



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 02:14 AM UTC

PDB ID : 8WXJ / pdb_00008wxj
EMDB ID : EMD-37909
Title : human CLC-1 D136G closed state
Authors : Zhang, M.F.
Deposited on : 2023-10-29
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 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

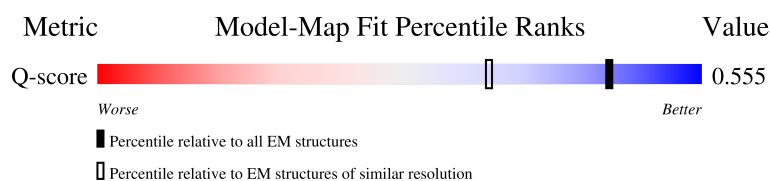
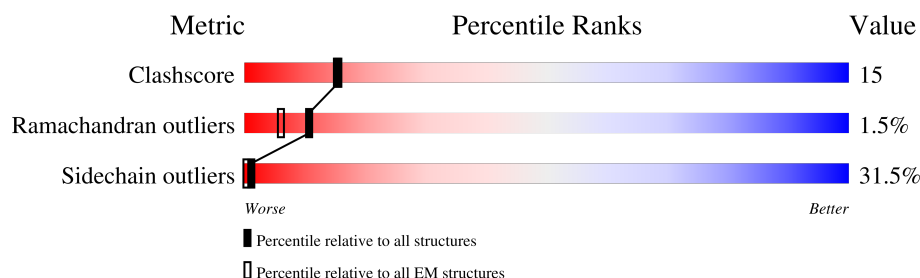
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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	9255 (2.18 - 3.18)

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	988	 5% 28% 15% • 53%
1	B	988	 5% 28% 15% • 53%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SCN	A	1001	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 7188 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.

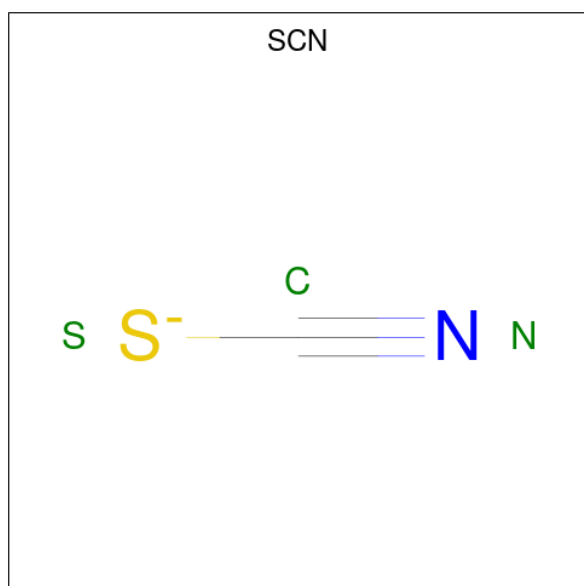
- Molecule 1 is a protein called Chloride channel protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	467	Total	C	N	O	S	0	0
			3585	2394	567	595	29		
1	B	467	Total	C	N	O	S	0	0
			3585	2394	567	595	29		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	GLY	ASP	engineered mutation	UNP P35523
B	136	GLY	ASP	engineered mutation	UNP P35523

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS) (labeled as "Ligand of Interest" by depositor).



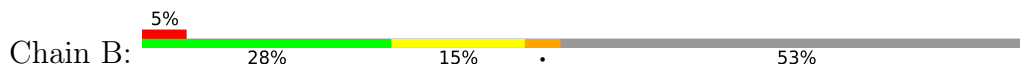
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	S	0
			3	1	1	1	

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Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total 3	C 1	N 1	S 1	0
2	A	1	Total 3	C 1	N 1	S 1	0
2	B	1	Total 3	C 1	N 1	S 1	0
2	B	1	Total 3	C 1	N 1	S 1	0
2	B	1	Total 3	C 1	N 1	S 1	0

- Molecule 1: Chloride channel protein 1



ILE	TYR	GLY	HIS	HIS	LYS	GLU	GLN	PHE	SER	ASP	ARG	GLU	GLN	ASP	ILE	GLY	MET	PRO	LYS	LYS	THR	GLY	SER	SER	SER	THR	THR	VAL	ASP	SER	SER	LYS	ASP	GLU	ASP	HIS	TYR	SER	SER	LYS	CYS	CYS	GLN	ASP	ASP	CYS	ILE	HIS	ARG	LEU	GLY	GLN	VAL	VAL	ARG	ARG	LYS	LYS	LEU	GLI5	GLI6	DI17	L121
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L123	L124	G125	L126	L127	M128	M135	S139	L140	K141	S142	L143	K147	Q152	L157	P158	L159	L162	F167	P168	L173	L177	L181	Q185	S189	G190	I191	M194	K195	T196	L197	L198	G199	R200	V201	V202	L203	R204	V206	V206	L207	K210	A211	F212	K215
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L219	K231	E232	G233	P234	F235	V236	H237	L241	C242	L246	S247	K248	F249	M250	V252	F253	CY5	GLY	VAL	TYR	GLU	GLN	PR0	TYR	V262	V263	S264	D265	L266	L267	T268	V273	G274	V275	T281	P282	L283	L287	F288	L290	E291	V292	T293	S294	T295	V296	F297	A298	V299	P300
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N301	N302	N303	N304	N305	N306	N307	N308	N309	N310	N311	N312	N313	N314	N315	N316	N317	N318	N319	N320	N321	N322	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	N500	N501	N502	N503	N504	N505	N506	N507	N508	N509	N510	N511	N512	N513	N514	N515	N516	N517	N518	N519	N520	N521	N522	N523	N524	N525	N526	N527	N528	N529	N530	N531	N532	N533	N534	N535	N536	N537	N538	N539	N540	N541	N542	N543	N544	N545	N546	N547	N548	N549	N550	N551	N552	N553	N554	N555	N556	N557	N558	N559	N560	N561	N562	N563	N564	N565	N566	N567	N568	N569	N570	N571	N572	N573	N574	N575	N576	N577	N578	N579	N580	N581	N582	N583	N584	N585	N586	N587	N588	N589	N590	N591	N592	N593	N594	N595	N596	N597	N598	N599	N600	N601	N602	N603	N604	N605	N606	N607	N608	N609	N610	N611	N612	N613	N614	N615	N616	N617	N618	N619	N620	N621	N622	N623	N624	N625	N626	N627	N628	N629	N630	N631	N632	N633	N634	N635	N636	N637	N638	N639	N640	N641	N642	N643	N644	N645	N646	N647	N648	N649	N650	N651	N652	N653	N654	N655	N656	N657	N658	N659	N660	N661	N662	N663	N664	N665	N666	N667	N668	N669	N670	N671	N672	N673	N674	N675	N676	N677	N678	N679	N680	N681	N682	N683	N684	N685	N686	N687	N688	N689	N690	N691	N692	N693	N694	N695	N696	N697	N698	N699	N700	N701	N702	N703	N704	N705	N706	N707	N708	N709	N710	N711	N712	N713	N714	N715	N716	N717	N718	N719	N720	N721	N722	N723	N724	N725	N726	N727	N728	N729	N730	N731	N732	N733	N734	N735	N736	N737	N738	N739	N740	N741	N742	N743	N744	N745	N746	N747	N748	N749	N750	N751	N752	N753	N754	N755	N756	N757	N758	N759	N760	N761	N762	N763	N764	N765	N766	N767	N768	N769	N770	N771	N772	N773	N774	N775	N776	N777	N778	N779	N780	N781	N782	N783	N784	N785	N786	N787	N788	N789	N790	N791	N792	N793	N794	N795	N796	N797	N798	N799	N800	N801	N802	N803	N804	N805	N806	N807	N808	N809	N810	N811	N812	N813	N814	N815	N816	N817	N818	N819	N820	N821	N822	N823	N824	N825	N826	N827	N828	N829	N830	N831	N832	N833	N834	N835	N836	N837	N838	N839	N840	N841	N842	N843	N844	N845	N846	N847	N848	N849	N850	N851	N852	N853	N854	N855	N856	N857	N858	N859	N860	N861	N862	N863	N864	N865	N866	N867	N868	N869	N870	N871	N872	N873	N874	N875	N876	N877	N878	N879	N880	N881	N882	N883	N884	N885	N886	N887	N888	N889	N890	N891	N892	N893	N894	N895	N896	N897	N898	N899	N900	N901	N902	N903	N904	N905	N906	N907	N908	N909	N910	N911	N912	N913	N914	N915	N916	N917	N918	N919	N920	N921	N922	N923	N924	N925	N926	N927	N928	N929	N930	N931	N932	N933	N934	N935	N936	N937	N938	N939	N940	N941	N942	N943	N944	N945	N946	N947	N948	N949	N950	N951	N952	N953	N954	N955	N956	N957	N958	N959	N960	N961	N962	N963	N964	N965	N966	N967	N968	N969	N970	N971	N972	N973	N974	N975	N976	N977	N978	N979	N980	N981	N982	N983	N984	N985	N986	N987	N988	N989	N990	N991	N992	N993	N994	N995	N996	N997	N998	N999	N1000
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A387 K388 K389 R390 R391 L392 L393 I401 P407 M410 L418 M419 P420 R421 I424 A425 T426 D429 N430 W433 V434 K435 H436 A437 G438 D439 P440 E441 S442 L443 G444 Q445 S446 A447 V448 W449 I450 R453 V456 I459 L462 M466 K467 M470 S471 I472

P480	F484	F488	V489	L497	M502	A503	M504	G508	G509	L510	L511	F512	D513	D514	L515	L516	L519	L520	L527	L532	V536	T539	V540	S541	T542	A543	V544	L545	C546	F547	F548	L549	T550	G551	Q552	L553	A554	H555	L556	L557	F558	H559	M560	L564	O571
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Year	Value	Category
1576	1576	LEU
1577	1577	PRO
1578	1578	ASP
1579	1579	LEU
1580	1580	GLY
1581	1581	TRP
1582	1582	ASN
1583	1583	GLN
1584	1584	LEU
1585	1585	SER
1586	1586	LYS
1587	1587	TYR
1588	1588	THR
1589	1589	ILE
1590	1590	PHE
1591	1591	VAL
1592	1592	GLU
1593	1593	ASP
1594	1594	ASP
1595	1595	ILE
1596	1596	MET
1597	1597	VAL
1598	1598	ARG
1599	1599	VAL
1600	1600	ASP
1601	1601	VAL
1602	1602	LYS
1603	1603	PHE
1604	1604	VAL
1605	1605	SER
1606	1606	ALA
1607	1607	SER
1608	1608	TYR
1609	1609	THR
1610	1610	TYR
1611	1611	GLY
1612	1612	GLU
1613	1613	LEU
1614	1614	ARG
1615	1615	THR
1616	1616	LEU
1617	1617	LEU
1618	1618	GLN
1619	1619	THR
1620	1620	THR
1621	1621	THR
1622	1622	VAL
1623	1623	LYS

[illegible]

