



## Full wwPDB EM Validation Report ⓘ

Aug 28, 2025 – 01:21 pm BST

PDB ID : 9HMS / pdb\_00009hms  
EMDB ID : EMD-52297  
Title : Cryo-EM structure of human separase bound to SCC1 (310-550 aa) and SA2  
Authors : Yu, J.; Schmidt, S.; Botto, M.; Boland, A.  
Deposited on : 2024-12-09  
Resolution : 3.40 Å (reported)  
Based on initial models : 4PJU, 7NJ1

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev126  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

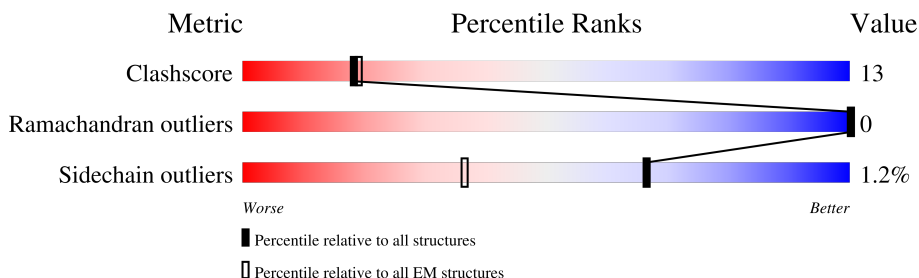
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1271	
2	B	241	
3	C	2172	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16909 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 Cohesin subunit SA-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	933	Total	C	N	O	S	0	0
			7178	4547	1230	1360	41		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1232	SER	-	expression tag	UNP Q8N3U4
A	1233	SER	-	expression tag	UNP Q8N3U4
A	1234	LEU	-	expression tag	UNP Q8N3U4
A	1235	ALA	-	expression tag	UNP Q8N3U4
A	1236	GLU	-	expression tag	UNP Q8N3U4
A	1237	GLU	-	expression tag	UNP Q8N3U4
A	1238	ASN	-	expression tag	UNP Q8N3U4
A	1239	LEU	-	expression tag	UNP Q8N3U4
A	1240	TYR	-	expression tag	UNP Q8N3U4
A	1241	PHE	-	expression tag	UNP Q8N3U4
A	1242	GLN	-	expression tag	UNP Q8N3U4
A	1243	SER	-	expression tag	UNP Q8N3U4
A	1244	TRP	-	expression tag	UNP Q8N3U4
A	1245	SER	-	expression tag	UNP Q8N3U4
A	1246	HIS	-	expression tag	UNP Q8N3U4
A	1247	PRO	-	expression tag	UNP Q8N3U4
A	1248	GLN	-	expression tag	UNP Q8N3U4
A	1249	PHE	-	expression tag	UNP Q8N3U4
A	1250	GLU	-	expression tag	UNP Q8N3U4
A	1251	LYS	-	expression tag	UNP Q8N3U4
A	1252	GLY	-	expression tag	UNP Q8N3U4
A	1253	GLY	-	expression tag	UNP Q8N3U4
A	1254	GLY	-	expression tag	UNP Q8N3U4
A	1255	SER	-	expression tag	UNP Q8N3U4
A	1256	GLY	-	expression tag	UNP Q8N3U4
A	1257	GLY	-	expression tag	UNP Q8N3U4
A	1258	GLY	-	expression tag	UNP Q8N3U4
A	1259	SER	-	expression tag	UNP Q8N3U4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1260	GLY	-	expression tag	UNP Q8N3U4
A	1261	GLY	-	expression tag	UNP Q8N3U4
A	1262	GLY	-	expression tag	UNP Q8N3U4
A	1263	SER	-	expression tag	UNP Q8N3U4
A	1264	TRP	-	expression tag	UNP Q8N3U4
A	1265	SER	-	expression tag	UNP Q8N3U4
A	1266	HIS	-	expression tag	UNP Q8N3U4
A	1267	PRO	-	expression tag	UNP Q8N3U4
A	1268	GLN	-	expression tag	UNP Q8N3U4
A	1269	PHE	-	expression tag	UNP Q8N3U4
A	1270	GLU	-	expression tag	UNP Q8N3U4
A	1271	LYS	-	expression tag	UNP Q8N3U4

- Molecule 2 is a protein called Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			869	552	145	168	4		

- Molecule 3 is a protein called Separin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1141	Total	C	N	O	S	0	0
			8861	5652	1536	1632	41		

There are 113 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-54	MET	-	initiating methionine	UNP Q14674
C	-53	ASP	-	expression tag	UNP Q14674
C	-52	TYR	-	expression tag	UNP Q14674
C	-51	LYS	-	expression tag	UNP Q14674
C	-50	ASP	-	expression tag	UNP Q14674
C	-49	HIS	-	expression tag	UNP Q14674
C	-48	ASP	-	expression tag	UNP Q14674
C	-47	GLY	-	expression tag	UNP Q14674
C	-46	ASP	-	expression tag	UNP Q14674
C	-45	TYR	-	expression tag	UNP Q14674
C	-44	LYS	-	expression tag	UNP Q14674
C	-43	ASP	-	expression tag	UNP Q14674
C	-42	HIS	-	expression tag	UNP Q14674
C	-41	ASP	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-40	ILE	-	expression tag	UNP Q14674
C	-39	ASP	-	expression tag	UNP Q14674
C	-38	TYR	-	expression tag	UNP Q14674
C	-37	LYS	-	expression tag	UNP Q14674
C	-36	ASP	-	expression tag	UNP Q14674
C	-35	ASP	-	expression tag	UNP Q14674
C	-34	ASP	-	expression tag	UNP Q14674
C	-33	ASP	-	expression tag	UNP Q14674
C	-32	LYS	-	expression tag	UNP Q14674
C	-31	SER	-	expression tag	UNP Q14674
C	-30	GLY	-	expression tag	UNP Q14674
C	-29	PRO	-	expression tag	UNP Q14674
C	-28	GLY	-	expression tag	UNP Q14674
C	-27	GLY	-	expression tag	UNP Q14674
C	-26	SER	-	expression tag	UNP Q14674
C	-25	GLY	-	expression tag	UNP Q14674
C	-24	GLY	-	expression tag	UNP Q14674
C	-23	SER	-	expression tag	UNP Q14674
C	-22	GLY	-	expression tag	UNP Q14674
C	-21	GLY	-	expression tag	UNP Q14674
C	-20	GLY	-	expression tag	UNP Q14674
C	-19	SER	-	expression tag	UNP Q14674
C	-18	GLY	-	expression tag	UNP Q14674
C	-17	GLY	-	expression tag	UNP Q14674
C	-16	GLY	-	expression tag	UNP Q14674
C	-15	SER	-	expression tag	UNP Q14674
C	-14	GLY	-	expression tag	UNP Q14674
C	-13	GLU	-	expression tag	UNP Q14674
C	-12	ASN	-	expression tag	UNP Q14674
C	-11	LEU	-	expression tag	UNP Q14674
C	-10	TYR	-	expression tag	UNP Q14674
C	-9	PHE	-	expression tag	UNP Q14674
C	-8	GLN	-	expression tag	UNP Q14674
C	-7	GLY	-	expression tag	UNP Q14674
C	-6	GLY	-	expression tag	UNP Q14674
C	-5	GLY	-	expression tag	UNP Q14674
C	-4	SER	-	expression tag	UNP Q14674
C	-3	GLY	-	expression tag	UNP Q14674
C	-2	GLY	-	expression tag	UNP Q14674
C	-1	SER	-	expression tag	UNP Q14674
C	0	GLY	-	expression tag	UNP Q14674
C	25	ASP	ALA	conflict	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	116	VAL	ALA	conflict	UNP Q14674
C	1372	SER	ARG	conflict	UNP Q14674
C	1525	GLY	-	linker	UNP Q14674
C	1526	LEU	-	linker	UNP Q14674
C	1527	GLU	-	linker	UNP Q14674
C	1528	VAL	-	linker	UNP Q14674
C	1529	LEU	-	linker	UNP Q14674
C	1530	PHE	-	linker	UNP Q14674
C	1531	GLN	-	linker	UNP Q14674
C	1532	GLY	-	linker	UNP Q14674
C	1533	PRO	-	linker	UNP Q14674
C	1534	GLY	-	linker	UNP Q14674
C	1535	SER	-	linker	UNP Q14674
C	1536	GLY	-	linker	UNP Q14674
C	1561	GLN	ARG	conflict	UNP Q14674
C	2029	SER	CYS	conflict	UNP Q14674
C	2037	HIS	ARG	conflict	UNP Q14674
C	2121	SER	-	expression tag	UNP Q14674
C	2122	SER	-	expression tag	UNP Q14674
C	2123	LEU	-	expression tag	UNP Q14674
C	2124	ALA	-	expression tag	UNP Q14674
C	2125	GLU	-	expression tag	UNP Q14674
C	2126	GLU	-	expression tag	UNP Q14674
C	2127	ASN	-	expression tag	UNP Q14674
C	2128	LEU	-	expression tag	UNP Q14674
C	2129	TYR	-	expression tag	UNP Q14674
C	2130	PHE	-	expression tag	UNP Q14674
C	2131	GLN	-	expression tag	UNP Q14674
C	2132	SER	-	expression tag	UNP Q14674
C	2133	TRP	-	expression tag	UNP Q14674
C	2134	SER	-	expression tag	UNP Q14674
C	2135	HIS	-	expression tag	UNP Q14674
C	2136	PRO	-	expression tag	UNP Q14674
C	2137	GLN	-	expression tag	UNP Q14674
C	2138	PHE	-	expression tag	UNP Q14674
C	2139	GLU	-	expression tag	UNP Q14674
C	2140	LYS	-	expression tag	UNP Q14674
C	2141	GLY	-	expression tag	UNP Q14674
C	2142	GLY	-	expression tag	UNP Q14674
C	2143	GLY	-	expression tag	UNP Q14674
C	2144	SER	-	expression tag	UNP Q14674
C	2145	GLY	-	expression tag	UNP Q14674

