



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:04 PM UTC

PDB ID : 8SSL / pdb_00008ssl
EMDB ID : EMD-40751
Title : Isobutyryl-CoA mutase fused Q341A in the presence of GTP
Authors : Vaccaro, F.A.; Drennan, C.L.
Deposited on : 2023-05-08
Resolution : 4.60 Å (reported)
Based on initial model : 4XC6

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

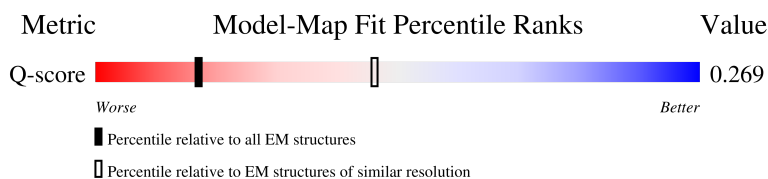
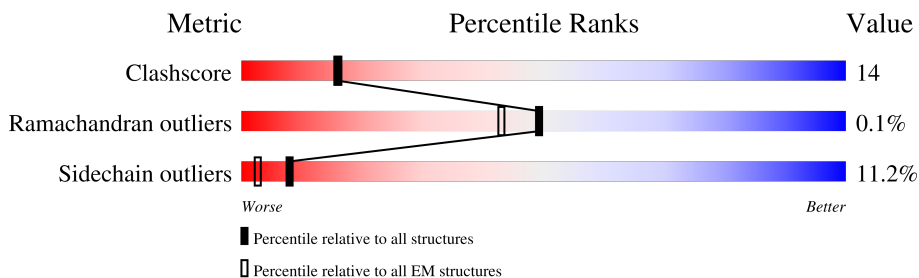
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2407 (4.10 - 5.10)

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	1113	<p>61% 30% 5% .</p>
1	B	1113	<p>65% 28% . .</p>
1	C	1113	<p>7% 64% 28% 5% .</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 24672 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 Fused isobutyryl-CoA mutase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1072	8193	5107	1479	1570	37	0	0
1	B	1072	8197	5110	1480	1570	37	0	0
1	C	1072	8197	5110	1480	1570	37	0	0

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q1LRY0
A	-18	GLY	-	expression tag	UNP Q1LRY0
A	-17	SER	-	expression tag	UNP Q1LRY0
A	-16	SER	-	expression tag	UNP Q1LRY0
A	-15	HIS	-	expression tag	UNP Q1LRY0
A	-14	HIS	-	expression tag	UNP Q1LRY0
A	-13	HIS	-	expression tag	UNP Q1LRY0
A	-12	HIS	-	expression tag	UNP Q1LRY0
A	-11	HIS	-	expression tag	UNP Q1LRY0
A	-10	HIS	-	expression tag	UNP Q1LRY0
A	-9	SER	-	expression tag	UNP Q1LRY0
A	-8	SER	-	expression tag	UNP Q1LRY0
A	-7	GLY	-	expression tag	UNP Q1LRY0
A	-6	LEU	-	expression tag	UNP Q1LRY0
A	-5	VAL	-	expression tag	UNP Q1LRY0
A	-4	PRO	-	expression tag	UNP Q1LRY0
A	-3	ARG	-	expression tag	UNP Q1LRY0
A	-2	GLY	-	expression tag	UNP Q1LRY0
A	-1	SER	-	expression tag	UNP Q1LRY0
A	0	HIS	-	expression tag	UNP Q1LRY0
A	341	ALA	GLN	engineered mutation	UNP Q1LRY0
B	-19	MET	-	initiating methionine	UNP Q1LRY0
B	-18	GLY	-	expression tag	UNP Q1LRY0
B	-17	SER	-	expression tag	UNP Q1LRY0

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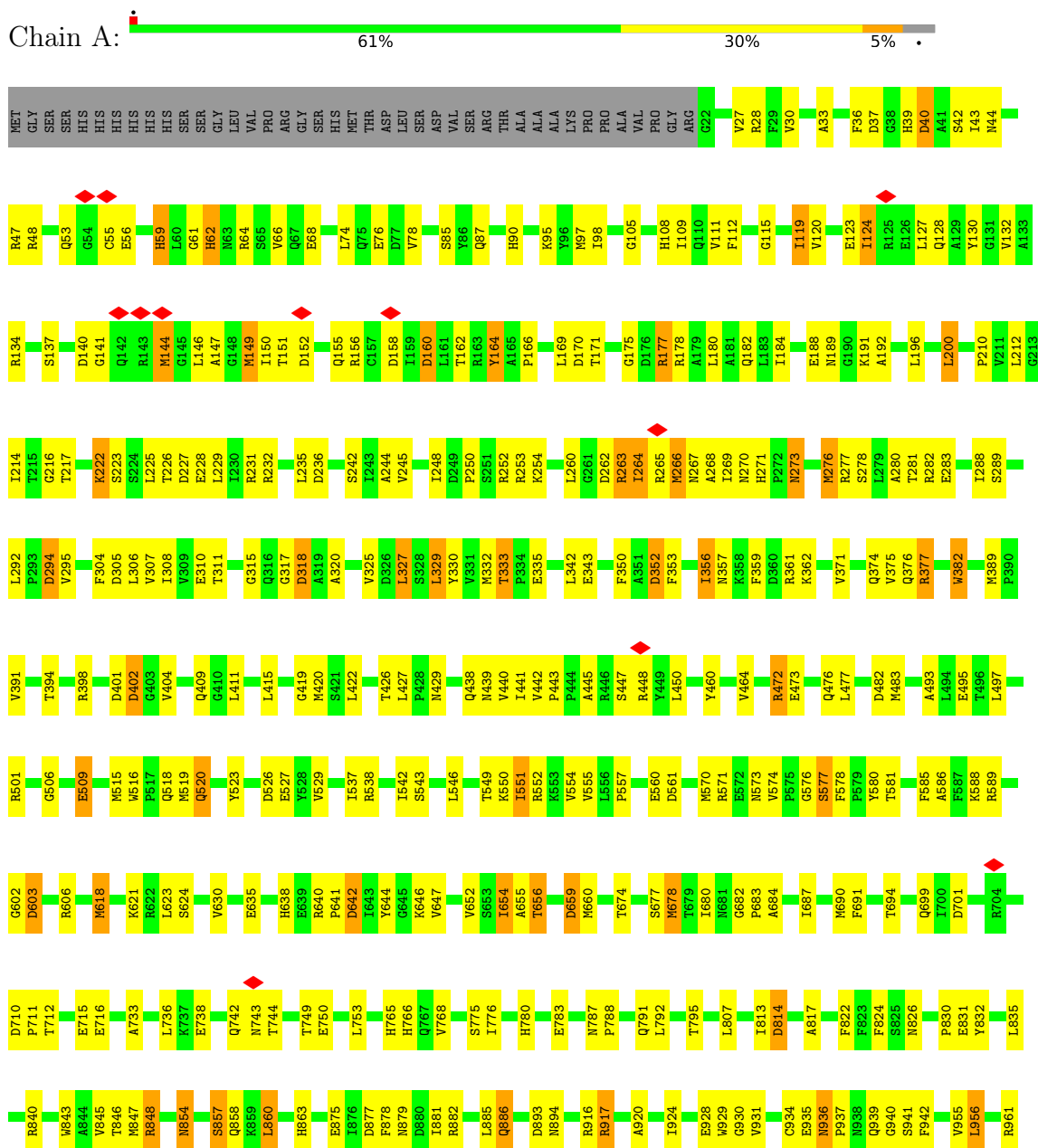
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q1LRY0
B	-15	HIS	-	expression tag	UNP Q1LRY0
B	-14	HIS	-	expression tag	UNP Q1LRY0
B	-13	HIS	-	expression tag	UNP Q1LRY0
B	-12	HIS	-	expression tag	UNP Q1LRY0
B	-11	HIS	-	expression tag	UNP Q1LRY0
B	-10	HIS	-	expression tag	UNP Q1LRY0
B	-9	SER	-	expression tag	UNP Q1LRY0
B	-8	SER	-	expression tag	UNP Q1LRY0
B	-7	GLY	-	expression tag	UNP Q1LRY0
B	-6	LEU	-	expression tag	UNP Q1LRY0
B	-5	VAL	-	expression tag	UNP Q1LRY0
B	-4	PRO	-	expression tag	UNP Q1LRY0
B	-3	ARG	-	expression tag	UNP Q1LRY0
B	-2	GLY	-	expression tag	UNP Q1LRY0
B	-1	SER	-	expression tag	UNP Q1LRY0
B	0	HIS	-	expression tag	UNP Q1LRY0
B	341	ALA	GLN	engineered mutation	UNP Q1LRY0
C	-19	MET	-	initiating methionine	UNP Q1LRY0
C	-18	GLY	-	expression tag	UNP Q1LRY0
C	-17	SER	-	expression tag	UNP Q1LRY0
C	-16	SER	-	expression tag	UNP Q1LRY0
C	-15	HIS	-	expression tag	UNP Q1LRY0
C	-14	HIS	-	expression tag	UNP Q1LRY0
C	-13	HIS	-	expression tag	UNP Q1LRY0
C	-12	HIS	-	expression tag	UNP Q1LRY0
C	-11	HIS	-	expression tag	UNP Q1LRY0
C	-10	HIS	-	expression tag	UNP Q1LRY0
C	-9	SER	-	expression tag	UNP Q1LRY0
C	-8	SER	-	expression tag	UNP Q1LRY0
C	-7	GLY	-	expression tag	UNP Q1LRY0
C	-6	LEU	-	expression tag	UNP Q1LRY0
C	-5	VAL	-	expression tag	UNP Q1LRY0
C	-4	PRO	-	expression tag	UNP Q1LRY0
C	-3	ARG	-	expression tag	UNP Q1LRY0
C	-2	GLY	-	expression tag	UNP Q1LRY0
C	-1	SER	-	expression tag	UNP Q1LRY0
C	0	HIS	-	expression tag	UNP Q1LRY0
C	341	ALA	GLN	engineered mutation	UNP Q1LRY0

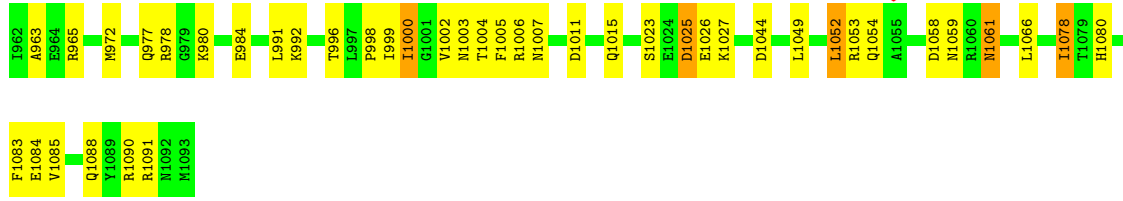
- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂) (labeled as "Ligand of Interest" by depositor).

3 Residue-property plots

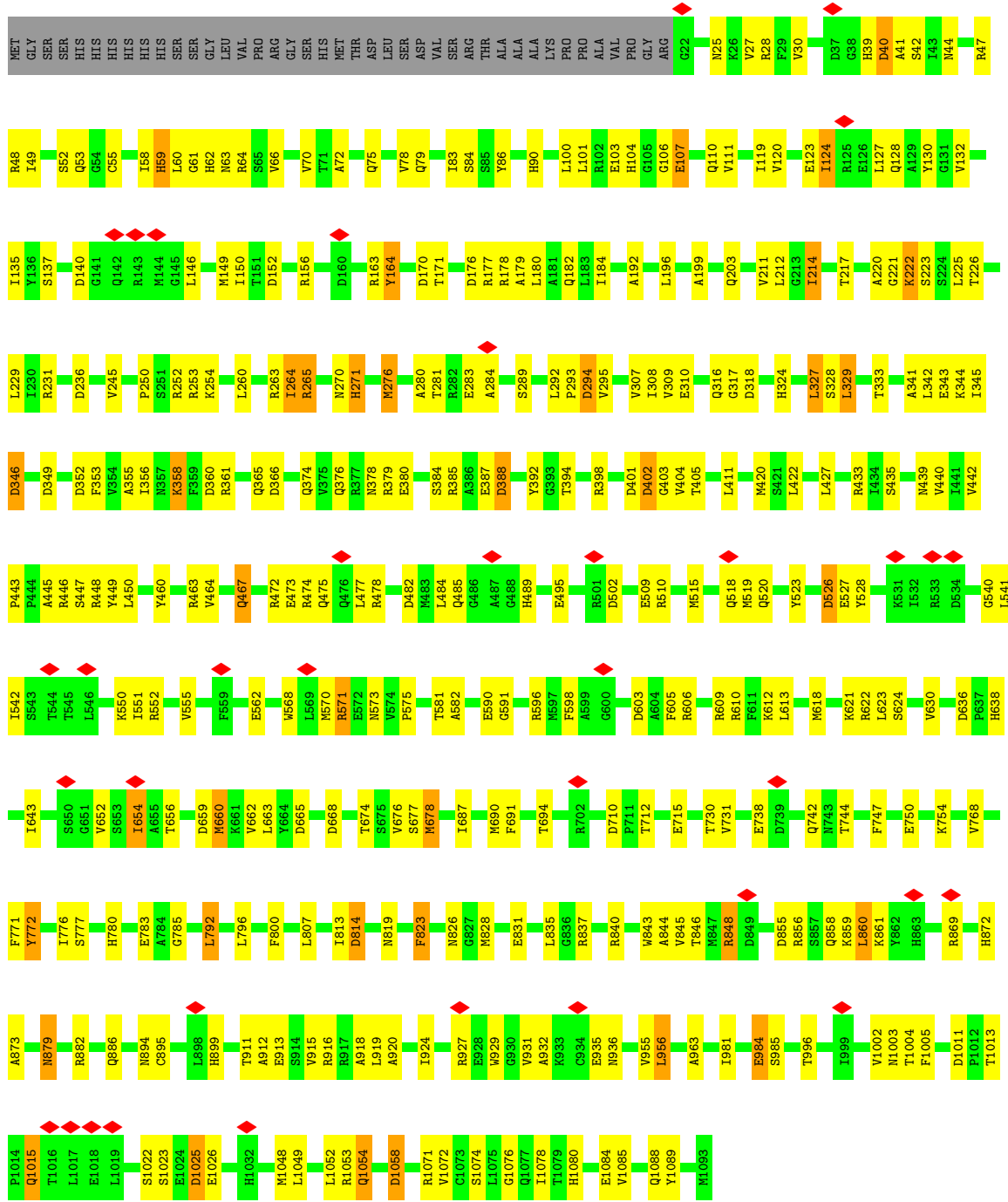
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Fused isobutyryl-CoA mutase





• Molecule 1: Fused isobutyryl-CoA mutase



● Molecule 1: Fused isobutyryl-CoA mutase



MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	PRO	ARG	ARG	GLY	SER	SER	HIS	HIS	MET	THR	ASP	ASP	LEU	LEU	SER	SER	ASP	VAL	VAL	SER	SER	ARG	ARG	THR	THR	ALA	ALA	ALA	LYS	PRO	PRO	ALA	ALA	VAL	PRO	GLY	ARG	G22	R25	R26	V27	R28	F29	V30	F31	A32	A33	S34	L35	G38	H39	D40	A41	S42	I43	M44	I45	M46	R47	R48	I49	L50	O53	S54	C55	E56	L60	G61	H62	M63	R64	S65	F68	V69	V70	A73	L74	L75	Q75	E76	Q79	A82	I83	S84	S85	Y86	Q87	G88	G89	H90	L100	L101	H104	E107	Q110	Q111	G114	G117	V118	I119	D122	E123	I124	R125	Q128	A129	V132	A133	R134	I135	F136	S137	F138	E139	D140	R143	M144	G145	A146	A147	G148	M149	I150	T151	D152	Q157	D160	Y164	A165	P166	T171	A174	R178	A179	L180	A181	I184	F185	F186	L187	E188	M189	G190	L200	A208	V209	F210	L211	L212	G216	T217	G218	G219	A220	G221	K222	S223	S224	K226	D227	E228	R231	R232	F233	R234	L235	M236	Q237	A240	G241	L241	V245	I246	S247	L248	D249	G257	A258	G261	D262	R263	I264	R265	M266	N267	A268	I269	N270	H271	P272	M273	I274	F275	M276	R277	A280	T281	E283	A284	G285	R286	K362	G363	L282	V295	I296	C299	K300	A301	A302	R303	F304	D305	L306	V307	V309	E310	T311	S312	G313	I314	G315	A320	I321	V322	P323	H324	L327	S328	M332	T333	P334	A338	A341	K344	D349	F350	A351	D352	F353	V354	A355	L356	N357	K358	F359	D360	R361	K362	G363	D366	A367	W368	R369	D370	V371	Q374	N378	W382	H383	R385	A386	M389	V391	Y392	G393	T394	R398	D401	D402	G403	V404	T405	L415	G416	A417	M420	S421	L422	T426	M429	L430	R433	N439	V440	I441	V442	L450	Y460	H461	V464	R472	Q476	L477	F478	A479	D482	M483	L484	Q485	E495	T496	V508	E509	E512	Q520	Y523	S524	Y528	K531	E536	G537	R538	L541	I542	S547	K550	I551	R552	V555	L556	P557	R558	F559	E560	W568	L569	M570	S571	E572	N573	V574	S577	M578	T579	N581	P685	I686	L687	L688	A689	M690	Q699	R702	F703	R704	N707	T712	D734	E738	D739	Q742	N743	T744	F747	E750	K754	G757	D758	I759	V768	Y772	H780	E783	P788	Y806	L807	I813	D814	D815	F816	A817	P818	N819	F822	N826	D829	P830	E831	Y832	L835	R840	W843	A844	T846	R847	R848	D849	K850	Y851	D855	R856	S857	Q858	K859	L860	H863	H872	E875	F878	N879	D880	I881	R882	T883	L884	L885	Q886	D893	M894	C895	H899	T911	A912	E913	S914	V915	R916	R917	I921	I924	E928	N929	G930	Y931	C934	E935	N936	P937	N938	Q939	C940	S941	F942	L943	L956	A963	L969	M972	Q977	R978	G979	Q988	V989	R990	I991	L991	L997	I1000	G1001	V1002	M1003	T1004	F1005	R1006	N1007	Q1015	T1016	L1017	A1020	S1023	E1024	D1025	E1026	K1027	Q1028	D1044	M1048	L1049	A1050	R1051	L1052	R1053	Q1054	I1057	V1065	C1073	S1074	G1075	G1076	Q1077	I1078	T1079	H1080	A1081	L1082	F1083	E1084	V1085	G1086	G1087	Q1088	V1089	R1090	I1091	N1092	M1093
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59335	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58.71	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3100	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	14.743	Depositor
Minimum map value	0.000	Depositor
Average map value	0.260	Depositor
Map value standard deviation	0.795	Depositor
Recommended contour level	2.69	Depositor
Map size (\AA)	313.5608, 313.5608, 313.5608	wwPDB
Map dimensions	196, 196, 196	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.5998, 1.5998, 1.5998	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: GDP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/8336	0.37	0/11289
1	B	0.18	0/8340	0.36	0/11293
1	C	0.18	0/8340	0.39	1/11293 (0.0%)
All	All	0.19	0/25016	0.37	1/33875 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	312	SER	CB-CA-C	-6.22	109.39	116.54

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	8193	0	7948	282	0
1	B	8197	0	7959	207	0
1	C	8197	0	7959	276	0
2	A	28	0	12	1	0
2	B	28	0	12	5	0
2	C	28	0	12	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24672	0	23902	699	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 14.