ALA	PRO	GLU	PRO	ALA	GLY	GLN	ARG	PRO	SER	ILE	PHE	GLN	SER	LEU	LEU	HIS	CYS	LEU	LEU	GLY	ARG	ALA	ALA	ARG	PRO	THR	LYS	LYS	LYS	THR	THR	GLN	ASP	ASP	SER	THR	ASP	LEU	LEU	VAL	ASP	ASN	MET	SER	PRO	GLU	GLU	ILE	GLU	ALA	TRP	GLN	GLN	GLU	GLN	LEU	SER	GLN	PRO	VAL	VAL	CYS	PHE
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GLY	ASP
PRO	SER
PRO	CYS
LEU	ILE
SER	ARG
LEU	PRO
ALA	GLN
PRO	SER
GLY	PRO
LYS	PHE
VAL	GLN
GLU	LEU
GLY	VAL
LEU	GLU
GLU	GLN
GLU	THR
GLU	THR
GLU	ARG
GLU	LEU
LEU	HIS
LEU	LYS
VAL	THR
GLU	THR
SER	GLY
PRO	ALA
GLY	PRO
LEU	PHE
GLU	SER
GLU	SER
GLU	LEU
LEU	ALA
LEU	GLY
ALA	ASN
ASP	LEU
ILE	HIS
LEU	ASP
GLN	TRP
GLY	ASN
PRO	LEU
GLY	ALA
SER	PRO
LEU	TYR
ARG	VAL
LEU	GLU
THR	ASP
ASP	THR
GLU	SER
ARG	MET
SER	GLY
THR	LYS
THR	LEU
GLY	ARG
GLY	THR
ASP	GLY
GLU	VAL
ASP	LEU
GLU	ALA
ASP	ILE
ASP	LEU
GLU	ALA
LEU	GLU
ILE	SER
LEU	PRO
LEU	GLN
	LYS
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	GLU
	PRO
	GLY
	HIS
	THR
	LYS
	SER
	PRO

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36886	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.212	Depositor
Minimum map value	-0.127	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	252.0, 252.0, 252.0	wwPDB
Map dimensions	720, 720, 720	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.35, 0.35, 0.35	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: SCN

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	0.51	0/3685	0.76	2/5013 (0.0%)
1	B	0.51	0/3685	0.76	1/5013 (0.0%)
All	All	0.51	0/7370	0.76	3/10026 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	VAL	N-CA-C	-5.99	104.47	111.00
1	A	407	PRO	N-CA-C	5.38	117.26	110.70
1	B	407	PRO	N-CA-C	5.38	117.26	110.70

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	3585	0	3697	156	0
1	B	3585	0	3697	157	0
2	A	9	0	0	3	0
2	B	9	0	0	2	0
All	All	7188	0	7394	214	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 15.