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2146	GLY	-	expression tag	UNP Q14674
C	2147	GLY	-	expression tag	UNP Q14674
C	2148	SER	-	expression tag	UNP Q14674
C	2149	GLY	-	expression tag	UNP Q14674
C	2150	GLY	-	expression tag	UNP Q14674
C	2151	GLY	-	expression tag	UNP Q14674
C	2152	SER	-	expression tag	UNP Q14674
C	2153	TRP	-	expression tag	UNP Q14674
C	2154	SER	-	expression tag	UNP Q14674
C	2155	HIS	-	expression tag	UNP Q14674
C	2156	PRO	-	expression tag	UNP Q14674
C	2157	GLN	-	expression tag	UNP Q14674
C	2158	PHE	-	expression tag	UNP Q14674
C	2159	GLU	-	expression tag	UNP Q14674
C	2160	LYS	-	expression tag	UNP Q14674

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

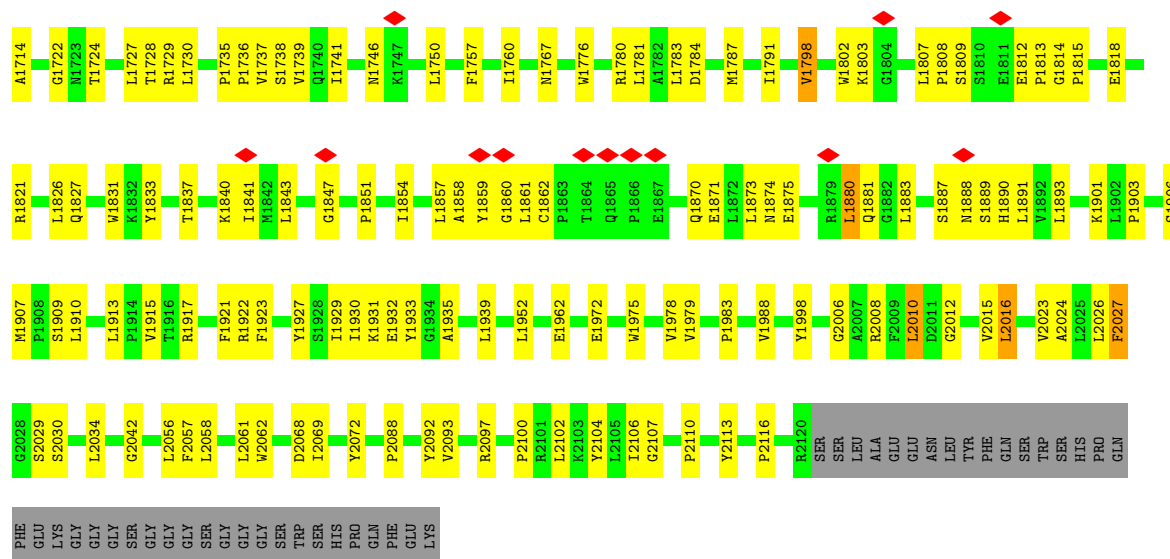
Mol	Chain	Residues	Atoms		AltConf
4	C	1	Total 1	Zn 1	0











## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177878	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	22.198	Depositor
Minimum map value	-0.111	Depositor
Average map value	-0.022	Depositor
Map value standard deviation	0.291	Depositor
Recommended contour level	4.4	Depositor
Map size (Å)	462.0288, 462.0288, 462.0288	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9024, 0.9024, 0.9024	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: ZN

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	0.52	0/7292	0.75	2/9865 (0.0%)
2	B	0.53	0/882	0.74	1/1188 (0.1%)
3	C	0.46	0/9036	0.67	3/12290 (0.0%)
All	All	0.49	0/17210	0.71	6/23343 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	730	TYR	N-CA-C	-6.66	105.31	113.50
2	B	395	PRO	N-CA-CB	6.60	110.26	103.00
3	C	2027	PHE	N-CA-CB	-5.93	101.77	110.49
1	A	479	TYR	CB-CA-C	5.35	119.95	110.85
3	C	1798	VAL	N-CA-C	5.35	116.01	110.82
1	A	224	MET	N-CA-C	-5.22	105.48	111.07

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	7178	0	6844	174	0
2	B	869	0	878	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8861	0	9021	245	0
4	C	1	0	0	0	0
All	All	16909	0	16743	434	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 13.