All (699) 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:338:ALA:HB1	1:C:341:ALA:HB3	1.55	0.89
1:C:402:ASP:OD1	1:C:402:ASP:N	2.12	0.82
1:C:366:ASP:OD1	1:C:366:ASP:N	2.11	0.82
1:B:358:LYS:HD3	1:B:360:ASP:HB2	1.61	0.81
1:C:28:ARG:HB2	1:C:79:GLN:HG2	1.63	0.79
1:A:940:GLY:N	1:C:941:SER:H	1.81	0.79
1:B:463:ARG:HE	1:B:467:GLN:HE22	1.32	0.78
1:A:940:GLY:H	1:C:940:GLY:H	1.28	0.78
1:A:362:LYS:H	1:B:361:ARG:HH12	1.32	0.78
1:A:894:ASN:HD21	1:A:935:GLU:HB3	1.50	0.76
1:A:641:PRO:HA	1:A:644:TYR:HB3	1.66	0.76
1:A:294:ASP:OD1	1:A:294:ASP:N	2.19	0.76
1:A:377:ARG:HD3	1:B:48:ARG:HD3	1.68	0.76
1:B:294:ASP:N	1:B:294:ASP:OD1	2.19	0.75
1:B:439:ASN:HD21	1:B:754:LYS:HD3	1.52	0.74
1:C:523:TYR:O	1:C:552:ARG:NH1	2.20	0.73
1:C:398:ARG:NH2	1:C:439:ASN:O	2.21	0.73
1:A:210:PRO:HG3	1:A:420:MET:HG2	1.70	0.73
1:C:441:ILE:HG21	1:C:969:LEU:CD2	2.19	0.73
1:A:546:LEU:HD21	1:C:997:LEU:HD22	1.70	0.73
1:A:252:ARG:NH2	1:B:343:GLU:O	2.22	0.73
1:C:1051:ARG:HH21	1:C:1065:VAL:HA	1.54	0.72
1:A:40:ASP:OD1	1:A:40:ASP:N	2.22	0.72
1:A:941:SER:H	1:C:940:GLY:N	1.87	0.72
1:B:264:ILE:HG23	1:B:265:ARG:HD3	1.71	0.72
1:A:62:HIS:O	1:A:1091:ARG:NH2	2.23	0.72
1:A:74:LEU:HD11	1:A:178:ARG:HD3	1.71	0.71
1:A:940:GLY:H	1:C:940:GLY:N	1.87	0.71
1:A:678:MET:SD	1:A:678:MET:N	2.64	0.71
1:C:699:GLN:HE22	1:C:702:ARG:HE	1.38	0.71
1:A:1025:ASP:OD1	1:A:1025:ASP:N	2.21	0.71
1:A:523:TYR:O	1:A:552:ARG:NH1	2.24	0.70
1:A:318:ASP:N	1:A:318:ASP:OD1	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:807:LEU:HD12	1:A:813:ILE:HD11	1.72	0.70
1:A:212:LEU:HB3	1:A:308:ILE:HD13	1.72	0.70
1:A:450:LEU:HB2	1:A:963:ALA:HB2	1.74	0.70
1:A:743:ASN:OD1	1:A:978:ARG:NH2	2.24	0.70
1:B:49:ILE:O	1:B:53:GLN:NE2	2.24	0.70
1:C:366:ASP:HA	1:C:369:ARG:HH11	1.56	0.70
1:B:388:ASP:N	1:B:388:ASP:OD1	2.24	0.69
1:B:678:MET:SD	1:B:678:MET:N	2.65	0.69
1:A:576:GLY:HA3	1:A:586:ALA:HA	1.74	0.69
1:C:217:THR:OG1	1:C:315:GLY:O	2.11	0.69
1:A:222:LYS:NZ	1:A:262:ASP:OD2	2.25	0.69
1:A:940:GLY:N	1:C:940:GLY:H	1.90	0.69
1:B:40:ASP:OD1	1:B:40:ASP:N	2.22	0.69
1:C:281:THR:HG22	1:C:283:GLU:H	1.57	0.69
1:C:68:GLU:OE1	1:C:270:ASN:ND2	2.27	0.68
1:A:398:ARG:NH2	1:A:439:ASN:O	2.25	0.68
1:A:972:MET:HA	1:A:977:GLN:HE22	1.59	0.68
1:C:314:ILE:HG22	1:C:315:GLY:H	1.59	0.68
1:A:877:ASP:O	1:C:917:ARG:NH2	2.27	0.67
1:C:223:SER:O	1:C:227:ASP:N	2.23	0.67
1:A:561:ASP:OD1	1:C:472:ARG:NH1	2.28	0.67
1:B:807:LEU:HD12	1:B:813:ILE:HD11	1.74	0.67
1:B:1025:ASP:OD1	1:B:1025:ASP:N	2.27	0.67
1:C:160:ASP:OD1	1:C:160:ASP:N	2.27	0.67
1:A:448:ARG:NH1	1:B:447:SER:OG	2.27	0.66
1:A:581:THR:O	1:A:840:ARG:NH1	2.28	0.66
1:C:542:ILE:HD11	1:C:550:LYS:HB2	1.76	0.66
1:B:44:ASN:OD1	1:B:48:ARG:NH2	2.29	0.66
1:A:448:ARG:HG2	1:B:448:ARG:HH11	1.60	0.66
1:A:738:GLU:OE2	1:A:744:THR:OG1	2.12	0.66
1:B:398:ARG:HH22	1:B:440:VAL:HG23	1.59	0.66
1:A:273:ASN:OD1	1:A:273:ASN:N	2.28	0.66
1:B:475:GLN:OE1	1:B:562:GLU:N	2.28	0.66
1:A:780:HIS:HA	1:A:783:GLU:HB3	1.78	0.65
1:A:343:GLU:O	1:B:252:ARG:NH2	2.28	0.65
1:C:738:GLU:OE2	1:C:744:THR:OG1	2.14	0.65
1:C:357:ASN:ND2	2:C:1101:GDP:O6	2.29	0.65
1:C:840:ARG:NH2	1:C:893:ASP:O	2.29	0.65
1:C:104:HIS:O	1:C:178:ARG:NH2	2.29	0.65
1:A:164:TYR:O	1:A:182:GLN:NE2	2.30	0.65
1:A:105:GLY:O	1:A:178:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:HB1	1:A:196:LEU:HD12	1.78	0.64
1:B:245:VAL:HG22	1:B:308:ILE:HB	1.80	0.64
1:B:612:LYS:NZ	1:B:665:ASP:O	2.31	0.64
1:B:214:ILE:HG23	1:B:329:LEU:HB3	1.78	0.64
1:C:441:ILE:HG21	1:C:969:LEU:HD22	1.78	0.64
1:C:855:ASP:OD1	1:C:855:ASP:N	2.28	0.64
1:B:606:ARG:NH2	1:B:1022:SER:OG	2.30	0.64
1:A:401:ASP:OD2	1:A:404:VAL:N	2.31	0.64
1:B:192:ALA:HB1	1:B:196:LEU:HD12	1.80	0.64
1:B:502:ASP:O	1:B:510:ARG:NH1	2.31	0.64
1:B:231:ARG:NH1	1:B:1084:GLU:O	2.31	0.63
1:C:807:LEU:HD12	1:C:813:ILE:HD11	1.81	0.63
1:A:791:GLN:HE21	1:A:824:PHE:HB2	1.64	0.63
1:B:184:ILE:HD12	1:B:295:VAL:HG23	1.81	0.63
1:C:245:VAL:HG22	1:C:308:ILE:HB	1.80	0.63
1:C:573:ASN:OD1	1:C:574:VAL:N	2.27	0.63
1:A:1000:ILE:HG21	1:C:924:ILE:HA	1.81	0.62
1:A:940:GLY:H	1:C:939:GLN:HA	1.64	0.62
1:B:39:HIS:CE1	1:B:42:SER:H	2.17	0.62
1:C:35:LEU:HA	1:C:63:ASN:HA	1.81	0.62
1:A:398:ARG:HH21	1:A:441:ILE:HG12	1.63	0.62
1:B:270:ASN:O	1:B:271:HIS:ND1	2.22	0.62
1:C:1051:ARG:NH2	1:C:1065:VAL:HA	2.14	0.62
1:A:33:ALA:HB2	1:A:43:ILE:HD11	1.80	0.62
1:B:450:LEU:HB2	1:B:963:ALA:HB2	1.82	0.62
1:B:581:THR:O	1:B:840:ARG:NH1	2.32	0.62
1:A:573:ASN:OD1	1:A:574:VAL:N	2.29	0.62
1:A:588:LYS:NZ	1:A:589:ARG:O	2.29	0.61
1:C:392:TYR:HE1	1:C:433:ARG:HA	1.65	0.61
1:A:495:GLU:OE1	1:A:495:GLU:N	2.32	0.61
1:C:65:SER:HB2	1:C:68:GLU:HB3	1.82	0.61
1:C:222:LYS:HD3	1:C:310:GLU:HB3	1.82	0.61
1:A:448:ARG:HH11	1:B:448:ARG:HG2	1.65	0.61
1:C:495:GLU:N	1:C:495:GLU:OE1	2.31	0.61
1:C:843:TRP:O	1:C:846:THR:OG1	2.16	0.61
1:B:776:ILE:O	1:B:823:PHE:N	2.34	0.61
1:C:247:SER:HA	1:C:310:GLU:HB2	1.83	0.61
1:C:699:GLN:O	1:C:702:ARG:HB3	2.00	0.61
1:C:911:THR:OG1	1:C:912:ALA:N	2.34	0.61
1:C:678:MET:SD	1:C:678:MET:N	2.73	0.61
1:C:880:ASP:O	1:C:883:THR:OG1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:GLU:OE2	1:B:744:THR:OG1	2.19	0.60
1:C:656:THR:N	1:C:659:ASP:OD2	2.28	0.60
1:A:342:LEU:HD21	1:A:371:VAL:HA	1.82	0.60
1:A:854:ASN:N	1:A:854:ASN:OD1	2.33	0.60
1:B:1071:ARG:HG2	1:B:1072:VAL:HG13	1.84	0.60
1:A:276:MET:SD	1:A:277:ARG:N	2.75	0.60
1:A:814:ASP:N	1:A:814:ASP:OD1	2.31	0.60
1:B:128:GLN:HA	1:B:132:VAL:HG12	1.84	0.59
1:C:222:LYS:N	2:C:1101:GDP:O2B	2.35	0.59
1:C:450:LEU:HB2	1:C:963:ALA:HB2	1.84	0.59
1:A:382:TRP:CD1	1:A:382:TRP:H	2.18	0.59
1:C:354:VAL:HG11	1:C:391:VAL:HG13	1.84	0.59
1:A:654:ILE:HG22	1:A:659:ASP:HB2	1.85	0.59
1:B:402:ASP:OD1	1:B:402:ASP:N	2.35	0.59
1:B:528:TYR:HB2	1:B:541:LEU:HD11	1.85	0.59
1:B:831:GLU:OE1	1:B:831:GLU:N	2.33	0.59
1:A:362:LYS:H	1:B:361:ARG:NH1	2.01	0.59
1:A:227:ASP:OD2	1:A:1090:ARG:NH2	2.36	0.59
1:A:621:LYS:H	1:A:674:THR:HG22	1.68	0.58
1:C:1002:VAL:O	1:C:1006:ARG:NE	2.28	0.58
1:A:356:ILE:HB	1:A:359:PHE:HE1	1.67	0.58
1:A:402:ASP:OD1	1:A:402:ASP:N	2.34	0.58
1:A:245:VAL:HB	1:A:276:MET:HG2	1.84	0.58
1:A:602:GLY:HA3	1:A:606:ARG:HH21	1.67	0.58
1:B:199:ALA:O	1:B:203:GLN:HG2	2.03	0.58
1:A:787:ASN:ND2	1:C:547:SER:OG	2.36	0.58
1:B:28:ARG:HB2	1:B:79:GLN:HG2	1.85	0.58
1:C:621:LYS:HB2	1:C:674:THR:HG22	1.85	0.58
1:A:64:ARG:HE	1:A:1091:ARG:NH2	2.02	0.57
1:C:137:SER:HB2	1:C:140:ASP:HB3	1.85	0.57
1:C:334:PRO:HG3	1:C:358:LYS:HB2	1.86	0.57
1:C:352:ASP:OD2	1:C:353:PHE:N	2.36	0.57
1:C:509:GLU:CD	1:C:509:GLU:H	2.10	0.57
1:B:495:GLU:OE1	1:B:495:GLU:N	2.33	0.57
1:A:39:HIS:CE1	1:A:42:SER:H	2.23	0.57
1:B:318:ASP:OD1	1:B:318:ASP:N	2.35	0.57
1:C:441:ILE:HG22	1:C:442:VAL:HG12	1.84	0.57
1:C:329:LEU:HA	1:C:352:ASP:OD2	2.03	0.57
1:C:578:PHE:CE2	1:C:848:ARG:HG3	2.39	0.57
1:A:266:MET:SD	1:A:268:ALA:N	2.75	0.57
1:B:281:THR:HG22	1:B:283:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:GLU:OE1	1:C:509:GLU:N	2.31	0.57
1:C:685:PRO:O	1:C:688:LEU:HB3	2.04	0.57
1:C:817:ALA:HB3	1:C:857:SER:HB3	1.87	0.56
1:C:341:ALA:O	1:C:344:LYS:NZ	2.33	0.56
1:C:936:ASN:N	1:C:936:ASN:OD1	2.38	0.56
1:A:137:SER:HB2	1:A:140:ASP:HB3	1.85	0.56
1:B:75:GLN:HE22	1:B:276:MET:H	1.52	0.56
1:C:847:MET:HB2	1:C:858:GLN:HG3	1.86	0.56
1:C:39:HIS:CE1	1:C:42:SER:H	2.23	0.56
1:B:358:LYS:N	1:B:394:THR:O	2.36	0.56
1:C:415:LEU:HG	1:C:420:MET:HG2	1.86	0.56
1:A:557:PRO:HA	1:C:942:PHE:HE1	1.69	0.56
1:B:691:PHE:O	1:B:694:THR:OG1	2.18	0.56
1:A:226:THR:OG1	1:A:310:GLU:OE2	2.24	0.56
1:A:352:ASP:OD1	1:A:352:ASP:N	2.39	0.56
1:B:222:LYS:NZ	2:B:1101:GDP:O3B	2.28	0.56
1:C:555:VAL:H	1:C:936:ASN:HD21	1.52	0.56
1:A:644:TYR:O	1:A:1027:LYS:NZ	2.26	0.56
1:B:176:ASP:OD2	1:B:179:ALA:N	2.29	0.56
1:A:1007:ASN:OD1	1:C:916:ARG:NH2	2.39	0.55
1:A:1052:LEU:HD21	1:A:1066:LEU:HD22	1.88	0.55
1:B:107:GLU:O	1:B:110:GLN:NE2	2.39	0.55
1:C:441:ILE:HG21	1:C:969:LEU:HD21	1.87	0.55
1:A:119:ILE:HB	1:A:124:ILE:HB	1.88	0.55
1:C:1051:ARG:HE	1:C:1065:VAL:HG13	1.71	0.55
1:A:281:THR:HG22	1:A:283:GLU:H	1.71	0.55
1:A:840:ARG:NH2	1:A:893:ASP:O	2.39	0.55
1:B:72:ALA:HB1	1:B:263:ARG:HH22	1.72	0.55
1:C:128:GLN:HA	1:C:132:VAL:HG13	1.88	0.55
1:B:814:ASP:OD1	1:B:814:ASP:N	2.37	0.55
1:A:939:GLN:C	1:C:941:SER:H	2.15	0.55
1:C:181:ALA:HA	1:C:277:ARG:HH12	1.72	0.55
1:B:226:THR:OG1	1:B:310:GLU:OE2	2.23	0.55
1:C:641:PRO:HA	1:C:644:TYR:HB3	1.89	0.55
1:A:509:GLU:CD	1:A:509:GLU:H	2.13	0.55
1:B:30:VAL:HG23	1:B:78:VAL:HG11	1.89	0.55
1:C:576:GLY:HA3	1:C:586:ALA:HA	1.89	0.55
1:A:68:GLU:OE1	1:A:270:ASN:ND2	2.39	0.54
1:A:329:LEU:HD22	1:A:353:PHE:HB2	1.89	0.54
1:A:555:VAL:H	1:A:936:ASN:HD21	1.54	0.54
1:A:691:PHE:O	1:A:694:THR:OG1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:SER:HB2	1:B:140:ASP:HB3	1.89	0.54
1:C:146:LEU:O	1:C:150:ILE:HG12	2.07	0.54
1:A:59:HIS:CD2	1:A:61:GLY:H	2.26	0.54
1:A:765:HIS:O	1:A:765:HIS:ND1	2.40	0.54
1:B:27:VAL:HB	1:B:55:CYS:HB3	1.89	0.54
1:B:920:ALA:O	1:B:924:ILE:N	2.35	0.54
1:B:1023:SER:HB3	1:B:1026:GLU:HG3	1.88	0.54
1:A:543:SER:HB3	1:A:551:ILE:HG23	1.88	0.54
1:A:578:PHE:HE2	1:A:848:ARG:HG3	1.72	0.54
1:B:75:GLN:NE2	1:B:276:MET:H	2.06	0.54
1:B:403:GLY:H	1:B:435:SER:HB2	1.73	0.54
1:B:915:VAL:O	1:B:919:LEU:N	2.35	0.54
1:A:30:VAL:HG23	1:A:78:VAL:HG11	1.89	0.54
1:B:101:LEU:O	1:B:106:GLY:N	2.40	0.54
1:A:941:SER:HA	1:C:937:PRO:HA	1.89	0.54
1:B:402:ASP:O	1:B:405:THR:OG1	2.21	0.54
1:B:527:GLU:HG2	1:B:540:GLY:HA2	1.89	0.54
1:B:289:SER:HB3	1:B:292:LEU:HB2	1.90	0.54
1:C:625:THR:HB	1:C:678:MET:HB3	1.88	0.54
1:A:881:ILE:HG13	1:C:917:ARG:HE	1.73	0.53
1:C:829:ASP:OD1	1:C:829:ASP:N	2.41	0.53
1:C:972:MET:HA	1:C:977:GLN:HE22	1.73	0.53
1:A:64:ARG:HE	1:A:1091:ARG:HH21	1.55	0.53
1:B:860:LEU:HD22	1:B:861:LYS:H	1.74	0.53
1:C:429:ASN:H	1:C:429:ASN:HD22	1.54	0.53
1:A:108:HIS:CE1	1:A:109:ILE:HG13	2.43	0.53
1:B:630:VAL:HG22	1:B:643:ILE:HD11	1.91	0.53
1:C:30:VAL:O	1:C:82:ALA:N	2.34	0.53
1:C:831:GLU:OE1	1:C:831:GLU:N	2.40	0.53
1:C:210:PRO:HB2	1:C:306:LEU:HD13	1.89	0.53
1:C:384:SER:OG	1:C:385:ARG:N	2.41	0.53
1:C:934:CYS:SG	1:C:935:GLU:N	2.82	0.53
1:A:577:SER:O	1:A:580:TYR:N	2.39	0.53
1:A:111:VAL:HB	1:A:132:VAL:HG23	1.90	0.53
1:B:911:THR:OG1	1:B:912:ALA:N	2.42	0.53
1:C:25:ASN:OD1	1:C:25:ASN:N	2.35	0.53
1:C:1044:ASP:OD1	1:C:1044:ASP:N	2.42	0.53
1:A:242:SER:HB2	1:A:305:ASP:H	1.73	0.53
1:A:317:GLY:C	1:B:253:ARG:HH21	2.17	0.53
1:A:630:VAL:HG21	1:A:647:VAL:HG23	1.91	0.53
1:A:939:GLN:HA	1:C:940:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ILE:HA	1:B:690:MET:HE2	1.90	0.53
1:C:62:HIS:O	1:C:1091:ARG:NH2	2.21	0.53
1:C:90:HIS:CD2	1:C:90:HIS:H	2.27	0.53
1:A:85:SER:O	1:A:115:GLY:HA2	2.10	0.53
1:B:981:ILE:HA	1:B:984:GLU:HG2	1.90	0.52
1:C:636:ASP:HB2	1:C:1076:GLY:HA3	1.91	0.52
1:C:863:HIS:HE1	1:C:899:HIS:CE1	2.28	0.52
1:A:160:ASP:OD1	1:A:160:ASP:N	2.36	0.52
1:C:913:GLU:O	1:C:916:ARG:HB2	2.10	0.52
1:A:742:GLN:HB3	1:A:744:THR:HG23	1.90	0.52
1:C:872:HIS:O	1:C:879:ASN:ND2	2.36	0.52
1:A:27:VAL:HB	1:A:55:CYS:HB3	1.92	0.52
1:A:184:ILE:HD12	1:A:295:VAL:HG23	1.92	0.52
1:A:929:TRP:NE1	1:A:931:VAL:HB	2.23	0.52
1:B:636:ASP:OD2	1:B:1074:SER:OG	2.27	0.52
1:C:283:GLU:HG2	1:C:285:GLY:H	1.75	0.52
1:A:169:LEU:HD11	1:A:200:LEU:HD22	1.91	0.52
1:B:265:ARG:N	1:B:265:ARG:CD	2.72	0.52
1:B:843:TRP:O	1:B:846:THR:OG1	2.25	0.52
1:C:288:ILE:HG21	1:C:292:LEU:HD22	1.91	0.52
1:C:512:LEU:HG	1:C:569:LEU:HD13	1.92	0.52
1:A:936:ASN:N	1:A:936:ASN:OD1	2.42	0.52
1:C:578:PHE:HE2	1:C:858:GLN:HE22	1.56	0.52
1:A:44:ASN:HA	1:A:47:ARG:HG2	1.92	0.52
1:A:1011:ASP:OD1	1:A:1011:ASP:N	2.42	0.52
1:B:656:THR:N	1:B:659:ASP:OD2	2.36	0.52
1:A:929:TRP:HE1	1:A:931:VAL:HB	1.75	0.52
1:A:942:PHE:CE1	1:C:557:PRO:HA	2.45	0.52
1:B:180:LEU:O	1:B:184:ILE:HG12	2.10	0.52
1:B:621:LYS:H	1:B:674:THR:HG22	1.75	0.52
1:A:37:ASP:OD1	1:A:87:GLN:NE2	2.39	0.51
1:A:252:ARG:NH1	1:B:346:ASP:OD1	2.43	0.51
1:A:817:ALA:HB3	1:A:857:SER:HB3	1.91	0.51
1:C:588:LYS:NZ	1:C:589:ARG:O	2.43	0.51
1:B:211:VAL:HG22	1:B:307:VAL:HB	1.92	0.51
1:B:515:MET:HB3	1:B:519:MET:HE2	1.91	0.51
1:A:236:ASP:HB2	1:A:427:LEU:HD11	1.92	0.51
1:A:875:GLU:HB3	1:A:878:PHE:CD1	2.45	0.51
1:C:283:GLU:OE1	1:C:286:SER:OG	2.24	0.51
1:C:362:LYS:HD3	1:C:363:GLY:H	1.75	0.51
1:C:1007:ASN:OD1	1:C:1007:ASN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:MET:SD	1:A:267:ASN:N	2.84	0.51
1:A:965:ARG:NH2	1:B:366:ASP:OD1	2.27	0.51
1:B:772:TYR:HB3	1:B:819:ASN:HB3	1.93	0.51
1:C:228:GLU:O	1:C:232:ARG:HG2	2.11	0.51
1:C:826:ASN:C	1:C:886:GLN:HE22	2.18	0.51
1:C:1025:ASP:N	1:C:1025:ASP:OD1	2.41	0.51
1:B:49:ILE:HG21	1:B:150:ILE:HG13	1.93	0.51
1:B:1004:THR:OG1	1:B:1005:PHE:N	2.42	0.51
1:C:28:ARG:HA	1:C:56:GLU:O	2.11	0.51
1:C:349:ASP:HB2	1:C:378:ASN:CG	2.36	0.51
1:C:848:ARG:HH12	1:C:849:ASP:HB3	1.76	0.51
1:C:1048:MET:SD	1:C:1048:MET:N	2.83	0.51
1:A:542:ILE:HD11	1:A:550:LYS:HB3	1.92	0.51
1:A:941:SER:H	1:C:939:GLN:C	2.19	0.51
1:A:992:LYS:HG3	1:A:999:ILE:HD12	1.93	0.51
1:A:28:ARG:HA	1:A:56:GLU:O	2.11	0.51
1:A:920:ALA:O	1:A:924:ILE:HG13	2.10	0.51
1:B:401:ASP:OD2	1:B:404:VAL:N	2.39	0.51
1:A:529:VAL:HA	1:A:537:ILE:O	2.11	0.51
1:A:623:LEU:O	1:A:677:SER:OG	2.23	0.51
1:C:401:ASP:OD2	1:C:404:VAL:N	2.40	0.51
1:A:253:ARG:HH22	1:B:317:GLY:C	2.18	0.50
1:B:260:LEU:HD11	1:B:280:ALA:HB2	1.93	0.50
1:C:180:LEU:O	1:C:184:ILE:HG12	2.11	0.50
1:C:632:LEU:HG	1:C:680:ILE:HG13	1.92	0.50
1:B:349:ASP:HA	1:B:378:ASN:HD21	1.76	0.50
1:B:374:GLN:O	1:B:374:GLN:NE2	2.44	0.50
1:B:750:GLU:OE1	1:B:750:GLU:N	2.30	0.50
1:B:25:ASN:OD1	1:B:25:ASN:N	2.44	0.50
1:A:39:HIS:HE1	1:A:42:SER:H	1.56	0.50
1:C:276:MET:SD	1:C:277:ARG:N	2.84	0.50
1:A:402:ASP:OD2	1:A:438:GLN:NE2	2.44	0.50
1:C:557:PRO:HB3	1:C:559:PHE:HD2	1.76	0.50
1:A:214:ILE:HG12	1:A:329:LEU:HB3	1.93	0.50
1:A:231:ARG:NH1	1:A:1084:GLU:O	2.45	0.50
1:B:111:VAL:HB	1:B:132:VAL:HG23	1.93	0.50
1:B:523:TYR:O	1:B:552:ARG:NH1	2.39	0.50
1:B:101:LEU:HD12	1:B:106:GLY:HA3	1.94	0.50
1:B:828:MET:SD	1:B:882:ARG:NH2	2.85	0.50
1:C:856:ARG:HA	1:C:859:LYS:HD3	1.94	0.50
1:B:283:GLU:HG2	1:B:284:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:MET:HG2	1:C:266:MET:O	2.11	0.49
1:C:1049:LEU:O	1:C:1053:ARG:HG3	2.12	0.49
1:C:1053:ARG:O	1:C:1057:ILE:HG12	2.12	0.49
1:A:1049:LEU:O	1:A:1053:ARG:HG3	2.12	0.49
1:B:596:ARG:HG2	1:B:622:ARG:HB3	1.94	0.49
1:C:464:VAL:HG22	1:C:570:MET:HG2	1.93	0.49
1:C:267:ASN:HD21	1:C:1088:GLN:HG3	1.76	0.49
1:C:1023:SER:HB3	1:C:1026:GLU:HG3	1.94	0.49
1:A:315:GLY:N	1:A:318:ASP:OD2	2.37	0.49
1:C:249:ASP:O	1:C:281:THR:N	2.45	0.49
1:C:568:TRP:HZ2	1:C:938:ASN:HD22	1.60	0.49
1:A:250:PRO:HA	1:A:281:THR:OG1	2.12	0.49
1:B:826:ASN:O	1:B:886:GLN:NE2	2.46	0.49
1:A:571:ARG:HE	1:A:571:ARG:HA	1.78	0.49
1:B:463:ARG:NE	1:B:467:GLN:HE22	2.08	0.49
1:A:64:ARG:HH21	1:A:1091:ARG:NE	2.11	0.49
1:C:39:HIS:HE1	1:C:42:SER:H	1.61	0.49
1:A:266:MET:HE1	1:A:268:ALA:HB3	1.94	0.49
1:A:831:GLU:N	1:A:831:GLU:OE1	2.41	0.49
1:B:52:SER:OG	1:B:53:GLN:NE2	2.46	0.49
1:A:175:GLY:O	1:A:177:ARG:NE	2.45	0.48
1:A:939:GLN:H	1:C:942:PHE:N	2.11	0.48
1:C:265:ARG:HH22	2:C:1101:GDP:PB	2.36	0.48
1:C:398:ARG:CZ	1:C:440:VAL:HA	2.43	0.48
1:A:120:VAL:O	1:A:124:ILE:HG22	2.14	0.48
1:A:917:ARG:NH1	1:C:878:PHE:HA	2.28	0.48
1:A:156:ARG:O	1:A:156:ARG:NE	2.47	0.48
1:A:244:ALA:HB3	1:A:307:VAL:HG22	1.95	0.48
1:A:476:GLN:OE1	1:C:476:GLN:HA	2.13	0.48
1:C:929:TRP:HE1	1:C:931:VAL:HB	1.78	0.48
1:C:987:TYR:CZ	1:C:991:LEU:HD11	2.48	0.48
1:A:263:ARG:HH11	1:A:263:ARG:HB3	1.77	0.48
1:A:483:MET:HE2	1:A:483:MET:HB3	1.77	0.48
1:B:872:HIS:CG	1:B:873:ALA:H	2.31	0.48
1:C:265:ARG:NH2	2:C:1101:GDP:O3B	2.41	0.48
1:C:374:GLN:O	1:C:374:GLN:NE2	2.46	0.48