All (214) 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:560:MET:HE2	1:B:306:PHE:CZ	1.54	1.41
1:A:306:PHE:CZ	1:B:560:MET:HE2	1.54	1.39
1:A:310:THR:CG2	1:B:560:MET:HG2	1.56	1.35
1:A:560:MET:HG2	1:B:310:THR:CG2	1.56	1.34
1:A:560:MET:CE	1:B:306:PHE:HZ	1.52	1.22
1:A:306:PHE:HZ	1:B:560:MET:CE	1.52	1.21
1:A:552:GLN:HG3	1:B:552:GLN:CG	1.74	1.17
1:A:552:GLN:CG	1:B:552:GLN:HG3	1.74	1.16
1:A:310:THR:HG21	1:B:560:MET:HG2	1.29	1.08
1:A:552:GLN:HG3	1:B:552:GLN:HG3	1.07	1.05
1:A:560:MET:CE	1:B:306:PHE:CZ	2.33	1.05
1:A:560:MET:HG2	1:B:310:THR:HG21	1.29	1.03
1:A:306:PHE:CZ	1:B:560:MET:HG3	1.97	1.00
1:A:560:MET:HG3	1:B:306:PHE:CZ	1.97	1.00
1:A:306:PHE:CZ	1:B:560:MET:CE	2.33	0.99
1:A:310:THR:HG22	1:B:560:MET:HG2	1.47	0.95
1:A:560:MET:HG2	1:B:310:THR:HG22	1.47	0.92
1:A:307:PHE:HD1	1:B:564:ILE:HG21	1.35	0.91
1:A:564:ILE:HG21	1:B:307:PHE:HD1	1.35	0.90
1:A:560:MET:CG	1:B:310:THR:CG2	2.49	0.89
1:A:306:PHE:CZ	1:B:560:MET:CG	2.56	0.89
1:A:560:MET:CG	1:B:306:PHE:CZ	2.56	0.89
1:A:310:THR:CG2	1:B:560:MET:CG	2.49	0.88
1:A:283:LEU:HD11	1:B:544:VAL:HG22	1.56	0.86
1:A:550:THR:O	1:B:553:ILE:CD1	2.24	0.85
1:A:553:ILE:CD1	1:B:550:THR:O	2.24	0.85
1:A:544:VAL:HG22	1:B:283:LEU:HD11	1.56	0.84
1:A:560:MET:CG	1:B:310:THR:HG21	2.06	0.84
1:A:310:THR:HG21	1:B:560:MET:CG	2.06	0.82
1:A:283:LEU:CD1	1:B:544:VAL:HG22	2.09	0.82
1:A:296:TYR:CE1	1:B:298:ALA:HB2	2.14	0.82
1:A:298:ALA:HB2	1:B:296:TYR:CE1	2.14	0.82
1:A:306:PHE:CE1	1:B:560:MET:HE2	2.15	0.81
1:A:544:VAL:HG22	1:B:283:LEU:CD1	2.09	0.80
1:A:564:ILE:HG21	1:B:307:PHE:CD1	2.17	0.80
1:A:560:MET:HE2	1:B:306:PHE:CE1	2.15	0.80
1:A:291:GLU:OE1	1:B:302:TYR:CE2	2.36	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:PHE:CD1	1:B:564:ILE:HG21	2.17	0.79
1:A:302:TYR:CE2	1:B:291:GLU:OE1	2.36	0.78
1:A:421:ARG:HD3	2:A:1003:SCN:N	2.02	0.75
1:A:544:VAL:CG2	1:B:283:LEU:HD11	2.17	0.74
1:A:283:LEU:HD11	1:B:544:VAL:CG2	2.17	0.74
1:B:421:ARG:HD3	2:B:1003:SCN:N	2.02	0.74
1:A:306:PHE:HZ	1:B:560:MET:HE2	0.94	0.73
1:A:553:ILE:HD11	1:B:550:THR:O	1.89	0.72
1:A:552:GLN:HE22	1:B:548:GLU:HA	1.54	0.72
1:A:556:ILE:HD12	1:B:548:GLU:HG2	1.71	0.72
1:A:548:GLU:HA	1:B:552:GLN:HE22	1.54	0.71
1:A:560:MET:HE2	1:B:306:PHE:HZ	0.94	0.71
1:A:306:PHE:CZ	1:B:560:MET:SD	2.84	0.70
1:A:560:MET:SD	1:B:306:PHE:CZ	2.84	0.70
1:B:338:ARG:HH11	1:B:430:ASN:HB2	1.55	0.70
1:A:338:ARG:HH11	1:A:430:ASN:HB2	1.55	0.70
1:A:548:GLU:HG2	1:B:556:ILE:HD12	1.71	0.70
1:A:550:THR:O	1:B:553:ILE:HD11	1.89	0.70
1:A:302:TYR:HE2	1:B:291:GLU:CD	2.01	0.69
1:A:291:GLU:CD	1:B:302:TYR:HE2	2.01	0.68
1:A:552:GLN:HG3	1:B:552:GLN:CD	2.19	0.66
1:A:302:TYR:HE2	1:B:291:GLU:OE1	1.78	0.66
1:A:552:GLN:CD	1:B:552:GLN:HG3	2.19	0.66
1:A:291:GLU:OE1	1:B:302:TYR:HE2	1.78	0.66
1:A:560:MET:CG	1:B:310:THR:HG22	2.23	0.65
1:A:552:GLN:NE2	1:B:548:GLU:HA	2.12	0.64
1:A:345:LEU:HD11	1:B:317:ARG:HB3	1.80	0.64
1:A:548:GLU:HA	1:B:552:GLN:NE2	2.12	0.64
1:A:287:LEU:HD11	1:B:287:LEU:HD11	1.81	0.63
1:A:310:THR:HG22	1:B:560:MET:CG	2.23	0.62
1:A:317:ARG:HB3	1:B:345:LEU:HD11	1.80	0.62
1:A:302:TYR:CE2	1:B:291:GLU:CD	2.78	0.61
1:A:550:THR:O	1:B:553:ILE:HD13	2.01	0.60
1:A:299:VAL:HG11	1:B:291:GLU:HA	1.84	0.59
1:A:560:MET:HG3	1:B:306:PHE:CE2	2.37	0.59
1:A:291:GLU:CD	1:B:302:TYR:CE2	2.78	0.59
1:A:291:GLU:HA	1:B:299:VAL:HG11	1.84	0.59
1:A:306:PHE:CE2	1:B:560:MET:HG3	2.37	0.57
1:A:553:ILE:HD13	1:B:550:THR:O	2.01	0.57
1:A:564:ILE:HD13	1:B:307:PHE:HA	1.86	0.57
1:A:307:PHE:HA	1:B:564:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD12	1:B:560:MET:HE2	1.86	0.56
1:A:560:MET:HE2	1:B:283:LEU:HD12	1.86	0.56
1:A:560:MET:CE	1:B:283:LEU:HD12	2.36	0.56
1:B:547:PHE:HB3	1:B:552:GLN:HG2	1.88	0.56
1:A:283:LEU:HD12	1:B:560:MET:CE	2.36	0.55
1:A:547:PHE:HB3	1:A:552:GLN:HG2	1.88	0.55
1:A:299:VAL:HG21	1:B:294:SER:O	2.07	0.55
1:B:268:THR:HG21	1:B:301:ASN:HB3	1.88	0.54
1:A:294:SER:O	1:B:299:VAL:HG21	2.07	0.54
1:B:281:THR:HG21	1:B:545:ILE:HA	1.89	0.54
1:A:281:THR:HG21	1:A:545:ILE:HA	1.89	0.54
1:B:167:PHE:HB3	1:B:168:PRO:HD3	1.90	0.54
1:A:167:PHE:HB3	1:A:168:PRO:HD3	1.90	0.53
1:A:298:ALA:HB2	1:B:296:TYR:HE1	1.69	0.53
1:A:344:ASP:HB3	1:A:347:GLU:HG2	1.92	0.52
1:A:544:VAL:HG22	1:B:283:LEU:HD13	1.91	0.52
1:B:344:ASP:HB3	1:B:347:GLU:HG2	1.92	0.52
1:B:290:ILE:HG12	1:B:297:PHE:CE1	2.46	0.51
1:A:296:TYR:HE1	1:B:298:ALA:HB2	1.69	0.51
1:A:542:THR:HA	1:A:545:ILE:HD12	1.92	0.51
1:B:542:THR:HA	1:B:545:ILE:HD12	1.92	0.50
1:A:290:ILE:HG12	1:A:297:PHE:CE1	2.46	0.50
1:A:548:GLU:CA	1:B:552:GLN:HE22	2.24	0.50
1:A:552:GLN:HE22	1:B:548:GLU:CA	2.24	0.50
1:A:306:PHE:HZ	1:B:560:MET:SD	2.26	0.49
1:B:124:LEU:HD23	1:B:246:LEU:HD23	1.95	0.48
1:B:436:HIS:HB2	1:B:443:LEU:HD21	1.96	0.48
1:A:436:HIS:HB2	1:A:443:LEU:HD21	1.96	0.48
1:B:527:ILE:HG23	1:B:559:MET:HA	1.96	0.48
1:A:124:LEU:HD23	1:A:246:LEU:HD23	1.95	0.48
1:B:433:TRP:HB3	1:B:456:VAL:HG11	1.96	0.48
1:B:345:LEU:HB2	1:B:512:PHE:CZ	2.49	0.48
1:A:586:LYS:HB2	1:A:586:LYS:HE2	1.57	0.47
1:B:384:GLN:HE21	1:B:384:GLN:HB3	1.50	0.47
1:A:443:LEU:HD13	1:A:450:ILE:HD13	1.97	0.47
1:A:552:GLN:CG	1:B:552:GLN:CG	2.59	0.47
1:A:560:MET:SD	1:B:306:PHE:CE1	3.08	0.47
1:B:215:LYS:HE3	1:B:480:PRO:HB3	1.97	0.47
1:A:306:PHE:CE1	1:B:560:MET:SD	3.08	0.47
1:A:345:LEU:HB2	1:A:512:PHE:CZ	2.49	0.47
1:A:380:LYS:HA	1:A:380:LYS:HD2	1.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LEU:HD13	1:B:450:ILE:HD13	1.97	0.47
1:A:527:ILE:HG23	1:A:559:MET:HA	1.96	0.46
1:A:306:PHE:CE1	1:B:560:MET:CE	2.89	0.46
1:A:433:TRP:HB3	1:A:456:VAL:HG11	1.96	0.46
1:A:204:LYS:HD3	1:A:204:LYS:HA	1.45	0.46
1:B:204:LYS:HB3	1:B:205:GLU:H	1.52	0.46
1:A:298:ALA:HB2	1:B:296:TYR:CD1	2.49	0.46
1:A:384:GLN:HE21	1:A:384:GLN:HB3	1.50	0.46
1:A:283:LEU:HD13	1:B:544:VAL:HG22	1.91	0.46
1:A:296:TYR:CD1	1:B:298:ALA:HB2	2.49	0.46
1:B:324:LYS:HA	1:B:324:LYS:HD3	1.53	0.45
1:B:198:LEU:HD12	1:B:198:LEU:HA	1.82	0.45
1:B:392:LEU:HD22	1:B:392:LEU:HA	1.77	0.45
1:A:540:VAL:HG22	1:B:303:TRP:CD1	2.52	0.45
1:A:547:PHE:CZ	1:A:556:ILE:HA	2.51	0.45
1:A:231:LYS:N	2:A:1001:SCN:S	2.77	0.45
1:A:418:LEU:HG	1:A:448:VAL:HG21	1.97	0.45
1:B:291:GLU:HB3	1:B:539:THR:HG22	1.98	0.45
1:A:117:ASP:O	1:A:121:LEU:HG	2.17	0.45
1:A:215:LYS:HE3	1:A:480:PRO:HB3	1.97	0.45
1:A:392:LEU:HD22	1:A:392:LEU:HA	1.77	0.45
1:B:141:LYS:HD3	1:B:141:LYS:HA	1.65	0.45
1:A:388:LYS:HB2	1:A:388:LYS:HE2	1.54	0.45
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.79	0.45
1:B:484:PHE:HB3	2:B:1001:SCN:S	2.57	0.45
1:A:141:LYS:HA	1:A:141:LYS:HD3	1.65	0.45
1:A:303:TRP:CD1	1:B:540:VAL:HG22	2.52	0.45
1:B:547:PHE:CZ	1:B:556:ILE:HA	2.51	0.45
1:A:300:ARG:NH1	1:B:296:TYR:OH	2.49	0.44
1:B:290:ILE:HG12	1:B:297:PHE:CZ	2.52	0.44
1:B:377:ARG:H	1:B:377:ARG:HG3	1.71	0.44
1:B:418:LEU:HG	1:B:448:VAL:HG21	1.97	0.44
1:B:586:LYS:HB2	1:B:586:LYS:HE2	1.57	0.44
1:A:296:TYR:OH	1:B:300:ARG:NH1	2.49	0.44
1:B:117:ASP:O	1:B:121:LEU:HG	2.17	0.44
1:B:177:LEU:HD12	1:B:177:LEU:HA	1.83	0.44
1:A:484:PHE:HB3	2:A:1001:SCN:S	2.57	0.44
1:B:292:VAL:HG23	1:B:293:THR:HG23	1.99	0.44
1:B:250:MET:HE3	1:B:250:MET:HB2	1.87	0.44
1:B:388:LYS:HE2	1:B:388:LYS:HB2	1.54	0.44
1:A:290:ILE:HG12	1:A:297:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:VAL:HG23	1:A:293:THR:HG23	1.99	0.44
1:B:288:PHE:O	1:B:292:VAL:HG22	2.18	0.44
1:B:401:ILE:HG12	1:B:470:MET:HG2	2.00	0.44
1:A:553:ILE:H	1:A:553:ILE:HG12	1.35	0.43
1:A:157:LEU:HD22	1:A:157:LEU:HA	1.77	0.43
1:A:298:ALA:CB	1:B:296:TYR:CE1	2.95	0.43
1:A:173:LEU:HD12	1:A:173:LEU:HA	1.79	0.43
1:A:291:GLU:HB3	1:A:539:THR:HG22	1.98	0.43
1:B:380:LYS:HD2	1:B:380:LYS:HA	1.48	0.43
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.82	0.43
1:A:426:THR:O	1:A:429:ASP:HB2	2.19	0.43
1:A:502:MET:HB3	1:A:519:ILE:HD12	2.01	0.43
1:A:190:GLY:HA3	1:A:237:HIS:HB2	2.01	0.42
1:A:288:PHE:O	1:A:292:VAL:HG22	2.18	0.42
1:A:401:ILE:HG12	1:A:470:MET:HG2	2.00	0.42
1:B:582:ILE:HA	1:B:587:LEU:HD12	2.00	0.42
1:B:190:GLY:HA3	1:B:237:HIS:HB2	2.01	0.42
1:B:212:PHE:HB2	1:B:241:ILE:HG21	2.01	0.42
1:B:502:MET:HB3	1:B:519:ILE:HD12	2.01	0.42
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.76	0.42
1:A:177:LEU:HD12	1:A:177:LEU:HA	1.83	0.42
1:A:377:ARG:H	1:A:377:ARG:HG3	1.71	0.42
1:A:582:ILE:HA	1:A:587:LEU:HD12	2.00	0.42
1:B:426:THR:O	1:B:429:ASP:HB2	2.19	0.42
1:B:382:LEU:HD12	1:B:382:LEU:HA	1.79	0.42
1:A:135:MET:HB2	1:A:135:MET:HE2	1.54	0.42
1:B:339:MET:HE2	1:B:339:MET:HB2	1.92	0.42
1:B:246:LEU:HD12	1:B:246:LEU:HA	1.77	0.42
1:A:212:PHE:HB2	1:A:241:ILE:HG21	2.01	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.89	0.41
1:A:372:VAL:HG12	1:A:476:THR:HG21	2.02	0.41
1:B:485:MET:O	1:B:489:VAL:HG13	2.20	0.41
1:A:485:MET:O	1:A:489:VAL:HG13	2.20	0.41
1:B:215:LYS:HE2	1:B:234:PRO:HA	2.03	0.41
1:B:370:ARG:HE	1:B:580:SER:HB2	1.85	0.41
1:A:357:CYS:HA	1:A:360:LEU:HD12	2.02	0.41
1:B:204:LYS:HA	1:B:204:LYS:HD3	1.45	0.41
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.93	0.41
1:A:370:ARG:HE	1:A:580:SER:HB2	1.85	0.41
1:A:419:MET:O	1:A:420:PRO:C	2.64	0.41
1:A:462:LEU:HD12	1:A:462:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HG12	1:B:476:THR:HG21	2.02	0.41
1:B:419:MET:O	1:B:420:PRO:C	2.64	0.41
1:A:324:LYS:HA	1:A:324:LYS:HD3	1.53	0.40
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.89	0.40
1:B:357:CYS:HA	1:B:360:LEU:HD12	2.02	0.40
1:B:549:LEU:HD23	1:B:549:LEU:HA	1.95	0.40
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.80	0.40
1:A:366:VAL:HG12	1:A:370:ARG:HH21	1.86	0.40
1:A:560:MET:CE	1:B:306:PHE:CE1	2.89	0.40
1:B:467:LYS:HA	1:B:470:MET:HB2	2.03	0.40
1:A:250:MET:HE3	1:A:250:MET:HB2	1.87	0.40
1:B:424:ILE:HD13	1:B:488:PHE:HD2	1.86	0.40
1:B:292:VAL:HG13	1:B:539:THR:HG21	2.03	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	463/988 (47%)	423 (91%)	33 (7%)	7 (2%)	8	19
1	B	463/988 (47%)	423 (91%)	33 (7%)	7 (2%)	8	19
All	All	926/1976 (47%)	846 (91%)	66 (7%)	14 (2%)	11	19

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	204	LYS
1	B	204	LYS
1	A	190	GLY
1	A	282	PRO
1	A	325	ASP

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Mol	Chain	Res	Type
1	A	343	PHE
1	B	190	GLY
1	B	282	PRO
1	B	325	ASP
1	B	343	PHE
1	A	329	ILE
1	B	329	ILE
1	A	440	PRO
1	B	440	PRO

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	381/837 (46%)	261 (68%)	120 (32%)	0	1
1	B	381/837 (46%)	261 (68%)	120 (32%)	0	1
All	All	762/1674 (46%)	522 (68%)	240 (32%)	1	1

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	GLU
1	A	123	LEU
1	A	124	LEU
1	A	126	LEU
1	A	127	LEU
1	A	128	MET
1	A	135	MET
1	A	139	SER
1	A	143	LEU
1	A	147	LYS
1	A	152	GLN
1	A	157	LEU
1	A	162	LEU
1	A	173	LEU

