



Full wwPDB EM Validation Report ⓘ

Nov 6, 2022 – 12:16 AM JST

PDB ID : 7XJ2
EMDB ID : EMD-33217
Title : Structure of human TRPV3_G573S in complex with Trpvicin in C4 symmetry
Authors : Fan, J.; Yue, Z.; Jiang, D.; Lei, X.
Deposited on : 2022-04-14
Resolution : 3.64 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

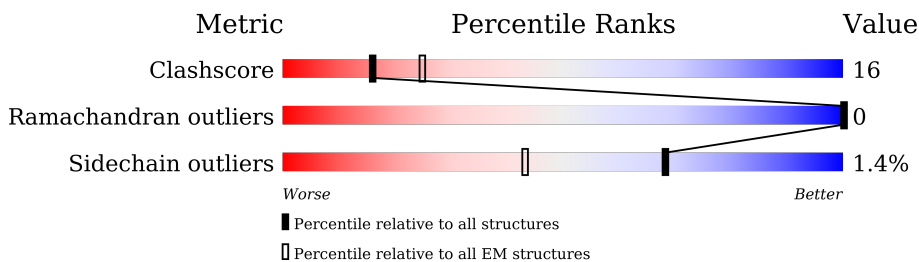
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1061	<div> <div>6%</div> <div>39% 18% 43%</div> </div>
1	B	1061	<div> <div>7%</div> <div>39% 18% 43%</div> </div>
1	C	1061	<div> <div>6%</div> <div>39% 18% 43%</div> </div>
1	D	1061	<div> <div>6%</div> <div>39% 18% 43%</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EQK	A	1101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EQK	B	1101	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18438 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 Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	607	Total	C	N	O	S	0	0
			4585	3015	763	780	27		
1	C	607	Total	C	N	O	S	0	0
			4575	3011	762	775	27		
1	A	607	Total	C	N	O	S	0	0
			4571	3006	763	775	27		
1	D	607	Total	C	N	O	S	0	0
			4575	3011	762	775	27		

There are 24 discrepancies between the modelled and reference sequences:

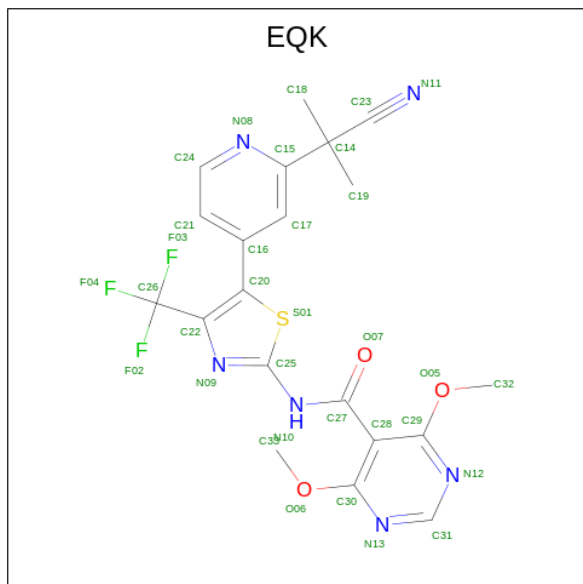
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ILE	VAL	conflict	UNP B2KYM6
B	117	ARG	GLY	conflict	UNP B2KYM6
B	246	LYS	ARG	conflict	UNP B2KYM6
B	247	GLY	GLU	conflict	UNP B2KYM6
B	573	SER	GLY	conflict	UNP B2KYM6
B	772	ASN	ASP	conflict	UNP B2KYM6
C	25	ILE	VAL	conflict	UNP B2KYM6
C	117	ARG	GLY	conflict	UNP B2KYM6
C	246	LYS	ARG	conflict	UNP B2KYM6
C	247	GLY	GLU	conflict	UNP B2KYM6
C	573	SER	GLY	conflict	UNP B2KYM6
C	772	ASN	ASP	conflict	UNP B2KYM6
A	25	ILE	VAL	conflict	UNP B2KYM6
A	117	ARG	GLY	conflict	UNP B2KYM6
A	246	LYS	ARG	conflict	UNP B2KYM6
A	247	GLY	GLU	conflict	UNP B2KYM6
A	573	SER	GLY	conflict	UNP B2KYM6
A	772	ASN	ASP	conflict	UNP B2KYM6
D	25	ILE	VAL	conflict	UNP B2KYM6
D	117	ARG	GLY	conflict	UNP B2KYM6
D	246	LYS	ARG	conflict	UNP B2KYM6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	247	GLY	GLU	conflict	UNP B2KYM6
D	573	SER	GLY	conflict	UNP B2KYM6
D	772	ASN	ASP	conflict	UNP B2KYM6

- Molecule 2 is N-[5-[2-(2-cyanopropan-2-yl)pyridin-4-yl]-4-(trifluoromethyl)-1,3-thiazol-2-yl]-4,6-dimethoxy-pyrimidine-5-carboxamide (three-letter code: EQK) (formula: C₂₀H₁₇F₃N₆O₃S) (labeled as "Ligand of Interest" by depositor).

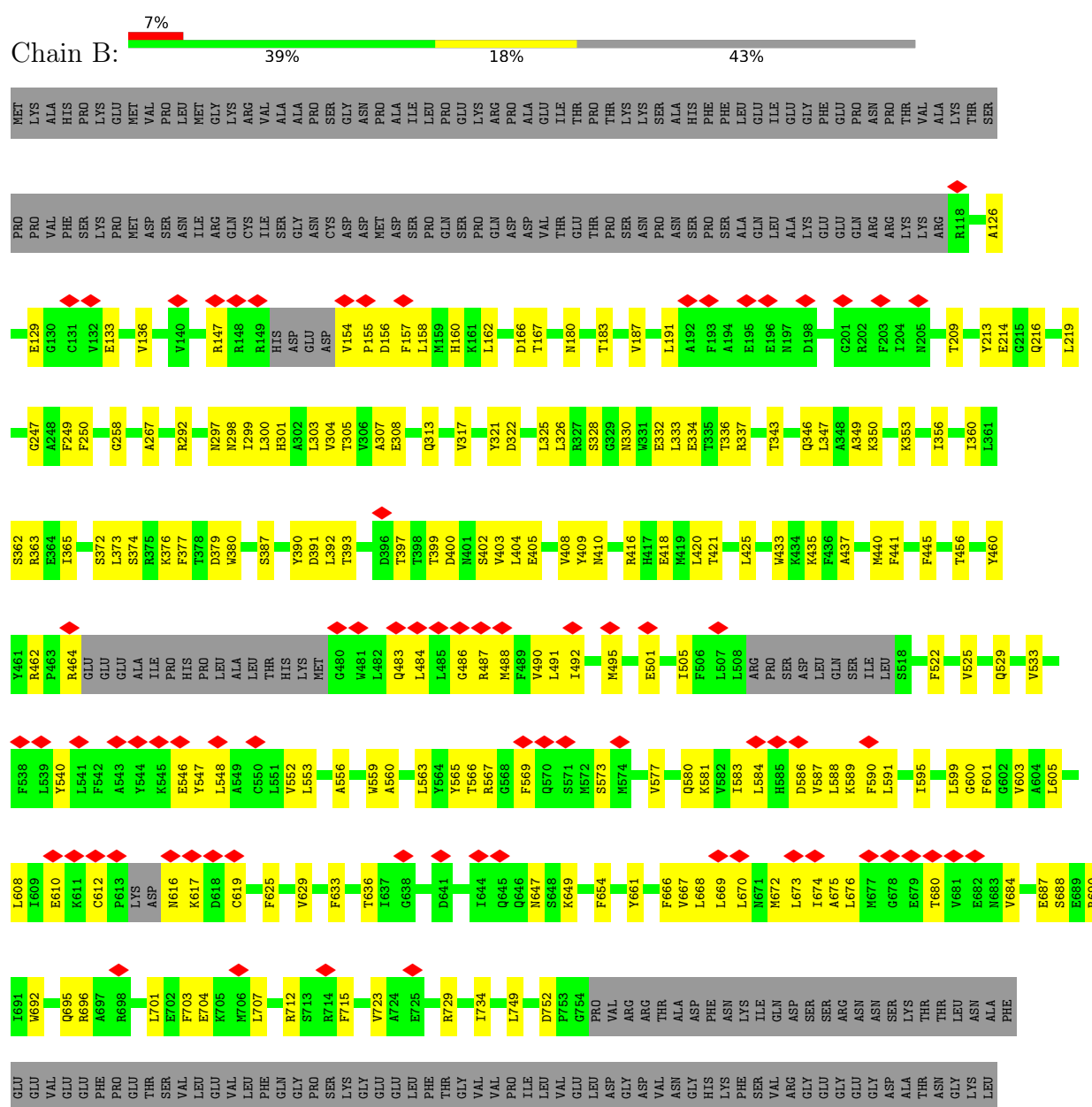


Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	
2	C	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	
2	A	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	
2	D	1	Total	C	F	N	O	S	0
			33	20	3	6	3	1	

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: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP



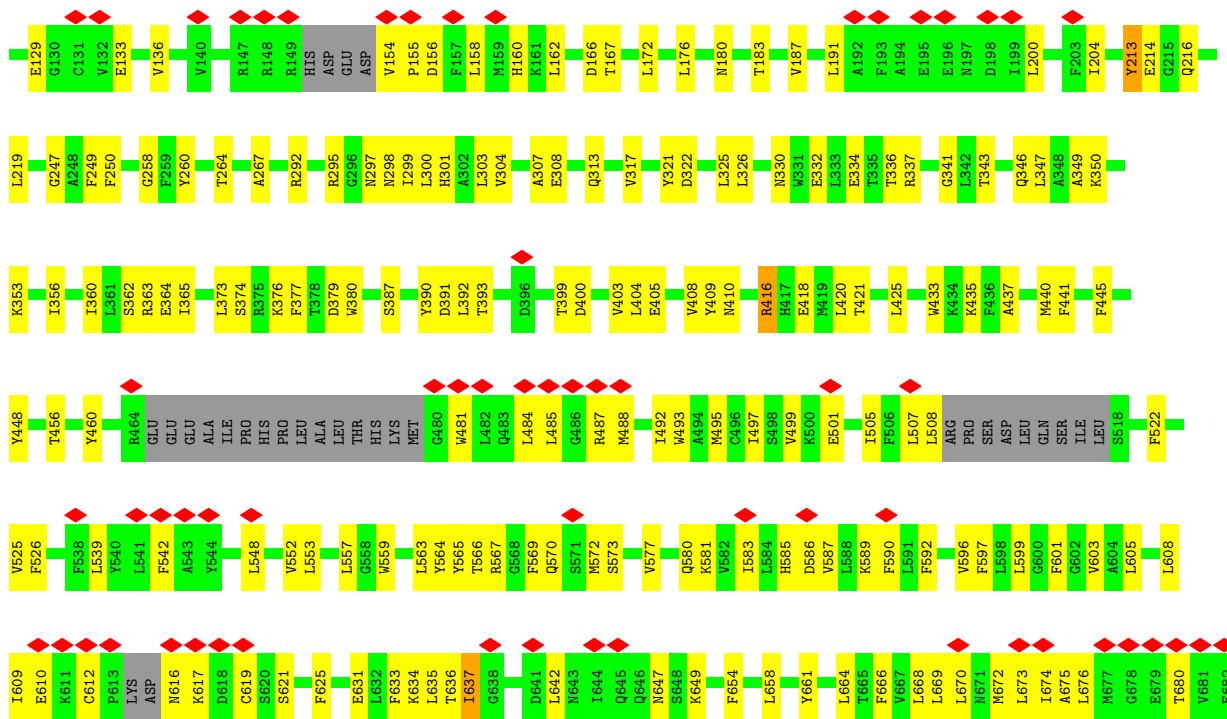
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- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP



MET	LYS	ALA	HIS	PRO	LYS	GLU	MET	LEU	GLY	LYS	ARG	VAL	ALA	ALA	PRO	SER	GLY	ASN	PRO	ALA	ILE	LEU	GLU	LYS	ARG	PRO	ALA	ALA	GLU	ILE	THR	PRO	THR	LYS	LYS	SER	ALA	HIS	PHE	PHE	LEU	GLU	ILE	GLU	GLY	PHE	GLU	PRO	PRO	ASN	PRO	THR	VAL	ALA	LYS	THR	SER
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PRO VAL PHE SER LYS PRO MET ASP SER ASN ILE ARG GLN CYS ILE SER GLY ASN CYS ASP ASP MET ASP SER PRO GLN ASP ASP VAL THR THR GLU PRO SER ASN PRO ASN SER PRO SER ALA ALA LEU ALA LYS GLU GLU GLN ARG ARG LYS LYS ARG R118



W683	W684	W685	W686	W687	W688	W689	W690	W691	W692	W693	W694	W695	W696	W697	W698	W699	W700	W701	W702	W703	W704	W705	W706	W707	W708	W709	W710	W711	W712	W713	W714	W715	W716	W717	W718	W719	W720	W721	W722	W723	W724	W725	W726	W727	W728	W729	W730	W731	W732	W733	W734	W735	W736	W737	W738	W739	W740	W741	W742	W743	W744	W745	W746	W747	W748	W749	W750	W751	W752	W753	W754	W755	W756	W757	W758	W759	W760	W761	W762	W763	W764	W765	W766	W767	W768	W769	W770	W771	W772	W773	W774	W775	W776	W777	W778	W779	W780	W781	W782	W783	W784	W785	W786	W787	W788	W789	W790	W791	W792	W793	W794	W795	W796	W797	W798	W799	W800	W801	W802	W803	W804	W805	W806	W807	W808	W809	W810	W811	W812	W813	W814	W815	W816	W817	W818	W819	W820	W821	W822	W823	W824	W825	W826	W827	W828	W829	W830	W831	W832	W833	W834	W835	W836	W837	W838	W839	W840	W841	W842	W843	W844	W845	W846	W847	W848	W849	W850	W851	W852	W853	W854	W855	W856	W857	W858	W859	W860	W861	W862	W863	W864	W865	W866	W867	W868	W869	W870	W871	W872	W873	W874	W875	W876	W877	W878	W879	W880	W881	W882	W883	W884	W885	W886	W887	W888	W889	W890	W891	W892	W893	W894	W895	W896	W897	W898	W899	W900	W901	W902	W903	W904	W905	W906	W907	W908	W909	W910	W911	W912	W913	W914	W915	W916	W917	W918	W919	W920	W921	W922	W923	W924	W925	W926	W927	W928	W929	W930	W931	W932	W933	W934	W935	W936	W937	W938	W939	W940	W941	W942	W943	W944	W945	W946	W947	W948	W949	W950	W951	W952	W953	W954	W955	W956	W957	W958	W959	W960	W961	W962	W963	W964	W965	W966	W967	W968	W969	W970	W971	W972	W973	W974	W975	W976	W977	W978	W979	W980	W981	W982	W983	W984	W985	W986	W987	W988	W989	W990	W991	W992	W993	W994	W995	W996	W997	W998	W999	W1000
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[illegible]

- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP



PRO	ASN	GLU	LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	HIS	GLY	MET	ASP	GLU	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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- Chain D:  6% 39% 18% 43%

PRO	PRO	VAL	PHE	SER	LYS	PRO	MET	ASP	SER	ASN	ILE	ARG	GLN	CYS	ILE	SER	GLY	ASN	CYS	ASP	MET	ASP	SER	PRO	GLN	GLM	SER	PRO	PRO	GLN	ASP	ASP	THR	VAL	ASP	GLU	THR	PRO	SER	SER	PRO	ALA	GLN	GLM	LEU	ALA	LYS	GLU	GLU	GLN	GLM	ARG	ARG	LYS	LYS	LYS	ARG
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Q227	I230	F249	F250	G258	F259	Y260	T264	A267	L268	D288	S291	R292	R295	G296	T297	N298	I299	L300	L301	H301	A302	L303	V304	A307	E308	Q313	V317	Y321	L326	R327	S328	G329	N330	E331	E332	L333	E334	T335	T336	R337	T343	Q346	L347	S348	I349
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K350	K353	I356	I360	K363	E364	I365	L373	S374	F377	D378	W380	S387	Y390	D391	L392	T393	D396	V403	L404	E405	V408	Y409	N410	R416	H417	E418	H419	L420	T421	L425	K432	W433	K434	K435	F436	F437	M440	F441	S444	F445
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L608	L609	E610	K611	C612	P613	LYS	ASP	N616	K617	D618	C619	S620	S621	Y622	F625	A628	E631	L632	T636	G638	L639	G640	D641	T644	G645	G646	M647	G648	K649	F654	Y661	L664	T665	F666	F667	L668	L669	L670	M671	M672	L673	L674	A675	L676	M677	G678	E679	T680	V681	F682
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E687	R690	I691	W692	Q695	R696	A697	R698	L701	F702	F703	E704	L707	W710	L711	L712	S713	R714	F715	R716	M717	V723	A724	E725	R729	I734	L749	G75A	PRO	VAL	ARG	ARG	THR	THR	ALA	ASP	PHE	ASN	LYS	ILE	GLN	ASP	SER	SER	ARG	ASN	ASN	SER	LYS	THR
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[illegible]

LYS	ASN	GLY	ILE	LYS	ALA	ASP	ASN	LYS	ILE	ARG	HIS	ASN	ASN	VAL	GLU	ASP	GLY	SER	VAL	GLN	LEU	ALA	ASP	HIS	THR	GLN	ASN	ASN	THR	PRO	PRO	ILE	GLY	GLY	PRO	VAL	LEU	LEU	PRO	PRO	ASP	ASN	HIS	THR	LEU	SER	THR	GLN	SER	VAL	VAL	LEU	SER	LYS	ASP	ASN	ASN	GLU	ARG	LYS	THR	ASP	HIS
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MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	HIS	GLY	MET	ASP	GLU	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	GLY	SER	GLY	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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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	48492	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.076	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: EQK

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	0.30	0/4668	0.45	0/6353
1	B	0.28	0/4683	0.43	0/6373
1	C	0.28	0/4673	0.43	0/6360
1	D	0.30	0/4673	0.43	0/6360
All	All	0.29	0/18697	0.43	0/25446