All (434) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HE3	1:A:400:SER:HB3	1.64	0.78
3:C:1682:LEU:HD13	3:C:1690:PRO:HA	1.67	0.75
3:C:894:SER:HB3	3:C:897:TRP:HD1	1.50	0.75
1:A:970:ILE:HD11	1:A:1006:PHE:HB3	1.69	0.73
3:C:1880:LEU:HD12	3:C:1883:LEU:HD11	1.71	0.71
3:C:759:THR:HG22	3:C:759:THR:O	1.92	0.70
1:A:659:ASP:OD1	1:A:706:TRP:NE1	2.28	0.65
3:C:1728:THR:HG22	3:C:1738:SER:HB3	1.78	0.65
1:A:913:ILE:O	1:A:917:LYS:HG2	1.97	0.65
1:A:220:THR:HG21	1:A:304:ILE:HG23	1.79	0.64
3:C:1601:CYS:HB2	3:C:1623:SER:HB3	1.79	0.64
1:A:219:SER:O	1:A:223:ALA:N	2.22	0.64
1:A:714:LYS:O	1:A:718:THR:HG23	1.97	0.64
1:A:472:GLU:HG2	1:A:472:GLU:O	1.97	0.64
3:C:1206:LEU:HB3	3:C:1208:HIS:CD2	2.33	0.64
1:A:529:ILE:HG23	1:A:563:ILE:HD13	1.80	0.64
1:A:731:ILE:HG22	1:A:735:GLN:HE21	1.63	0.64
3:C:701:ARG:NH1	3:C:961:THR:O	2.31	0.64
3:C:882:LEU:HD21	3:C:926:GLN:HB3	1.79	0.63
3:C:1055:LEU:HD11	3:C:1139:PHE:HE1	1.63	0.63
3:C:1203:GLN:NE2	3:C:1210:THR:O	2.30	0.63
3:C:1618:PHE:HB2	3:C:1695:PHE:CG	2.34	0.63
2:B:380:LEU:HD22	2:B:385:LEU:HD23	1.81	0.63
1:A:299:ASP:O	1:A:305:ARG:NH1	2.28	0.62
1:A:272:LYS:O	1:A:276:GLU:HG3	2.00	0.62
1:A:285:MET:HE1	1:A:323:PHE:HZ	1.64	0.62
3:C:1714:ALA:HB3	3:C:1724:THR:HB	1.80	0.62
3:C:1891:LEU:HD21	3:C:1893:LEU:HG	1.81	0.62
3:C:731:SER:HA	3:C:734:ALA:HB3	1.82	0.62
3:C:1199:THR:HG23	3:C:1212:PRO:HG2	1.82	0.62
1:A:283:ASN:HA	1:A:286:ASN:HD22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ILE:HG12	1:A:703:LEU:HD22	1.81	0.61
3:C:1837:THR:O	3:C:1841:ILE:HG12	2.01	0.61
3:C:954:MET:HE1	3:C:984:LEU:HD11	1.83	0.60
3:C:1151:CYS:O	3:C:1197:ARG:NH1	2.34	0.60
1:A:214:ALA:O	1:A:218:THR:HG22	2.01	0.60
3:C:1815:PRO:HG3	3:C:1843:LEU:HB2	1.83	0.60
3:C:1670:LEU:O	3:C:1674:GLN:HG2	2.01	0.60
1:A:1020:VAL:HG21	3:C:1781:LEU:HD21	1.83	0.59
3:C:946:LEU:HB3	3:C:987:VAL:HG22	1.84	0.59
3:C:1791:ILE:HD13	3:C:1906:SER:HB2	1.84	0.59
3:C:1617:ALA:HB1	3:C:1730:LEU:HD21	1.85	0.59
1:A:904:MET:HA	1:A:907:THR:HG22	1.85	0.59
1:A:303:GLU:O	1:A:307:ILE:HG12	2.02	0.59
1:A:316:MET:HB3	1:A:354:LEU:HD21	1.83	0.59
1:A:890:MET:HG2	1:A:951:LEU:HD13	1.83	0.59
1:A:899:ILE:O	1:A:903:THR:HG23	2.02	0.59
3:C:908:VAL:HG21	3:C:932:TRP:HD1	1.69	0.58
3:C:1062:THR:HB	3:C:1150:LEU:HD13	1.85	0.58
3:C:1767:ASN:HD21	3:C:1776:TRP:HA	1.68	0.58
1:A:582:ALA:O	1:A:586:THR:HG23	2.03	0.58
3:C:1058:LEU:HB3	3:C:1150:LEU:HD21	1.84	0.58
1:A:332:VAL:HG13	1:A:347:CYS:HB3	1.84	0.58
3:C:1858:ALA:HB1	3:C:1870:GLN:HA	1.86	0.58
3:C:1713:LEU:HD21	3:C:1722:GLY:H	1.67	0.57
3:C:1952:LEU:HB3	3:C:1979:VAL:HG22	1.85	0.57
3:C:1978:VAL:HG11	3:C:1983:PRO:HB3	1.87	0.57
3:C:1184:LEU:HB3	3:C:1230:LEU:HD21	1.87	0.57
1:A:698:HIS:CD2	1:A:703:LEU:HB2	2.39	0.57
3:C:2034:LEU:HB3	3:C:2042:GLY:HA3	1.86	0.56
1:A:615:GLN:O	1:A:619:ILE:HG13	2.04	0.56
1:A:737:THR:HA	1:A:740:VAL:HG12	1.87	0.56
3:C:908:VAL:HG21	3:C:932:TRP:CD1	2.40	0.56
3:C:1686:HIS:O	3:C:1690:PRO:CD	2.53	0.56
3:C:1859:TYR:HE1	3:C:1870:GLN:HB2	1.69	0.56
1:A:781:THR:HA	1:A:784:LYS:HG2	1.87	0.56
3:C:1294:TRP:CD1	3:C:1860:GLY:HA3	2.41	0.56
3:C:2057:PHE:HB3	3:C:2113:TYR:HB2	1.88	0.56
1:A:87:VAL:O	1:A:92:LYS:N	2.39	0.56
3:C:1018:THR:HG21	3:C:1027:CYS:N	2.20	0.56
1:A:632:CYS:O	1:A:635:THR:HG22	2.06	0.55
1:A:230:LEU:HD13	1:A:285:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1760:ILE:HG23	3:C:1783:LEU:HD22	1.89	0.55
1:A:1016:ARG:O	1:A:1020:VAL:HG23	2.06	0.55
3:C:1581:LEU:HB2	3:C:1604:LEU:HD13	1.88	0.55
3:C:2024:ALA:HB1	3:C:2026:LEU:HD13	1.89	0.55
3:C:1831:TRP:NE1	3:C:1833:TYR:O	2.39	0.55
3:C:1827:GLN:HA	3:C:1831:TRP:HB3	1.89	0.54
3:C:1988:VAL:HB	3:C:2010:LEU:HD12	1.89	0.54
1:A:830:LEU:HD11	1:A:884:ASP:HB3	1.90	0.54
3:C:1741:ILE:HG21	3:C:1798:VAL:O	2.07	0.54
1:A:975:LYS:HB2	2:B:416:PHE:HE1	1.73	0.54
1:A:592:PRO:HA	1:A:595:PHE:CD2	2.43	0.54
1:A:281:ILE:O	1:A:285:MET:HG3	2.08	0.54
1:A:503:LEU:HD21	1:A:573:GLN:HB2	1.90	0.54
1:A:288:ILE:HG23	1:A:292:VAL:HB	1.90	0.54
1:A:309:ILE:O	1:A:312:ILE:HG22	2.08	0.54
3:C:762:GLN:CD	3:C:762:GLN:H	2.16	0.54
3:C:1930:ILE:HG23	3:C:1935:ALA:HB3	1.88	0.54
3:C:1818:GLU:HA	3:C:1821:ARG:HB3	1.89	0.54
2:B:349:THR:HG22	2:B:350:THR:H	1.73	0.53
3:C:954:MET:SD	3:C:958:ILE:HG21	2.49	0.53
3:C:829:PRO:HB2	3:C:871:HIS:HE1	1.72	0.53
3:C:1729:ARG:NH2	3:C:1809:SER:H	2.06	0.53
1:A:534:GLU:HB2	1:A:536:HIS:HD2	1.73	0.53
3:C:1618:PHE:CG	3:C:1695:PHE:HB2	2.44	0.53
1:A:1012:ARG:O	1:A:1016:ARG:HG3	2.09	0.53
3:C:778:ILE:HD13	3:C:977:LEU:HB3	1.90	0.53
3:C:1203:GLN:OE1	3:C:1212:PRO:HD3	2.09	0.53
3:C:1931:LYS:HE3	3:C:1939:LEU:HB3	1.91	0.53
1:A:285:MET:HE1	1:A:323:PHE:CZ	2.44	0.53
1:A:581:ASP:O	1:A:585:VAL:HG13	2.09	0.53
2:B:455:VAL:HG23	2:B:456:MET:HE2	1.91	0.52
3:C:1780:ARG:HB3	3:C:2102:LEU:HD11	1.90	0.52
3:C:1686:HIS:O	3:C:1690:PRO:CG	2.57	0.52
3:C:1688:PRO:HB3	3:C:1692:LYS:HE2	1.90	0.52
1:A:922:SER:O	1:A:925:GLN:HG2	2.09	0.52
3:C:731:SER:HA	3:C:734:ALA:CB	2.39	0.52
3:C:1741:ILE:CG2	3:C:1798:VAL:O	2.58	0.52
1:A:211:GLN:HB3	2:B:326:VAL:HG23	1.91	0.52
1:A:277:ASN:OD1	1:A:278:GLN:N	2.41	0.52
1:A:297:TYR:CE1	1:A:331:TYR:HB3	2.44	0.52
2:B:369:VAL:HA	2:B:372:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:GLN:HG3	1:A:393:LEU:HD12	1.92	0.52
1:A:786:GLN:NE2	2:B:378:GLN:OE1	2.39	0.52
3:C:1693:GLU:O	3:C:1697:GLU:HG2	2.11	0.52
3:C:1854:ILE:HG21	3:C:1874:ASN:HA	1.92	0.52
1:A:285:MET:O	1:A:286:ASN:C	2.52	0.51
3:C:979:GLN:O	3:C:983:VAL:HG12	2.09	0.51
1:A:484:MET:HE3	1:A:492:LEU:HD11	1.92	0.51
1:A:372:LYS:NZ	1:A:406:THR:HG23	2.25	0.51
1:A:890:MET:HG2	1:A:951:LEU:CD1	2.40	0.51
2:B:450:ARG:HG3	2:B:450:ARG:O	2.10	0.51
1:A:288:ILE:O	1:A:292:VAL:N	2.42	0.51
3:C:914:LEU:HD22	3:C:1259:PRO:HG2	1.93	0.51
3:C:1291:SER:O	3:C:1610:HIS:N	2.42	0.51
3:C:1044:ILE:HD12	3:C:1170:VAL:HG23	1.93	0.51
3:C:1181:LEU:O	3:C:1185:GLN:HG2	2.10	0.51
3:C:1235:LEU:HD21	3:C:1271:ILE:HG23	1.93	0.51
3:C:991:SER:O	3:C:995:VAL:HG23	2.10	0.50
3:C:1617:ALA:HB2	3:C:1736:PRO:HB3	1.93	0.50
1:A:727:GLU:O	1:A:731:ILE:HG13	2.12	0.50
3:C:1815:PRO:HB3	3:C:1840:LYS:HA	1.93	0.50
1:A:344:ARG:HH12	2:B:347:ILE:HB	1.77	0.50
1:A:1011:LEU:HD23	1:A:1011:LEU:H	1.77	0.50
3:C:775:SER:O	3:C:778:ILE:HG22	2.12	0.50
3:C:1276:LYS:HE2	3:C:1573:THR:HG23	1.94	0.50
3:C:1812:GLU:O	3:C:1815:PRO:HD2	2.11	0.50
1:A:1022:LEU:HG	1:A:1026:MET:HE2	1.93	0.50
3:C:781:ALA:HB1	3:C:981:TRP:HB2	1.94	0.50
1:A:156:SER:HA	2:B:323:LYS:HD2	1.94	0.49
3:C:1266:ALA:HB3	3:C:1596:LEU:HD21	1.94	0.49
3:C:608:CYS:HA	3:C:611:LEU:HD12	1.95	0.49
3:C:1181:LEU:HD21	3:C:1233:GLU:HG2	1.95	0.49
3:C:1735:PRO:HG2	3:C:1837:THR:HG21	1.92	0.49
1:A:648:ASN:O	1:A:652:ILE:HG13	2.11	0.49
1:A:388:VAL:HG22	1:A:424:VAL:HG12	1.93	0.49