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Mol	Chain	Res	Type
1	A	181	LEU
1	A	185	GLN
1	A	189	SER
1	A	191	ILE
1	A	194	MET
1	A	195	LYS
1	A	197	ILE
1	A	198	LEU
1	A	199	ARG
1	A	201	VAL
1	A	203	LEU
1	A	204	LYS
1	A	207	LEU
1	A	210	LYS
1	A	219	LEU
1	A	231	LYS
1	A	232	GLU
1	A	236	VAL
1	A	242	CYS
1	A	246	LEU
1	A	247	SER
1	A	248	LYS
1	A	250	MET
1	A	252	VAL
1	A	262	TYR
1	A	264	SER
1	A	267	LEU
1	A	268	THR
1	A	273	VAL
1	A	275	VAL
1	A	283	LEU
1	A	287	LEU
1	A	289	SER
1	A	295	THR
1	A	299	VAL
1	A	300	ARG
1	A	312	SER
1	A	325	ASP
1	A	327	VAL
1	A	328	THR
1	A	329	ILE
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	334	ARG
1	A	336	ASN
1	A	338	ARG
1	A	339	MET
1	A	343	PHE
1	A	345	LEU
1	A	346	LYS
1	A	368	LEU
1	A	371	GLN
1	A	373	MET
1	A	377	ARG
1	A	378	LYS
1	A	380	LYS
1	A	383	SER
1	A	384	GLN
1	A	386	LEU
1	A	392	LEU
1	A	410	MET
1	A	419	MET
1	A	421	ARG
1	A	424	ILE
1	A	429	ASP
1	A	434	VAL
1	A	435	LYS
1	A	441	GLU
1	A	445	GLN
1	A	446	SER
1	A	453	ARG
1	A	456	VAL
1	A	459	ILE
1	A	462	LEU
1	A	466	MET
1	A	472	ILE
1	A	485	MET
1	A	489	VAL
1	A	497	LEU
1	A	504	MET
1	A	508	ASP
1	A	510	ILE
1	A	511	LEU
1	A	513	ASP
1	A	514	ASP

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Mol	Chain	Res	Type
1	A	515	ILE
1	A	516	ILE
1	A	519	ILE
1	A	520	LEU
1	A	527	ILE
1	A	532	LEU
1	A	536	VAL
1	A	540	VAL
1	A	541	SER
1	A	544	VAL
1	A	552	GLN
1	A	553	ILE
1	A	555	HIS
1	A	556	ILE
1	A	557	LEU
1	A	560	MET
1	A	571	GLN
1	A	576	SER
1	A	577	LEU
1	A	580	SER
1	A	585	LYS
1	A	586	LYS
1	B	116	GLU
1	B	123	LEU
1	B	124	LEU
1	B	126	LEU
1	B	127	LEU
1	B	128	MET
1	B	135	MET
1	B	139	SER
1	B	143	LEU
1	B	147	LYS
1	B	152	GLN
1	B	157	LEU
1	B	162	LEU
1	B	173	LEU
1	B	181	LEU
1	B	185	GLN
1	B	189	SER
1	B	191	ILE
1	B	194	MET
1	B	195	LYS

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Mol	Chain	Res	Type
1	B	197	ILE
1	B	198	LEU
1	B	199	ARG
1	B	201	VAL
1	B	203	LEU
1	B	204	LYS
1	B	207	LEU
1	B	210	LYS
1	B	219	LEU
1	B	231	LYS
1	B	232	GLU
1	B	236	VAL
1	B	242	CYS
1	B	246	LEU
1	B	247	SER
1	B	248	LYS
1	B	250	MET
1	B	252	VAL
1	B	262	TYR
1	B	264	SER
1	B	267	LEU
1	B	268	THR
1	B	273	VAL
1	B	275	VAL
1	B	283	LEU
1	B	287	LEU
1	B	289	SER
1	B	295	THR
1	B	299	VAL
1	B	300	ARG
1	B	312	SER
1	B	325	ASP
1	B	327	VAL
1	B	328	THR
1	B	329	ILE
1	B	332	LEU
1	B	334	ARG
1	B	336	ASN
1	B	338	ARG
1	B	339	MET
1	B	343	PHE
1	B	345	LEU

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Mol	Chain	Res	Type
1	B	346	LYS
1	B	368	LEU
1	B	371	GLN
1	B	373	MET
1	B	377	ARG
1	B	378	LYS
1	B	380	LYS
1	B	383	SER
1	B	384	GLN
1	B	386	LEU
1	B	392	LEU
1	B	410	MET
1	B	419	MET
1	B	421	ARG
1	B	424	ILE
1	B	429	ASP
1	B	434	VAL
1	B	435	LYS
1	B	441	GLU
1	B	445	GLN
1	B	446	SER
1	B	453	ARG
1	B	456	VAL
1	B	459	ILE
1	B	462	LEU
1	B	466	MET
1	B	472	ILE
1	B	485	MET
1	B	489	VAL
1	B	497	LEU
1	B	504	MET
1	B	508	ASP
1	B	510	ILE
1	B	511	LEU
1	B	513	ASP
1	B	514	ASP
1	B	515	ILE
1	B	516	ILE
1	B	519	ILE
1	B	520	LEU
1	B	527	ILE
1	B	532	LEU

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Mol	Chain	Res	Type
1	B	536	VAL
1	B	540	VAL
1	B	541	SER
1	B	544	VAL
1	B	552	GLN
1	B	553	ILE
1	B	555	HIS
1	B	556	ILE
1	B	557	LEU
1	B	560	MET
1	B	571	GLN
1	B	576	SER
1	B	577	LEU
1	B	580	SER
1	B	585	LYS
1	B	586	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	GLN
1	A	323	ASN
1	A	371	GLN
1	A	384	GLN
1	A	431	ASN
1	A	451	HIS
1	A	552	GLN
1	A	571	GLN
1	B	323	ASN
1	B	371	GLN
1	B	384	GLN
1	B	431	ASN
1	B	451	HIS
1	B	552	GLN
1	B	571	GLN

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

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	SCN	B	1003	-	1,2,2	0.23	0	0,1,1	-	-
2	SCN	B	1002	-	1,2,2	0.21	0	0,1,1	-	-
2	SCN	A	1002	-	1,2,2	0.21	0	0,1,1	-	-
2	SCN	A	1003	-	1,2,2	0.23	0	0,1,1	-	-
2	SCN	B	1001	-	1,2,2	0.15	0	0,1,1	-	-
2	SCN	A	1001	-	1,2,2	0.15	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

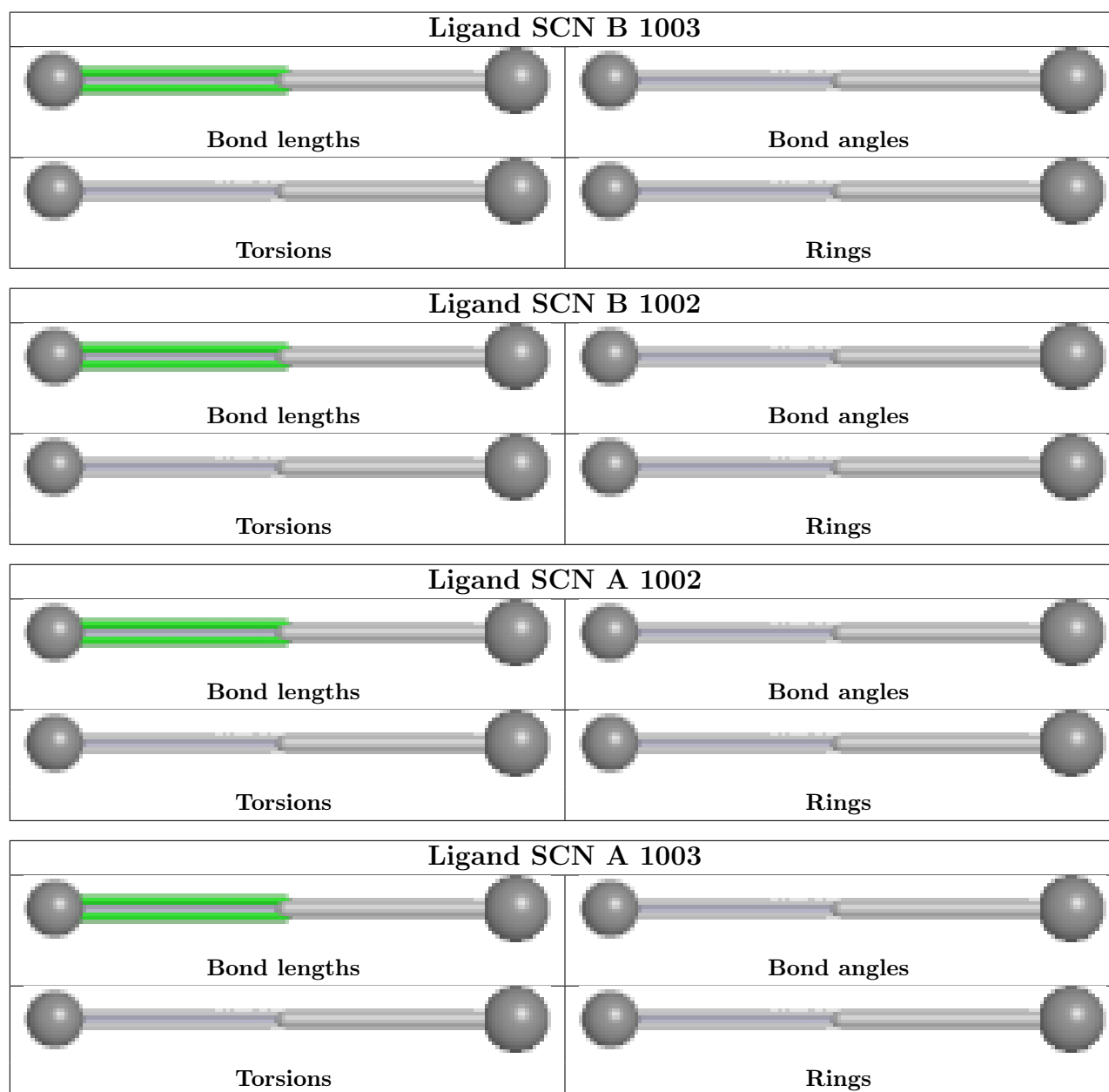
There are no torsion outliers.