1:B:124:ILE:HD11	1:B:135:ILE:HB	1.95	0.48
1:B:293:PRO:HG3	1:B:324:HIS:CE1	2.48	0.48
1:C:354:VAL:HG21	1:C:371:VAL:HG11	1.96	0.48
1:C:440:VAL:HG22	1:C:442:VAL:H	1.79	0.48
1:B:84:SER:HB2	1:B:86:TYR:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ALA:HA	1:C:389:MET:HG2	1.95	0.48
1:A:554:VAL:HA	1:A:936:ASN:HD21	1.79	0.48
1:B:571:ARG:HE	1:B:571:ARG:HA	1.79	0.48
1:A:216:GLY:HA2	1:A:330:TYR:CE1	2.49	0.48
1:B:376:GLN:NE2	1:B:384:SER:O	2.47	0.48
1:B:460:TYR:O	1:B:464:VAL:HG23	2.14	0.48
1:C:222:LYS:NZ	1:C:248:ILE:O	2.47	0.48
1:A:137:SER:O	1:A:141:GLY:N	2.38	0.47
1:A:188:GLU:OE2	1:A:282:ARG:NH2	2.47	0.47
1:A:222:LYS:HD2	1:A:223:SER:N	2.29	0.47
1:B:358:LYS:HB2	2:B:1101:GDP:HN1	1.80	0.47
1:C:266:MET:HG3	1:C:268:ALA:HB3	1.95	0.47
1:C:750:GLU:H	1:C:750:GLU:CD	2.22	0.47
1:C:703:PHE:O	1:C:707:ASN:N	2.43	0.47
1:A:361:ARG:HB3	1:B:361:ARG:NH1	2.30	0.47
1:A:640:ARG:HB3	1:A:642:ASP:OD2	2.14	0.47
1:A:518:GLN:H	1:A:518:GLN:NE2	2.11	0.47
1:B:623:LEU:HB2	1:B:676:VAL:HG22	1.97	0.47
1:B:929:TRP:NE1	1:B:931:VAL:HB	2.29	0.47
1:A:180:LEU:O	1:A:184:ILE:HG12	2.15	0.47
1:A:210:PRO:HD2	1:A:305:ASP:O	2.13	0.47
1:A:826:ASN:O	1:A:886:GLN:NE2	2.47	0.47
1:B:792:LEU:HB2	1:B:835:LEU:HD11	1.96	0.47
1:C:772:TYR:HB3	1:C:819:ASN:HB3	1.96	0.47
1:A:409:GLN:NE2	1:A:429:ASN:HB2	2.29	0.47
1:B:605:PHE:HB3	1:B:609:ARG:HH22	1.80	0.47
1:C:687:ILE:O	1:C:690:MET:HB2	2.14	0.47
1:C:912:ALA:O	1:C:915:VAL:HG22	2.15	0.47
1:A:98:ILE:HD11	1:A:132:VAL:HB	1.97	0.47
1:A:506:GLY:HA3	1:A:509:GLU:OE2	2.14	0.47
1:B:1058:ASP:OD1	1:B:1058:ASP:N	2.48	0.47
1:B:225:LEU:O	1:B:229:LEU:HG	2.15	0.47
1:B:341:ALA:O	1:B:344:LYS:HG2	2.15	0.47
1:A:170:ASP:OD1	1:A:171:THR:N	2.47	0.47
1:B:598:PHE:HA	1:B:624:SER:HB3	1.96	0.47
1:B:610:ARG:HD2	1:B:613:LEU:HD22	1.97	0.47
1:C:84:SER:HB2	1:C:86:TYR:HE1	1.80	0.47
1:C:875:GLU:HB3	1:C:878:PHE:CD1	2.50	0.47
1:A:357:ASN:HA	1:A:394:THR:O	2.15	0.46
1:A:398:ARG:CZ	1:A:440:VAL:HA	2.45	0.46
1:C:685:PRO:HB3	1:C:759:ILE:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:VAL:HG11	1:B:135:ILE:HD11	1.96	0.46
1:B:929:TRP:HD1	1:B:932:ALA:HB2	1.80	0.46
1:B:1054:GLN:HE21	1:B:1054:GLN:HB3	1.49	0.46
1:B:223:SER:OG	2:B:1101:GDP:O3B	2.31	0.46
1:A:36:PHE:HD2	1:A:646:LYS:HE3	1.80	0.46
1:A:242:SER:HB2	1:A:305:ASP:N	2.30	0.46
1:A:260:LEU:HD11	1:A:280:ALA:HB2	1.96	0.46
1:B:221:GLY:HA2	2:B:1101:GDP:H5''	1.96	0.46
1:A:939:GLN:O	1:C:942:PHE:HA	2.15	0.46
1:B:170:ASP:OD1	1:B:171:THR:N	2.48	0.46
1:B:509:GLU:H	1:B:509:GLU:CD	2.21	0.46
1:A:120:VAL:HG23	1:A:123:GLU:HB2	1.97	0.46
1:A:942:PHE:CD2	1:C:938:ASN:HB2	2.51	0.46
1:C:287:GLU:HB3	1:C:314:ILE:HD11	1.96	0.46
1:C:442:VAL:HG13	1:C:442:VAL:O	2.15	0.46
1:C:557:PRO:HB3	1:C:559:PHE:CD2	2.50	0.46
1:A:843:TRP:O	1:A:846:THR:OG1	2.27	0.46
1:A:930:GLY:HA3	1:C:830:PRO:HG3	1.97	0.46
1:B:265:ARG:HA	1:B:265:ARG:HD2	1.64	0.46
1:A:415:LEU:O	1:A:419:GLY:N	2.48	0.46
1:A:879:ASN:HA	1:A:882:ARG:HG2	1.98	0.46
1:C:88:GLY:HA2	1:C:90:HIS:CE1	2.51	0.46
1:A:644:TYR:O	1:A:647:VAL:HG12	2.16	0.46
1:A:655:ALA:N	1:A:659:ASP:OD1	2.45	0.46
1:B:484:LEU:HG	1:B:489:HIS:O	2.15	0.46
1:A:526:ASP:OD1	1:A:526:ASP:N	2.48	0.46
1:A:680:ILE:HD13	1:A:687:ILE:HG13	1.98	0.46
1:A:792:LEU:HB2	1:A:835:LEU:HD11	1.97	0.46
1:B:104:HIS:O	1:B:178:ARG:NH2	2.49	0.46
1:C:641:PRO:O	1:C:645:GLY:N	2.47	0.46
1:C:826:ASN:HA	1:C:832:TYR:CD1	2.51	0.46
1:A:289:SER:HB3	1:A:292:LEU:HB2	1.98	0.45
1:A:733:ALA:O	1:A:775:SER:OG	2.28	0.45
1:A:882:ARG:HE	1:A:1000:ILE:HD11	1.79	0.45
1:B:848:ARG:HG2	1:B:858:GLN:HE22	1.81	0.45
1:C:788:PRO:HG3	1:C:832:TYR:OH	2.16	0.45
1:A:227:ASP:HB2	1:A:266:MET:HG2	1.98	0.45
1:A:248:ILE:HB	1:A:311:THR:HA	1.98	0.45
1:A:792:LEU:HD12	1:A:955:VAL:HG21	1.98	0.45
1:C:275:PHE:CE2	1:C:277:ARG:HB2	2.52	0.45
1:C:1000:ILE:H	1:C:1000:ILE:HG13	1.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ASN:C	1:A:886:GLN:HE22	2.24	0.45
1:B:44:ASN:HA	1:B:47:ARG:HG2	1.97	0.45
1:B:856:ARG:HA	1:B:859:LYS:HD3	1.97	0.45
1:C:287:GLU:HG3	1:C:288:ILE:HG23	1.98	0.45
1:C:822:PHE:HE1	1:C:860:LEU:HD21	1.80	0.45
1:A:146:LEU:O	1:A:150:ILE:HG12	2.16	0.45
1:B:120:VAL:HG23	1:B:123:GLU:H	1.82	0.45
1:B:156:ARG:HA	1:B:156:ARG:HD2	1.81	0.45
1:C:44:ASN:HA	1:C:47:ARG:HG3	1.98	0.45
1:C:228:GLU:HB3	1:C:404:VAL:HG11	1.98	0.45
1:C:441:ILE:HA	1:C:441:ILE:HD12	1.60	0.45
1:C:788:PRO:HG3	1:C:832:TYR:CZ	2.51	0.45
1:A:830:PRO:HG3	1:C:930:GLY:C	2.41	0.45
1:C:747:PHE:HA	1:C:1087:GLY:O	2.17	0.45
1:C:757:GLY:HA2	1:C:806:TYR:HE1	1.81	0.45
1:C:528:TYR:HB2	1:C:541:LEU:HD11	1.98	0.45
1:C:943:LEU:HD23	1:C:943:LEU:H	1.81	0.45
1:C:956:LEU:HD13	1:C:956:LEU:HA	1.80	0.45
1:C:1082:LEU:O	1:C:1085:VAL:HG12	2.16	0.45
1:A:516:TRP:O	1:A:520:GLN:NE2	2.50	0.45
1:A:573:ASN:ND2	1:A:577:SER:OG	2.50	0.45
1:C:814:ASP:OD1	1:C:814:ASP:N	2.48	0.45
1:A:47:ARG:HG3	1:A:48:ARG:N	2.32	0.45
1:A:493:ALA:O	1:A:497:LEU:HG	2.16	0.45
1:A:776:ILE:O	1:A:822:PHE:HA	2.16	0.45
1:C:210:PRO:HD2	1:C:305:ASP:O	2.17	0.45
1:C:780:HIS:HA	1:C:783:GLU:HB3	1.98	0.45
1:A:244:ALA:HB2	1:A:304:PHE:CD2	2.52	0.45
1:A:375:VAL:HG21	1:A:391:VAL:HG21	1.99	0.45
1:A:847:MET:HB2	1:A:858:GLN:HG3	1.99	0.45
1:B:103:GLU:HG2	1:B:104:HIS:CD2	2.52	0.45
1:B:164:TYR:HD1	1:B:164:TYR:HA	1.68	0.45
1:B:526:ASP:O	1:B:541:LEU:N	2.40	0.45
1:B:915:VAL:HA	1:B:918:ALA:HB3	1.99	0.45
1:A:189:ASN:HB3	1:A:191:LYS:HZ1	1.81	0.44
1:A:788:PRO:HG3	1:A:832:TYR:CZ	2.52	0.44
1:B:777:SER:HA	1:B:823:PHE:O	2.17	0.44
1:A:228:GLU:OE1	1:A:232:ARG:NH1	2.50	0.44
1:A:327:LEU:HD22	1:A:327:LEU:HA	1.73	0.44
1:B:49:ILE:O	1:B:52:SER:OG	2.23	0.44
1:B:70:VAL:HG11	1:B:100:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:678:MET:HE2	1:B:731:VAL:HG22	1.99	0.44
1:B:796:LEU:O	1:B:800:PHE:HD2	1.99	0.44
1:C:245:VAL:HA	1:C:308:ILE:O	2.17	0.44
1:B:327:LEU:HA	1:B:327:LEU:HD22	1.80	0.44
1:B:984:GLU:HG3	1:B:985:SER:N	2.32	0.44
1:C:681:ASN:OD1	1:C:681:ASN:N	2.48	0.44
1:B:236:ASP:OD1	1:B:427:LEU:N	2.50	0.44
1:B:329:LEU:HD22	1:B:353:PHE:HB2	2.00	0.44
1:A:160:ASP:HB2	1:A:162:THR:HG23	2.00	0.44
1:B:217:THR:OG1	1:B:220:ALA:HB2	2.16	0.44
1:B:464:VAL:HG22	1:B:570:MET:HG2	1.99	0.44
1:A:942:PHE:HA	1:C:939:GLN:O	2.18	0.44
1:B:379:ARG:O	1:B:380:GLU:HB2	2.17	0.44
1:C:76:GLU:OE1	1:C:277:ARG:HD2	2.17	0.44
1:C:341:ALA:O	1:C:344:LYS:HG3	2.17	0.44
1:C:739:ASP:O	1:C:978:ARG:NH2	2.29	0.44
1:A:265:ARG:NE	2:A:1101:GDP:O2A	2.50	0.44
1:A:788:PRO:HD2	1:C:547:SER:OG	2.17	0.44
1:C:306:LEU:HD21	1:C:308:ILE:HD11	1.98	0.44
1:C:357:ASN:HA	1:C:394:THR:O	2.17	0.44
1:B:127:LEU:HA	1:B:130:TYR:HB2	1.99	0.44
1:B:844:ALA:O	1:B:858:GLN:NE2	2.45	0.44
1:C:70:VAL:HG21	1:C:100:LEU:HD23	2.00	0.44
1:C:263:ARG:HD3	1:C:276:MET:SD	2.58	0.44
1:A:680:ILE:HG12	1:A:683:PRO:HD2	1.99	0.43
1:A:687:ILE:HA	1:A:690:MET:HE2	1.99	0.43
1:A:937:PRO:CA	1:C:941:SER:HA	2.48	0.43
1:C:60:LEU:HD13	1:C:64:ARG:HG3	2.00	0.43
1:C:430:LEU:HD23	1:C:430:LEU:HA	1.80	0.43
1:C:884:THR:HG23	1:C:921:ILE:HD11	2.00	0.43
1:A:288:ILE:HD13	1:A:320:ALA:HB1	2.00	0.43
1:A:442:VAL:O	1:A:442:VAL:HG13	2.18	0.43
1:B:591:GLY:HA3	1:B:927:ARG:NH1	2.33	0.43
1:C:222:LYS:C	1:C:223:SER:HG	2.26	0.43
1:C:699:GLN:HE22	1:C:702:ARG:NE	2.12	0.43
1:C:850:LYS:HG3	1:C:851:TYR:CZ	2.53	0.43
1:A:473:GLU:HG3	1:C:483:MET:SD	2.58	0.43
1:A:555:VAL:H	1:A:936:ASN:ND2	2.15	0.43
1:A:937:PRO:HA	1:C:941:SER:HA	2.00	0.43
1:B:555:VAL:H	1:B:936:ASN:HD21	1.66	0.43
1:C:524:SER:O	1:C:552:ARG:NH2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:571:ARG:HE	1:C:571:ARG:HA	1.83	0.43
1:C:659:ASP:O	1:C:662:VAL:HG12	2.19	0.43
1:C:1028:GLN:HE21	1:C:1028:GLN:HB2	1.49	0.43
1:A:939:GLN:CA	1:C:940:GLY:H	2.31	0.43
1:B:792:LEU:HD12	1:B:955:VAL:HG21	2.00	0.43
1:C:42:SER:HA	1:C:45:ILE:HD12	1.99	0.43
1:A:155:GLN:HA	1:A:158:ASP:OD2	2.18	0.43
1:A:1061:ASN:OD1	1:A:1061:ASN:N	2.50	0.43
1:B:70:VAL:HG21	1:B:100:LEU:HD23	2.00	0.43
1:B:636:ASP:CG	1:B:1076:GLY:H	2.27	0.43
1:B:582:ALA:HA	1:B:837:ARG:HH12	1.82	0.43
1:B:731:VAL:HG23	1:B:771:PHE:HZ	1.82	0.43
1:C:822:PHE:CD1	1:C:860:LEU:HD11	2.53	0.43
1:A:476:GLN:OE1	1:C:479:ALA:HB3	2.18	0.43
1:A:618:MET:O	1:A:621:LYS:NZ	2.50	0.43
1:A:940:GLY:HA3	1:C:941:SER:O	2.19	0.43
1:C:227:ASP:HB2	1:C:266:MET:HB3	2.00	0.43
1:C:332:MET:HE3	1:C:332:MET:HB2	1.91	0.43
1:A:144:MET:SD	1:A:149:MET:HG3	2.59	0.43
1:A:147:ALA:O	1:A:151:THR:HG23	2.18	0.43
1:B:712:THR:N	1:B:715:GLU:OE2	2.34	0.43
1:C:460:TYR:O	1:C:464:VAL:HG23	2.18	0.43
1:C:654:ILE:HD13	1:C:690:MET:HE1	2.00	0.43
1:A:443:PRO:C	1:A:445:ALA:N	2.76	0.43
1:A:460:TYR:O	1:A:464:VAL:HG23	2.19	0.43
1:A:1004:THR:OG1	1:A:1005:PHE:N	2.52	0.43
1:B:474:ARG:NH2	1:B:478:ARG:HH21	2.17	0.43
1:C:70:VAL:HG11	1:C:100:LEU:HG	2.01	0.43
1:C:234:ARG:HH21	1:C:271:HIS:CE1	2.37	0.43
1:C:1088:GLN:HE21	1:C:1088:GLN:HB3	1.61	0.43
1:A:128:GLN:HG2	1:A:132:VAL:O	2.19	0.43
1:A:254:LYS:HA	1:A:254:LYS:HD2	1.95	0.43
1:A:939:GLN:HB3	1:C:942:PHE:CD1	2.53	0.43
1:B:250:PRO:HA	1:B:281:THR:OG1	2.18	0.43
1:B:659:ASP:OD1	1:B:660:MET:N	2.52	0.43
1:A:374:GLN:OE1	1:A:377:ARG:NE	2.29	0.42
1:A:656:THR:H	1:A:659:ASP:CG	2.25	0.42
1:A:881:ILE:HG12	1:C:917:ARG:HH21	1.83	0.42
1:B:894:ASN:HD21	1:B:935:GLU:HB3	1.84	0.42
2:B:1101:GDP:H8	2:B:1101:GDP:H2'	1.61	0.42
1:C:186:ALA:O	1:C:190:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:PRO:HG3	1:C:420:MET:HG3	2.01	0.42
1:C:237:GLN:HE21	1:C:240:ALA:HB3	1.83	0.42
1:C:296:ILE:O	1:C:300:LYS:HG3	2.19	0.42
1:A:76:GLU:OE2	1:A:278:SER:N	2.51	0.42
1:A:483:MET:HE1	1:C:477:LEU:HD11	2.01	0.42
1:A:940:GLY:H	1:C:939:GLN:CA	2.30	0.42
1:A:1003:ASN:HA	1:A:1006:ARG:HH21	1.84	0.42
1:B:59:HIS:CD2	1:B:61:GLY:H	2.37	0.42
1:B:837:ARG:HG2	1:B:840:ARG:HH12	1.84	0.42
1:C:63:ASN:N	1:C:63:ASN:OD1	2.51	0.42
1:C:119:ILE:H	1:C:119:ILE:HG13	1.53	0.42
1:C:581:THR:O	1:C:840:ARG:HD2	2.19	0.42
1:C:350:PHE:HD1	1:C:350:PHE:HA	1.68	0.42
1:C:815:ASP:OD1	1:C:815:ASP:N	2.52	0.42
1:A:123:GLU:O	1:A:127:LEU:HG	2.20	0.42
1:A:621:LYS:N	1:A:674:THR:HG22	2.33	0.42
1:B:482:ASP:O	1:B:485:GLN:HG2	2.20	0.42
1:B:654:ILE:HG22	1:B:659:ASP:HB2	2.02	0.42
1:B:879:ASN:O	1:B:882:ARG:HG2	2.20	0.42
1:C:624:SER:HA	1:C:677:SER:O	2.19	0.42
1:A:376:GLN:HG3	1:A:389:MET:HE3	2.00	0.42
1:A:472:ARG:NH2	1:C:560:GLU:HB2	2.34	0.42
1:A:916:ARG:NH2	1:C:1007:ASN:OD1	2.51	0.42
1:B:146:LEU:O	1:B:150:ILE:HG12	2.20	0.42
1:B:780:HIS:O	1:B:783:GLU:HG2	2.20	0.42
1:B:1011:ASP:OD1	1:B:1011:ASP:N	2.52	0.42
1:C:754:LYS:HE3	1:C:754:LYS:HB3	1.93	0.42
1:A:832:TYR:HA	1:A:835:LEU:HB2	2.02	0.42
1:B:446:ARG:O	1:B:449:TYR:HD1	2.02	0.42
1:B:575:PRO:HD3	1:B:582:ALA:HB3	2.02	0.42
1:A:941:SER:O	1:C:940:GLY:HA3	2.19	0.42
1:B:124:ILE:HG12	1:B:135:ILE:HD12	2.02	0.42
1:C:482:ASP:O	1:C:485:GLN:HG2	2.19	0.42
1:C:608:ASN:ND2	1:C:663:LEU:O	2.53	0.42
1:A:848:ARG:NH1	1:A:848:ARG:HB3	2.35	0.42
1:A:1058:ASP:OD1	1:A:1058:ASP:N	2.52	0.42
1:B:473:GLU:O	1:B:477:LEU:HG	2.20	0.42
1:B:747:PHE:O	1:B:1089:TYR:HB2	2.20	0.42
1:B:785:GLY:HA2	1:B:869:ARG:NE	2.35	0.42
1:B:855:ASP:OD1	1:B:856:ARG:N	2.51	0.42
1:A:222:LYS:H	1:A:222:LYS:HG3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LEU:HA	1:A:956:LEU:HD13	1.75	0.42
1:A:965:ARG:HH22	1:B:365:GLN:HB2	1.85	0.42
1:A:998:PRO:HB2	1:C:928:GLU:OE1	2.20	0.42
1:B:316:GLN:NE2	1:B:345:ILE:HG12	2.34	0.42
1:B:568:TRP:CZ3	1:B:573:ASN:HA	2.54	0.42
1:C:323:PRO:HG2	1:C:324:HIS:CD2	2.55	0.42
1:C:832:TYR:HA	1:C:835:LEU:HB2	2.02	0.42
1:A:264:ILE:HG23	1:A:265:ARG:HD2	2.02	0.41
1:A:560:GLU:HB2	1:C:472:ARG:NH2	2.35	0.41
1:A:1023:SER:N	1:A:1026:GLU:OE1	2.50	0.41
1:B:913:GLU:O	1:B:916:ARG:HB2	2.19	0.41
1:C:840:ARG:NH2	1:C:894:ASN:HB2	2.35	0.41
1:A:76:GLU:CD	1:A:277:ARG:HD2	2.46	0.41
1:A:940:GLY:N	1:C:939:GLN:HA	2.31	0.41
1:B:152:ASP:O	1:B:156:ARG:HB2	2.20	0.41
1:B:392:TYR:CE1	1:B:433:ARG:HA	2.55	0.41
1:B:956:LEU:HD13	1:B:956:LEU:HA	1.84	0.41
1:B:1049:LEU:O	1:B:1053:ARG:HG3	2.20	0.41
1:C:366:ASP:HA	1:C:369:ARG:NH1	2.29	0.41
1:A:95:LYS:HE3	1:A:130:TYR:CE2	2.56	0.41
1:A:736:LEU:HD21	1:A:753:LEU:HD21	2.02	0.41
1:B:62:HIS:ND1	1:B:63:ASN:OD1	2.39	0.41
1:B:63:ASN:O	1:B:64:ARG:HD3	2.20	0.41
1:C:64:ARG:HH21	1:C:1091:ARG:HG3	1.84	0.41
1:C:429:ASN:H	1:C:429:ASN:ND2	2.16	0.41
1:A:350:PHE:CE2	1:B:254:LYS:HE2	2.56	0.41
1:A:603:ASP:OD1	1:A:606:ARG:N	2.38	0.41
1:A:937:PRO:C	1:C:941:SER:HA	2.46	0.41
1:A:965:ARG:NH2	1:B:365:GLN:HB2	2.36	0.41
1:B:385:ARG:NH1	1:B:387:GLU:OE2	2.53	0.41
1:C:306:LEU:HD12	1:C:307:VAL:H	1.85	0.41
1:C:742:GLN:OE1	1:C:744:THR:OG1	2.30	0.41
1:A:477:LEU:HD11	1:C:483:MET:HE1	2.03	0.41
1:A:843:TRP:CD1	1:A:860:LEU:HB2	2.56	0.41
1:B:398:ARG:HH12	1:B:440:VAL:HB	1.86	0.41
1:C:322:VAL:N	1:C:323:PRO:HD2	2.36	0.41
1:C:327:LEU:HD13	1:C:327:LEU:HA	1.95	0.41
1:A:112:PHE:CD1	1:A:134:ARG:HB2	2.56	0.41
1:B:355:ALA:HA	1:B:392:TYR:O	2.20	0.41
1:B:1013:THR:O	1:B:1015:GLN:HG3	2.20	0.41
1:A:266:MET:SD	1:A:269:ILE:HG23	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:H	1:A:715:GLU:HG2	1.64	0.41
1:C:219:GLY:HA3	1:C:333:THR:HB	2.03	0.41
1:C:344:LYS:HE2	1:C:344:LYS:HB2	1.87	0.41
1:C:604:ALA:HB1	1:C:663:LEU:HA	2.01	0.41
1:A:39:HIS:HE1	1:A:42:SER:N	2.18	0.41
1:A:464:VAL:HG22	1:A:570:MET:HG2	2.02	0.41
1:A:515:MET:HB3	1:A:519:MET:HE2	2.02	0.41
1:A:624:SER:HA	1:A:677:SER:O	2.20	0.41
1:A:749:THR:OG1	1:A:750:GLU:N	2.53	0.41
1:A:1023:SER:HB3	1:A:1026:GLU:CD	2.46	0.41
1:B:443:PRO:C	1:B:445:ALA:H	2.29	0.41
1:B:1048:MET:SD	1:B:1048:MET:N	2.94	0.41
1:C:200:LEU:HD13	1:C:200:LEU:HA	1.89	0.41
1:C:231:ARG:NH1	1:C:1083:PHE:O	2.54	0.41
1:C:402:ASP:O	1:C:405:THR:OG1	2.31	0.41
1:C:531:LYS:HA	1:C:536:GLU:HA	2.02	0.41
1:C:590:GLU:OE1	1:C:591:GLY:N	2.53	0.41
1:C:656:THR:H	1:C:659:ASP:CG	2.24	0.41
1:C:987:TYR:CE2	1:C:991:LEU:HD11	2.55	0.41
1:A:332:MET:HG2	1:A:333:THR:H	1.85	0.41
1:A:443:PRO:C	1:A:445:ALA:H	2.29	0.41
1:A:830:PRO:HG3	1:C:930:GLY:HA3	2.03	0.41
1:A:1078:ILE:HD12	1:A:1078:ILE:HA	1.88	0.41
1:C:140:ASP:O	1:C:144:MET:HG2	2.21	0.41
1:A:225:LEU:O	1:A:229:LEU:HG	2.21	0.40
1:A:830:PRO:HG3	1:C:930:GLY:CA	2.51	0.40
1:C:216:GLY:HA3	1:C:220:ALA:HA	2.02	0.40
1:C:846:THR:O	1:C:850:LYS:HB3	2.20	0.40
1:C:1054:GLN:HE21	1:C:1054:GLN:HB3	1.63	0.40
1:A:447:SER:HB3	1:B:448:ARG:HH12	1.86	0.40
1:A:710:ASP:HA	1:A:711:PRO:HD3	1.97	0.40
1:B:30:VAL:HG22	1:B:58:ILE:HB	2.02	0.40
1:B:39:HIS:CD2	1:B:41:ALA:H	2.39	0.40
1:B:542:ILE:HD11	1:B:550:LYS:HB3	2.04	0.40
1:C:360:ASP:OD1	1:C:360:ASP:N	2.50	0.40
1:A:66:VAL:HG13	1:A:97:MET:SD	2.61	0.40
1:A:682:GLY:C	1:A:684:ALA:H	2.30	0.40
1:A:917:ARG:CZ	1:C:881:ILE:HD12	2.52	0.40
1:A:991:LEU:HD23	1:A:991:LEU:HA	1.97	0.40
1:B:385:ARG:HG3	1:B:388:ASP:OD1	2.21	0.40
1:B:472:ARG:O	1:B:475:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:SER:HB3	1:B:730:THR:HB	2.02	0.40
1:A:318:ASP:N	1:B:253:ARG:HH21	2.20	0.40
1:C:357:ASN:ND2	1:C:358:LYS:H	2.19	0.40
1:C:483:MET:HE2	1:C:483:MET:HB3	1.78	0.40
1:A:166:PRO:HD3	1:A:182:GLN:HG2	2.03	0.40
1:A:242:SER:H	1:A:305:ASP:HB2	1.87	0.40
1:A:935:GLU:N	1:A:935:GLU:OE1	2.54	0.40
1:B:328:SER:HB2	1:B:352:ASP:H	1.85	0.40
1:C:184:ILE:HD12	1:C:295:VAL:HG23	2.03	0.40
1:C:222:LYS:O	1:C:224:SER:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1070/1113 (96%)	1004 (94%)	66 (6%)	0	100	100
1	B	1070/1113 (96%)	999 (93%)	70 (6%)	1 (0%)	48	83
1	C	1070/1113 (96%)	997 (93%)	72 (7%)	1 (0%)	48	83
All	All	3210/3339 (96%)	3000 (94%)	208 (6%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	LYS
1	C	937	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	834/905 (92%)	734 (88%)	100 (12%)	5	18
1	B	835/905 (92%)	756 (90%)	79 (10%)	8	25
1	C	835/905 (92%)	734 (88%)	101 (12%)	5	18
All	All	2504/2715 (92%)	2224 (89%)	280 (11%)	8	20