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4571	0	4409	155	0
1	B	4585	0	4422	143	0
1	C	4575	0	4412	155	0
1	D	4575	0	4412	147	0
2	A	33	0	0	10	0
2	B	33	0	0	11	0
2	C	33	0	0	7	0
2	D	33	0	0	0	0
All	All	18438	0	17655	579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (579) 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:B:583:ILE:HG23	2:B:1101:EQK:C18	1.76	1.15
1:A:620:SER:OG	1:A:646:GLN:HA	1.54	1.06
1:B:583:ILE:HD12	2:B:1101:EQK:C18	1.89	1.02
1:B:583:ILE:CG2	2:B:1101:EQK:C18	2.42	0.97
1:A:620:SER:HG	1:A:646:GLN:HA	1.31	0.94
1:A:583:ILE:HG23	2:A:1101:EQK:C18	1.99	0.91
1:A:377:PHE:CE2	1:A:723:VAL:HG21	2.06	0.90
1:D:462:ARG:HD2	1:D:548:LEU:HD13	1.54	0.90
1:A:620:SER:OG	1:A:646:GLN:CA	2.21	0.88
1:A:583:ILE:CG2	2:A:1101:EQK:C18	2.57	0.83
1:C:692:TRP:HE1	1:C:696:ARG:HH21	1.27	0.81
1:A:692:TRP:HE1	1:A:696:ARG:HH21	1.31	0.78
1:C:612:CYS:SG	1:C:619:CYS:HB2	2.26	0.76
1:D:692:TRP:HE1	1:D:696:ARG:HH21	1.32	0.75
1:A:463:PRO:HD3	1:A:487:ARG:HH22	1.50	0.75
1:A:573:SER:OG	1:A:692:TRP:HB2	1.87	0.75
1:D:462:ARG:HD3	1:D:548:LEU:HD11	1.68	0.75
1:C:616:ASN:CB	1:C:619:CYS:SG	2.75	0.75
1:A:377:PHE:CE1	1:A:723:VAL:HG11	2.23	0.73
1:C:334:GLU:OE2	1:C:363:ARG:NH2	2.22	0.72
1:A:297:ASN:HB3	1:A:301:HIS:HB2	1.70	0.72
1:A:559:TRP:O	2:A:1101:EQK:C33	2.37	0.72
1:B:334:GLU:OE2	1:B:363:ARG:NH2	2.23	0.72
1:B:616:ASN:CB	1:B:619:CYS:SG	2.78	0.71
1:A:260:TYR:OH	1:A:297:ASN:ND2	2.20	0.71
1:D:433:TRP:HA	1:D:437:ALA:HB3	1.72	0.71
1:C:379:ASP:HB2	1:C:749:LEU:HB2	1.73	0.70
1:A:433:TRP:HA	1:A:437:ALA:HB3	1.72	0.70
1:A:334:GLU:OE2	1:A:363:ARG:NH2	2.24	0.70
1:C:380:TRP:HB3	1:C:387:SER:HB3	1.73	0.70
1:B:379:ASP:HB2	1:B:749:LEU:HB2	1.72	0.70
1:A:445:PHE:HD1	1:A:565:TYR:HB3	1.56	0.70
1:B:612:CYS:HB2	1:B:617:LYS:HA	1.73	0.70
1:D:334:GLU:OE2	1:D:363:ARG:NH2	2.23	0.70
1:D:612:CYS:SG	1:D:647:ASN:OD1	2.49	0.70
1:D:379:ASP:HB2	1:D:749:LEU:HB2	1.74	0.69
1:B:552:VAL:HG11	1:C:608:LEU:HD21	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ASP:HB2	1:A:749:LEU:HB2	1.74	0.69
1:B:433:TRP:HA	1:B:437:ALA:HB3	1.72	0.69
1:B:608:LEU:HD21	1:A:552:VAL:HG11	1.75	0.69
1:A:583:ILE:HD12	2:A:1101:EQK:C18	2.22	0.69
1:D:606:ALA:HA	1:D:609:ILE:CD1	2.24	0.68
1:D:462:ARG:CD	1:D:548:LEU:HD13	2.23	0.68
1:C:433:TRP:HA	1:C:437:ALA:HB3	1.74	0.68
1:A:156:ASP:O	1:A:160:HIS:ND1	2.26	0.68
1:C:156:ASP:O	1:C:160:HIS:ND1	2.27	0.68
1:A:380:TRP:HB3	1:A:387:SER:HB3	1.76	0.68
1:D:156:ASP:O	1:D:160:HIS:ND1	2.27	0.67
1:D:569:PHE:O	1:D:573:SER:N	2.27	0.67
1:C:365:ILE:N	1:C:374:SER:OG	2.27	0.67
1:D:462:ARG:CD	1:D:548:LEU:CD1	2.72	0.67
1:B:156:ASP:O	1:B:160:HIS:ND1	2.27	0.66
1:D:380:TRP:HB3	1:D:387:SER:HB3	1.77	0.66
1:B:380:TRP:HB3	1:B:387:SER:HB3	1.78	0.66
1:B:343:THR:OG1	1:B:346:GLN:NE2	2.30	0.65
1:B:350:LYS:O	1:B:410:ASN:ND2	2.28	0.65
1:C:633:PHE:HE2	1:C:637:ILE:HD13	1.62	0.65
1:D:350:LYS:O	1:D:410:ASN:ND2	2.30	0.65
1:D:586:ASP:HA	1:D:589:LYS:HE2	1.78	0.65
1:D:586:ASP:HB3	1:D:672:MET:SD	2.37	0.64
1:A:343:THR:OG1	1:A:346:GLN:NE2	2.29	0.64
1:A:350:LYS:O	1:A:410:ASN:ND2	2.30	0.64
1:C:445:PHE:HD1	1:C:565:TYR:HB3	1.61	0.64
1:C:612:CYS:HB3	1:C:617:LYS:HA	1.80	0.64
1:D:343:THR:OG1	1:D:346:GLN:NE2	2.30	0.64
1:B:445:PHE:HD1	1:B:565:TYR:HB3	1.61	0.64
1:A:365:ILE:H	1:A:374:SER:HG	1.46	0.64
1:D:462:ARG:HD3	1:D:548:LEU:CD1	2.27	0.64
1:C:377:PHE:HZ	1:C:729:ARG:HH21	1.45	0.64
1:D:304:VAL:O	1:D:353:LYS:NZ	2.31	0.63
1:C:633:PHE:CE2	1:C:637:ILE:HD13	2.32	0.63
1:B:583:ILE:HG22	1:B:584:LEU:HD22	1.81	0.63
1:C:616:ASN:CB	1:C:619:CYS:HG	2.11	0.63
1:A:304:VAL:O	1:A:353:LYS:NZ	2.32	0.63
1:C:633:PHE:O	1:C:637:ILE:HG12	1.99	0.63
1:D:567:ARG:NE	1:D:695:GLN:OE1	2.32	0.63
1:B:649:LYS:HD2	1:A:548:LEU:HD23	1.81	0.63
1:C:304:VAL:O	1:C:353:LYS:NZ	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LYS:O	1:C:410:ASN:ND2	2.32	0.62
1:D:445:PHE:HD1	1:D:565:TYR:HB3	1.64	0.62
1:B:616:ASN:CB	1:B:619:CYS:HG	2.11	0.62
1:C:484:LEU:HD12	1:C:487:ARG:HD2	1.81	0.62
1:C:552:VAL:HG11	1:D:608:LEU:HD21	1.82	0.62
1:C:567:ARG:NH1	1:C:580:GLN:OE1	2.32	0.62
1:B:304:VAL:O	1:B:353:LYS:NZ	2.32	0.62
1:B:365:ILE:N	1:B:374:SER:OG	2.26	0.62
1:C:569:PHE:O	1:C:573:SER:N	2.31	0.62
1:D:365:ILE:N	1:D:374:SER:OG	2.29	0.62
1:B:365:ILE:H	1:B:374:SER:HG	1.47	0.62
1:C:577:VAL:HG21	1:C:691:ILE:HG21	1.82	0.62
1:D:674:ILE:HG13	1:D:675:ALA:N	2.15	0.62
1:C:343:THR:OG1	1:C:346:GLN:NE2	2.31	0.62
1:C:636:THR:HG1	1:C:661:TYR:HH	1.48	0.62
1:B:556:ALA:O	2:B:1101:EQK:N10	2.32	0.61
1:A:462:ARG:HD3	1:A:548:LEU:HD13	1.81	0.61
1:B:522:PHE:HA	1:B:525:VAL:HG12	1.83	0.61
1:D:522:PHE:HA	1:D:525:VAL:HG12	1.83	0.61
1:A:692:TRP:HE1	1:A:696:ARG:NH2	1.99	0.61
1:D:698:ARG:O	1:D:702:GLU:HG3	2.00	0.61
1:A:608:LEU:HD21	1:D:552:VAL:HG11	1.83	0.60
1:C:583:ILE:HD11	1:D:667:VAL:HG11	1.83	0.60
1:B:583:ILE:HG21	2:B:1101:EQK:C23	2.32	0.60
1:C:633:PHE:HD2	1:C:637:ILE:HD11	1.67	0.60
1:B:187:VAL:O	1:B:191:LEU:HG	2.02	0.59
1:C:187:VAL:O	1:C:191:LEU:HG	2.02	0.59
1:A:612:CYS:SG	1:A:619:CYS:HB2	2.42	0.59
1:D:187:VAL:O	1:D:191:LEU:HG	2.02	0.59
1:C:557:LEU:HD13	2:C:1101:EQK:F03	1.92	0.59
1:A:377:PHE:CZ	1:A:723:VAL:HG11	2.38	0.59
1:A:672:MET:O	1:A:676:LEU:HG	2.02	0.59
1:C:522:PHE:HA	1:C:525:VAL:HG12	1.84	0.59
1:C:672:MET:O	1:C:676:LEU:HG	2.03	0.59
1:A:365:ILE:N	1:A:374:SER:OG	2.30	0.59
1:A:522:PHE:HA	1:A:525:VAL:HG12	1.83	0.59
1:D:432:LYS:HG2	1:D:717:MET:HG3	1.85	0.59
1:C:563:LEU:HA	1:C:566:THR:HG22	1.84	0.59
1:D:590:PHE:HE1	1:D:668:LEU:HB3	1.68	0.59
1:C:408:VAL:HG21	1:C:701:LEU:HG	1.85	0.59
1:A:667:VAL:HG11	1:D:583:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:ARG:NH1	1:C:373:LEU:O	2.36	0.58
1:D:577:VAL:HG21	1:D:691:ILE:HG21	1.84	0.58
1:B:483:GLN:O	1:B:487:ARG:HB2	2.03	0.58
1:C:216:GLN:HB2	1:C:250:PHE:HE2	1.69	0.58
1:C:337:ARG:NH2	1:C:341:GLY:O	2.37	0.58
1:A:216:GLN:HB2	1:A:250:PHE:HE2	1.69	0.58
1:A:620:SER:OG	1:A:646:GLN:NE2	2.37	0.58
1:D:452:ASN:HD21	1:D:559:TRP:HA	1.69	0.58
1:B:462:ARG:NH1	1:B:464:ARG:O	2.36	0.58
1:A:187:VAL:O	1:A:191:LEU:HG	2.03	0.58
1:A:583:ILE:HG22	1:A:584:LEU:HD22	1.86	0.58
1:C:685:SER:O	1:C:689:GLU:HG2	2.03	0.57
1:A:583:ILE:HG21	2:A:1101:EQK:C18	2.34	0.57
1:B:583:ILE:HG21	2:B:1101:EQK:C18	2.30	0.57
1:C:292:ARG:NH1	1:C:337:ARG:O	2.36	0.57
1:D:605:LEU:O	1:D:609:ILE:HG13	2.03	0.57
1:B:586:ASP:OD1	1:B:587:VAL:N	2.37	0.57
1:B:216:GLN:HB2	1:B:250:PHE:HE2	1.69	0.57
1:B:491:LEU:O	1:B:495:MET:HG2	2.04	0.57
1:D:606:ALA:HA	1:D:609:ILE:HD12	1.87	0.57
1:C:559:TRP:O	2:C:1101:EQK:C33	2.52	0.56
1:A:432:LYS:HG2	1:A:717:MET:HG3	1.86	0.56
1:B:267:ALA:HA	1:B:299:ILE:HD13	1.88	0.56
1:B:672:MET:O	1:B:676:LEU:HG	2.04	0.56
1:C:559:TRP:HB3	2:C:1101:EQK:C30	2.35	0.56
1:C:559:TRP:HB3	2:C:1101:EQK:N13	2.21	0.56
1:A:687:GLU:HA	1:A:690:ARG:HG2	1.86	0.56
1:D:636:THR:OG1	1:D:661:TYR:OH	2.22	0.56
1:A:267:ALA:HA	1:A:299:ILE:HD13	1.88	0.56
1:A:363:ARG:NH1	1:A:373:LEU:O	2.39	0.56
1:D:599:LEU:HD13	1:D:625:PHE:HZ	1.70	0.56
1:C:539:LEU:HA	1:C:542:PHE:HB2	1.88	0.56
1:A:612:CYS:SG	1:A:619:CYS:SG	3.04	0.55
1:B:408:VAL:HG21	1:B:701:LEU:HG	1.89	0.55
1:D:304:VAL:HG22	1:D:356:ILE:HG21	1.89	0.55
1:B:460:TYR:HB2	1:C:603:VAL:HG23	1.88	0.55
1:B:674:ILE:HG13	1:B:675:ALA:N	2.22	0.55
1:A:292:ARG:NH1	1:A:337:ARG:O	2.35	0.55
1:A:636:THR:OG1	1:A:661:TYR:OH	2.25	0.55
1:B:372:SER:O	1:B:729:ARG:NH2	2.37	0.55
1:A:408:VAL:HG21	1:A:701:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:PHE:O	1:A:573:SER:N	2.40	0.55
1:C:267:ALA:HA	1:C:299:ILE:HD13	1.88	0.54
1:D:710:TRP:O	1:D:714:ARG:HG3	2.07	0.54
1:B:563:LEU:HA	1:B:566:THR:HG22	1.89	0.54
1:B:636:THR:HG1	1:B:661:TYR:HH	1.53	0.54
1:B:559:TRP:HB3	2:B:1101:EQK:C31	2.37	0.54
1:C:692:TRP:HE1	1:C:696:ARG:NH2	2.03	0.54
1:D:363:ARG:NH1	1:D:373:LEU:O	2.40	0.54
1:A:304:VAL:HG22	1:A:356:ILE:HG21	1.90	0.54
1:B:304:VAL:HG22	1:B:356:ILE:HG21	1.90	0.54
1:B:610:GLU:O	1:B:647:ASN:ND2	2.40	0.54
1:C:610:GLU:O	1:C:647:ASN:ND2	2.41	0.54
1:A:129:GLU:O	1:A:180:ASN:ND2	2.41	0.54
1:D:573:SER:OG	1:D:692:TRP:HB2	2.07	0.54
1:B:577:VAL:HG11	1:B:688:SER:HA	1.88	0.54
1:D:216:GLN:HB2	1:D:250:PHE:HE2	1.73	0.54
1:D:408:VAL:HG21	1:D:701:LEU:HG	1.90	0.54
1:C:129:GLU:O	1:C:180:ASN:ND2	2.41	0.54
1:D:180:ASN:O	1:D:183:THR:HG23	2.09	0.53
1:C:633:PHE:CD2	1:C:637:ILE:HD11	2.42	0.53
1:A:606:ALA:HA	1:A:609:ILE:HD12	1.91	0.53
1:B:180:ASN:O	1:B:183:THR:HG23	2.08	0.53
1:C:399:THR:HG22	1:C:400:ASP:H	1.74	0.53
1:C:670:LEU:O	1:C:674:ILE:HG23	2.09	0.53
1:A:180:ASN:O	1:A:183:THR:HG23	2.09	0.53
1:A:435:LYS:NZ	1:A:715:PHE:O	2.40	0.53
1:D:303:LEU:HD22	1:D:317:VAL:HG23	1.90	0.53
1:C:180:ASN:O	1:C:183:THR:HG23	2.09	0.53
1:C:304:VAL:HG22	1:C:356:ILE:HG21	1.91	0.53
1:C:356:ILE:O	1:C:360:ILE:HG13	2.09	0.52
1:A:303:LEU:HD22	1:A:317:VAL:HG23	1.90	0.52
1:D:666:PHE:O	1:D:670:LEU:HG	2.09	0.52
1:B:363:ARG:NH1	1:B:373:LEU:O	2.41	0.52
1:B:666:PHE:O	1:B:670:LEU:HG	2.09	0.52
1:C:616:ASN:O	1:C:619:CYS:SG	2.67	0.52
1:A:356:ILE:O	1:A:360:ILE:HG13	2.10	0.52
1:C:586:ASP:OD2	1:C:587:VAL:N	2.43	0.52
1:A:404:LEU:HD13	1:A:425:LEU:HD22	1.92	0.52
1:B:129:GLU:O	1:B:180:ASN:ND2	2.41	0.52
1:C:303:LEU:HD22	1:C:317:VAL:HG23	1.91	0.52
1:A:666:PHE:O	1:A:670:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:MET:O	1:C:492:ILE:HG13	2.09	0.52
1:A:391:ASP:OD1	1:A:392:LEU:N	2.43	0.52
1:D:183:THR:O	1:D:187:VAL:HG22	2.10	0.52
1:B:356:ILE:O	1:B:360:ILE:HG13	2.10	0.52
1:B:687:GLU:HA	1:B:690:ARG:HG2	1.91	0.52
1:A:577:VAL:HG21	1:A:691:ILE:HG21	1.91	0.52
1:C:183:THR:O	1:C:187:VAL:HG22	2.10	0.52
1:B:603:VAL:HG11	1:A:456:THR:HG23	1.92	0.52
1:B:249:PHE:CE1	1:B:258:GLY:HA2	2.46	0.51
1:C:633:PHE:CD2	1:C:637:ILE:CD1	2.93	0.51
1:A:603:VAL:HG11	1:D:456:THR:HG23	1.92	0.51
1:B:435:LYS:NZ	1:B:715:PHE:O	2.39	0.51
1:C:435:LYS:NZ	1:C:715:PHE:O	2.40	0.51
1:A:183:THR:O	1:A:187:VAL:HG22	2.10	0.51
1:A:249:PHE:CE1	1:A:258:GLY:HA2	2.45	0.51
1:C:377:PHE:CZ	1:C:723:VAL:HG21	2.45	0.51
1:D:404:LEU:HD13	1:D:425:LEU:HD22	1.91	0.51
1:C:460:TYR:HB2	1:D:603:VAL:HG23	1.92	0.51
1:C:669:LEU:O	1:C:673:LEU:HG	2.11	0.51
1:B:616:ASN:O	1:B:619:CYS:SG	2.69	0.51
1:D:129:GLU:O	1:D:180:ASN:ND2	2.43	0.51
1:D:300:LEU:HD12	1:D:321:TYR:CZ	2.45	0.51
1:A:581:LYS:O	1:A:585:HIS:HB2	2.11	0.51
1:B:183:THR:O	1:B:187:VAL:HG22	2.10	0.51
1:B:391:ASP:OD1	1:B:392:LEU:N	2.44	0.51
1:C:249:PHE:CE1	1:C:258:GLY:HA2	2.45	0.51
1:C:599:LEU:HD13	1:C:625:PHE:HZ	1.75	0.51
1:A:563:LEU:HA	1:A:566:THR:HG22	1.91	0.51
1:D:249:PHE:CE1	1:D:258:GLY:HA2	2.46	0.50
1:D:620:SER:OG	1:D:646:GLN:C	2.49	0.50
1:B:303:LEU:HD22	1:B:317:VAL:HG23	1.92	0.50
1:D:343:THR:O	1:D:347:LEU:N	2.39	0.50
1:D:621:SER:OG	1:D:631:GLU:CD	2.49	0.50
1:D:687:GLU:HA	1:D:690:ARG:HG2	1.93	0.50
1:B:456:THR:HG23	1:C:603:VAL:HG11	1.94	0.50
1:C:666:PHE:O	1:C:670:LEU:HG	2.10	0.50
1:B:300:LEU:HD12	1:B:321:TYR:CZ	2.47	0.50
1:A:533:VAL:HG22	1:A:554:ALA:HB1	1.93	0.50
1:C:635:LEU:CD1	1:C:658:LEU:HD11	2.42	0.50
1:D:692:TRP:HE1	1:D:696:ARG:NH2	2.03	0.50
1:C:493:TRP:O	1:C:497:ILE:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:570:GLN:HE22	1:D:696:ARG:HH22	1.57	0.50
1:B:399:THR:HG22	1:B:400:ASP:H	1.77	0.50
1:D:377:PHE:CE1	1:D:723:VAL:HG21	2.47	0.50
1:B:692:TRP:NE1	1:B:696:ARG:HD2	2.27	0.49
1:A:300:LEU:HD12	1:A:321:TYR:CZ	2.47	0.49
1:A:343:THR:O	1:A:347:LEU:N	2.40	0.49
1:A:450:PHE:HA	1:A:453:ILE:HG22	1.94	0.49
1:A:559:TRP:O	2:A:1101:EQK:O06	2.30	0.49
1:A:723:VAL:HG22	1:A:749:LEU:HD21	1.92	0.49
1:D:356:ILE:O	1:D:360:ILE:HG13	2.11	0.49
1:A:288:ASP:O	1:A:291:SER:OG	2.27	0.49
1:D:391:ASP:OD1	1:D:392:LEU:N	2.45	0.49
1:A:392:LEU:HD13	1:A:396:ASP:HB3	1.93	0.49
1:D:300:LEU:CD2	1:D:333:LEU:HD13	2.43	0.49
1:B:391:ASP:OD1	1:B:393:THR:N	2.46	0.49
1:C:680:THR:HG22	1:C:684:VAL:HB	1.95	0.49
1:B:397:THR:HA	1:B:402:SER:HB3	1.95	0.49
1:A:559:TRP:HB3	2:A:1101:EQK:N13	2.28	0.49
1:C:343:THR:O	1:C:347:LEU:N	2.39	0.49
1:C:391:ASP:OD1	1:C:392:LEU:N	2.46	0.49
1:A:462:ARG:HG3	1:A:464:ARG:HD2	1.94	0.49
1:A:391:ASP:OD1	1:A:393:THR:N	2.45	0.49
1:D:158:LEU:O	1:D:162:LEU:HB2	2.13	0.49
1:D:444:SER:OG	1:D:565:TYR:OH	2.24	0.49
1:B:377:PHE:CZ	1:B:723:VAL:HG21	2.48	0.49
1:D:435:LYS:NZ	1:D:715:PHE:O	2.38	0.49
1:B:377:PHE:CE1	1:B:723:VAL:HG21	2.48	0.48
1:B:600:GLY:HA3	2:A:1101:EQK:N12	2.27	0.48
1:C:300:LEU:HD12	1:C:321:TYR:CZ	2.48	0.48
1:C:391:ASP:OD1	1:C:393:THR:N	2.46	0.48
1:D:637:ILE:HG23	1:D:639:LEU:HD23	1.96	0.48
1:B:680:THR:HG22	1:B:684:VAL:HB	1.94	0.48
1:D:484:LEU:O	1:D:488:MET:HG2	2.13	0.48
1:C:586:ASP:O	1:C:589:LYS:HG2	2.13	0.48
2:C:1101:EQK:N12	1:D:600:GLY:HA3	2.29	0.48
1:D:391:ASP:O	1:D:392:LEU:HD23	2.14	0.48
1:B:391:ASP:O	1:B:392:LEU:HD23	2.14	0.48
1:D:599:LEU:O	1:D:603:VAL:HG12	2.14	0.48
1:B:612:CYS:SG	1:B:619:CYS:HB2	2.53	0.48
1:D:292:ARG:NH1	1:D:337:ARG:O	2.40	0.48
2:B:1101:EQK:S01	1:C:664:LEU:HD11	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:LEU:O	1:B:673:LEU:HG	2.13	0.48
1:C:300:LEU:HD12	1:C:321:TYR:CE2	2.49	0.48
1:D:484:LEU:HA	1:D:487:ARG:HG3	1.94	0.48
1:B:391:ASP:OD2	1:B:729:ARG:HD2	2.14	0.48
1:B:440:MET:SD	1:B:707:LEU:HD21	2.54	0.48
1:C:391:ASP:O	1:C:392:LEU:HD23	2.13	0.48
1:A:440:MET:SD	1:A:707:LEU:HD21	2.54	0.48
1:A:586:ASP:OD1	1:A:587:VAL:N	2.47	0.48
1:A:501:GLU:O	1:A:505:ILE:HG13	2.14	0.47