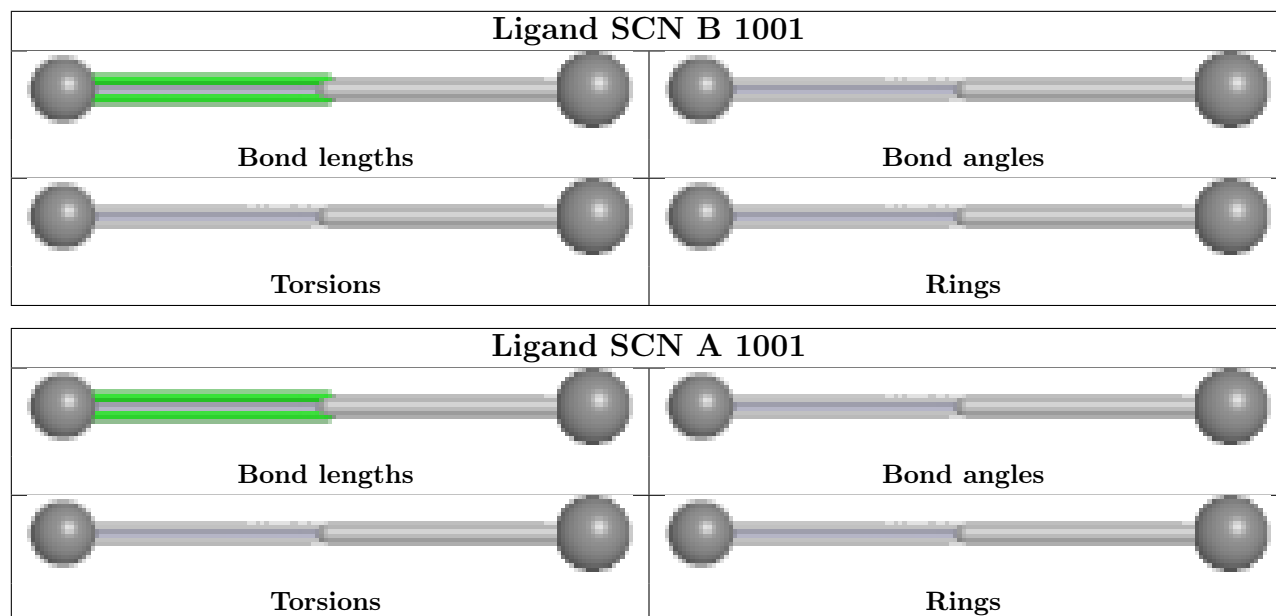
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1003	SCN	1	0
2	A	1003	SCN	1	0
2	B	1001	SCN	1	0
2	A	1001	SCN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

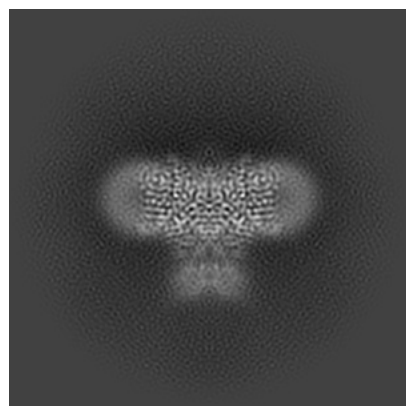
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37909. These allow visual inspection of the internal detail of the map and identification of artifacts.

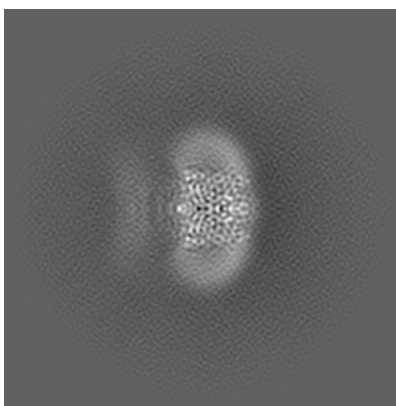
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

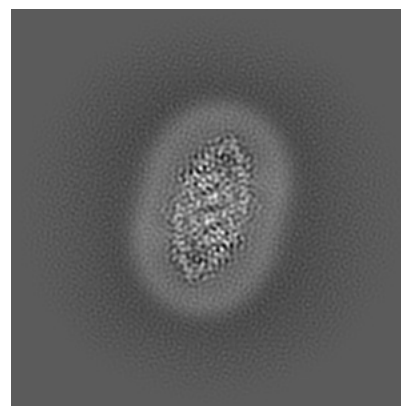
6.1.1 Primary map



X

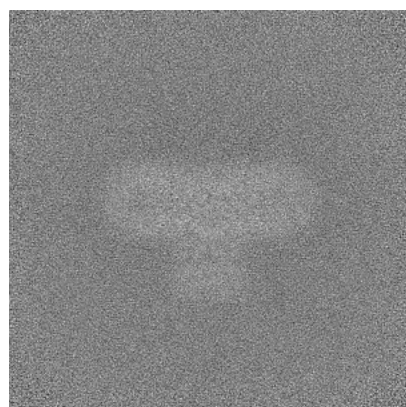


Y

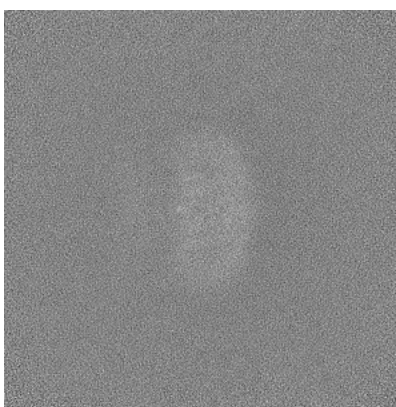


Z

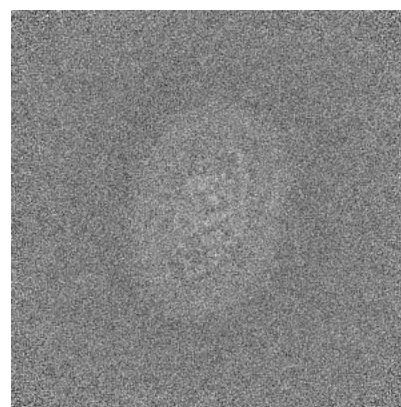
6.1.2 Raw map



X



Y

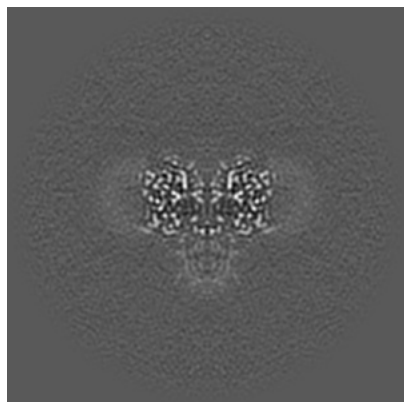


Z

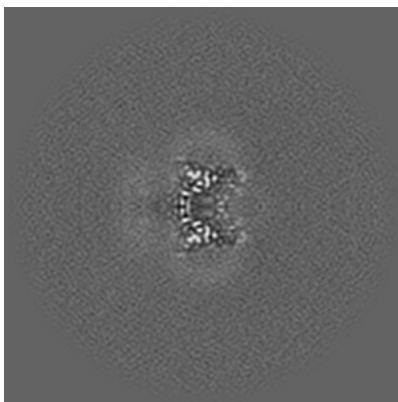
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

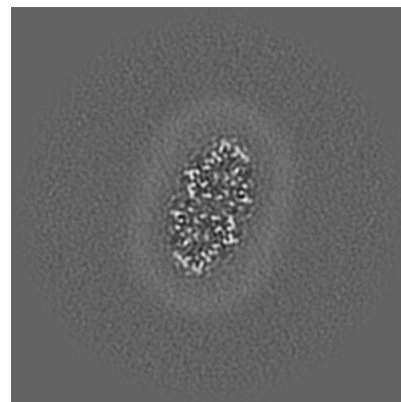
6.2.1 Primary map



X Index: 360

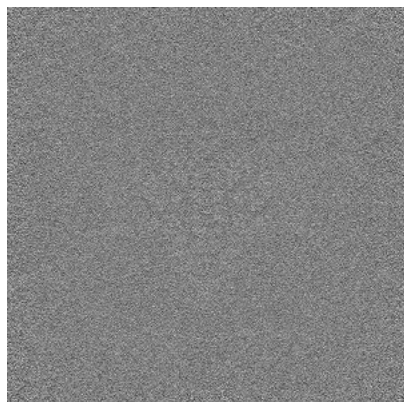


Y Index: 360

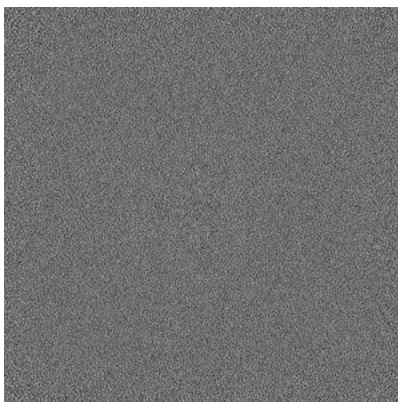


Z Index: 360

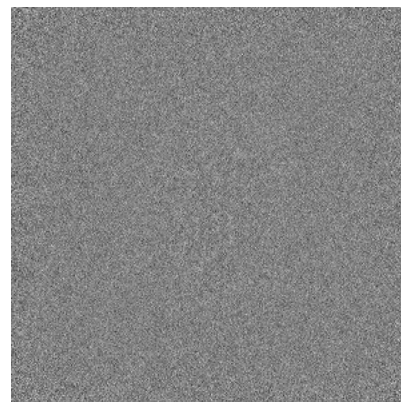
6.2.2 Raw map



X Index: 360



Y Index: 360

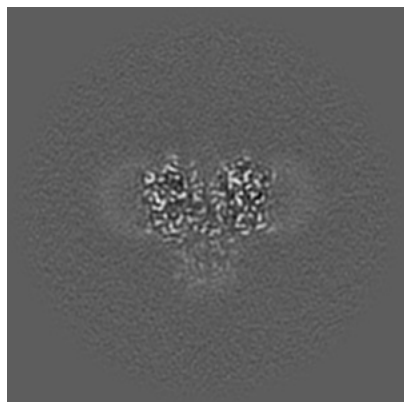


Z Index: 360

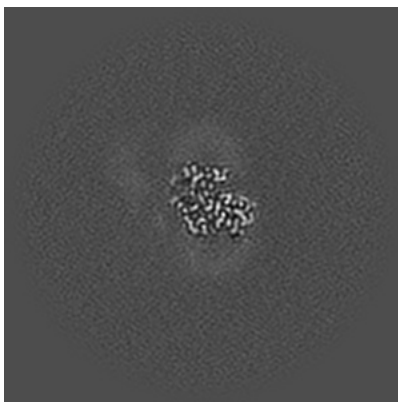
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