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	53	GLN
1	A	59	HIS
1	A	62	HIS
1	A	90	HIS
1	A	119	ILE
1	A	124	ILE
1	A	144	MET
1	A	149	MET
1	A	152	ASP
1	A	160	ASP
1	A	164	TYR
1	A	177	ARG
1	A	200	LEU
1	A	217	THR
1	A	222	LYS
1	A	235	LEU
1	A	263	ARG
1	A	264	ILE
1	A	266	MET
1	A	271	HIS
1	A	273	ASN
1	A	276	MET
1	A	294	ASP
1	A	306	LEU
1	A	318	ASP

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Mol	Chain	Res	Type
1	A	325	VAL
1	A	327	LEU
1	A	329	LEU
1	A	333	THR
1	A	335	GLU
1	A	352	ASP
1	A	356	ILE
1	A	377	ARG
1	A	382	TRP
1	A	402	ASP
1	A	411	LEU
1	A	422	LEU
1	A	426	THR
1	A	472	ARG
1	A	482	ASP
1	A	501	ARG
1	A	509	GLU
1	A	520	GLN
1	A	527	GLU
1	A	538	ARG
1	A	549	THR
1	A	551	ILE
1	A	577	SER
1	A	585	PHE
1	A	603	ASP
1	A	618	MET
1	A	635	GLU
1	A	638	HIS
1	A	642	ASP
1	A	652	VAL
1	A	654	ILE
1	A	656	THR
1	A	659	ASP
1	A	660	MET
1	A	678	MET
1	A	699	GLN
1	A	701	ASP
1	A	712	THR
1	A	716	GLU
1	A	766	HIS
1	A	768	VAL
1	A	795	THR