1:C:507:LEU:O	1:C:508:LEU:HG	2.14	0.47
1:C:599:LEU:O	1:C:603:VAL:HG12	2.13	0.47
1:B:404:LEU:HD13	1:B:425:LEU:HD22	1.96	0.47
1:C:605:LEU:HG	1:C:654:PHE:CE1	2.49	0.47
1:D:440:MET:SD	1:D:707:LEU:HD21	2.54	0.47
1:B:126:ALA:HB1	1:B:136:VAL:HG12	1.96	0.47
1:A:557:LEU:HD13	2:A:1101:EQK:F03	2.04	0.47
1:D:126:ALA:HB1	1:D:136:VAL:HG12	1.96	0.47
1:D:674:ILE:HG13	1:D:675:ALA:H	1.79	0.47
1:B:633:PHE:HE2	1:C:642:LEU:HD22	1.80	0.47
1:C:332:GLU:O	1:C:336:THR:HG23	2.14	0.47
1:A:300:LEU:HD12	1:A:321:TYR:CE2	2.50	0.47
1:B:292:ARG:NH1	1:B:337:ARG:O	2.42	0.47
1:D:391:ASP:OD1	1:D:393:THR:N	2.46	0.47
1:D:566:THR:HB	1:D:572:MET:HG3	1.96	0.47
1:D:687:GLU:O	1:D:691:ILE:HG22	2.15	0.47
1:C:440:MET:SD	1:C:707:LEU:HD21	2.55	0.47
1:C:601:PHE:CG	1:C:661:TYR:HB2	2.50	0.47
1:D:590:PHE:CE1	1:D:668:LEU:HB3	2.50	0.47
1:A:620:SER:OG	1:A:646:GLN:C	2.54	0.47
1:D:267:ALA:HA	1:D:299:ILE:HD13	1.97	0.47
1:A:529:GLN:O	1:A:533:VAL:HG23	2.15	0.47
1:A:601:PHE:CG	1:A:661:TYR:HB2	2.50	0.47
1:A:507:LEU:HD23	1:A:508:LEU:H	1.80	0.47
1:D:300:LEU:HD23	1:D:333:LEU:HD13	1.97	0.47
1:D:436:PHE:CZ	1:D:704:GLU:OE1	2.68	0.47
1:D:495:MET:O	1:D:499:VAL:HG23	2.15	0.47
1:B:605:LEU:HG	1:B:654:PHE:CE1	2.50	0.46
1:A:295:ARG:HB3	1:A:297:ASN:ND2	2.31	0.46
1:A:612:CYS:SG	1:A:619:CYS:CB	3.03	0.46
1:B:300:LEU:HD12	1:B:321:TYR:CE2	2.49	0.46
1:B:332:GLU:O	1:B:336:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLU:O	1:A:691:ILE:HG22	2.15	0.46
1:D:377:PHE:HZ	1:D:729:ARG:NH2	2.14	0.46
1:C:126:ALA:HB1	1:C:136:VAL:HG12	1.96	0.46
1:A:391:ASP:O	1:A:392:LEU:HD23	2.14	0.46
1:A:605:LEU:HG	1:A:654:PHE:CE1	2.51	0.46
1:D:418:GLU:O	1:D:421:THR:OG1	2.33	0.46
1:C:621:SER:OG	1:C:631:GLU:HG3	2.15	0.46
1:D:332:GLU:O	1:D:336:THR:HG23	2.16	0.46
1:D:622:TYR:HD1	1:D:628:ALA:HA	1.81	0.46
1:C:322:ASP:O	1:C:326:LEU:HG	2.16	0.46
1:C:570:GLN:HE22	1:C:696:ARG:NH2	2.13	0.46
1:D:408:VAL:O	1:D:416:ARG:NH1	2.49	0.46
1:A:147:ARG:HA	1:A:157:PHE:HE2	1.80	0.46
1:A:362:SER:O	1:A:362:SER:OG	2.31	0.46
1:D:195:GLU:HA	1:D:200:LEU:HD11	1.97	0.46
1:D:328:SER:O	1:D:328:SER:OG	2.29	0.46
1:B:349:ALA:HB2	1:B:403:VAL:HG13	1.98	0.46
1:C:501:GLU:O	1:C:505:ILE:HG13	2.15	0.46
1:A:227:GLN:HB3	1:A:230:ILE:HD13	1.97	0.46
1:C:377:PHE:CE1	1:C:723:VAL:HG21	2.51	0.46
1:C:448:TYR:CZ	1:C:526:PHE:HE1	2.34	0.46
1:A:201:GLY:O	1:A:205:ASN:HB2	2.16	0.46
1:A:448:TYR:CZ	1:A:526:PHE:HE1	2.34	0.46
1:D:297:ASN:HB3	1:D:301:HIS:HB2	1.96	0.46
1:C:481:TRP:O	1:C:485:LEU:HG	2.16	0.46
1:A:377:PHE:CD2	1:A:723:VAL:HG21	2.51	0.46
1:B:147:ARG:HA	1:B:157:PHE:HE2	1.81	0.46
1:C:158:LEU:O	1:C:162:LEU:HB2	2.16	0.46
1:A:332:GLU:O	1:A:336:THR:HG23	2.15	0.46
1:A:418:GLU:O	1:A:421:THR:OG1	2.34	0.46
1:B:362:SER:O	1:B:362:SER:OG	2.32	0.45
1:A:322:ASP:O	1:A:326:LEU:HG	2.16	0.45
1:B:297:ASN:HB3	1:B:301:HIS:HB2	1.98	0.45
1:B:563:LEU:HD21	1:B:580:GLN:CG	2.47	0.45
1:B:612:CYS:SG	1:B:647:ASN:ND2	2.90	0.45
1:B:308:GLU:H	1:B:313:GLN:NE2	2.13	0.45
1:C:297:ASN:HB3	1:C:301:HIS:HB2	1.98	0.45
1:C:330:ASN:OD1	1:C:330:ASN:N	2.49	0.45
1:B:599:LEU:O	1:B:603:VAL:HG12	2.17	0.45
1:C:404:LEU:HD13	1:C:425:LEU:HD22	1.97	0.45
1:C:559:TRP:HB3	2:C:1101:EQK:C31	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:GLU:O	1:C:691:ILE:HG22	2.16	0.45
1:A:682:GLU:O	1:A:686:LYS:NZ	2.32	0.45
1:B:328:SER:O	1:B:328:SER:OG	2.30	0.45
1:B:501:GLU:O	1:B:505:ILE:HG13	2.15	0.45
1:C:484:LEU:O	1:C:488:MET:HG2	2.16	0.45
1:A:405:GLU:O	1:A:409:TYR:HB2	2.15	0.45
1:B:569:PHE:O	1:B:573:SER:OG	2.34	0.45
1:C:569:PHE:O	1:C:573:SER:OG	2.32	0.45
1:A:408:VAL:HG12	1:A:420:LEU:HD11	1.99	0.45
1:D:300:LEU:HD12	1:D:321:TYR:CE2	2.52	0.45
1:D:529:GLN:O	1:D:533:VAL:HG23	2.17	0.45
1:B:486:GLY:O	1:B:490:VAL:HG13	2.17	0.45
1:B:488:MET:O	1:B:492:ILE:HG12	2.16	0.45
1:B:590:PHE:HE1	1:B:668:LEU:HB3	1.82	0.45
1:A:195:GLU:HA	1:A:200:LEU:HD11	1.98	0.45
1:A:611:LYS:HA	1:A:611:LYS:HD3	1.42	0.45
1:D:671:ASN:HA	1:D:674:ILE:HG12	1.99	0.45
1:B:322:ASP:O	1:B:326:LEU:HG	2.16	0.45
1:B:330:ASN:N	1:B:330:ASN:OD1	2.50	0.45
1:A:444:SER:OG	1:A:565:TYR:OH	2.24	0.45
1:D:330:ASN:N	1:D:330:ASN:OD1	2.50	0.45
1:B:601:PHE:CG	1:B:661:TYR:HB2	2.52	0.44
1:B:670:LEU:O	1:B:674:ILE:HG23	2.17	0.44
1:C:200:LEU:O	1:C:204:ILE:HG22	2.17	0.44
1:B:581:LYS:HA	1:B:581:LYS:HD3	1.72	0.44
1:B:133:GLU:O	1:B:136:VAL:HG22	2.17	0.44
1:B:560:ALA:HB2	2:B:1101:EQK:C25	2.47	0.44
1:C:166:ASP:OD1	1:C:167:THR:N	2.47	0.44
1:C:349:ALA:HB2	1:C:403:VAL:HG13	1.99	0.44
1:C:590:PHE:HE1	1:C:668:LEU:HB3	1.82	0.44
1:D:288:ASP:O	1:D:291:SER:OG	2.26	0.44
1:D:405:GLU:O	1:D:409:TYR:HB2	2.17	0.44
1:D:533:VAL:HG22	1:D:554:ALA:HB1	1.99	0.44
1:D:583:ILE:HA	1:D:587:VAL:HG12	1.99	0.44
1:C:133:GLU:O	1:C:136:VAL:HG22	2.17	0.44
1:A:330:ASN:OD1	1:A:330:ASN:N	2.50	0.44
1:A:674:ILE:HD13	1:A:674:ILE:HA	1.81	0.44
1:B:704:GLU:O	1:B:712:ARG:HD2	2.18	0.44
1:C:308:GLU:H	1:C:313:GLN:NE2	2.16	0.44
1:A:200:LEU:O	1:A:204:ILE:HG22	2.17	0.44
1:C:321:TYR:HE1	1:C:325:LEU:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:605:LEU:HG	1:D:654:PHE:CE1	2.52	0.44
1:C:162:LEU:HD12	1:C:162:LEU:HA	1.89	0.43
1:C:572:MET:HB2	1:C:572:MET:HE2	1.87	0.43
1:D:308:GLU:H	1:D:313:GLN:NE2	2.16	0.43
1:B:376:LYS:HB2	1:B:390:TYR:CD1	2.53	0.43
1:B:603:VAL:HG23	1:A:460:TYR:HB2	1.99	0.43
1:A:133:GLU:O	1:A:136:VAL:HG22	2.17	0.43
1:A:451:TYR:OH	1:A:533:VAL:HG21	2.18	0.43
1:A:588:LEU:HD23	1:A:588:LEU:HA	1.82	0.43
1:B:343:THR:O	1:B:347:LEU:N	2.40	0.43
1:B:567:ARG:NH2	1:B:695:GLN:HB3	2.34	0.43
1:B:586:ASP:O	1:B:589:LYS:HG2	2.19	0.43
1:A:441:PHE:HB2	1:A:703:PHE:HE2	1.82	0.43
1:D:540:TYR:HB2	1:D:547:TYR:CD2	2.53	0.43
1:A:321:TYR:HE1	1:A:325:LEU:HD22	1.83	0.43
1:A:599:LEU:O	1:A:603:VAL:HG12	2.18	0.43
1:A:663:ILE:HG22	1:A:664:LEU:HD23	2.00	0.43
1:D:292:ARG:HA	1:D:297:ASN:O	2.18	0.43
1:C:567:ARG:NH1	1:C:577:VAL:HG23	2.33	0.43
1:D:227:GLN:HB3	1:D:230:ILE:HD13	2.01	0.43
1:B:540:TYR:HB2	1:B:547:TYR:CD2	2.53	0.43
1:C:583:ILE:HD12	2:C:1101:EQK:C18	2.48	0.43
1:A:156:ASP:OD1	1:A:156:ASP:N	2.51	0.43
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.74	0.43
1:A:408:VAL:O	1:A:416:ARG:NH1	2.52	0.43
1:A:595:ILE:HD13	1:A:595:ILE:HA	1.87	0.43
1:D:441:PHE:HB2	1:D:703:PHE:HE2	1.83	0.43
1:D:581:LYS:HA	1:D:581:LYS:HD3	1.54	0.43
1:D:612:CYS:SG	1:D:647:ASN:CG	2.97	0.43
1:C:154:VAL:HB	1:C:155:PRO:HD3	2.01	0.43
1:C:418:GLU:O	1:C:421:THR:OG1	2.36	0.43
1:C:633:PHE:CE2	1:C:637:ILE:CD1	3.00	0.43
1:C:704:GLU:O	1:C:712:ARG:HD2	2.19	0.43
1:D:408:VAL:HG12	1:D:420:LEU:HD11	2.01	0.43
1:C:441:PHE:HB2	1:C:703:PHE:HE2	1.82	0.43
1:A:603:VAL:HG23	1:D:460:TYR:HB2	2.00	0.43
1:D:147:ARG:HA	1:D:157:PHE:HE2	1.83	0.43
1:B:405:GLU:O	1:B:409:TYR:HB2	2.18	0.43
1:B:588:LEU:HD23	1:B:588:LEU:HA	1.80	0.43
1:C:298:ASN:H	1:C:301:HIS:CD2	2.36	0.43
1:C:577:VAL:HG21	1:C:691:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:TYR:CZ	1:D:526:PHE:HE1	2.37	0.43
1:B:321:TYR:HE1	1:B:325:LEU:HD22	1.83	0.43
1:C:362:SER:O	1:C:362:SER:OG	2.29	0.43
1:C:390:TYR:CE2	1:C:734:ILE:HD12	2.54	0.43
1:C:410:ASN:O	1:C:416:ARG:NH1	2.51	0.43
1:A:548:LEU:O	1:A:552:VAL:HG12	2.19	0.43
1:D:582:VAL:HG22	1:D:676:LEU:HD11	2.01	0.43
1:B:156:ASP:N	1:B:156:ASP:OD1	2.51	0.42
1:B:625:PHE:O	1:B:629:VAL:HG23	2.18	0.42
1:B:667:VAL:HG11	1:A:583:ILE:HD11	2.01	0.42
1:C:260:TYR:CD1	1:C:295:ARG:NH2	2.87	0.42
1:A:625:PHE:O	1:A:629:VAL:HG23	2.18	0.42
1:D:133:GLU:O	1:D:136:VAL:HG22	2.18	0.42
1:D:392:LEU:HD13	1:D:396:ASP:HB3	2.01	0.42
1:D:649:LYS:HB3	1:D:649:LYS:HE2	1.78	0.42
1:B:603:VAL:HG21	1:A:456:THR:HG23	2.01	0.42
1:B:666:PHE:HE2	1:A:669:LEU:HD11	1.84	0.42
1:C:292:ARG:HA	1:C:297:ASN:O	2.19	0.42
1:A:126:ALA:HB1	1:A:136:VAL:HG12	2.00	0.42
1:A:307:ALA:HB2	1:A:317:VAL:HG21	2.00	0.42
1:D:156:ASP:N	1:D:156:ASP:OD1	2.51	0.42
1:D:611:LYS:HA	1:D:611:LYS:HD3	1.48	0.42
1:B:390:TYR:CE2	1:B:734:ILE:HD12	2.54	0.42
1:B:408:VAL:HG12	1:B:420:LEU:HD11	2.01	0.42
1:D:223:ILE:HB	1:D:268:LEU:HD23	2.01	0.42
1:D:377:PHE:CZ	1:D:723:VAL:HG21	2.54	0.42
1:D:577:VAL:HG21	1:D:691:ILE:CG2	2.49	0.42
1:D:704:GLU:O	1:D:712:ARG:HD2	2.19	0.42
1:B:166:ASP:OD1	1:B:167:THR:N	2.47	0.42
1:B:591:LEU:O	1:B:595:ILE:HG12	2.19	0.42
1:C:674:ILE:HG13	1:C:675:ALA:N	2.34	0.42
1:A:298:ASN:H	1:A:301:HIS:CD2	2.38	0.42
1:D:154:VAL:HB	1:D:155:PRO:HD3	2.02	0.42
1:B:158:LEU:O	1:B:162:LEU:HB2	2.18	0.42
1:C:564:TYR:HE1	1:C:695:GLN:OE1	2.03	0.42
1:A:167:THR:O	1:A:209:THR:N	2.52	0.42
1:A:484:LEU:O	1:A:488:MET:HG2	2.19	0.42
1:D:390:TYR:CE2	1:D:734:ILE:HD12	2.54	0.42
1:D:562:MET:O	1:D:566:THR:HG23	2.19	0.42
1:B:456:THR:HG23	1:C:603:VAL:HG21	2.01	0.42
1:B:583:ILE:HG21	2:B:1101:EQK:C14	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ILE:HD13	1:B:583:ILE:HA	1.94	0.42
1:C:495:MET:O	1:C:499:VAL:HG23	2.20	0.42
1:D:597:PHE:CE2	1:D:664:LEU:HB3	2.54	0.42
1:C:634:LYS:HA	1:C:637:ILE:HG13	2.01	0.42
1:A:173:MET:O	1:A:177:LEU:HD12	2.20	0.42
1:B:441:PHE:HB2	1:B:703:PHE:HE2	1.84	0.42
1:B:636:THR:OG1	1:B:661:TYR:OH	2.27	0.42
1:A:308:GLU:H	1:A:313:GLN:NE2	2.16	0.42
1:B:219:LEU:HD23	1:B:219:LEU:HA	1.74	0.42
1:A:680:THR:HG22	1:A:684:VAL:HB	2.02	0.42
1:B:292:ARG:HA	1:B:297:ASN:O	2.20	0.41
1:B:300:LEU:CD2	1:B:333:LEU:HD13	2.50	0.41
1:B:418:GLU:O	1:B:421:THR:OG1	2.34	0.41
1:D:548:LEU:O	1:D:552:VAL:HG12	2.20	0.41
1:C:548:LEU:O	1:C:552:VAL:HG12	2.20	0.41
1:A:214:GLU:HB3	1:A:247:GLY:HA2	2.02	0.41
1:A:390:TYR:CE2	1:A:734:ILE:HD12	2.55	0.41
1:A:493:TRP:O	1:A:497:ILE:HG12	2.20	0.41
1:D:260:TYR:CD1	1:D:295:ARG:NH2	2.88	0.41
1:B:298:ASN:H	1:B:301:HIS:CD2	2.38	0.41
1:C:364:GLU:O	1:C:365:ILE:HD13	2.21	0.41
1:C:408:VAL:HG12	1:C:420:LEU:HD11	2.02	0.41
1:C:420:LEU:HD23	1:C:420:LEU:HA	1.83	0.41
1:A:200:LEU:HD12	1:A:200:LEU:H	1.86	0.41
1:D:307:ALA:HB2	1:D:317:VAL:HG21	2.02	0.41
1:D:598:LEU:CD1	1:D:632:LEU:HB3	2.51	0.41
1:D:620:SER:OG	1:D:646:GLN:HA	2.20	0.41
1:B:408:VAL:O	1:B:416:ARG:NH1	2.54	0.41
1:C:219:LEU:HD12	1:C:219:LEU:HA	1.80	0.41
1:C:307:ALA:HB2	1:C:317:VAL:HG21	2.01	0.41
1:D:199:ILE:HD12	1:D:199:ILE:HA	1.91	0.41
1:C:553:LEU:HD12	1:C:553:LEU:HA	1.92	0.41
1:A:154:VAL:HB	1:A:155:PRO:HD3	2.02	0.41
1:D:493:TRP:O	1:D:497:ILE:HG12	2.20	0.41
1:C:298:ASN:ND2	1:C:336:THR:OG1	2.53	0.41
1:A:504:ALA:O	1:A:507:LEU:HD22	2.20	0.41
1:D:298:ASN:H	1:D:301:HIS:CD2	2.38	0.41
1:D:598:LEU:HD11	1:D:632:LEU:HB2	2.02	0.41
1:B:484:LEU:HD23	1:B:484:LEU:HA	1.78	0.41
1:B:548:LEU:O	1:B:552:VAL:HG12	2.20	0.41
1:C:376:LYS:HB2	1:C:390:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:581:LYS:HA	1:C:581:LYS:HD3	1.51	0.41
1:D:162:LEU:HD12	1:D:162:LEU:HA	1.89	0.41
1:D:326:LEU:HD21	1:D:365:ILE:HG13	2.02	0.41
1:D:349:ALA:HB2	1:D:403:VAL:HG13	2.03	0.41
1:B:553:LEU:HD12	1:B:553:LEU:HA	1.91	0.41
1:B:752:ASP:HB2	1:C:213:TYR:OH	2.20	0.41
1:C:172:LEU:O	1:C:176:LEU:HG	2.21	0.41
1:C:214:GLU:HB3	1:C:247:GLY:HA2	2.02	0.41
1:C:456:THR:HG23	1:D:603:VAL:HG11	2.03	0.41
1:A:364:GLU:O	1:A:365:ILE:HD13	2.21	0.41
1:A:452:ASN:HD21	1:A:559:TRP:HA	1.86	0.41
1:D:169:LYS:HA	1:D:173:MET:SD	2.61	0.41
1:D:303:LEU:HD23	1:D:303:LEU:HA	1.90	0.41
1:B:154:VAL:HB	1:B:155:PRO:HD3	2.01	0.41
1:C:567:ARG:HH11	1:C:577:VAL:HG23	1.85	0.41
1:A:292:ARG:HA	1:A:297:ASN:O	2.20	0.41
1:A:591:LEU:HD13	1:A:591:LEU:HA	1.95	0.41
1:D:307:ALA:O	1:D:353:LYS:HD2	2.21	0.41
1:B:167:THR:O	1:B:209:THR:N	2.54	0.40
1:B:529:GLN:O	1:B:533:VAL:HG23	2.21	0.40
2:B:1101:EQK:S01	2:B:1101:EQK:O07	2.79	0.40
1:A:166:ASP:OD1	1:A:167:THR:N	2.49	0.40
1:A:377:PHE:HZ	1:A:729:ARG:NH2	2.19	0.40
1:A:570:GLN:O	1:A:573:SER:HB3	2.21	0.40
1:C:405:GLU:O	1:C:409:TYR:HB2	2.22	0.40
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.84	0.40
2:A:1101:EQK:O07	2:A:1101:EQK:S01	2.79	0.40
1:D:586:ASP:O	1:D:589:LYS:HG2	2.21	0.40
1:B:162:LEU:HD12	1:B:162:LEU:HA	1.89	0.40
1:B:301:HIS:O	1:B:305:THR:OG1	2.35	0.40
1:B:307:ALA:O	1:B:353:LYS:HD2	2.22	0.40
1:C:307:ALA:O	1:C:353:LYS:HD2	2.21	0.40
1:C:581:LYS:O	1:C:585:HIS:HB2	2.20	0.40
1:C:592:PHE:O	1:C:596:VAL:HG23	2.21	0.40
1:C:612:CYS:SG	1:C:619:CYS:CB	3.03	0.40
1:C:636:THR:OG1	1:C:661:TYR:OH	2.23	0.40
1:A:300:LEU:CD2	1:A:333:LEU:HD13	2.51	0.40
1:A:495:MET:O	1:A:499:VAL:HG23	2.21	0.40
1:D:637:ILE:HG13	1:D:637:ILE:O	2.21	0.40
1:B:633:PHE:HE2	1:C:642:LEU:CD2	2.33	0.40
1:C:493:TRP:HA	1:C:493:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:LYS:HB3	1:C:649:LYS:HE2	1.74	0.40
1:A:577:VAL:HG11	1:A:688:SER:HA	2.04	0.40
1:B:214:GLU:HB3	1:B:247:GLY:HA2	2.03	0.40
1:B:546:GLU:OE1	1:B:546:GLU:N	2.52	0.40
1:C:300:LEU:HA	1:C:300:LEU:HD13	1.88	0.40
1:A:307:ALA:O	1:A:353:LYS:HD2	2.21	0.40
1:A:328:SER:O	1:A:328:SER:OG	2.30	0.40
1:A:674:ILE:HD11	1:D:676:LEU:HG	2.03	0.40
1:D:545:LYS:HA	1:D:545:LYS:HD3	1.89	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	597/1061 (56%)	556 (93%)	41 (7%)	0	100	100
1	B	597/1061 (56%)	555 (93%)	42 (7%)	0	100	100
1	C	597/1061 (56%)	557 (93%)	40 (7%)	0	100	100
1	D	597/1061 (56%)	554 (93%)	43 (7%)	0	100	100
All	All	2388/4244 (56%)	2222 (93%)	166 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	433/934 (46%)	424 (98%)	9 (2%)	53	77
1	B	436/934 (47%)	435 (100%)	1 (0%)	93	98
1	C	433/934 (46%)	426 (98%)	7 (2%)	62	82
1	D	433/934 (46%)	425 (98%)	8 (2%)	59	80
All	All	1735/3736 (46%)	1710 (99%)	25 (1%)	68	84

