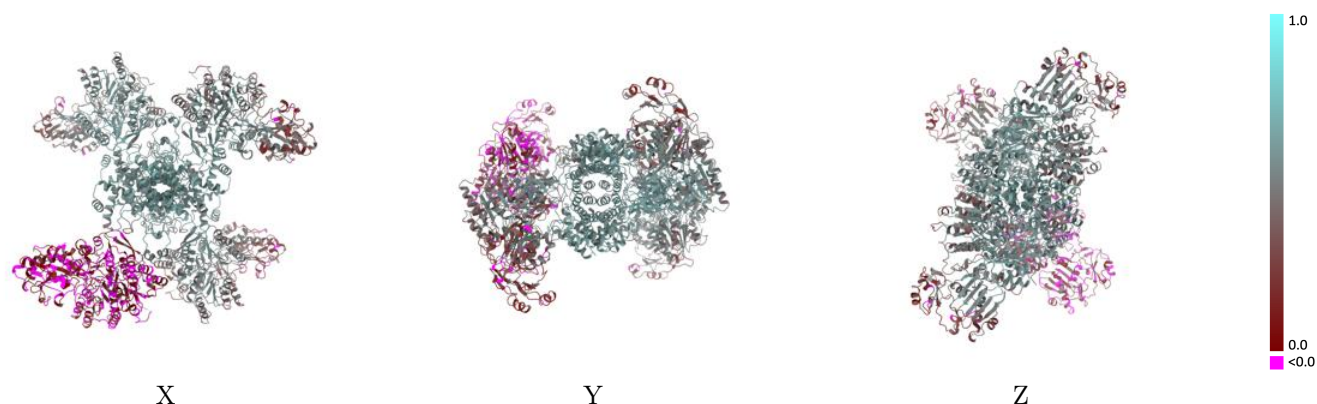
Y



Z

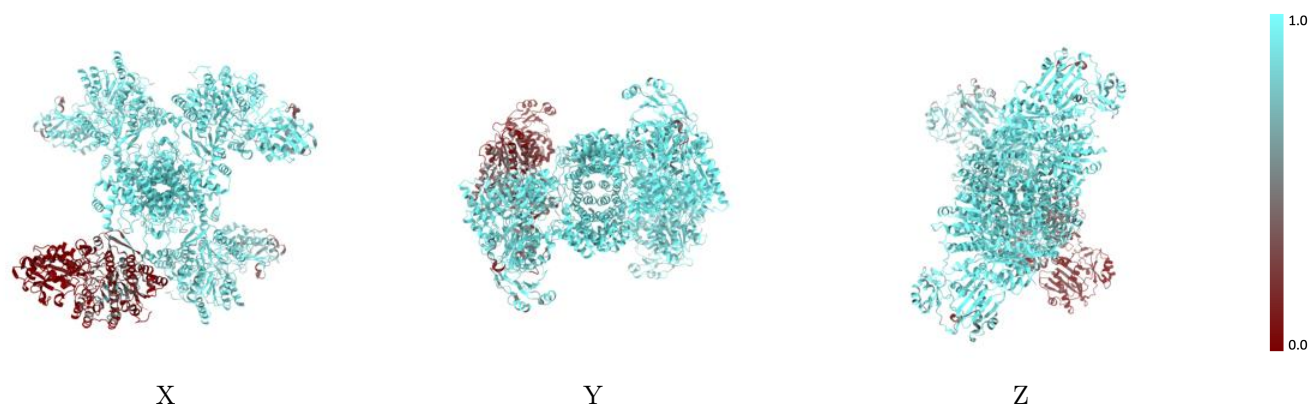
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