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Mol	Chain	Res	Type
1	A	814	ASP
1	A	845	VAL
1	A	848	ARG
1	A	854	ASN
1	A	857	SER
1	A	860	LEU
1	A	863	HIS
1	A	885	LEU
1	A	886	GLN
1	A	917	ARG
1	A	928	GLU
1	A	934	CYS
1	A	936	ASN
1	A	956	LEU
1	A	961	ARG
1	A	980	LYS
1	A	984	GLU
1	A	996	THR
1	A	1000	ILE
1	A	1002	VAL
1	A	1015	GLN
1	A	1025	ASP
1	A	1044	ASP
1	A	1052	LEU
1	A	1054	GLN
1	A	1059	ASN
1	A	1061	ASN
1	A	1078	ILE
1	A	1080	HIS
1	A	1083	PHE
1	A	1085	VAL
1	A	1088	GLN
1	B	40	ASP
1	B	59	HIS
1	B	60	LEU
1	B	66	VAL
1	B	83	ILE
1	B	90	HIS
1	B	107	GLU
1	B	119	ILE
1	B	124	ILE
1	B	149	MET

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Mol	Chain	Res	Type
1	B	163	ARG
1	B	164	TYR
1	B	177	ARG
1	B	182	GLN
1	B	212	LEU
1	B	214	ILE
1	B	222	LYS
1	B	264	ILE
1	B	265	ARG
1	B	271	HIS
1	B	276	MET
1	B	294	ASP
1	B	309	VAL
1	B	327	LEU
1	B	329	LEU
1	B	333	THR
1	B	342	LEU
1	B	346	ASP
1	B	356	ILE
1	B	388	ASP
1	B	402	ASP
1	B	411	LEU
1	B	420	MET
1	B	422	LEU
1	B	442	VAL
1	B	467	GLN
1	B	518	GLN
1	B	520	GLN
1	B	526	ASP
1	B	551	ILE
1	B	571	ARG
1	B	590	GLU
1	B	603	ASP
1	B	618	MET
1	B	638	HIS
1	B	652	VAL
1	B	654	ILE
1	B	660	MET
1	B	662	VAL
1	B	663	LEU
1	B	668	ASP
1	B	678	MET

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Mol	Chain	Res	Type
1	B	710	ASP
1	B	742	GLN
1	B	768	VAL
1	B	772	TYR
1	B	792	LEU
1	B	814	ASP
1	B	823	PHE
1	B	845	VAL
1	B	848	ARG
1	B	860	LEU
1	B	879	ASN
1	B	895	CYS
1	B	899	HIS
1	B	956	LEU
1	B	984	GLU
1	B	996	THR
1	B	1002	VAL
1	B	1003	ASN
1	B	1015	GLN
1	B	1025	ASP
1	B	1052	LEU
1	B	1054	GLN
1	B	1058	ASP
1	B	1078	ILE
1	B	1080	HIS
1	B	1085	VAL
1	B	1088	GLN
1	C	25	ASN
1	C	27	VAL
1	C	30	VAL
1	C	40	ASP
1	C	48	ARG
1	C	49	ILE
1	C	50	LEU
1	C	53	GLN
1	C	60	LEU
1	C	63	ASN
1	C	75	GLN
1	C	83	ILE
1	C	90	HIS
1	C	110	GLN
1	C	119	ILE

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Mol	Chain	Res	Type
1	C	124	ILE
1	C	152	ASP
1	C	160	ASP
1	C	164	TYR
1	C	171	THR
1	C	200	LEU
1	C	212	LEU
1	C	226	THR
1	C	235	LEU
1	C	237	GLN
1	C	262	ASP
1	C	264	ILE
1	C	266	MET
1	C	267	ASN
1	C	271	HIS
1	C	273	ASN
1	C	276	MET
1	C	309	VAL
1	C	311	THR
1	C	312	SER
1	C	327	LEU
1	C	344	LYS
1	C	350	PHE
1	C	353	PHE
1	C	356	ILE
1	C	362	LYS
1	C	366	ASP
1	C	382	TRP
1	C	401	ASP
1	C	402	ASP
1	C	422	LEU
1	C	426	THR
1	C	429	ASN
1	C	441	ILE
1	C	461	HIS
1	C	496	THR
1	C	508	VAL
1	C	520	GLN
1	C	536	GLU
1	C	538	ARG
1	C	550	LYS
1	C	551	ILE

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Mol	Chain	Res	Type
1	C	596	ARG
1	C	618	MET
1	C	635	GLU
1	C	639	GLU
1	C	652	VAL
1	C	656	THR
1	C	660	MET
1	C	670	THR
1	C	678	MET
1	C	712	THR
1	C	768	VAL
1	C	772	TYR
1	C	814	ASP
1	C	815	ASP
1	C	829	ASP
1	C	845	VAL
1	C	848	ARG
1	C	855	ASP
1	C	860	LEU
1	C	863	HIS
1	C	872	HIS
1	C	881	ILE
1	C	885	LEU
1	C	886	GLN
1	C	895	CYS
1	C	911	THR
1	C	928	GLU
1	C	936	ASN
1	C	956	LEU
1	C	980	LYS
1	C	1000	ILE
1	C	1002	VAL
1	C	1004	THR
1	C	1007	ASN
1	C	1015	GLN
1	C	1025	ASP
1	C	1028	GLN
1	C	1044	ASP
1	C	1074	SER
1	C	1078	ILE
1	C	1080	HIS
1	C	1085	VAL

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Mol	Chain	Res	Type
1	C	1088	GLN
1	C	1090	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	44	ASN
1	A	59	HIS
1	A	75	GLN
1	A	90	HIS
1	A	128	GLN
1	A	142	GLN
1	A	237	GLN
1	A	270	ASN
1	A	316	GLN
1	A	381	GLN
1	A	438	GLN
1	A	481	HIS
1	A	518	GLN
1	A	521	GLN
1	A	693	ASN
1	A	699	GLN
1	A	725	GLN
1	A	732	GLN
1	A	740	GLN
1	A	787	ASN
1	A	826	ASN
1	A	863	HIS
1	A	865	GLN
1	A	872	HIS
1	A	879	ASN
1	A	894	ASN
1	A	936	ASN
1	A	990	GLN
1	A	1028	GLN
1	A	1054	GLN
1	A	1088	GLN
1	B	53	GLN
1	B	59	HIS
1	B	75	GLN
1	B	90	HIS

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Mol	Chain	Res	Type
1	B	104	HIS
1	B	128	GLN
1	B	142	GLN
1	B	237	GLN
1	B	270	ASN
1	B	316	GLN
1	B	324	HIS
1	B	409	GLN
1	B	429	ASN
1	B	438	GLN
1	B	439	ASN
1	B	467	GLN
1	B	476	GLN
1	B	518	GLN
1	B	520	GLN
1	B	725	GLN
1	B	732	GLN
1	B	740	GLN
1	B	787	ASN
1	B	826	ASN
1	B	858	GLN
1	B	863	HIS
1	B	894	ASN
1	B	936	ASN
1	B	990	GLN
1	B	1003	ASN
1	B	1015	GLN
1	B	1028	GLN
1	B	1054	GLN
1	B	1088	GLN
1	B	1092	ASN
1	C	39	HIS
1	C	75	GLN
1	C	79	GLN
1	C	90	HIS
1	C	110	GLN
1	C	128	GLN
1	C	142	GLN
1	C	409	GLN
1	C	429	ASN
1	C	518	GLN
1	C	520	GLN