2:B:451:LEU:HG	3:C:948:SER:HB3	1.94	0.49
3:C:682:LEU:O	3:C:686:ILE:HG13	2.12	0.49
3:C:784:GLN:NE2	3:C:822:LEU:HD13	2.27	0.49
3:C:803:SER:OG	3:C:811:LYS:HB3	2.12	0.49
3:C:905:LEU:O	3:C:908:VAL:HG12	2.13	0.49
3:C:2072:TYR:OH	3:C:2093:VAL:HG13	2.12	0.49
1:A:765:MET:HG3	1:A:798:PHE:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:ASP:HA	1:A:887:LYS:HE2	1.94	0.49
3:C:1687:PHE:N	3:C:1688:PRO:HD2	2.27	0.49
2:B:356:PRO:HD2	2:B:360:LEU:HD12	1.94	0.49
3:C:1859:TYR:CE1	3:C:1870:GLN:HB2	2.47	0.49
3:C:934:THR:HG23	3:C:935:PRO:HD2	1.95	0.49
1:A:600:TYR:CE2	1:A:609:LEU:HD23	2.48	0.49
3:C:1818:GLU:N	3:C:1818:GLU:OE2	2.46	0.49
1:A:922:SER:O	1:A:926:LEU:HG	2.13	0.48
3:C:1757:PHE:HE2	3:C:1901:LYS:HB2	1.77	0.48
1:A:1026:MET:O	1:A:1027:THR:HB	2.12	0.48
3:C:618:THR:HG23	3:C:621:GLY:H	1.77	0.48
3:C:1061:CYS:HB2	3:C:1150:LEU:HD11	1.95	0.48
1:A:680:ASP:OD1	1:A:683:ASP:HB2	2.13	0.48
1:A:697:PHE:HD1	1:A:701:HIS:HD2	1.62	0.48
1:A:333:GLY:HA2	1:A:336:MET:HE3	1.94	0.48
3:C:1288:PHE:O	3:C:1291:SER:OG	2.30	0.48
3:C:2023:VAL:HG13	3:C:2056:LEU:HB3	1.95	0.48
1:A:277:ASN:O	1:A:280:GLU:HG3	2.13	0.48
1:A:986:ASN:ND2	1:A:992:HIS:HB2	2.29	0.48
3:C:735:PHE:O	3:C:736:ASN:C	2.55	0.48
1:A:297:TYR:OH	1:A:331:TYR:O	2.25	0.48
1:A:927:PHE:O	1:A:931:ILE:HG13	2.14	0.48
2:B:412:ASN:C	2:B:414:ASP:N	2.72	0.48
3:C:970:PHE:CZ	3:C:980:LYS:HD2	2.48	0.48
2:B:374:SER:HA	2:B:393:LEU:HD21	1.95	0.47
2:B:448:PRO:HB3	3:C:947:ARG:HB3	1.96	0.47
3:C:627:THR:O	3:C:630:VAL:HG12	2.14	0.47
3:C:633:ALA:O	3:C:637:CYS:HB2	2.14	0.47
3:C:890:LEU:HG	3:C:901:ARG:HG3	1.94	0.47
3:C:934:THR:CG2	3:C:935:PRO:HD2	2.44	0.47
3:C:2072:TYR:HE2	3:C:2097:ARG:HA	1.79	0.47
3:C:698:GLU:O	3:C:702:ARG:HG2	2.13	0.47
2:B:357:THR:HG22	2:B:360:LEU:HG	1.96	0.47
3:C:1614:TYR:HD1	3:C:1695:PHE:HE2	1.62	0.47
3:C:1693:GLU:O	3:C:1694:SER:C	2.56	0.47
3:C:1998:TYR:HD2	3:C:2026:LEU:HD11	1.79	0.47
1:A:720:ILE:HG12	1:A:774:HIS:CE1	2.49	0.47
1:A:1019:TYR:CE2	1:A:1045:ARG:HD2	2.49	0.47
1:A:213:ARG:HH12	1:A:216:ARG:CZ	2.27	0.47
1:A:374:ARG:O	1:A:378:MET:HG3	2.15	0.47
1:A:870:LYS:HE3	2:B:373:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:ASP:O	1:A:686:GLN:HG2	2.14	0.47
2:B:412:ASN:C	2:B:414:ASP:H	2.23	0.47
3:C:1901:LYS:HA	3:C:2061:LEU:HD21	1.96	0.47
1:A:213:ARG:HH22	1:A:216:ARG:HH22	1.62	0.47
1:A:371:PHE:O	1:A:375:ILE:HG13	2.14	0.47
3:C:988:LEU:HD22	3:C:1030:PHE:CE2	2.50	0.47
3:C:1295:GLN:N	3:C:1295:GLN:OE1	2.47	0.47
3:C:1693:GLU:O	3:C:1696:GLN:N	2.48	0.47
3:C:1910:LEU:HD23	3:C:1913:LEU:HD12	1.95	0.47
3:C:2012:GLY:O	3:C:2015:VAL:HG12	2.14	0.47
1:A:212:VAL:HG13	1:A:215:PHE:H	1.79	0.47
3:C:1784:ASP:HB2	3:C:2102:LEU:HD22	1.96	0.47
1:A:966:THR:O	1:A:970:ILE:HG22	2.15	0.47
1:A:742:LEU:HD23	1:A:742:LEU:HA	1.76	0.46
3:C:2006:GLY:C	3:C:2008:ARG:H	2.22	0.46
3:C:889:ALA:HB1	3:C:897:TRP:CH2	2.50	0.46
1:A:469:LEU:HD21	1:A:516:ARG:HE	1.80	0.46
1:A:245:GLN:HA	1:A:271:ARG:HH12	1.79	0.46
1:A:526:LEU:HD11	1:A:590:GLN:HB2	1.97	0.46
3:C:933:GLN:HE21	3:C:1678:SER:HB2	1.80	0.46
3:C:1288:PHE:HZ	3:C:1603:PHE:HE1	1.63	0.46
3:C:1011:CYS:SG	3:C:1034:LYS:HB2	2.56	0.46
3:C:1803:LYS:O	3:C:1807:LEU:HG	2.15	0.46
3:C:1851:PRO:HA	3:C:1854:ILE:HD12	1.97	0.46
3:C:2027:PHE:CE1	3:C:2058:LEU:HD23	2.51	0.46
1:A:666:ASN:O	1:A:670:GLU:HG3	2.16	0.46
1:A:755:LYS:HD2	1:A:755:LYS:HA	1.76	0.46
1:A:887:LYS:HB2	1:A:925:GLN:HE21	1.80	0.46
3:C:1291:SER:HB2	3:C:1608:LEU:O	2.14	0.46
3:C:1669:PRO:HB3	3:C:1933:TYR:CD2	2.50	0.46
1:A:273:GLU:HA	1:A:276:GLU:OE1	2.16	0.46
1:A:525:MET:O	1:A:529:ILE:HG12	2.16	0.46
3:C:829:PRO:HD2	3:C:1214:LEU:HB2	1.98	0.46
3:C:1604:LEU:HD12	3:C:1607:CYS:SG	2.56	0.46
3:C:1814:GLY:H	3:C:1815:PRO:HD2	1.81	0.46
1:A:325:ASN:O	1:A:328:TYR:N	2.44	0.46
3:C:1622:GLU:CD	3:C:1922:ARG:HH22	2.24	0.46
1:A:211:GLN:HG2	2:B:330:LYS:HD3	1.97	0.46
1:A:742:LEU:HD21	1:A:797:ILE:HD13	1.97	0.46
3:C:970:PHE:HZ	3:C:977:LEU:HA	1.81	0.46
3:C:1235:LEU:HD11	3:C:1271:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ARG:HE	1:A:501:LEU:HD12	1.81	0.45
2:B:354:ALA:HB1	2:B:355:PRO:HD2	1.98	0.45
1:A:1035:GLU:HB2	1:A:1038:TRP:HD1	1.80	0.45
3:C:685:TYR:HE2	3:C:782:LEU:HD22	1.82	0.45
3:C:1294:TRP:CG	3:C:1802:TRP:HZ2	2.34	0.45
1:A:293:PHE:HE1	1:A:308:CYS:HB3	1.80	0.45
1:A:305:ARG:O	1:A:309:ILE:HG12	2.17	0.45
1:A:395:THR:O	1:A:399:GLN:HG3	2.16	0.45
1:A:970:ILE:HG23	1:A:1010:LEU:HD23	1.97	0.45
3:C:1148:CYS:O	3:C:1152:ALA:N	2.41	0.45
1:A:748:ILE:HD12	1:A:748:ILE:HA	1.83	0.45
1:A:986:ASN:OD1	1:A:986:ASN:N	2.49	0.45
3:C:682:LEU:HD22	3:C:754:TRP:HH2	1.82	0.45
3:C:764:PRO:HD2	3:C:805:ARG:HD2	1.99	0.45
3:C:797:LEU:HD11	3:C:1206:LEU:HD23	1.99	0.45
3:C:1168:ALA:HB2	3:C:1183:LEU:HB2	1.99	0.45
3:C:855:LEU:HD12	3:C:897:TRP:CE2	2.51	0.45
3:C:943:HIS:NE2	3:C:991:SER:OG	2.50	0.45
3:C:1702:ILE:HG12	3:C:1921:PHE:CZ	2.51	0.45
2:B:354:ALA:O	2:B:355:PRO:C	2.60	0.45
3:C:1601:CYS:HB3	3:C:1619:LEU:O	2.17	0.45
3:C:1808:PRO:HB3	3:C:1889:SER:OG	2.17	0.45
1:A:731:ILE:HG23	1:A:786:GLN:HG2	1.99	0.45
3:C:1618:PHE:CD1	3:C:1695:PHE:HB2	2.52	0.45
3:C:1050:ASP:O	3:C:1054:VAL:HG23	2.17	0.45
3:C:1826:LEU:HD22	3:C:1862:CYS:SG	2.57	0.45
3:C:830:SER:O	3:C:834:LEU:HG	2.17	0.45
3:C:1142:HIS:CE1	3:C:1148:CYS:SG	3.10	0.45
3:C:1167:THR:O	3:C:1170:VAL:HG12	2.17	0.45
3:C:1923:PHE:O	3:C:1927:TYR:HD1	2.00	0.45
1:A:705:LYS:HD3	1:A:705:LYS:N	2.32	0.44
2:B:448:PRO:HD3	3:C:947:ARG:NH1	2.32	0.44
3:C:777:GLN:HG2	3:C:799:LEU:HD21	1.99	0.44
3:C:1927:TYR:O	3:C:1931:LYS:HB2	2.17	0.44
3:C:658:GLN:HA	3:C:661:ASP:OD2	2.17	0.44
3:C:2072:TYR:CE2	3:C:2097:ARG:HA	2.52	0.44
1:A:185:GLN:O	1:A:186:CYS:C	2.60	0.44
3:C:919:LEU:HG	3:C:920:SER:H	1.82	0.44
3:C:2100:PRO:HG2	3:C:2107:GLY:HA2	1.99	0.44
3:C:885:LEU:HD13	3:C:930:GLN:HE22	1.83	0.44
3:C:898:TYR:HB3	3:C:949:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1929:ILE:O	3:C:1932:GLU:HG2	2.17	0.44
1:A:321:ASP:O	1:A:322:ALA:C	2.60	0.44
3:C:874:VAL:O	3:C:878:VAL:HG23	2.17	0.44
3:C:1150:LEU:HD12	3:C:1156:LEU:HD13	1.99	0.44
3:C:1729:ARG:HH22	3:C:1809:SER:H	1.63	0.44
3:C:1812:GLU:HG2	3:C:1813:PRO:HD2	1.99	0.44
1:A:213:ARG:HH22	1:A:216:ARG:NH2	2.16	0.44
1:A:406:THR:OG1	1:A:408:GLU:OE1	2.31	0.44
3:C:692:LYS:HA	3:C:695:GLU:OE1	2.17	0.44
1:A:289:PHE:O	1:A:294:VAL:HG23	2.18	0.44
1:A:469:LEU:HD11	1:A:516:ARG:HG2	2.00	0.44
1:A:888:GLN:HB3	1:A:892:TYR:CD1	2.53	0.44
2:B:333:ASP:HB2	2:B:336:THR:HG23	2.00	0.44
3:C:754:TRP:CH2	3:C:775:SER:HB3	2.53	0.44
3:C:892:LYS:HD2	3:C:897:TRP:NE1	2.33	0.44
3:C:1746:ASN:C	3:C:1746:ASN:OD1	2.61	0.44
1:A:285:MET:C	1:A:287:ALA:N	2.75	0.44
1:A:942:SER:O	1:A:943:SER:OG	2.31	0.44
3:C:634:GLN:HG2	3:C:683:TRP:CE2	2.52	0.44