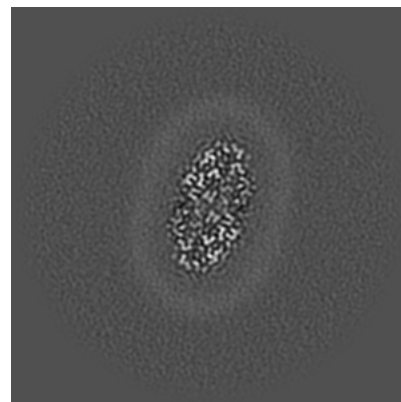
6.3.1 Primary map



X Index: 357

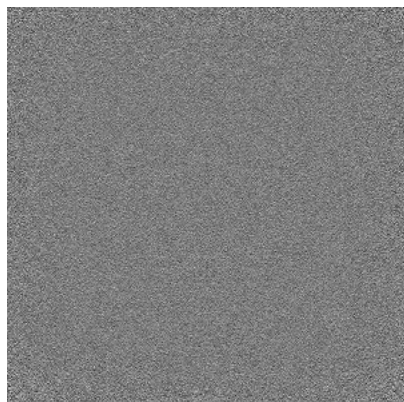


Y Index: 420

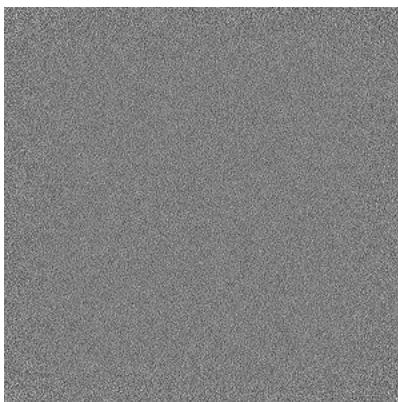


Z Index: 371

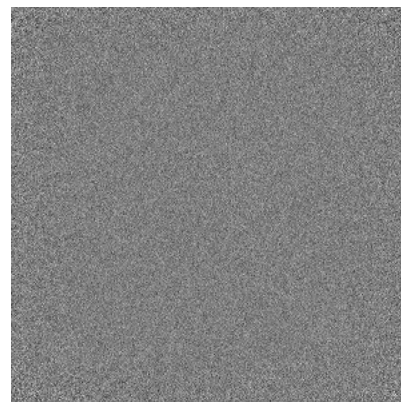
6.3.2 Raw map



X Index: 0



Y Index: 0

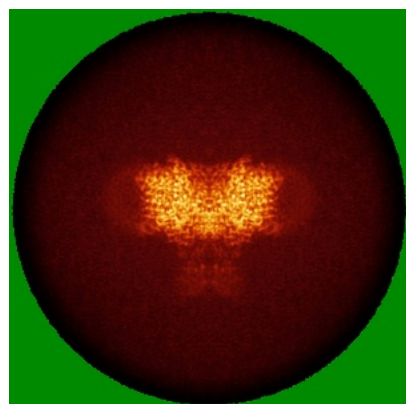


Z Index: 0

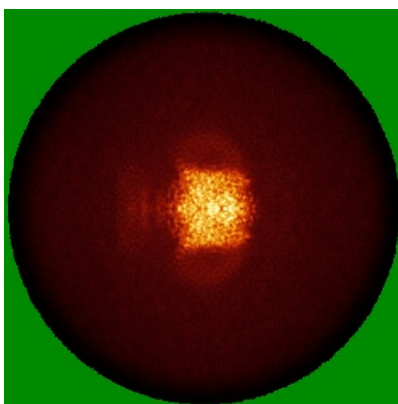
The images above show the largest variance slices of the map in three orthogonal directions.

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

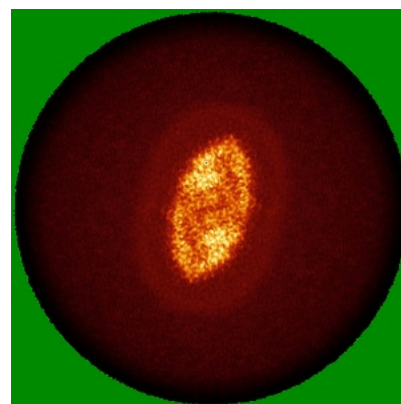
6.4.1 Primary map



X

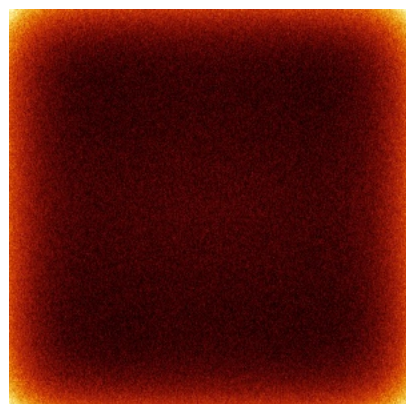


Y

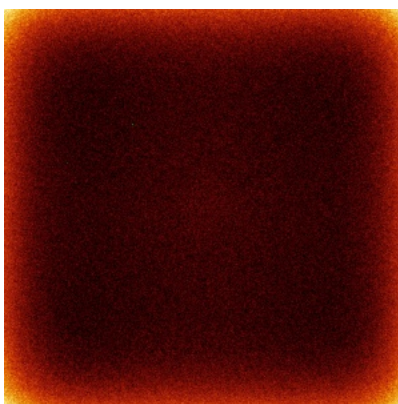


Z

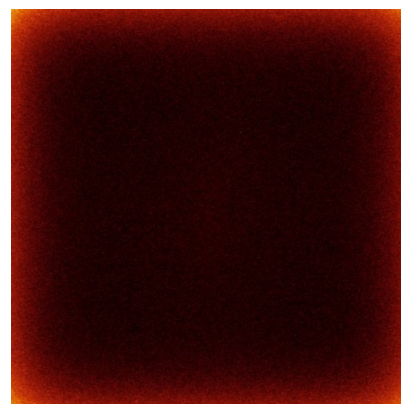
6.4.2 Raw map



X



Y

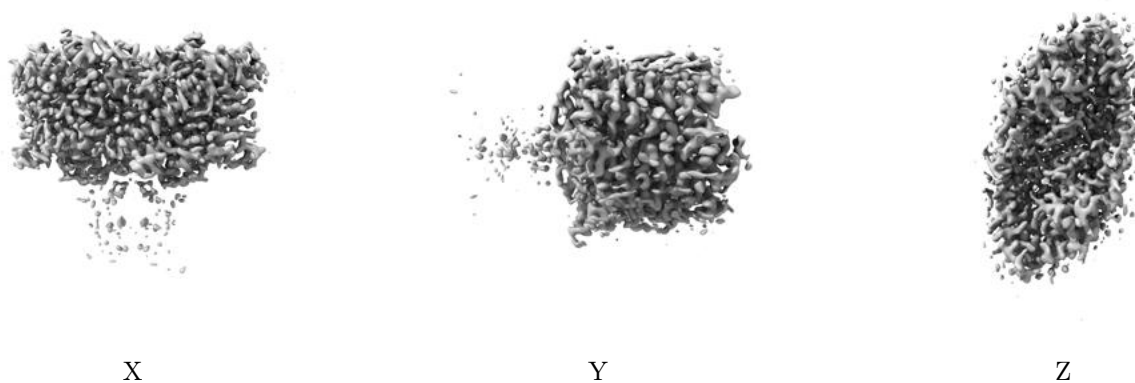


Z

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

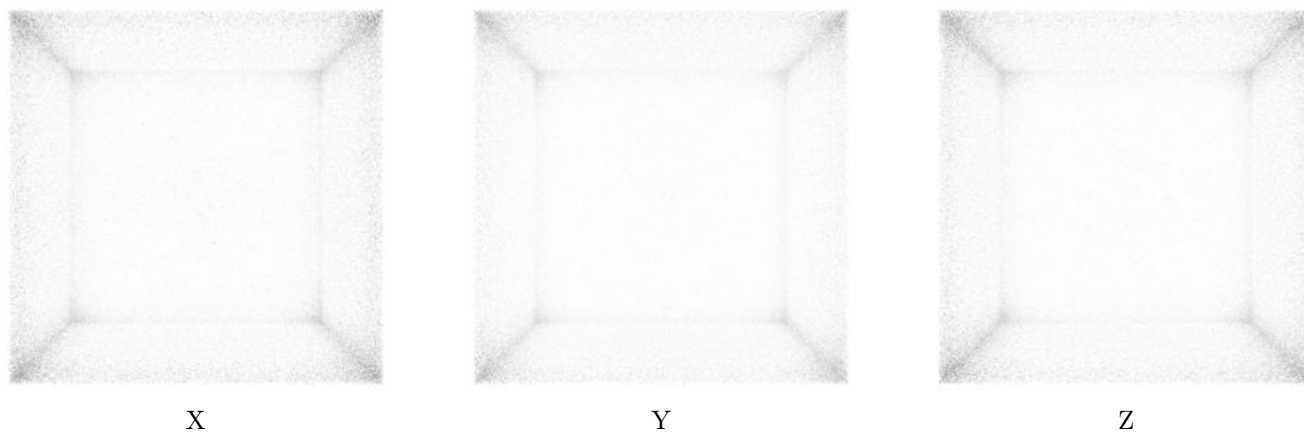
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

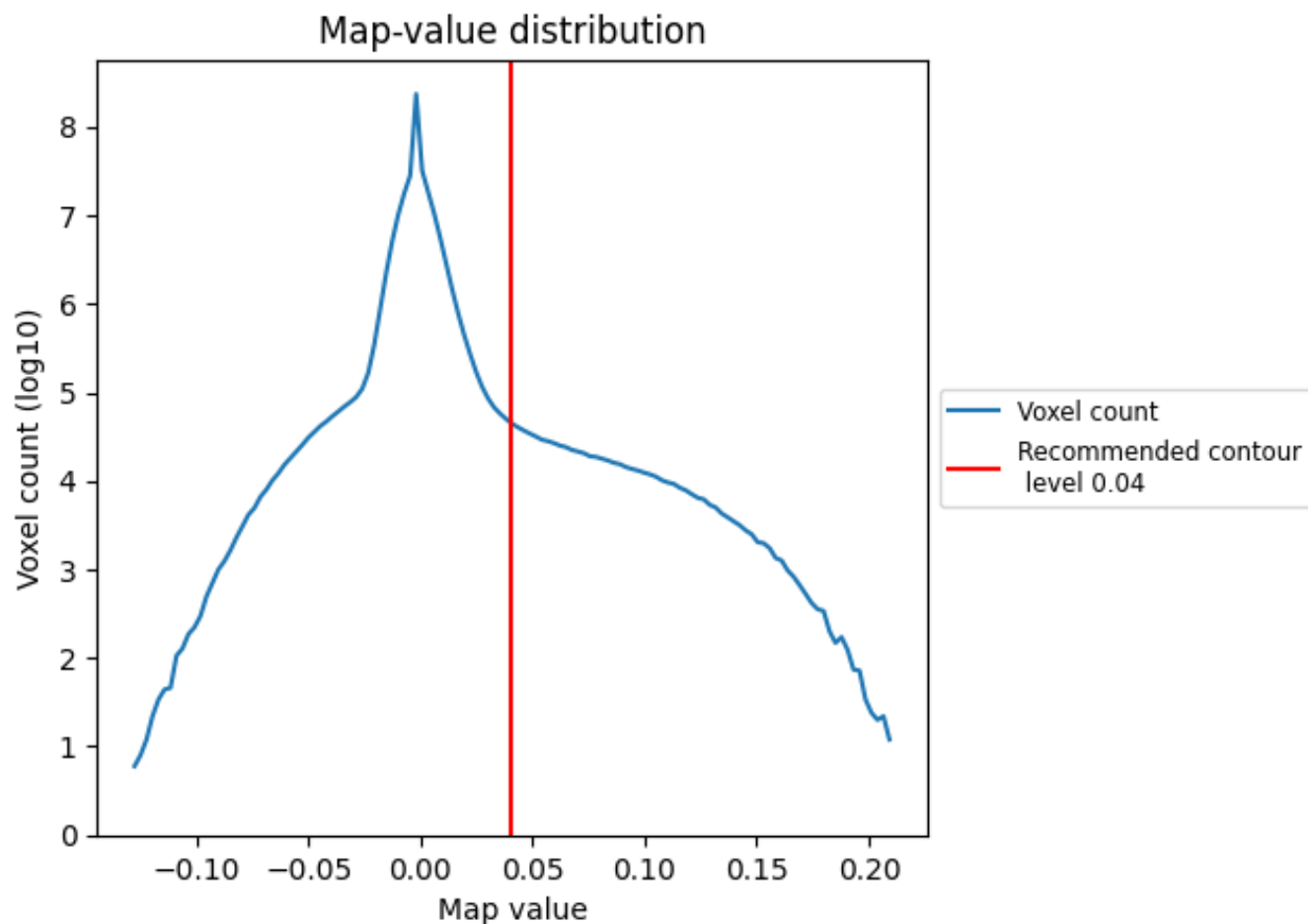
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