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Mol	Chain	Res	Type
1	C	638	HIS
1	C	699	GLN
1	C	725	GLN
1	C	732	GLN
1	C	743	ASN
1	C	770	ASN
1	C	812	HIS
1	C	826	ASN
1	C	863	HIS
1	C	872	HIS
1	C	936	ASN
1	C	990	GLN
1	C	1028	GLN
1	C	1054	GLN
1	C	1077	GLN
1	C	1092	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	GDP	C	1101	-	29,30,30	1.16	3 (10%)	45,47,47	1.77	7 (15%)
2	GDP	A	1101	3	29,30,30	1.16	4 (13%)	45,47,47	1.73	8 (17%)
2	GDP	B	1101	-	29,30,30	1.20	3 (10%)	45,47,47	1.73	8 (17%)

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	GDP	C	1101	-	-	5/16/32/32	0/3/3/3
2	GDP	A	1101	3	-	2/16/32/32	0/3/3/3
2	GDP	B	1101	-	-	5/16/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	GDP	C5-C4	3.05	1.47	1.38
2	C	1101	GDP	C5-C4	3.04	1.47	1.38
2	A	1101	GDP	C5-C4	2.94	1.46	1.38
2	B	1101	GDP	C6-N1	-2.89	1.33	1.38
2	A	1101	GDP	C6-N1	-2.60	1.34	1.38
2	C	1101	GDP	C6-N1	-2.59	1.34	1.38
2	B	1101	GDP	C5-N7	-2.28	1.34	1.39
2	A	1101	GDP	C5-N7	-2.24	1.34	1.39
2	C	1101	GDP	C5-N7	-2.18	1.34	1.39
2	A	1101	GDP	C4-N9	-2.05	1.32	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	GDP	C5-C4-N3	-6.16	118.58	128.39
2	B	1101	GDP	C5-C4-N3	-6.14	118.62	128.39
2	A	1101	GDP	C5-C4-N3	-5.84	119.10	128.39
2	B	1101	GDP	C2-N3-C4	4.89	120.72	112.30
2	C	1101	GDP	C2-N3-C4	4.89	120.72	112.30
2	A	1101	GDP	C2-N3-C4	4.69	120.39	112.30
2	B	1101	GDP	N9-C4-N3	4.62	135.20	125.95
2	C	1101	GDP	N9-C4-N3	4.61	135.17	125.95
2	A	1101	GDP	N9-C4-N3	4.37	134.70	125.95
2	A	1101	GDP	C6-C5-N7	3.13	135.99	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	GDP	C6-C5-N7	3.05	135.84	130.29
2	B	1101	GDP	C6-C5-N7	3.01	135.77	130.29
2	B	1101	GDP	C3'-C2'-C1'	2.54	106.27	101.46
2	A	1101	GDP	C4-C5-N7	-2.50	106.71	110.67
2	C	1101	GDP	C4-C5-N7	-2.46	106.77	110.67
2	B	1101	GDP	C4-C5-N7	-2.44	106.81	110.67
2	C	1101	GDP	O6-C6-C5	-2.39	120.22	126.53
2	A	1101	GDP	C3'-C2'-C1'	2.36	105.92	101.46
2	B	1101	GDP	C2'-C1'-N9	-2.34	106.74	113.25
2	A	1101	GDP	O6-C6-C5	-2.24	120.62	126.53
2	C	1101	GDP	C3'-C2'-C1'	2.24	105.70	101.46
2	A	1101	GDP	C2'-C1'-N9	-2.14	107.29	113.25
2	B	1101	GDP	O6-C6-C5	-2.04	121.15	126.53

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	GDP	C5'-O5'-PA-O3A
2	A	1101	GDP	C5'-O5'-PA-O1A
2	B	1101	GDP	C5'-O5'-PA-O3A
2	B	1101	GDP	C5'-O5'-PA-O1A
2	B	1101	GDP	C5'-O5'-PA-O2A
2	C	1101	GDP	C5'-O5'-PA-O3A
2	C	1101	GDP	C5'-O5'-PA-O2A
2	B	1101	GDP	C3'-C4'-C5'-O5'
2	C	1101	GDP	O4'-C4'-C5'-O5'
2	C	1101	GDP	C3'-C4'-C5'-O5'
2	B	1101	GDP	O4'-C4'-C5'-O5'
2	C	1101	GDP	PB-O3A-PA-O5'

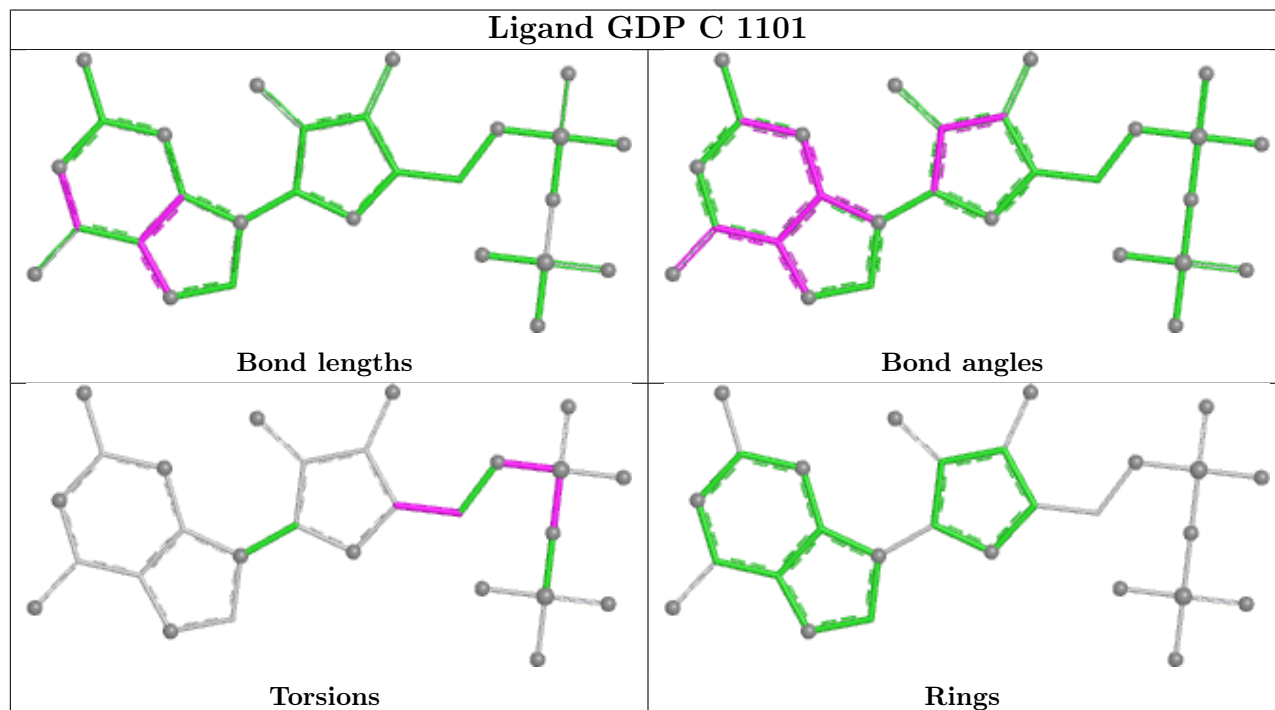
There are no ring outliers.

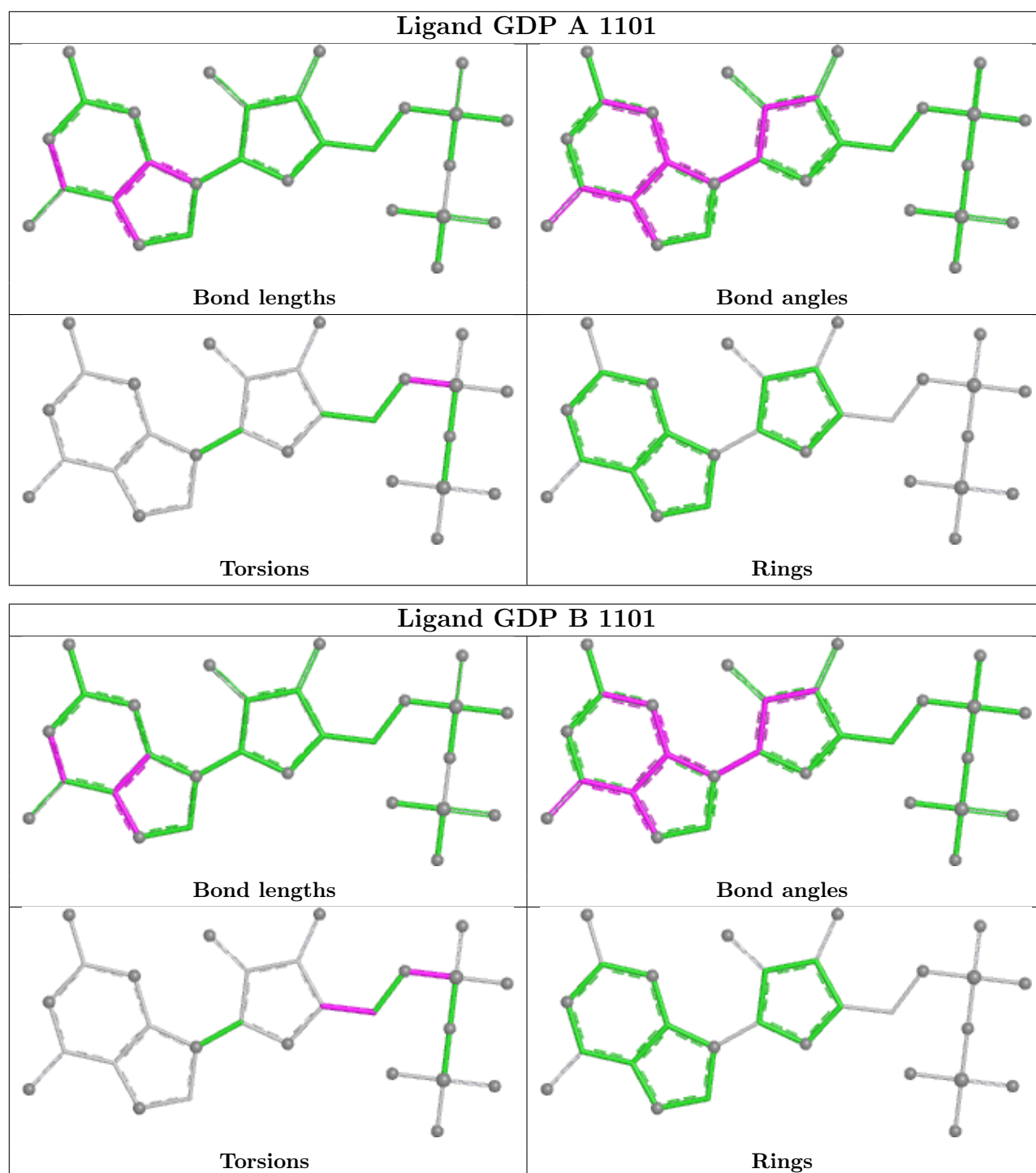
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	GDP	4	0
2	A	1101	GDP	1	0
2	B	1101	GDP	5	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.

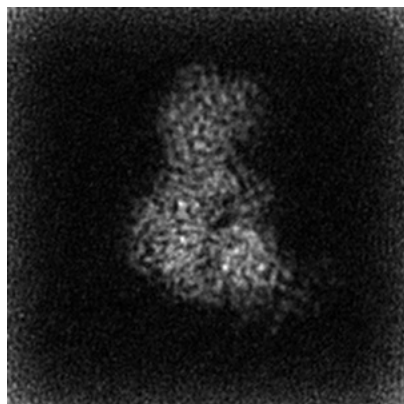
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40751. These allow visual inspection of the internal detail of the map and identification of artifacts.

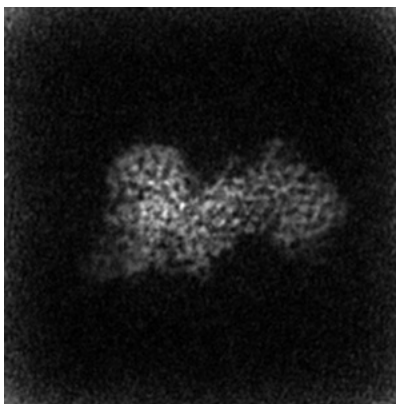
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

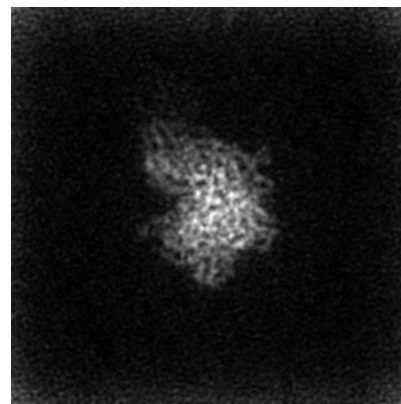
6.1.1 Primary map



X

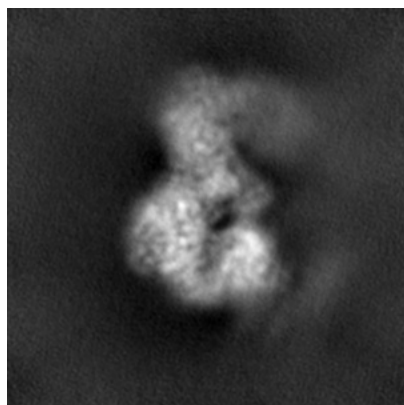


Y

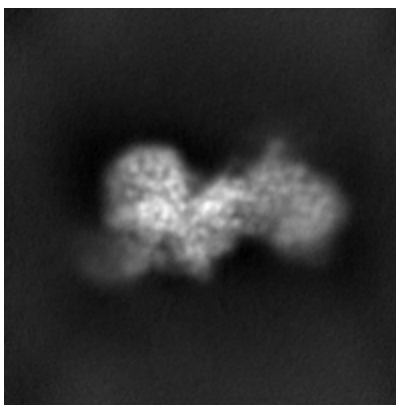


Z

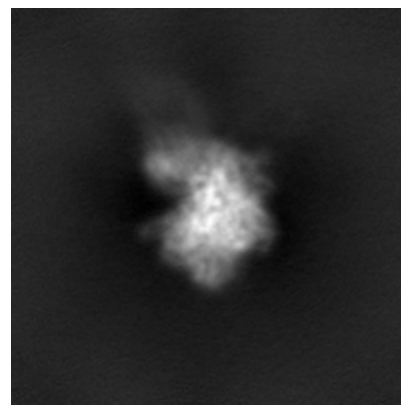
6.1.2 Raw map



X



Y

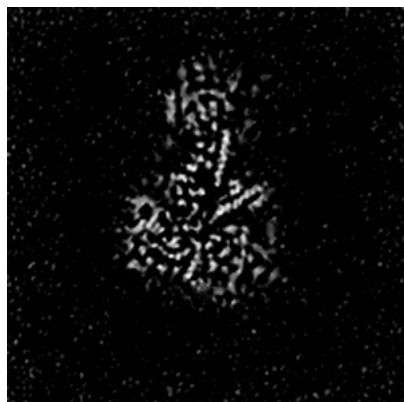


Z

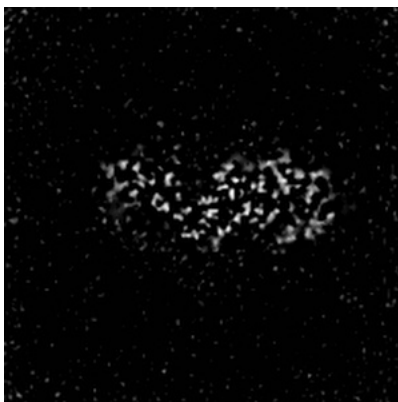
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