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	213	TYR
1	C	213	TYR
1	C	264	THR
1	C	416	ARG
1	C	597	PHE
1	C	609	ILE
1	C	637	ILE
1	C	692	TRP
1	A	213	TYR
1	A	264	THR
1	A	577	VAL
1	A	611	LYS
1	A	620	SER
1	A	671	ASN
1	A	676	LEU
1	A	692	TRP
1	A	704	GLU
1	D	213	TYR
1	D	264	THR
1	D	451	TYR
1	D	597	PHE
1	D	611	LYS
1	D	619	CYS
1	D	620	SER
1	D	692	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	205	ASN
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	284	HIS
1	B	301	HIS
1	B	313	GLN
1	B	346	GLN
1	B	452	ASN
1	B	483	GLN
1	B	647	ASN
1	C	178	ASN
1	C	244	HIS
1	C	279	GLN
1	C	284	HIS
1	C	301	HIS
1	C	313	GLN
1	C	346	GLN
1	C	452	ASN
1	C	570	GLN
1	C	646	GLN
1	A	279	GLN
1	A	284	HIS
1	A	297	ASN
1	A	301	HIS
1	A	313	GLN
1	A	346	GLN
1	A	452	ASN
1	A	570	GLN
1	A	646	GLN
1	D	205	ASN
1	D	279	GLN
1	D	284	HIS
1	D	301	HIS
1	D	313	GLN
1	D	346	GLN
1	D	452	ASN
1	D	570	GLN
1	D	646	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	EQK	C	1101	-	29,35,35	4.87	19 (65%)	33,52,52	2.33	13 (39%)
2	EQK	B	1101	-	29,35,35	4.87	19 (65%)	33,52,52	2.28	13 (39%)
2	EQK	A	1101	-	29,35,35	4.86	19 (65%)	33,52,52	2.28	13 (39%)
2	EQK	D	1101	-	29,35,35	4.81	19 (65%)	33,52,52	2.16	10 (30%)