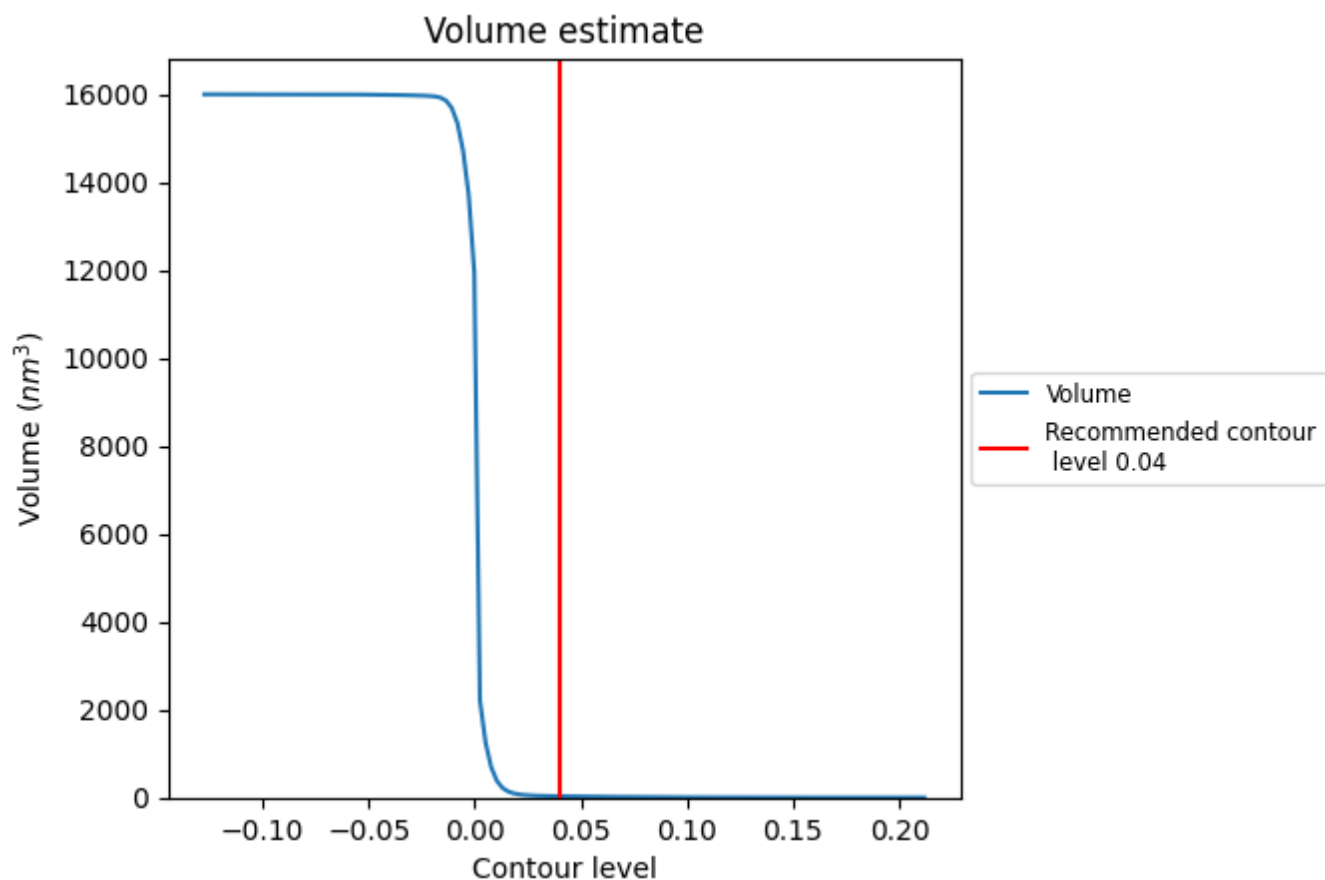
This section contains the results of statistical analysis of the map.

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.

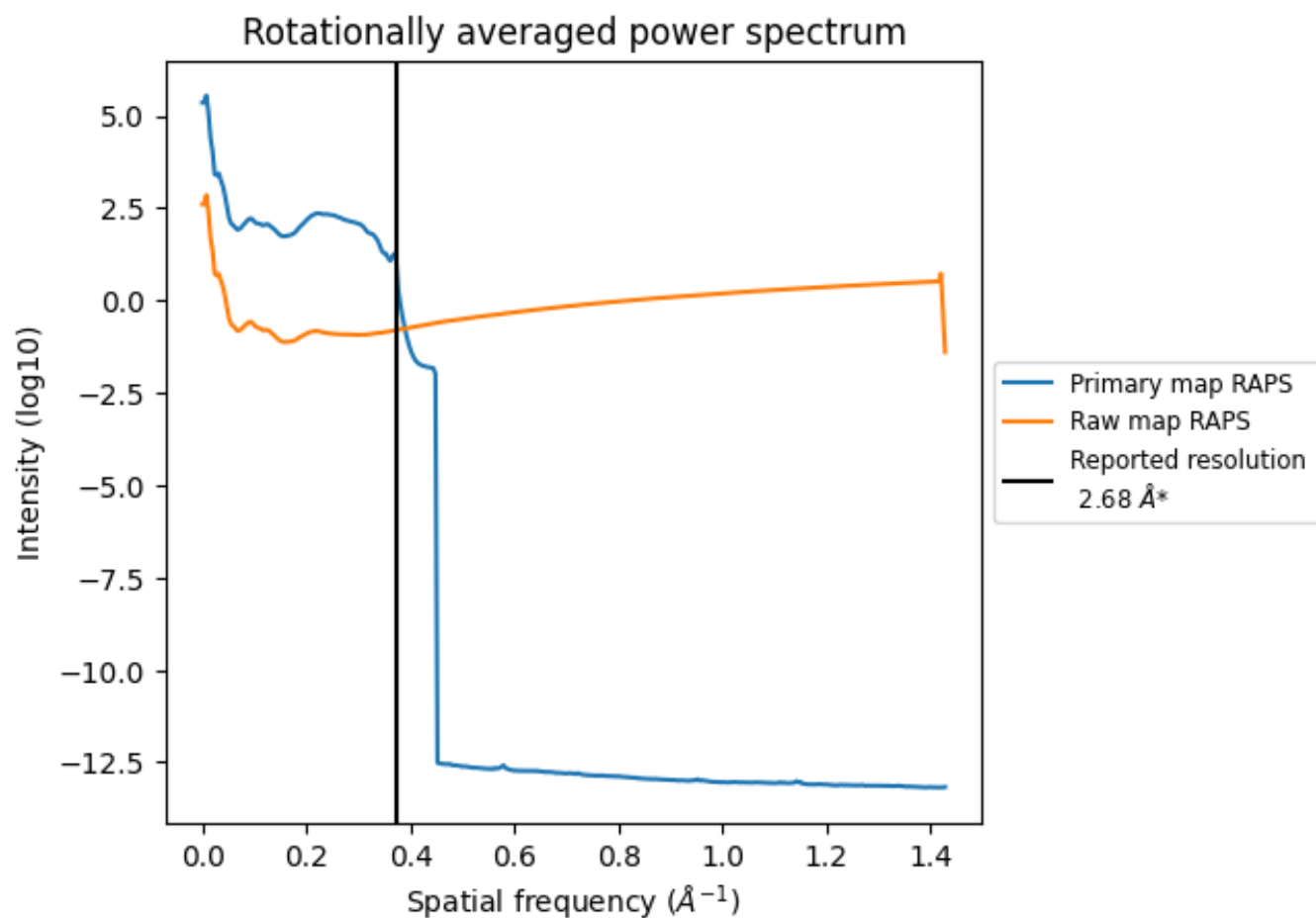
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 30 nm³; this corresponds to an approximate mass of 27 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 ⓘ