3:C:800:ARG:NH1	3:C:816:SER:OG	2.51	0.44
1:A:404:VAL:HG23	1:A:405:LEU:HD12	2.00	0.43
3:C:751:LEU:HD12	3:C:783:TYR:CE2	2.53	0.43
3:C:1791:ILE:HD12	3:C:2104:TYR:CD1	2.53	0.43
3:C:1952:LEU:O	3:C:1979:VAL:HA	2.17	0.43
1:A:312:ILE:HG13	1:A:315:TRP:CE3	2.53	0.43
1:A:473:LEU:HD12	1:A:473:LEU:HA	1.77	0.43
3:C:1602:ARG:O	3:C:1606:LEU:HG	2.19	0.43
3:C:1891:LEU:HD22	3:C:1915:VAL:HG22	1.99	0.43
1:A:1009:LYS:HD2	1:A:1009:LYS:N	2.33	0.43
3:C:954:MET:HG3	3:C:954:MET:O	2.18	0.43
3:C:1906:SER:O	3:C:1907:MET:C	2.60	0.43
1:A:396:LEU:HD12	1:A:396:LEU:HA	1.82	0.43
3:C:769:LEU:HG	3:C:802:VAL:HG13	1.99	0.43
3:C:1692:LYS:O	3:C:1695:PHE:HB3	2.18	0.43
3:C:1807:LEU:HD21	3:C:1909:SER:HB2	1.99	0.43
3:C:1887:SER:OG	3:C:1888:ASN:N	2.50	0.43
3:C:2088:PRO:O	3:C:2092:TYR:HD2	2.01	0.43
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.86	0.43
3:C:1757:PHE:CE2	3:C:1901:LYS:HB2	2.53	0.43
3:C:1972:GLU:HG2	3:C:1975:TRP:CE2	2.52	0.43
1:A:754:THR:OG1	1:A:755:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:MET:HE3	1:A:1038:TRP:CZ3	2.54	0.43
1:A:241:MET:O	1:A:245:GLN:N	2.49	0.43
3:C:858:LEU:HD22	3:C:884:VAL:HG13	2.00	0.43
3:C:1857:LEU:O	3:C:1861:LEU:HB2	2.19	0.43
1:A:887:LYS:HG3	1:A:926:LEU:HD21	2.01	0.43
1:A:776:LEU:O	1:A:776:LEU:HD23	2.19	0.43
1:A:1045:ARG:O	1:A:1049:LEU:HD13	2.19	0.43
2:B:350:THR:OG1	2:B:351:LEU:N	2.51	0.43
3:C:601:GLN:NE2	3:C:605:ASN:OD1	2.50	0.43
3:C:1588:ILE:HD11	3:C:1600:LEU:HD12	2.00	0.43
1:A:307:ILE:O	1:A:311:GLU:HG2	2.19	0.43
1:A:352:GLN:HE21	1:A:392:LYS:C	2.27	0.43
3:C:790:MET:HE3	3:C:1198:LEU:HD11	2.01	0.43
3:C:951:LEU:HA	3:C:955:GLY:O	2.19	0.43
3:C:1260:HIS:HB2	3:C:1261:LEU:HD12	2.00	0.43
3:C:1871:GLU:O	3:C:1875:GLU:HG2	2.19	0.43
1:A:688:LEU:O	1:A:692:LYS:HG3	2.18	0.42
3:C:760:LYS:HB2	3:C:762:GLN:OE1	2.19	0.42
3:C:2072:TYR:CZ	3:C:2110:PRO:HG2	2.53	0.42
1:A:312:ILE:HA	1:A:315:TRP:CE3	2.54	0.42
1:A:887:LYS:HG3	1:A:926:LEU:CD2	2.49	0.42
1:A:927:PHE:CD2	1:A:931:ILE:HD11	2.54	0.42
3:C:1727:LEU:O	3:C:1738:SER:HA	2.19	0.42
1:A:514:THR:OG1	1:A:517:GLN:HG3	2.18	0.42
1:A:648:ASN:OD1	1:A:649:ARG:N	2.51	0.42
3:C:607:ILE:HD12	3:C:607:ILE:HA	1.84	0.42
3:C:900:LEU:O	3:C:904:VAL:HG23	2.19	0.42
3:C:1218:LEU:HG	3:C:1219:LEU:HG	2.01	0.42
3:C:1952:LEU:HD21	3:C:1962:GLU:HA	2.00	0.42
1:A:296:ARG:HD3	1:A:296:ARG:HA	1.79	0.42
1:A:520:ALA:O	1:A:524:ILE:HG13	2.20	0.42
1:A:652:ILE:HG23	1:A:656:GLN:HE22	1.84	0.42
3:C:1182:ASP:O	3:C:1186:VAL:HG23	2.19	0.42
1:A:968:GLU:O	1:A:972:MET:HG2	2.20	0.42
3:C:2016:LEU:HA	3:C:2016:LEU:HD12	1.76	0.42
1:A:299:ASP:OD1	1:A:300:ALA:N	2.53	0.42
1:A:810:LEU:HB3	1:A:813:LEU:HD11	2.00	0.42
3:C:1689:GLN:HB2	3:C:1690:PRO:HD3	2.01	0.42
1:A:340:GLN:OE1	1:A:340:GLN:HA	2.19	0.42
1:A:567:PHE:O	1:A:571:LEU:HB2	2.20	0.42
1:A:697:PHE:HD1	1:A:701:HIS:CD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1622:GLU:OE2	3:C:1922:ARG:NH2	2.52	0.42
1:A:354:LEU:HB3	1:A:364:LEU:HD21	2.02	0.42
1:A:652:ILE:CG2	1:A:656:GLN:HE22	2.33	0.42
1:A:673:LEU:C	1:A:675:GLU:H	2.28	0.42
1:A:1028:PHE:CE1	1:A:1032:LEU:HD23	2.54	0.42
2:B:375:LEU:HD23	2:B:375:LEU:HA	1.90	0.42
1:A:582:ALA:O	1:A:585:VAL:HG22	2.20	0.42
3:C:1223:LEU:HD12	3:C:1223:LEU:HA	1.85	0.42
3:C:1702:ILE:HG12	3:C:1921:PHE:HZ	1.85	0.42
3:C:1907:MET:C	3:C:1909:SER:H	2.27	0.42
1:A:224:MET:O	1:A:225:LYS:C	2.62	0.42
1:A:698:HIS:NE2	1:A:703:LEU:HB2	2.35	0.42
1:A:949:LYS:NZ	1:A:1001:ASP:O	2.51	0.42
1:A:869:CYS:SG	1:A:903:THR:HG21	2.60	0.41
1:A:1026:MET:O	1:A:1030:MET:HB2	2.20	0.41
3:C:1008:LYS:HE2	3:C:1008:LYS:HB3	1.80	0.41
3:C:2006:GLY:C	3:C:2008:ARG:N	2.78	0.41
1:A:213:ARG:HH12	1:A:216:ARG:NH2	2.18	0.41
1:A:379:THR:HG22	1:A:391:ILE:HG12	2.02	0.41
1:A:1014:ASP:O	1:A:1018:VAL:HG23	2.20	0.41
3:C:755:LYS:HG3	3:C:798:LEU:HD11	2.03	0.41
3:C:1168:ALA:HB1	3:C:1184:LEU:HG	2.02	0.41
1:A:230:LEU:HA	1:A:233:VAL:HG23	2.01	0.41
1:A:774:HIS:CD2	1:A:774:HIS:C	2.99	0.41
1:A:914:GLN:O	1:A:918:THR:HG23	2.21	0.41
3:C:1903:PRO:HG3	3:C:2062:TRP:CH2	2.55	0.41
3:C:701:ARG:HD2	3:C:701:ARG:HA	1.89	0.41
3:C:1787:MET:HG2	3:C:2104:TYR:O	2.19	0.41
3:C:1847:GLY:HA2	3:C:1881:GLN:HG3	2.02	0.41
1:A:331:TYR:O	1:A:335:THR:HG22	2.21	0.41
1:A:411:GLU:HG3	1:A:415:HIS:NE2	2.36	0.41
1:A:436:LEU:O	1:A:436:LEU:HD23	2.20	0.41
1:A:992:HIS:HB3	1:A:993:PRO:HD2	2.03	0.41
3:C:1294:TRP:CD2	3:C:1802:TRP:HZ2	2.37	0.41
1:A:192:TYR:HA	1:A:280:GLU:OE2	2.19	0.41
3:C:751:LEU:HD13	3:C:791:GLN:HE21	1.84	0.41
2:B:456:MET:N	2:B:456:MET:SD	2.94	0.41
3:C:609:ASP:O	3:C:613:LEU:HB2	2.21	0.41
3:C:659:LEU:O	3:C:663:VAL:HG23	2.20	0.41
3:C:793:LEU:HD21	3:C:1206:LEU:HG	2.02	0.41
3:C:869:TRP:NE1	3:C:910:ALA:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:970:PHE:HE2	3:C:977:LEU:HD23	1.86	0.41
1:A:326:ASP:HA	1:A:329:LEU:HB3	2.03	0.41
1:A:364:LEU:HA	1:A:364:LEU:HD12	1.82	0.41
1:A:582:ALA:O	1:A:583:GLU:C	2.63	0.41
3:C:650:LEU:HA	3:C:653:ILE:HG22	2.03	0.41
3:C:970:PHE:CZ	3:C:977:LEU:HA	2.55	0.41
3:C:1242:SER:O	3:C:1245:LYS:HG2	2.21	0.41
3:C:1294:TRP:CD1	3:C:1802:TRP:HZ2	2.39	0.41
3:C:1609:GLY:O	3:C:1616:THR:OG1	2.26	0.41
3:C:1750:LEU:HD12	3:C:1750:LEU:HA	1.91	0.41
3:C:1854:ILE:HG23	3:C:1873:LEU:HD13	2.03	0.41
1:A:227:MET:HB2	1:A:288:ILE:HG21	2.02	0.41
1:A:880:ASN:HA	1:A:918:THR:HG22	2.02	0.41
3:C:1714:ALA:N	3:C:1724:THR:O	2.54	0.41
3:C:1055:LEU:HA	3:C:1055:LEU:HD12	1.81	0.40
1:A:334:TRP:C	1:A:336:MET:H	2.30	0.40
3:C:1055:LEU:HD12	3:C:1058:LEU:HD12	2.02	0.40
3:C:1883:LEU:HA	3:C:1883:LEU:HD23	1.87	0.40
3:C:1890:HIS:CD2	3:C:2116:PRO:HB3	2.55	0.40
3:C:2068:ASP:HB2	3:C:2106:ILE:HG21	2.03	0.40
1:A:948:ILE:HG21	1:A:1002:ILE:HD13	2.03	0.40
3:C:734:ALA:O	3:C:735:PHE:C	2.64	0.40
3:C:1858:ALA:HB2	3:C:1873:LEU:HD12	2.04	0.40
3:C:1917:ARG:O	3:C:2113:TYR:HA	2.21	0.40
1:A:982:PHE:CE2	1:A:994:PRO:HG3	2.56	0.40
3:C:831:TYR:OH	3:C:1210:THR:O	2.38	0.40
3:C:1972:GLU:HG2	3:C:1975:TRP:CZ2	2.57	0.40
3:C:2029:SER:O	3:C:2030:SER:C	2.64	0.40
3:C:2069:ILE:HA	3:C:2069:ILE:HD12	1.85	0.40
1:A:888:GLN:HG2	1:A:892:TYR:HE1	1.86	0.40
1:A:1037:VAL:HG23	1:A:1038:TRP:CD1	2.56	0.40
3:C:589:LEU:HD11	3:C:603:ARG:HA	2.04	0.40
3:C:946:LEU:HD13	3:C:987:VAL:HA	2.03	0.40
3:C:1160:CYS:O	3:C:1164:VAL:HG23	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	925/1271 (73%)	872 (94%)	53 (6%)	0	100	100
2	B	101/241 (42%)	94 (93%)	7 (7%)	0	100	100
3	C	1126/2172 (52%)	1053 (94%)	73 (6%)	0	100	100
All	All	2152/3684 (58%)	2019 (94%)	133 (6%)	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	725/1136 (64%)	717 (99%)	8 (1%)	70	81
2	B	100/224 (45%)	97 (97%)	3 (3%)	36	61
3	C	969/1814 (53%)	958 (99%)	11 (1%)	70	81
All	All	1794/3174 (56%)	1772 (99%)	22 (1%)	66	80