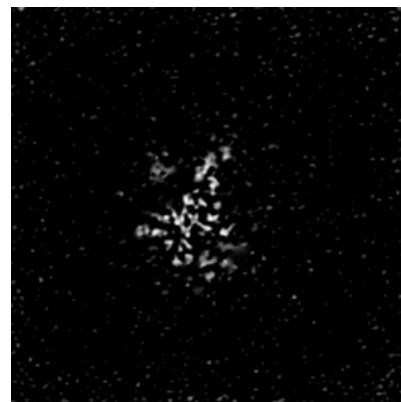
6.2.1 Primary map



X Index: 98

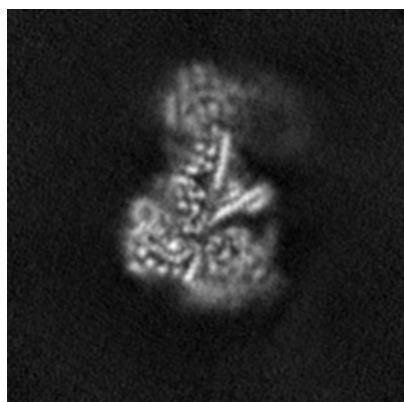


Y Index: 98

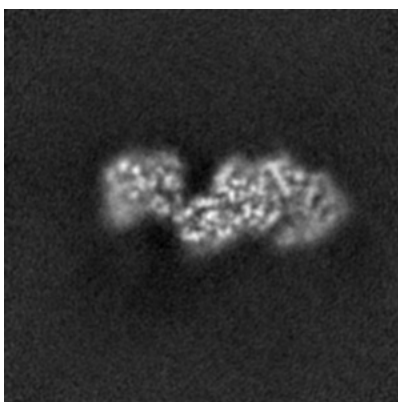


Z Index: 98

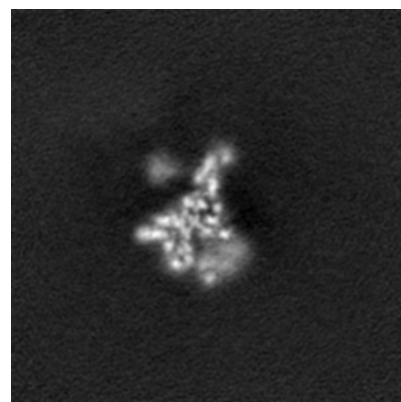
6.2.2 Raw map



X Index: 98



Y Index: 98

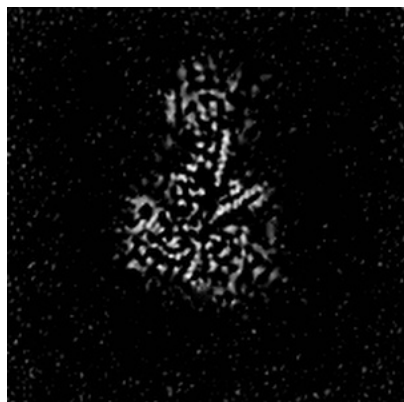


Z Index: 98

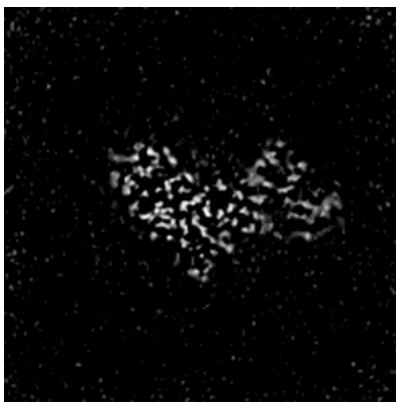
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

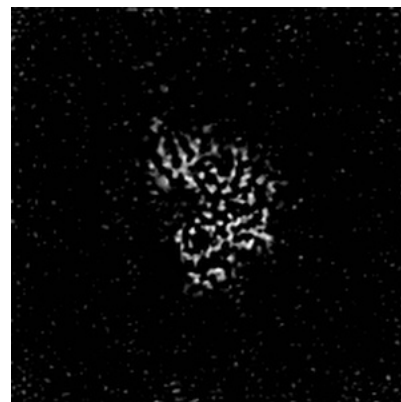
6.3.1 Primary map



X Index: 98

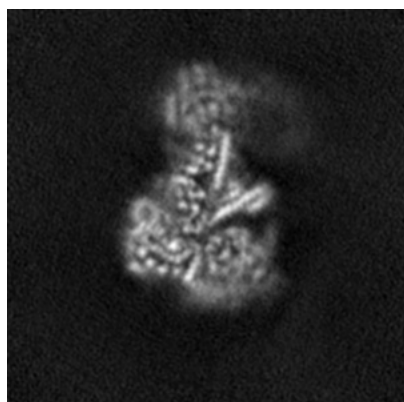


Y Index: 87

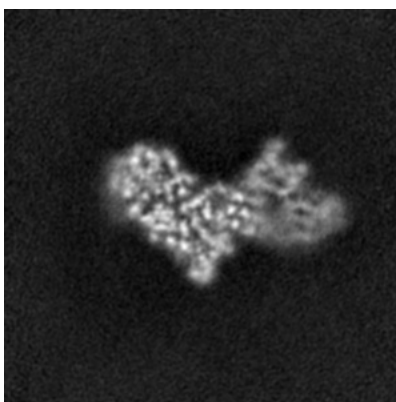


Z Index: 75

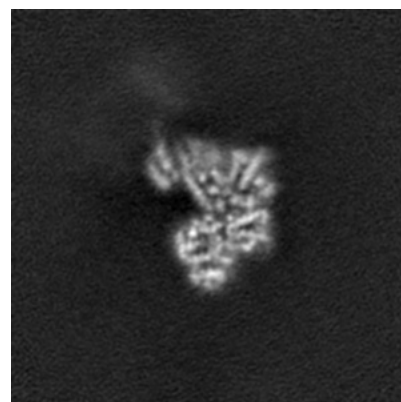
6.3.2 Raw map



X Index: 98



Y Index: 87

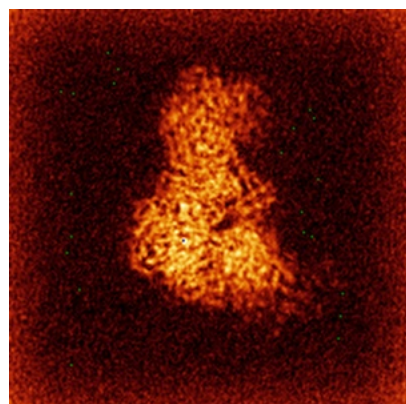


Z Index: 76

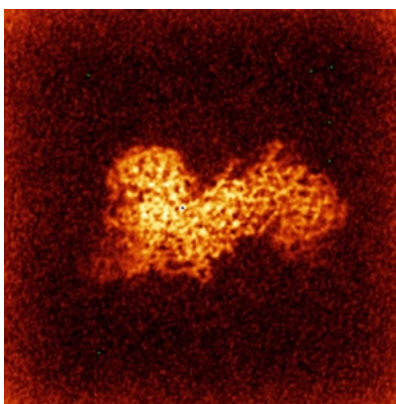
The images above show the largest variance slices of the map in three orthogonal directions.

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

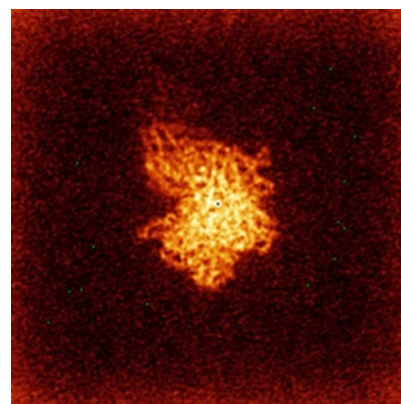
6.4.1 Primary map



X

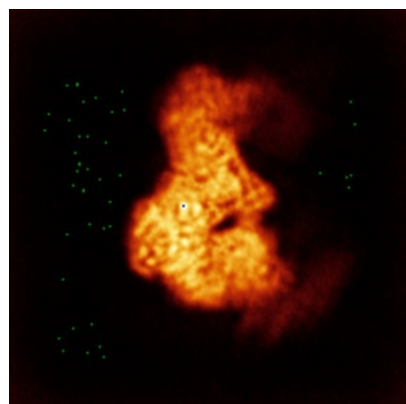


Y

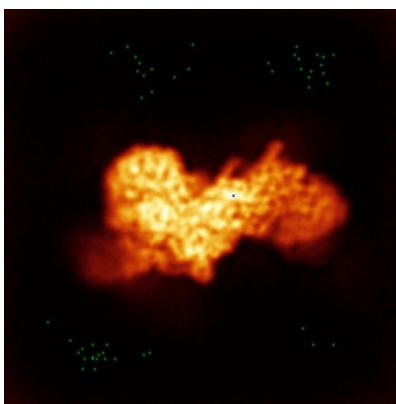


Z

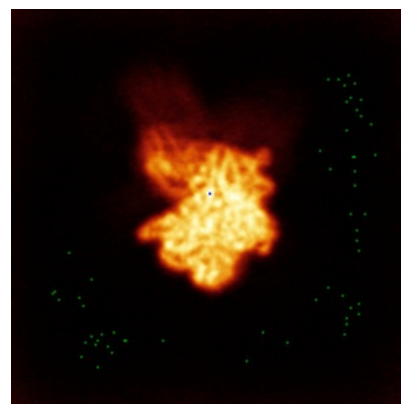
6.4.2 Raw map



X



Y

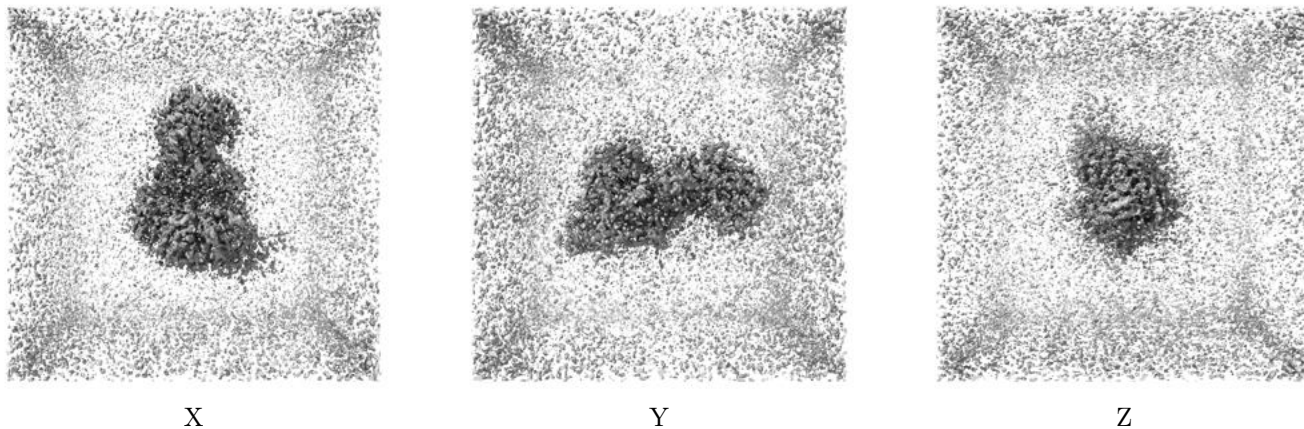


Z

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 2.69. 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.

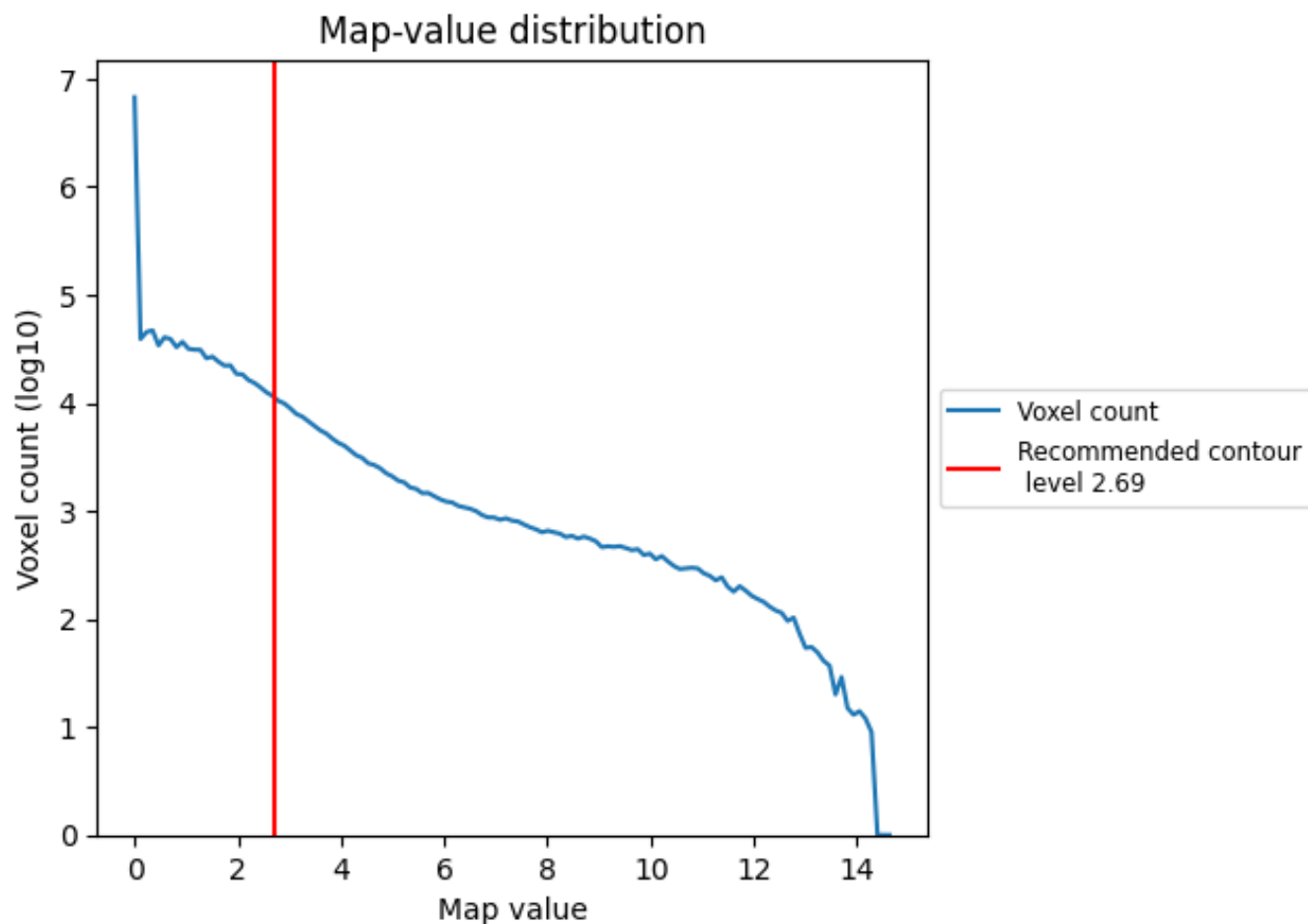
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

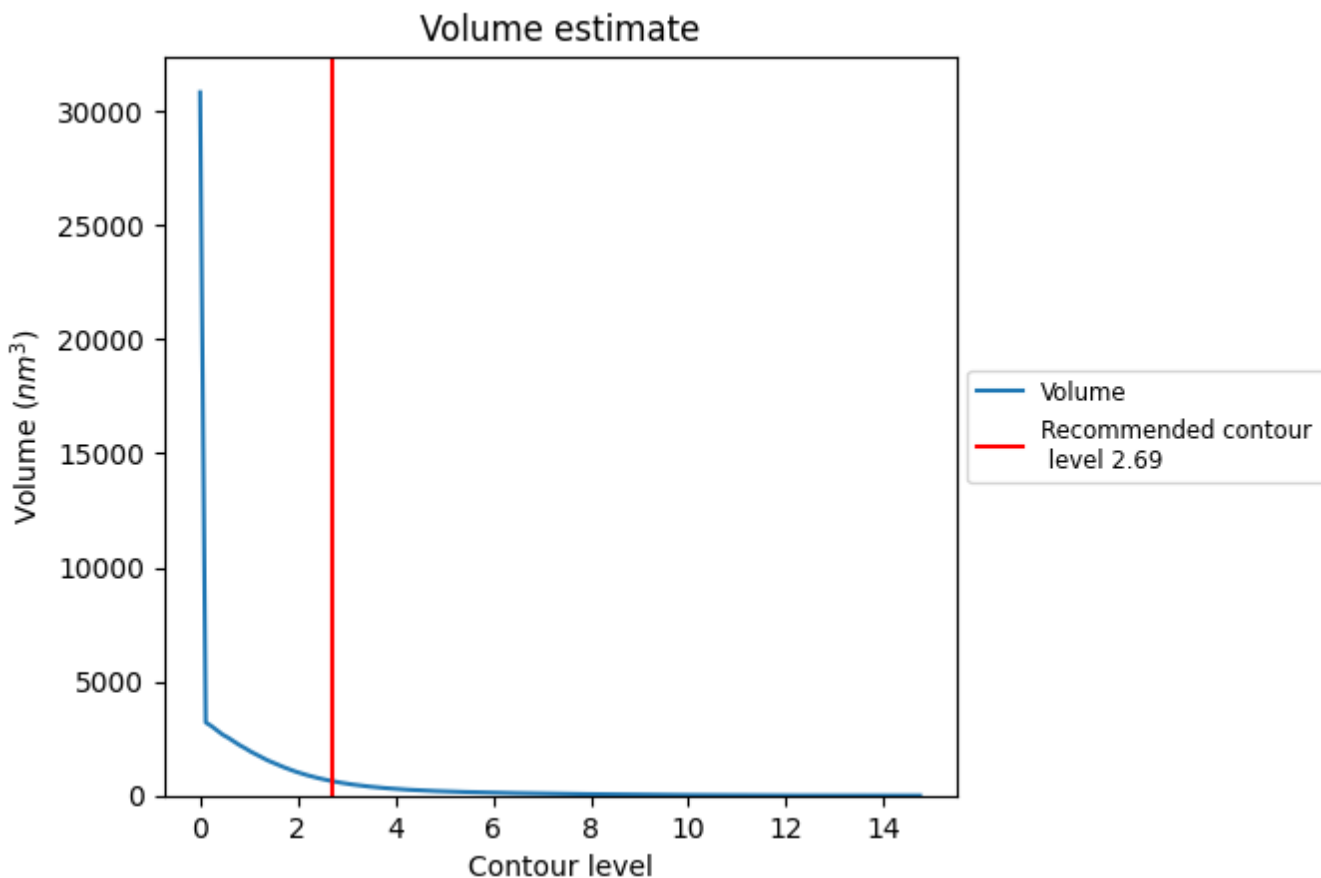
This section contains the results of statistical analysis of the map.