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	EQK	C	1101	-	-	3/26/31/31	0/3/3/3
2	EQK	B	1101	-	-	4/26/31/31	0/3/3/3
2	EQK	A	1101	-	-	6/26/31/31	0/3/3/3
2	EQK	D	1101	-	-	8/26/31/31	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	EQK	C31-N12	8.46	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	EQK	C31-N12	8.44	1.49	1.33
2	A	1101	EQK	C31-N12	8.44	1.49	1.33
2	C	1101	EQK	C31-N13	8.40	1.49	1.33
2	A	1101	EQK	C31-N13	8.40	1.49	1.33
2	D	1101	EQK	C31-N12	8.39	1.49	1.33
2	B	1101	EQK	C31-N13	8.36	1.49	1.33
2	D	1101	EQK	C31-N13	8.26	1.49	1.33
2	D	1101	EQK	C17-C15	7.83	1.53	1.39
2	C	1101	EQK	C17-C15	7.63	1.53	1.39
2	B	1101	EQK	C17-C15	7.59	1.53	1.39
2	A	1101	EQK	C17-C15	7.53	1.53	1.39
2	B	1101	EQK	C21-C24	7.21	1.53	1.38
2	C	1101	EQK	C21-C24	7.19	1.53	1.38
2	A	1101	EQK	C21-C24	7.18	1.53	1.38
2	B	1101	EQK	C30-N13	7.07	1.45	1.32
2	A	1101	EQK	C30-N13	7.07	1.45	1.32
2	C	1101	EQK	C30-N13	7.06	1.45	1.32
2	B	1101	EQK	C29-N12	6.98	1.45	1.32
2	D	1101	EQK	C21-C24	6.98	1.52	1.38
2	A	1101	EQK	C29-N12	6.97	1.45	1.32
2	C	1101	EQK	C29-N12	6.96	1.45	1.32
2	C	1101	EQK	C24-N08	6.88	1.49	1.34
2	D	1101	EQK	C29-N12	6.87	1.45	1.32
2	B	1101	EQK	C24-N08	6.86	1.49	1.34
2	A	1101	EQK	C15-N08	6.85	1.49	1.34
2	A	1101	EQK	C24-N08	6.85	1.49	1.34
2	B	1101	EQK	C15-N08	6.85	1.49	1.34
2	C	1101	EQK	C15-N08	6.84	1.49	1.34
2	D	1101	EQK	C30-N13	6.81	1.45	1.32
2	D	1101	EQK	C24-N08	6.78	1.48	1.34
2	D	1101	EQK	C15-N08	6.77	1.48	1.34
2	C	1101	EQK	C28-C29	5.89	1.49	1.41
2	A	1101	EQK	C28-C30	5.85	1.49	1.41
2	B	1101	EQK	C28-C29	5.84	1.49	1.41
2	C	1101	EQK	C28-C30	5.84	1.49	1.41
2	A	1101	EQK	C28-C29	5.82	1.49	1.41
2	B	1101	EQK	C28-C30	5.82	1.49	1.41
2	B	1101	EQK	C17-C16	5.72	1.49	1.39
2	A	1101	EQK	C17-C16	5.71	1.49	1.39
2	C	1101	EQK	C17-C16	5.70	1.49	1.39
2	D	1101	EQK	C28-C30	5.68	1.49	1.41
2	D	1101	EQK	C17-C16	5.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	EQK	C28-C29	5.57	1.48	1.41
2	D	1101	EQK	C25-N10	5.26	1.45	1.36
2	A	1101	EQK	C25-N10	5.21	1.45	1.36
2	B	1101	EQK	C25-N10	5.20	1.45	1.36
2	B	1101	EQK	C16-C20	5.13	1.53	1.48
2	D	1101	EQK	C16-C20	5.11	1.53	1.48
2	C	1101	EQK	C25-N10	5.09	1.45	1.36
2	A	1101	EQK	C16-C20	4.99	1.53	1.48
2	C	1101	EQK	C16-C20	4.99	1.53	1.48
2	C	1101	EQK	C21-C16	4.87	1.49	1.39
2	B	1101	EQK	C21-C16	4.82	1.49	1.39
2	A	1101	EQK	C21-C16	4.81	1.49	1.39
2	D	1101	EQK	C21-C16	4.71	1.49	1.39
2	B	1101	EQK	C22-N09	4.18	1.57	1.36
2	C	1101	EQK	C22-N09	4.18	1.57	1.36
2	A	1101	EQK	C22-N09	4.17	1.57	1.36
2	D	1101	EQK	C22-N09	4.04	1.56	1.36
2	D	1101	EQK	C27-N10	3.77	1.45	1.35
2	B	1101	EQK	C27-N10	3.74	1.45	1.35
2	A	1101	EQK	C27-N10	3.74	1.45	1.35
2	C	1101	EQK	C27-N10	3.71	1.45	1.35
2	A	1101	EQK	O05-C29	3.29	1.40	1.35
2	C	1101	EQK	O06-C30	3.28	1.40	1.35
2	B	1101	EQK	O05-C29	3.27	1.40	1.35
2	C	1101	EQK	O05-C29	3.27	1.40	1.35
2	B	1101	EQK	O06-C30	3.27	1.40	1.35
2	A	1101	EQK	O06-C30	3.24	1.40	1.35
2	D	1101	EQK	O05-C29	3.21	1.40	1.35
2	D	1101	EQK	O06-C30	3.01	1.39	1.35
2	D	1101	EQK	O07-C27	-2.39	1.18	1.23
2	A	1101	EQK	O07-C27	-2.22	1.18	1.23
2	B	1101	EQK	O07-C27	-2.21	1.18	1.23
2	C	1101	EQK	O07-C27	-2.17	1.18	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	EQK	N13-C31-N12	-5.78	119.55	128.60
2	C	1101	EQK	N13-C31-N12	-5.73	119.63	128.60
2	B	1101	EQK	N13-C31-N12	-5.71	119.67	128.60
2	A	1101	EQK	N13-C31-N12	-5.69	119.69	128.60
2	C	1101	EQK	C26-C22-N09	5.29	126.01	119.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	EQK	C26-C22-N09	5.17	125.87	119.69
2	B	1101	EQK	C26-C22-N09	5.17	125.87	119.69
2	D	1101	EQK	C33-O06-C30	-4.00	113.25	117.21
2	D	1101	EQK	C26-C22-N09	3.93	124.39	119.69
2	C	1101	EQK	C26-C22-C20	-3.64	125.83	129.29
2	D	1101	EQK	C21-C24-N08	-3.60	119.49	123.96
2	B	1101	EQK	C26-C22-C20	-3.42	126.04	129.29
2	B	1101	EQK	C33-O06-C30	-3.41	113.83	117.21
2	C	1101	EQK	C32-O05-C29	-3.40	113.84	117.21
2	A	1101	EQK	C26-C22-C20	-3.40	126.06	129.29
2	C	1101	EQK	C33-O06-C30	-3.36	113.88	117.21
2	B	1101	EQK	C32-O05-C29	-3.34	113.90	117.21
2	A	1101	EQK	C32-O05-C29	-3.34	113.90	117.21
2	A	1101	EQK	C33-O06-C30	-3.31	113.93	117.21
2	B	1101	EQK	C21-C24-N08	-3.23	119.94	123.96
2	A	1101	EQK	C21-C24-N08	-3.22	119.96	123.96
2	C	1101	EQK	C21-C24-N08	-3.21	119.97	123.96
2	D	1101	EQK	C32-O05-C29	-3.04	114.20	117.21
2	A	1101	EQK	C14-C15-N08	2.94	120.12	115.22
2	B	1101	EQK	C14-C15-N08	2.92	120.08	115.22
2	C	1101	EQK	C14-C15-N08	2.85	119.97	115.22
2	C	1101	EQK	C28-C27-N10	2.66	119.91	114.91
2	D	1101	EQK	C31-N13-C30	2.63	120.28	115.88
2	C	1101	EQK	C25-N10-C27	-2.60	120.21	126.64
2	A	1101	EQK	C31-N12-C29	2.57	120.19	115.88
2	C	1101	EQK	C31-N13-C30	2.56	120.18	115.88
2	C	1101	EQK	C31-N12-C29	2.56	120.17	115.88
2	B	1101	EQK	C31-N13-C30	2.55	120.15	115.88
2	D	1101	EQK	C31-N12-C29	2.54	120.14	115.88
2	B	1101	EQK	C31-N12-C29	2.53	120.12	115.88
2	B	1101	EQK	C28-C27-N10	2.52	119.65	114.91
2	A	1101	EQK	C31-N13-C30	2.52	120.11	115.88
2	A	1101	EQK	C28-C27-N10	2.50	119.61	114.91
2	D	1101	EQK	C26-C22-C20	-2.35	127.06	129.29
2	D	1101	EQK	C28-C27-N10	2.30	119.24	114.91
2	D	1101	EQK	C14-C15-N08	2.15	118.79	115.22
2	B	1101	EQK	C25-N10-C27	-2.12	121.40	126.64
2	A	1101	EQK	C25-N10-C27	-2.08	121.48	126.64
2	A	1101	EQK	C17-C15-N08	-2.08	119.93	123.31
2	C	1101	EQK	C24-N08-C15	2.06	120.31	117.49
2	C	1101	EQK	C17-C15-N08	-2.06	119.96	123.31
2	A	1101	EQK	C24-N08-C15	2.06	120.30	117.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	EQK	C24-N08-C15	2.05	120.29	117.49
2	B	1101	EQK	C17-C15-N08	-2.05	119.98	123.31