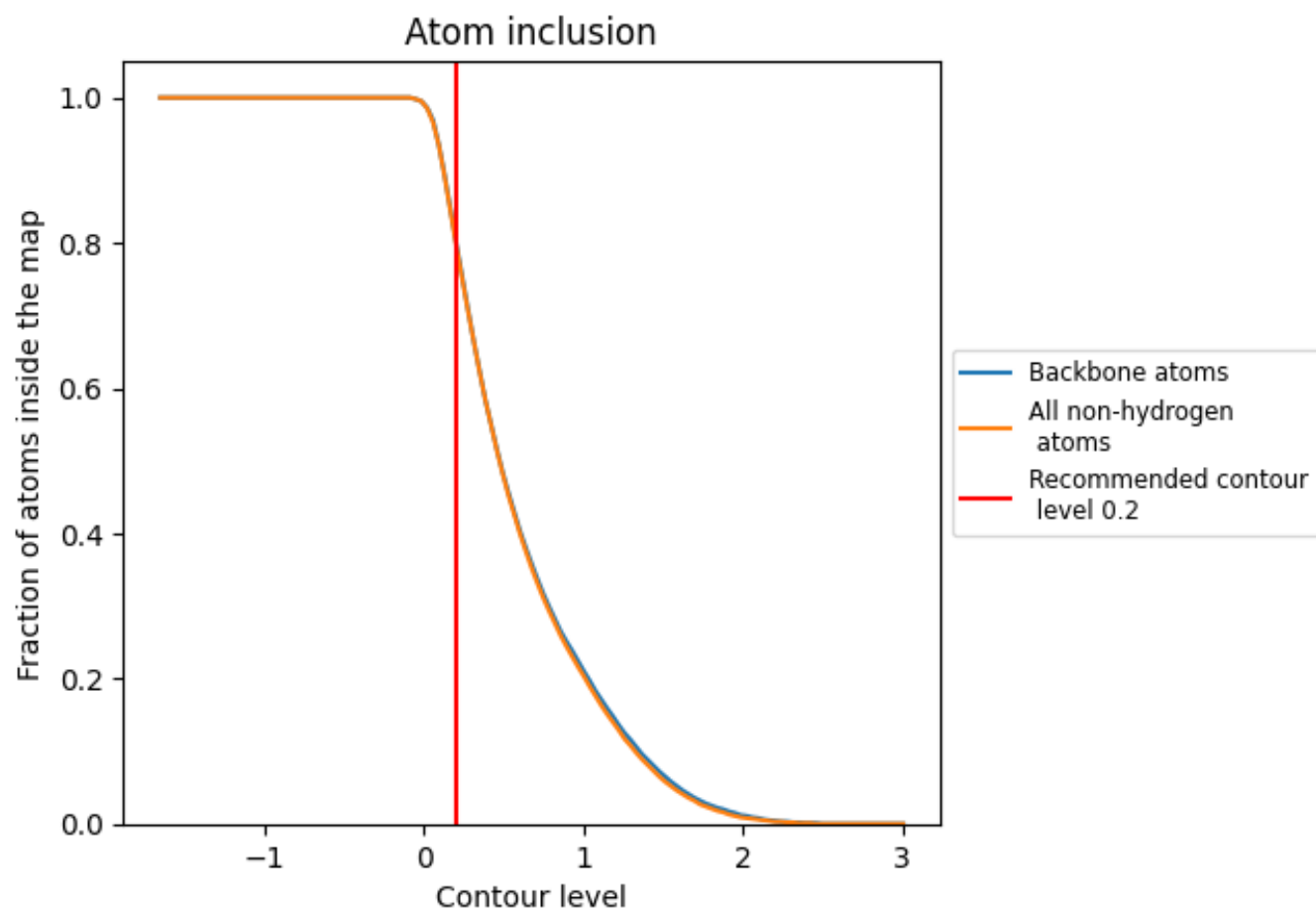
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7970	<div></div> 0.4240
A	<div></div> 0.4030	<div></div> 0.2090
B	<div></div> 0.9010	<div></div> 0.4570
C	<div></div> 0.9450	<div></div> 0.5150
D	<div></div> 0.9420	<div></div> 0.5120