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	TYR
1	A	364	LEU
1	A	482	ASP
1	A	622	LYS
1	A	745	LEU

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Mol	Chain	Res	Type
1	A	794	ILE
1	A	813	LEU
1	A	957	LEU
2	B	347	ILE
2	B	419	GLU
2	B	425	VAL
3	C	589	LEU
3	C	592	TYR
3	C	729	LEU
3	C	941	ASP
3	C	1055	LEU
3	C	1597	TYR
3	C	1737	VAL
3	C	1739	VAL
3	C	1880	LEU
3	C	2010	LEU
3	C	2016	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	ASN
1	A	236	ASN
1	A	243	ASN
1	A	275	GLN
1	A	278	GLN
1	A	286	ASN
1	A	399	GLN
1	A	517	GLN
1	A	536	HIS
1	A	556	GLN
1	A	587	ASN
1	A	735	GLN
1	A	738	HIS
1	A	888	GLN
1	A	988	GLN
2	B	412	ASN
3	C	679	GLN
3	C	704	GLN
3	C	771	GLN
3	C	784	GLN
3	C	791	GLN

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Mol	Chain	Res	Type
3	C	835	HIS
3	C	871	HIS
3	C	903	GLN
3	C	918	ASN
3	C	930	GLN
3	C	1177	GLN
3	C	1179	GLN
3	C	1208	HIS
3	C	1237	GLN
3	C	1248	GLN
3	C	1635	HIS
3	C	1637	HIS
3	C	1740	GLN
3	C	1767	ASN
3	C	1785	HIS
3	C	1890	HIS
3	C	1953	ASN
3	C	2013	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

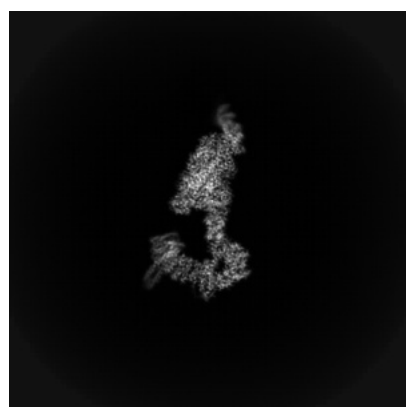
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52297. These allow visual inspection of the internal detail of the map and identification of artifacts.

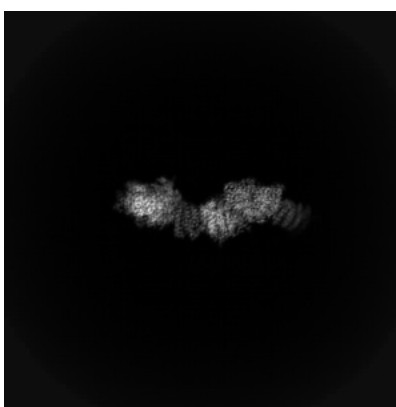
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

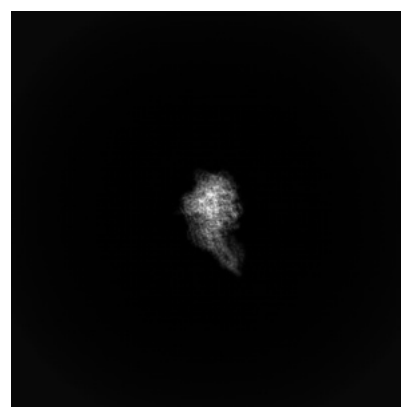
#### 6.1.1 Primary map



X



Y

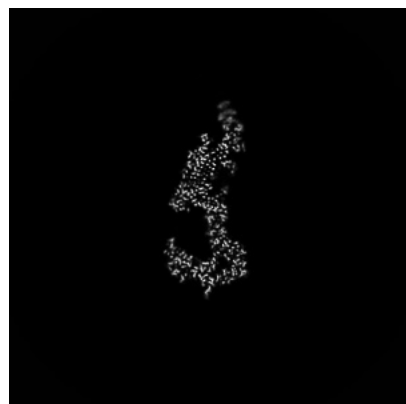


Z

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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 256



Y Index: 256

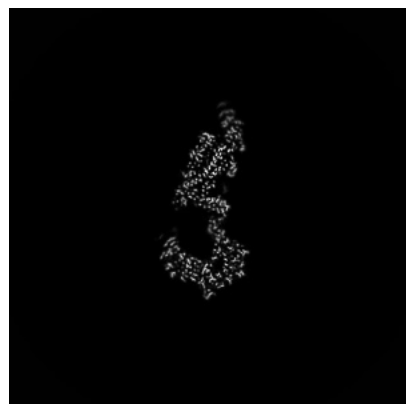


Z Index: 256

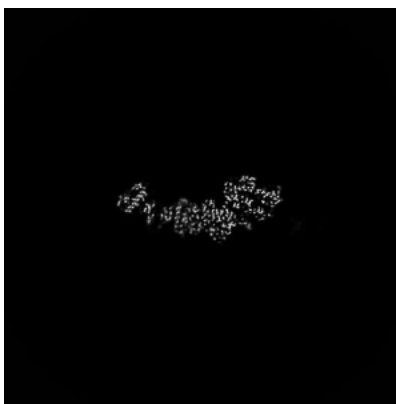
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 261



Y Index: 259



Z Index: 175

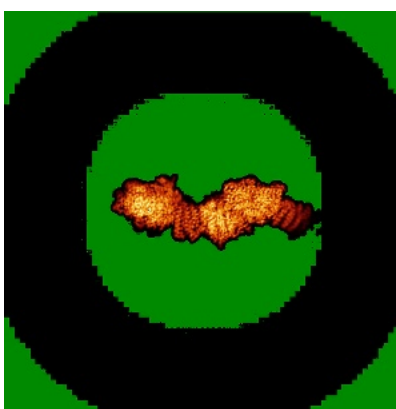
The images above show the largest variance slices of the map in three orthogonal directions.