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	EQK	N12-C29-O05-C32
2	C	1101	EQK	O07-C27-C28-C29
2	A	1101	EQK	C28-C29-O05-C32
2	D	1101	EQK	N09-C22-C26-F04
2	B	1101	EQK	C28-C29-O05-C32
2	A	1101	EQK	N12-C29-O05-C32
2	C	1101	EQK	N10-C27-C28-C29
2	D	1101	EQK	N10-C27-C28-C30
2	D	1101	EQK	N09-C22-C26-F03
2	A	1101	EQK	O07-C27-C28-C30
2	D	1101	EQK	O07-C27-C28-C30
2	A	1101	EQK	N10-C27-C28-C30
2	D	1101	EQK	N09-C22-C26-F02
2	B	1101	EQK	C21-C16-C20-S01
2	A	1101	EQK	C21-C16-C20-S01
2	C	1101	EQK	C18-C14-C15-N08
2	D	1101	EQK	C18-C14-C15-N08
2	D	1101	EQK	C19-C14-C15-C17
2	D	1101	EQK	O07-C27-C28-C29
2	B	1101	EQK	N10-C27-C28-C30
2	A	1101	EQK	N10-C27-C28-C29

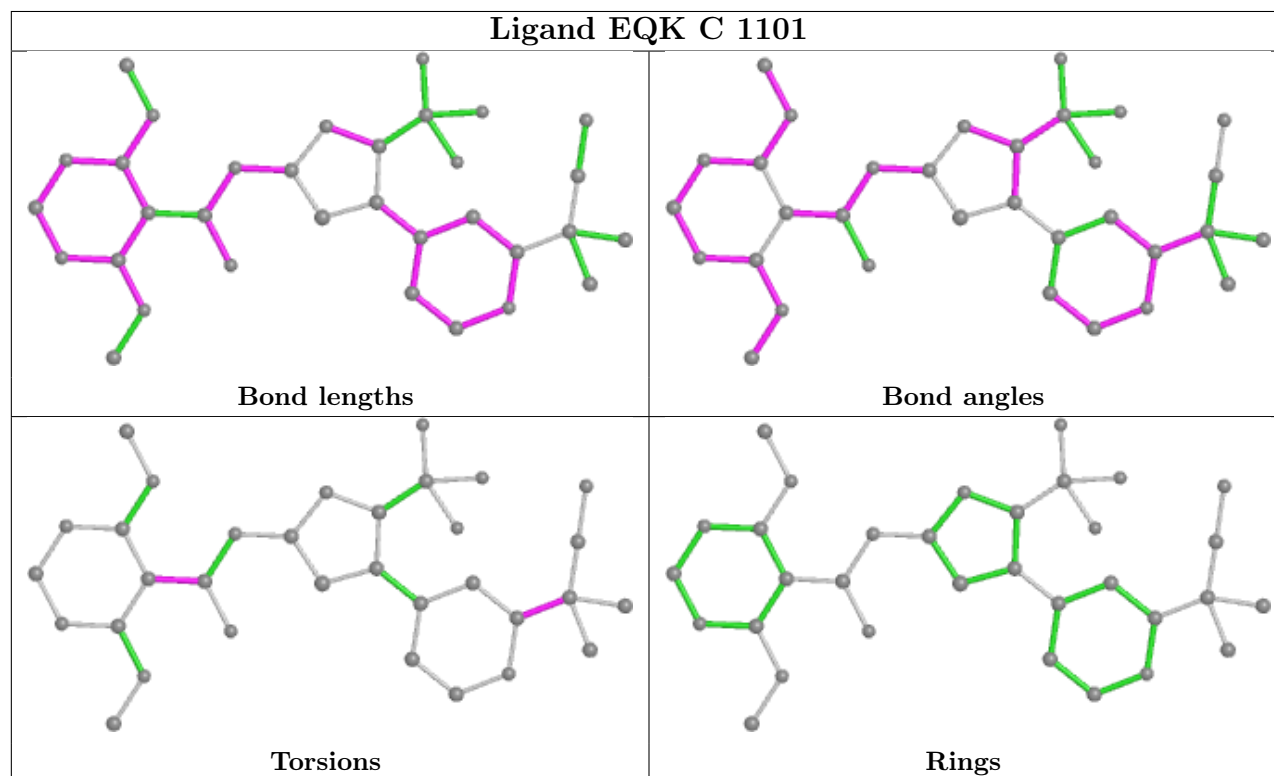
There are no ring outliers.