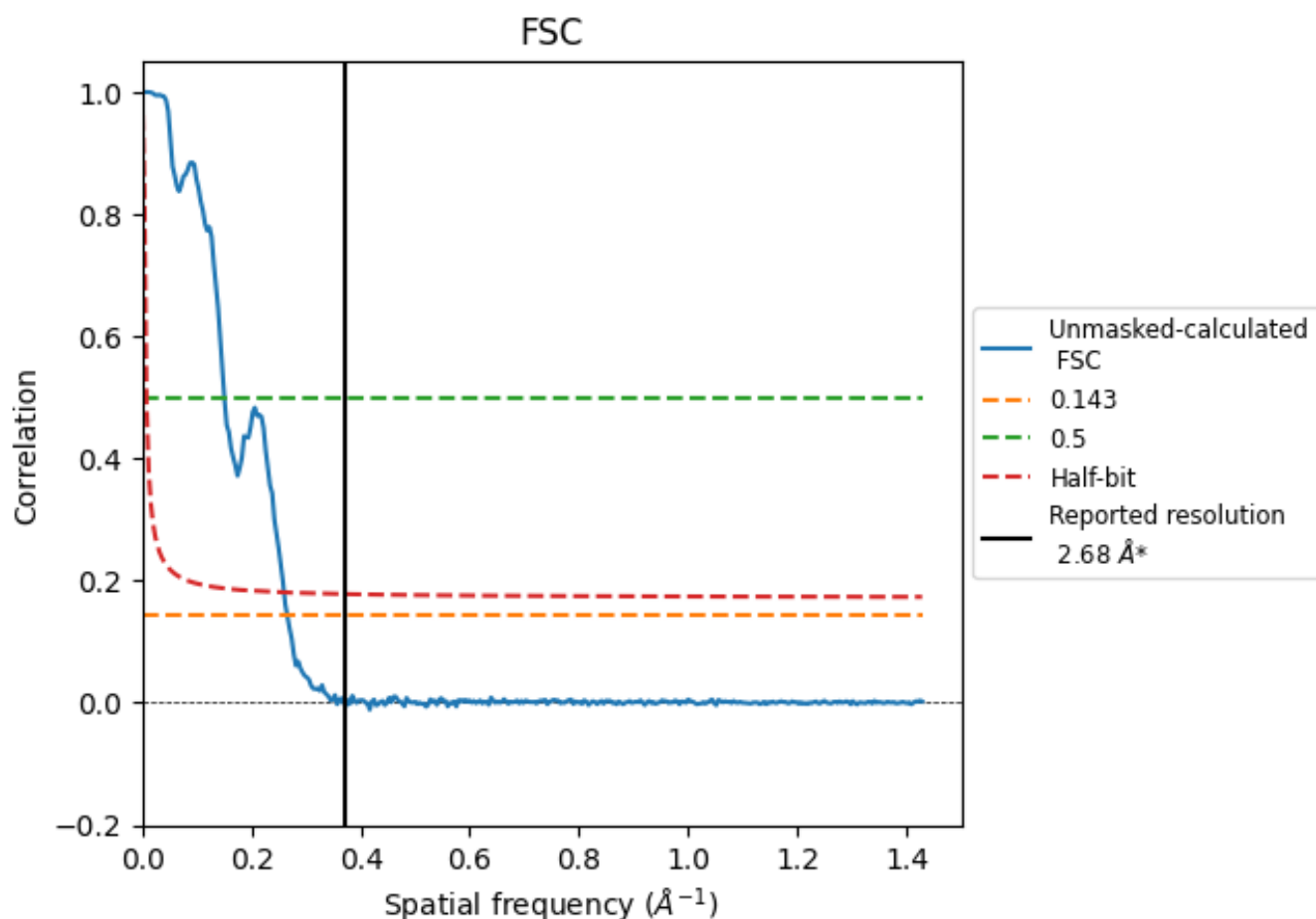


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 Å⁻¹

8.2 Resolution estimates [i](#)

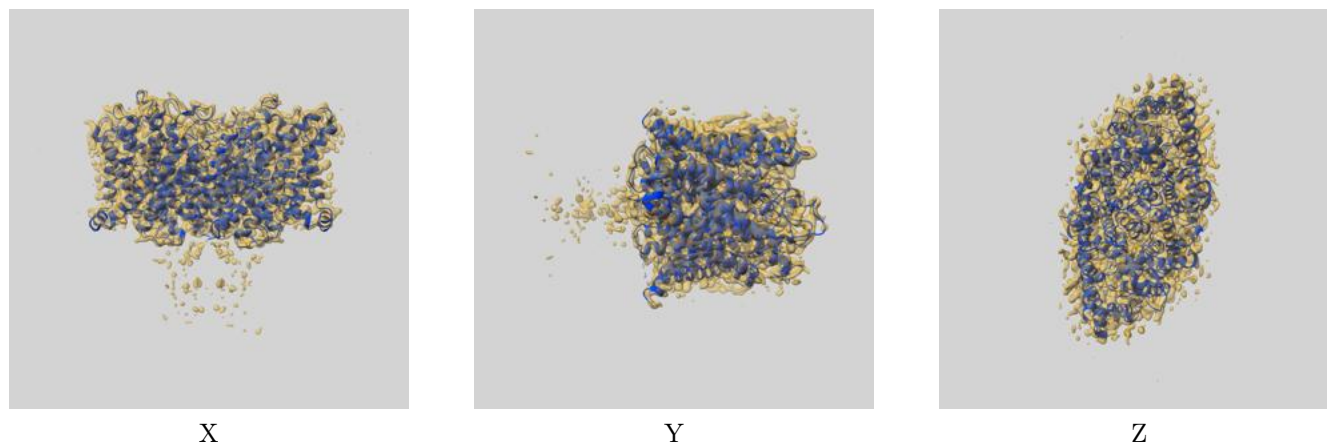
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.77	6.65	3.85

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.77 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

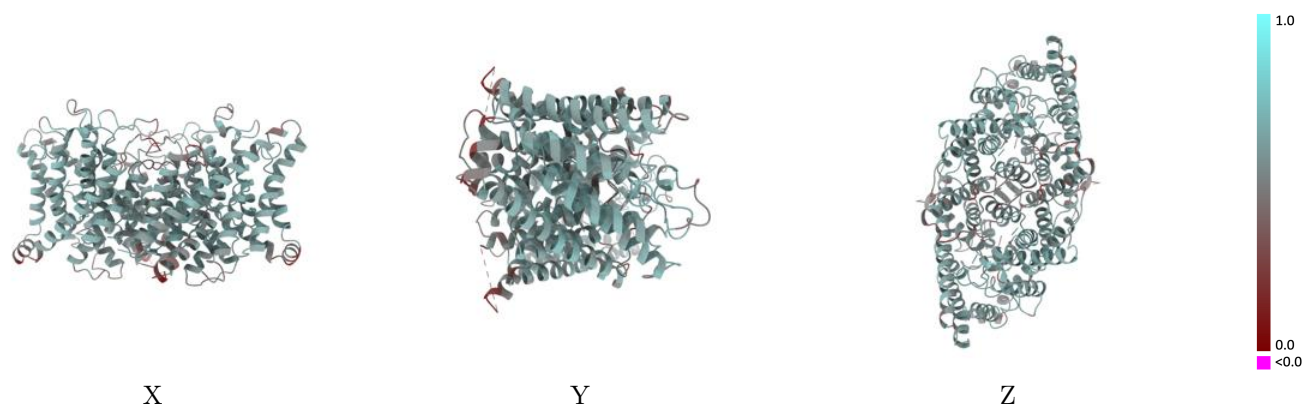
This section contains information regarding the fit between EMDB map EMD-37909 and PDB model 8WXJ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



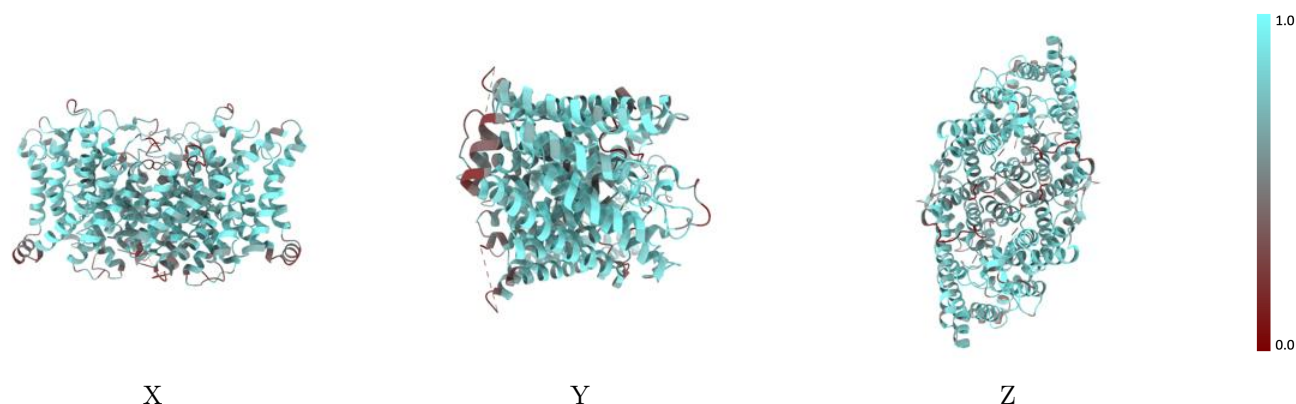
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



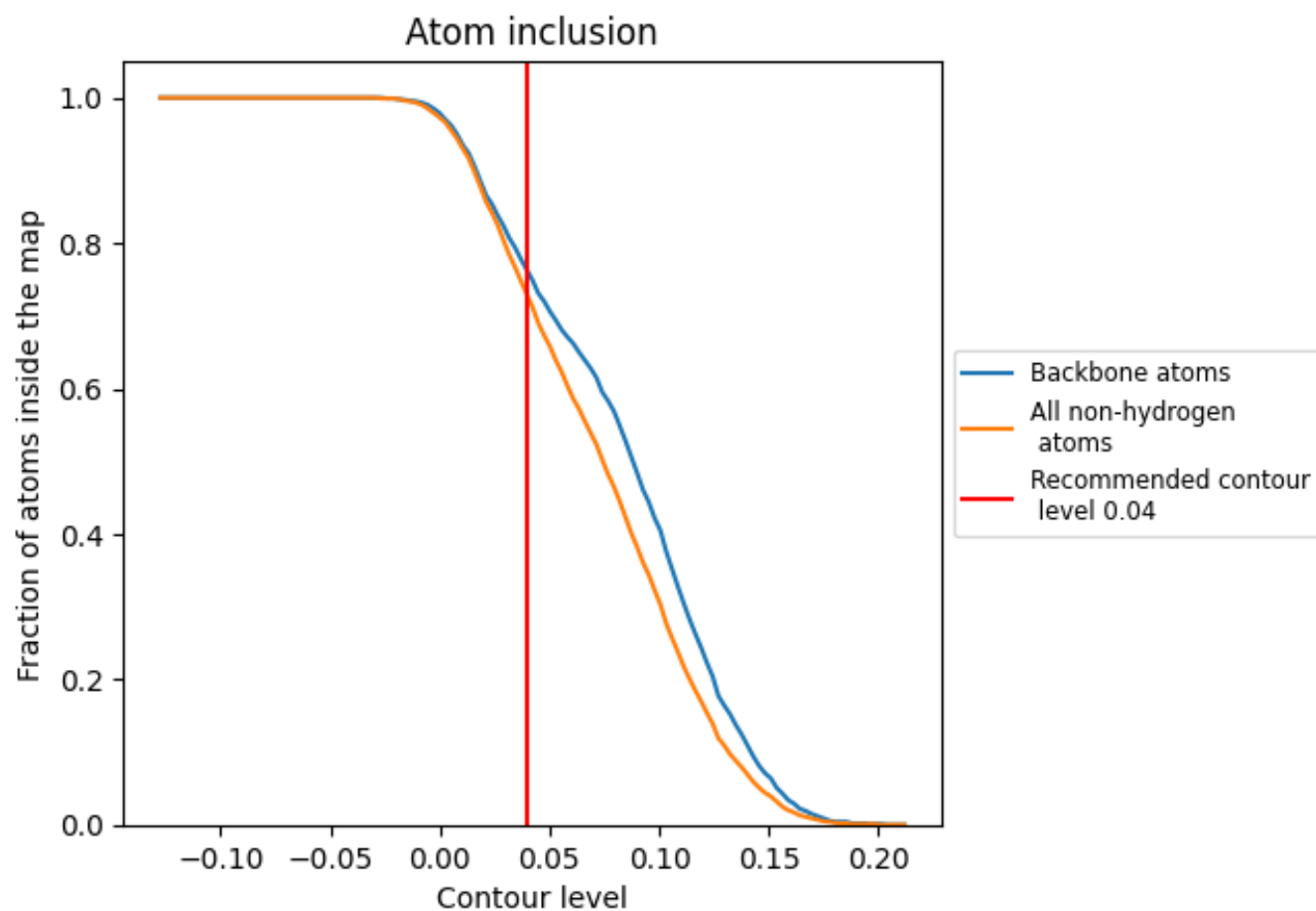
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7270	0.5550
A	0.7270	0.5560
B	0.7260	0.5550