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

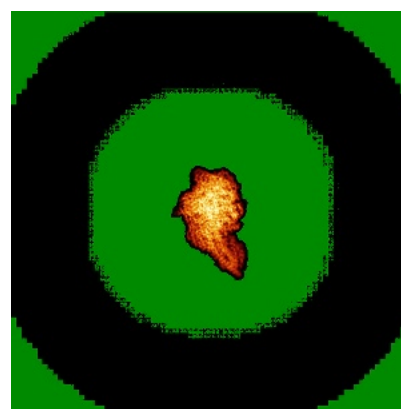
### 6.4.1 Primary map



X



Y

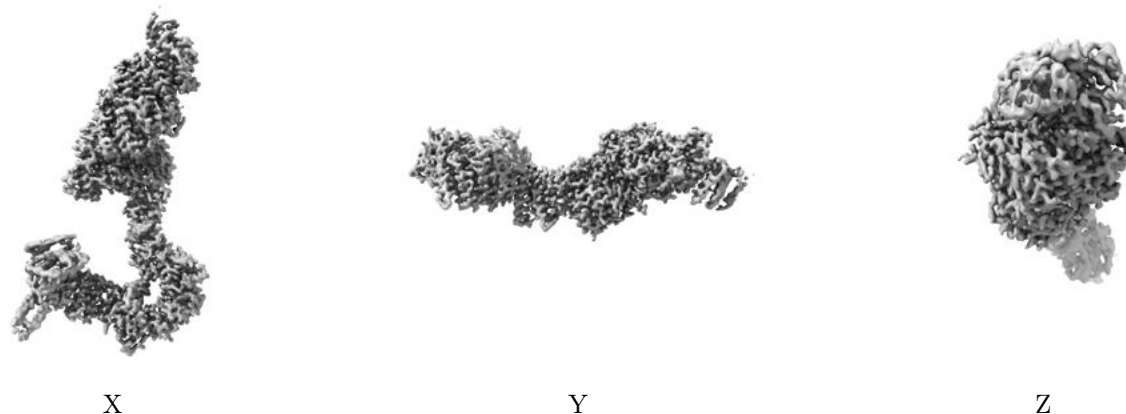


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

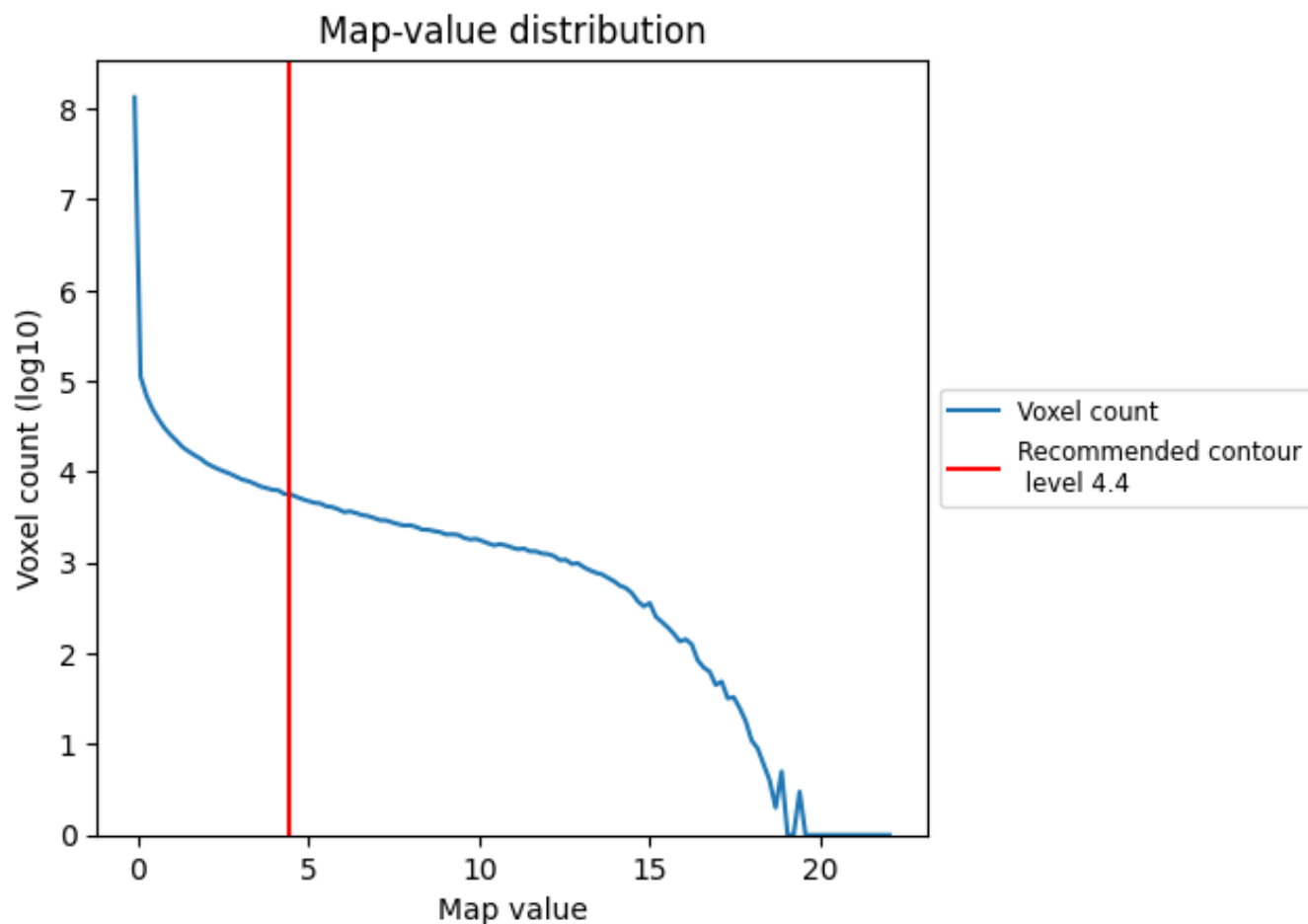
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

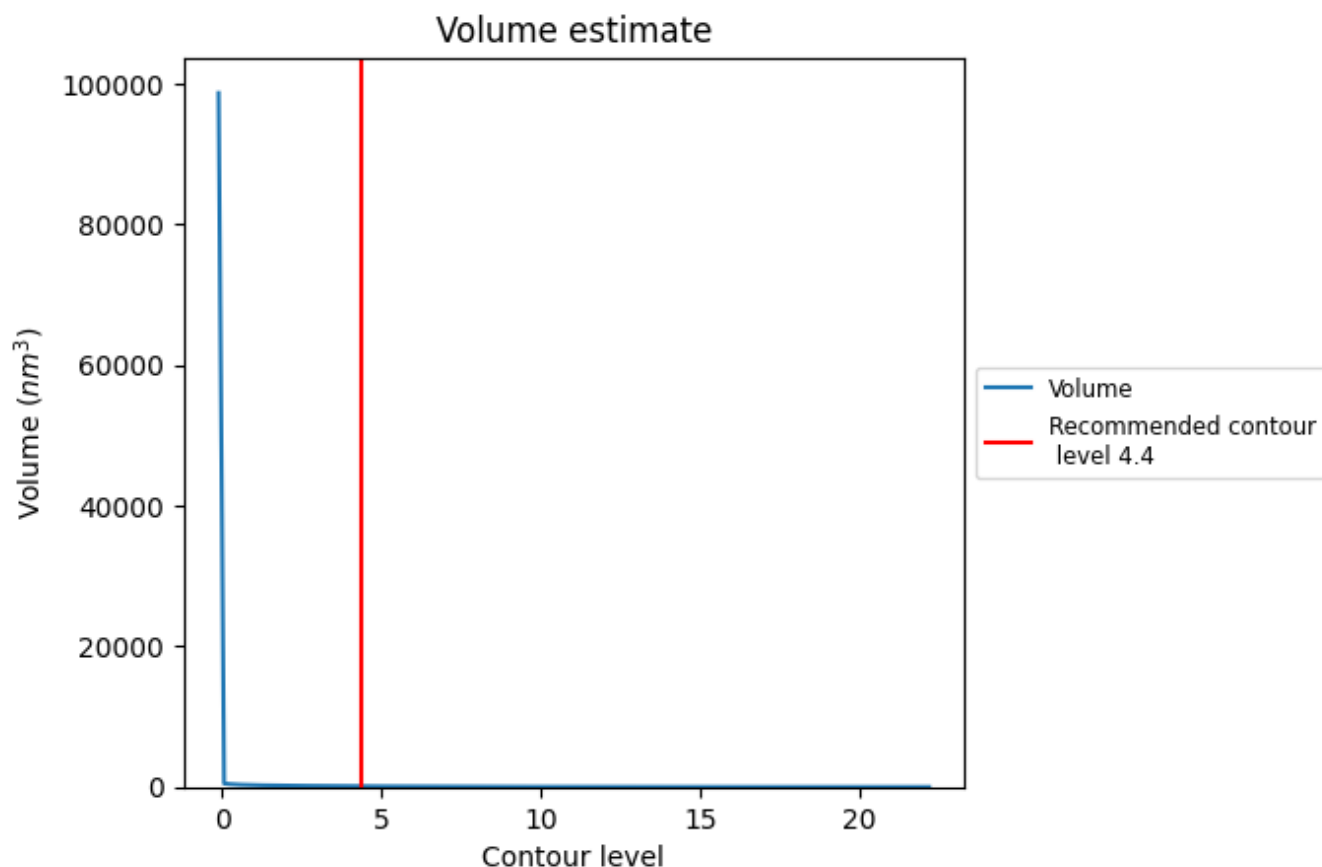
### 7.1 Map-value distribution [i](#)



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



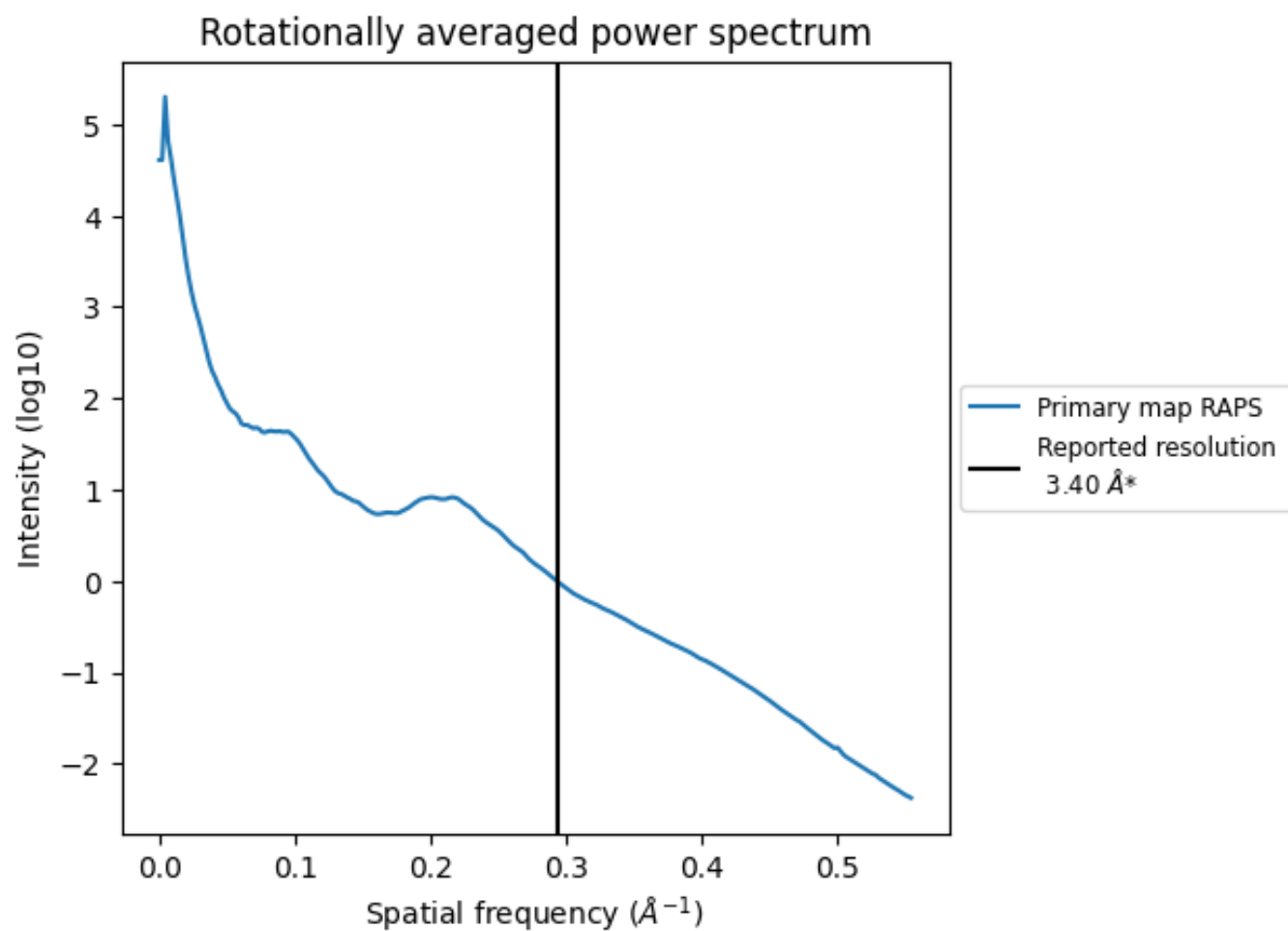
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100  $\text{nm}^3$ ; this corresponds to an approximate mass of 90 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