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.

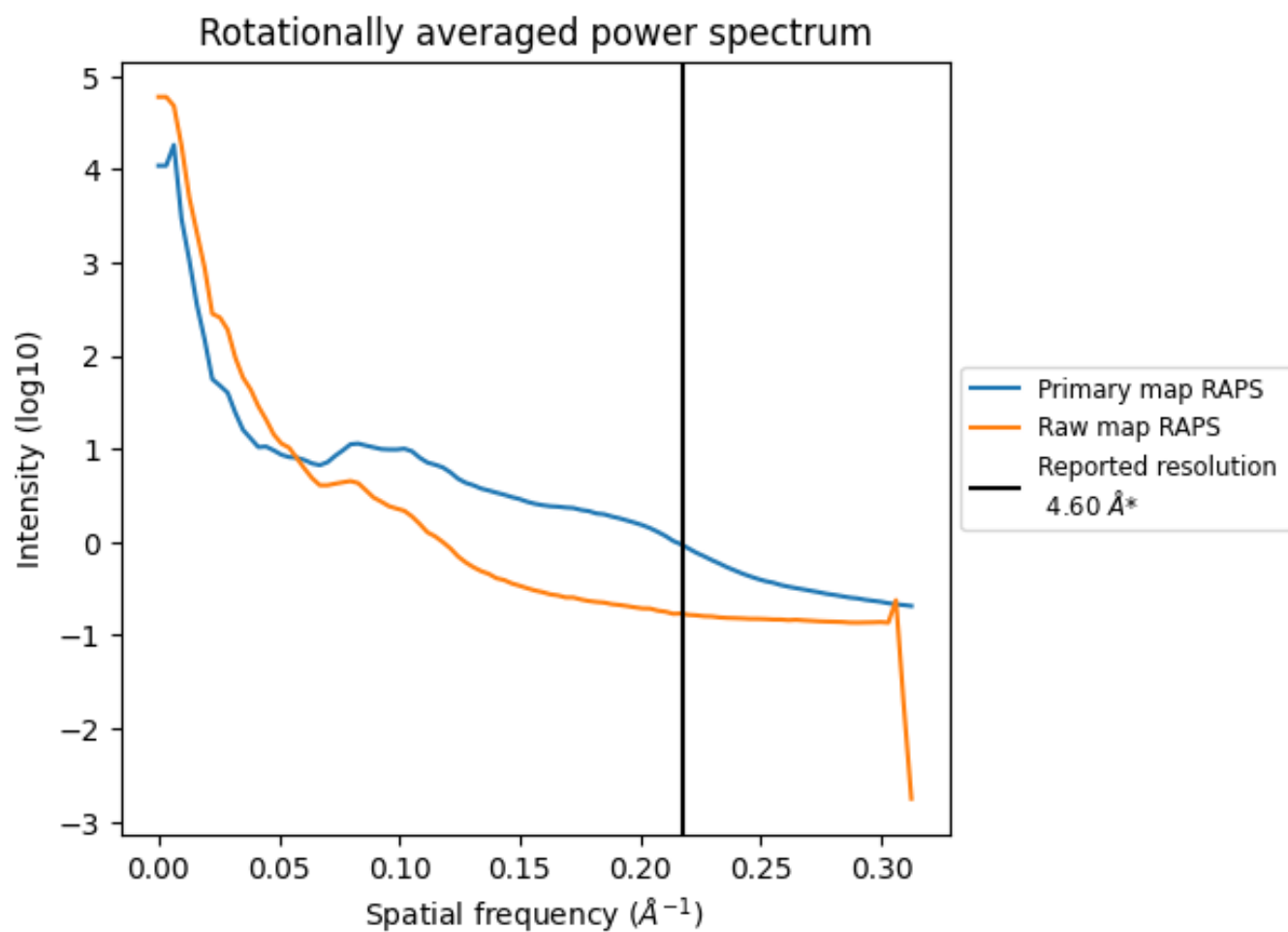
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 640 nm^3 ; this corresponds to an approximate mass of 578 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 i

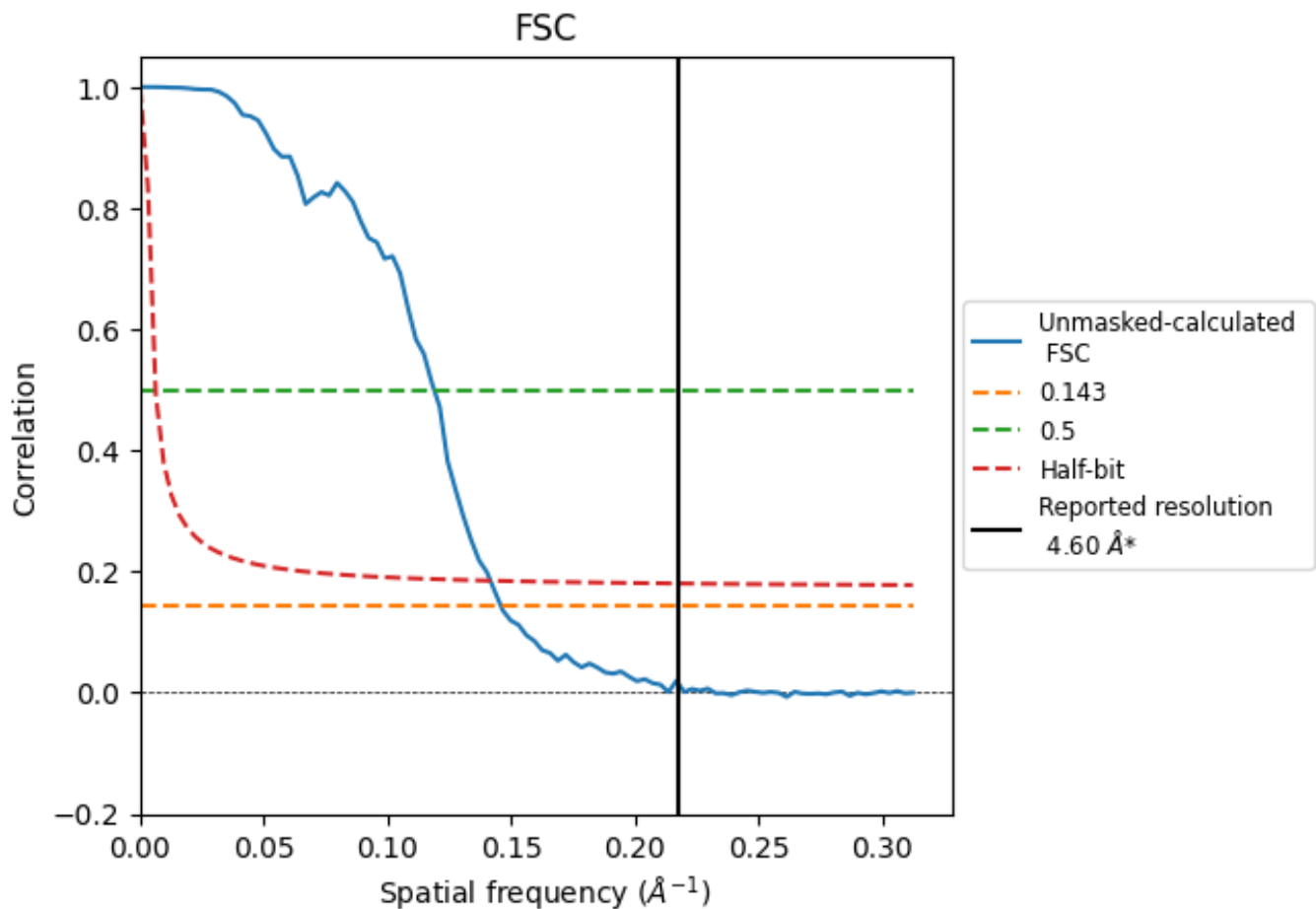


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [\(i\)](#)

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

8.1 FSC [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

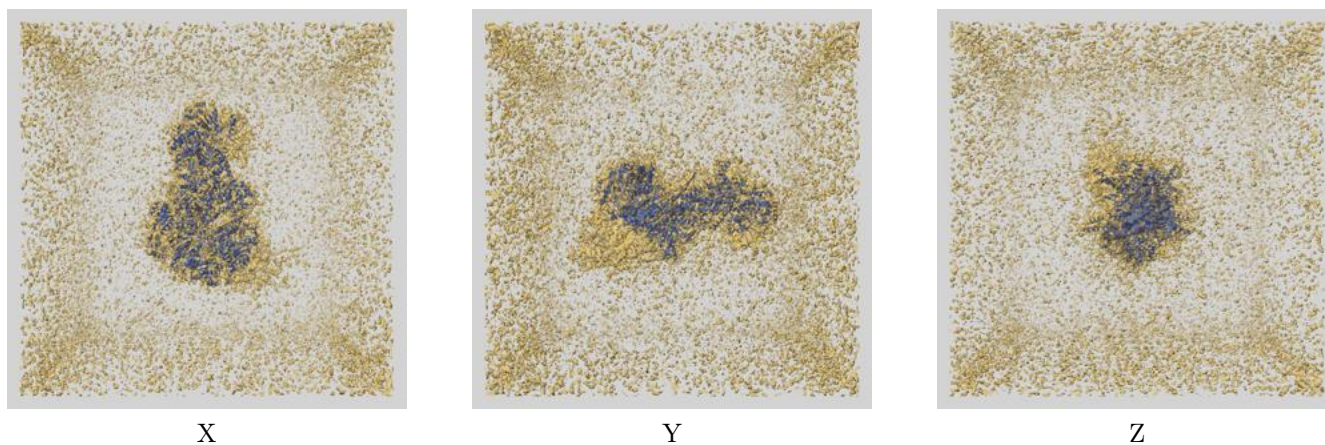
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.85	8.41	7.06

*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 6.85 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

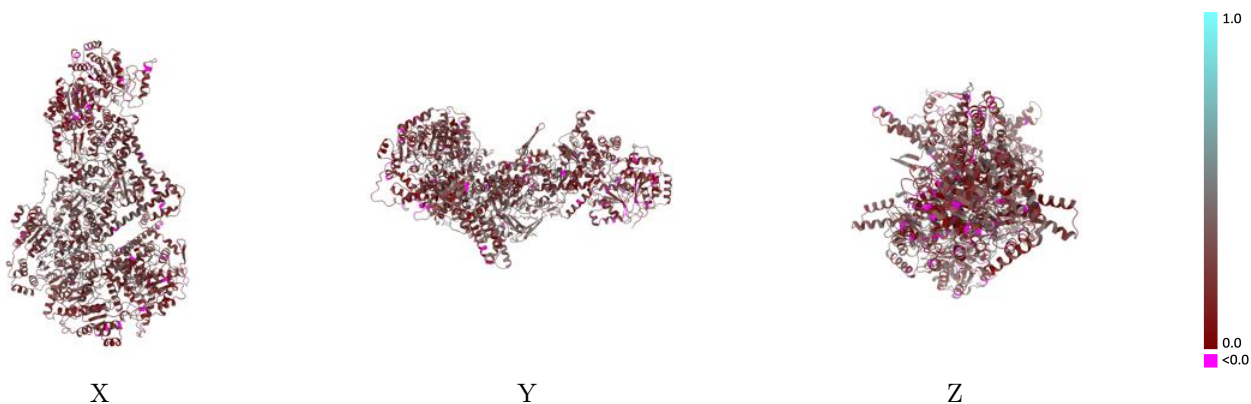
This section contains information regarding the fit between EMDB map EMD-40751 and PDB model 8SSL. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



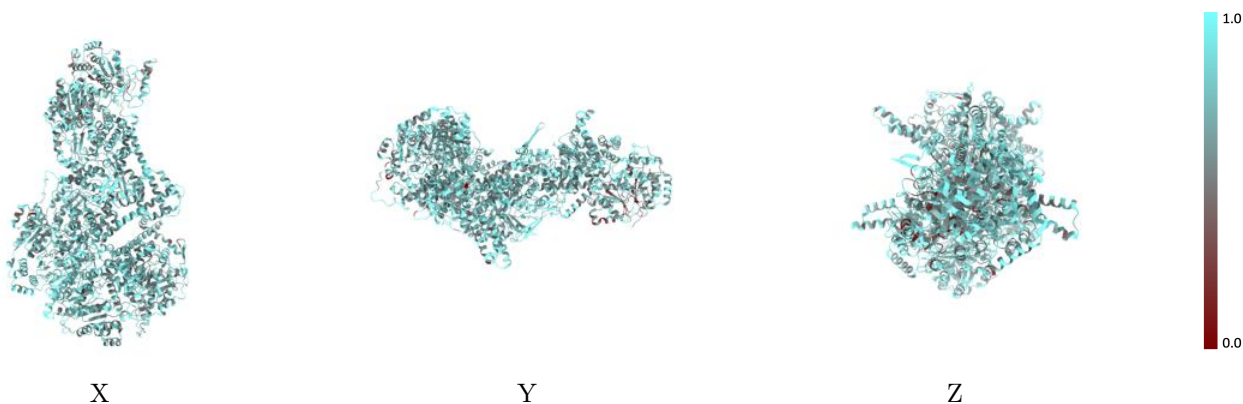
The images above show the 3D surface view of the map at the recommended contour level 2.69 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



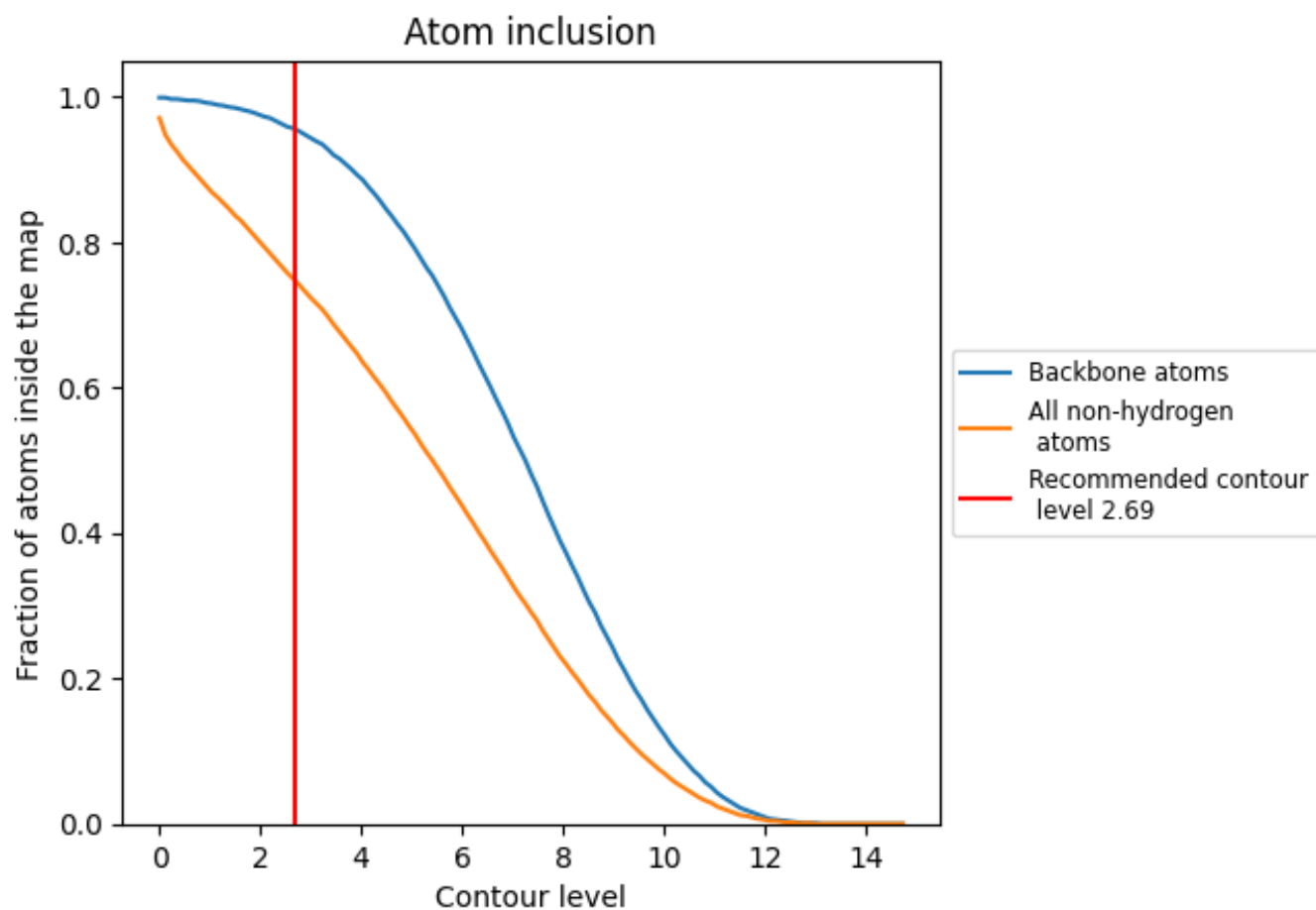
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.69).









9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 75% 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 (2.69) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7470	 0.2690
A	 0.7880	 0.3090
B	 0.7430	 0.2610
C	 0.7120	 0.2370