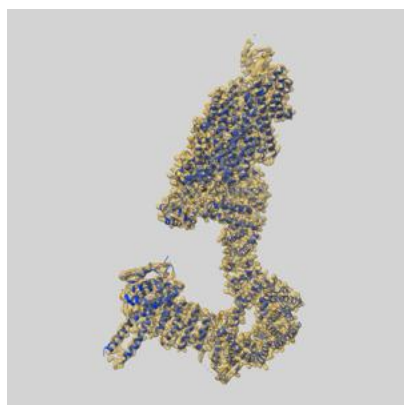
## 8 Fourier-Shell correlation

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

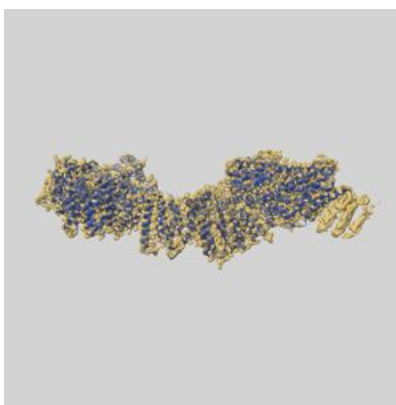
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52297 and PDB model 9HMS. Per-residue inclusion information can be found in section [3](#) on page [8](#).

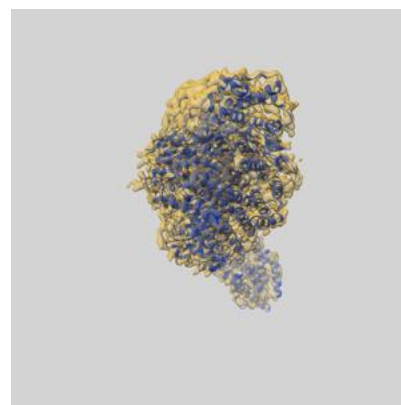
### 9.1 Map-model overlay [i](#)



X



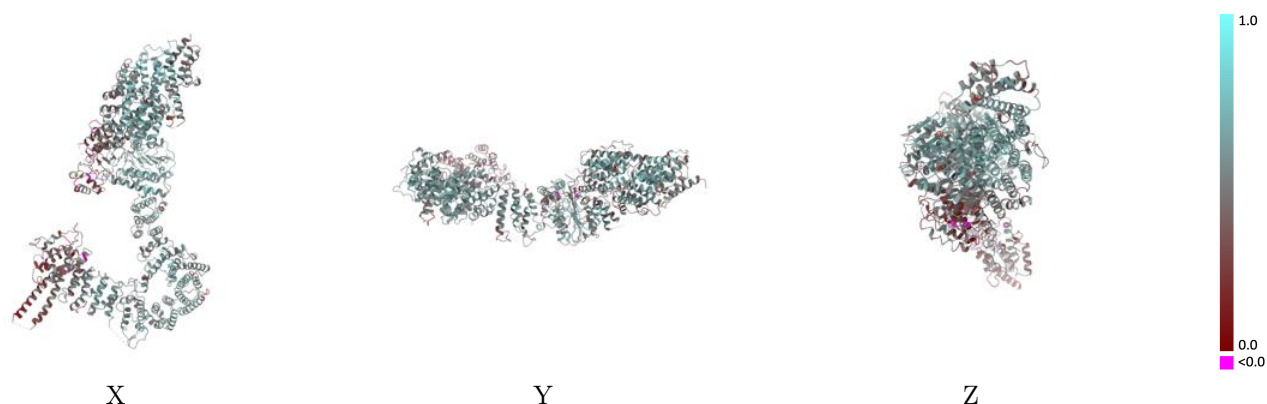
Y



Z

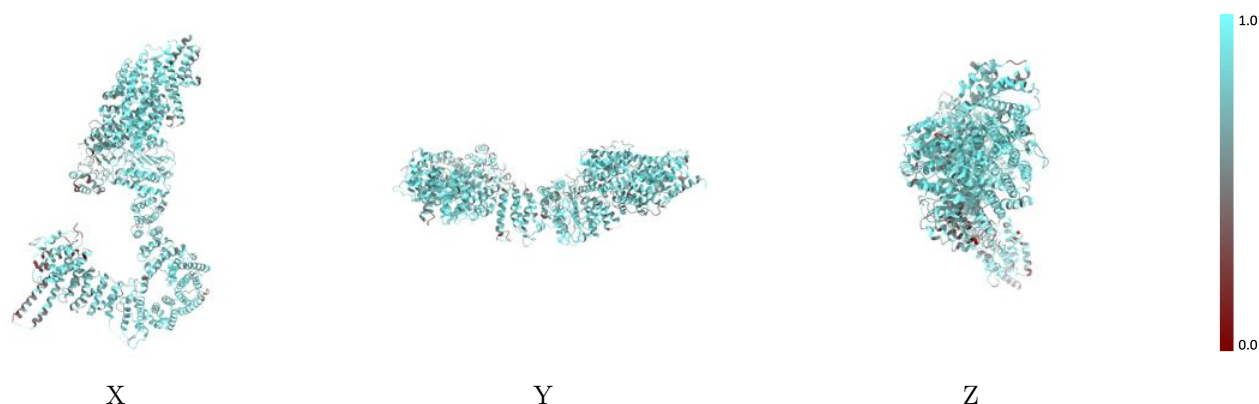
The images above show the 3D surface view of the map at the recommended contour level 4.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



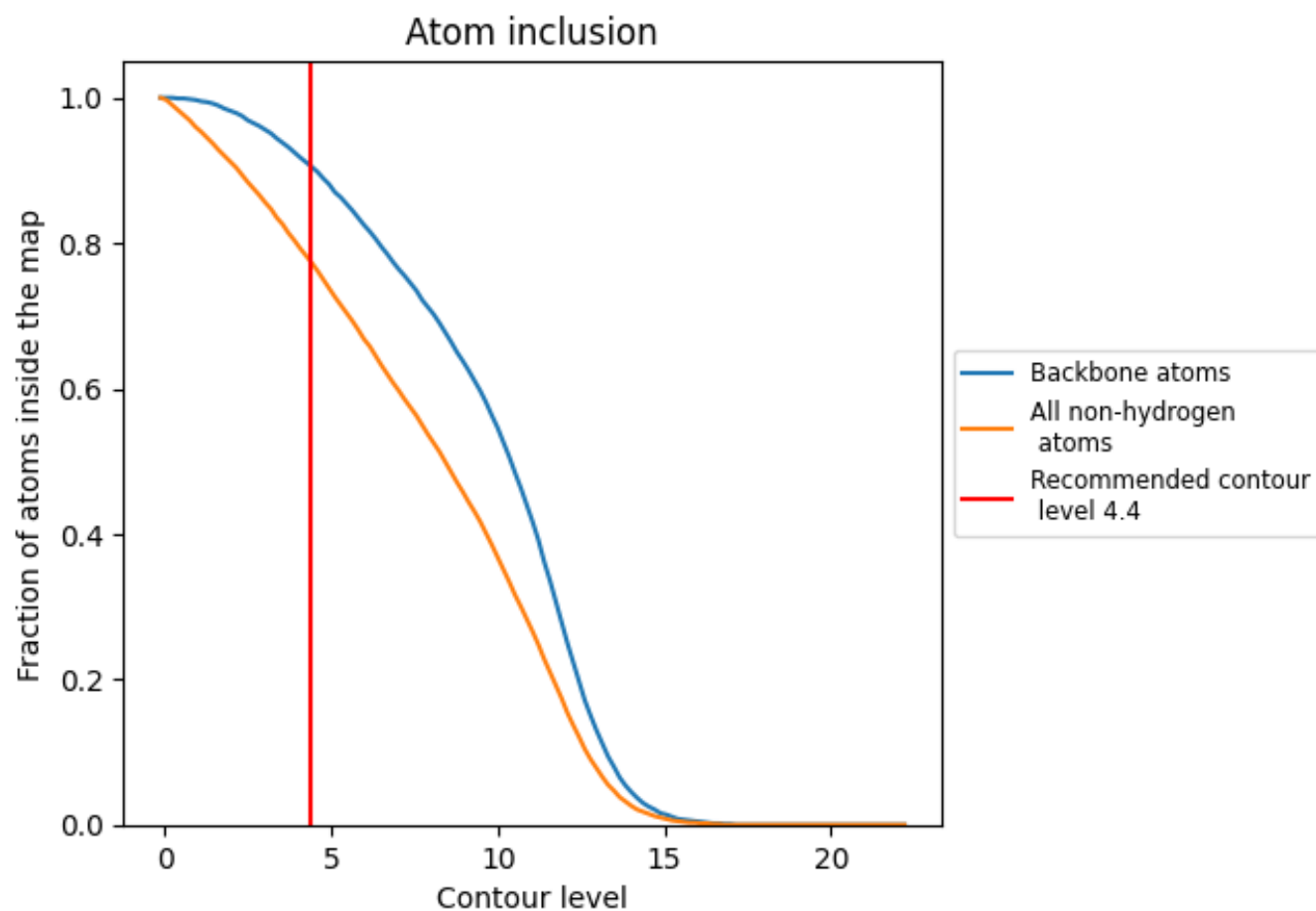
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.4).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 77% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7740	<div></div> 0.5010
A	<div></div> 0.7630	<div></div> 0.4940
B	<div></div> 0.6720	<div></div> 0.4640
C	<div></div> 0.7930	<div></div> 0.5090