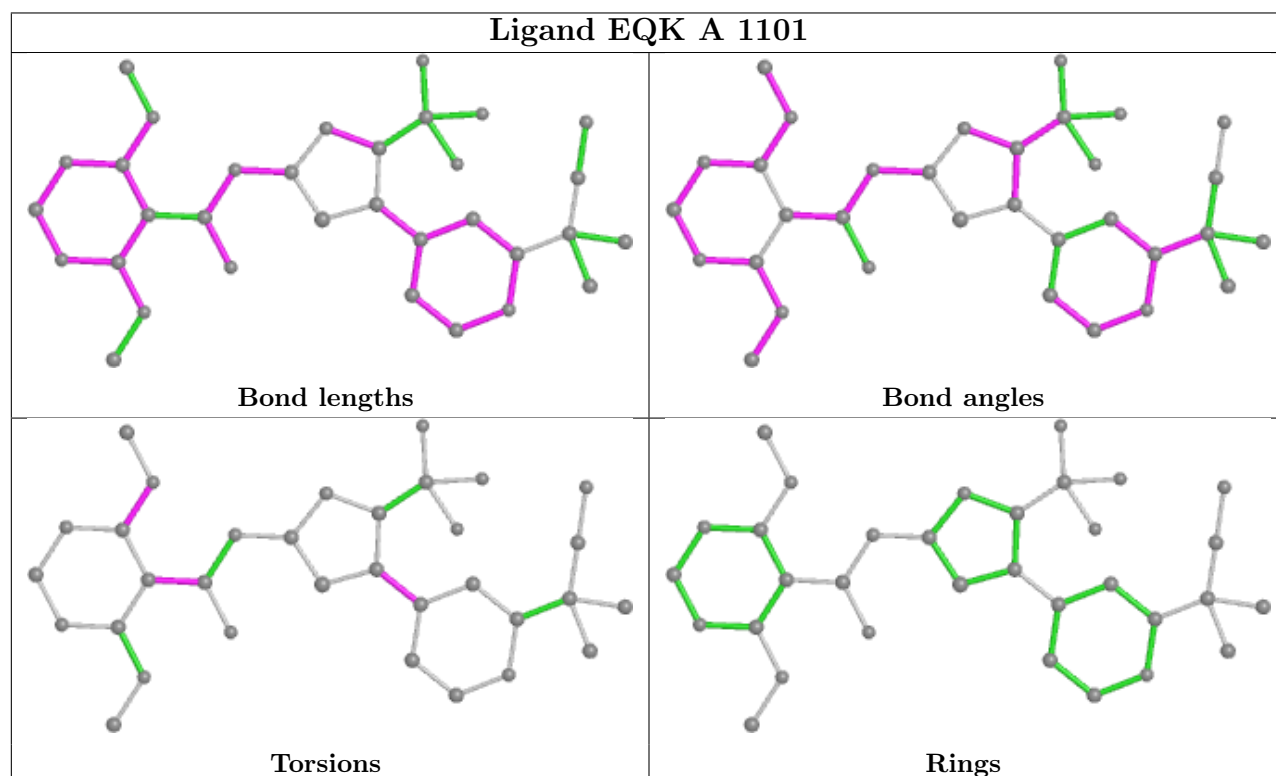
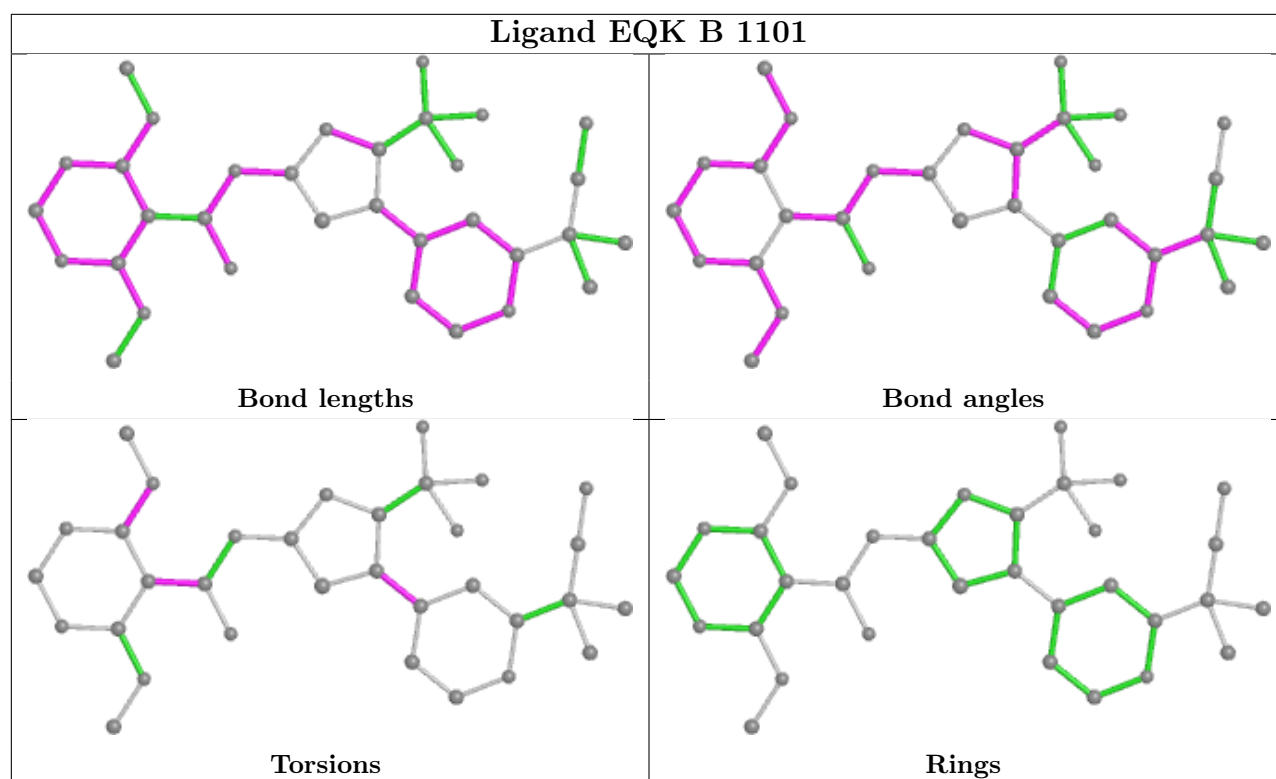
3 monomers are involved in 28 short contacts:

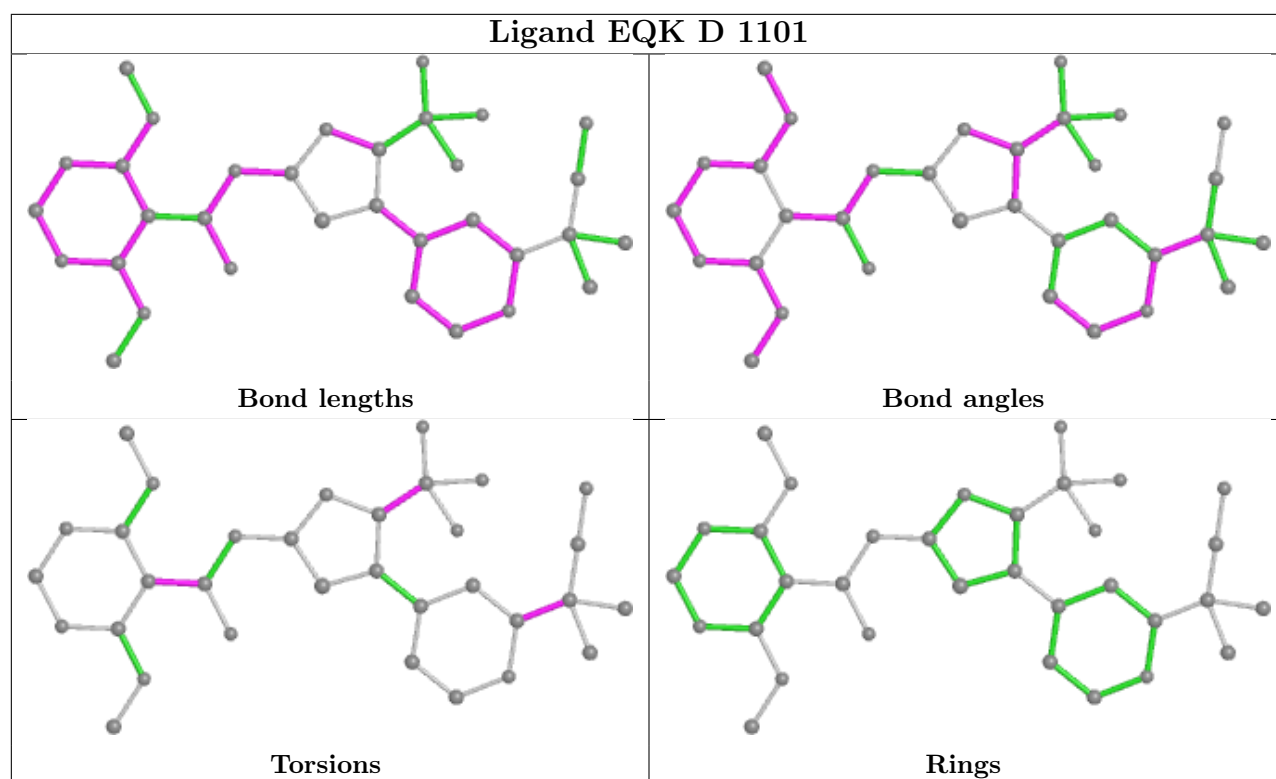
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	EQK	7	0
2	B	1101	EQK	11	0
2	A	1101	EQK	10	0

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.

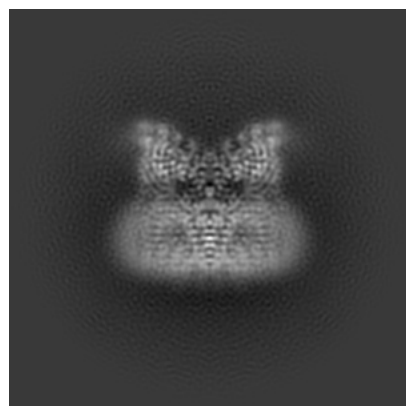
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33217. These allow visual inspection of the internal detail of the map and identification of artifacts.

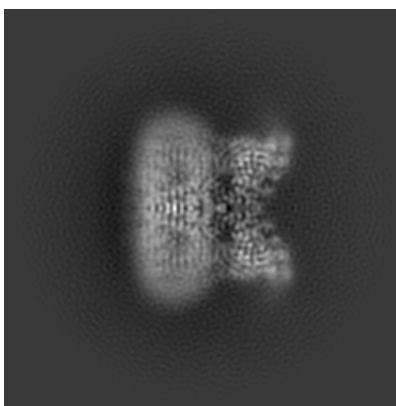
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

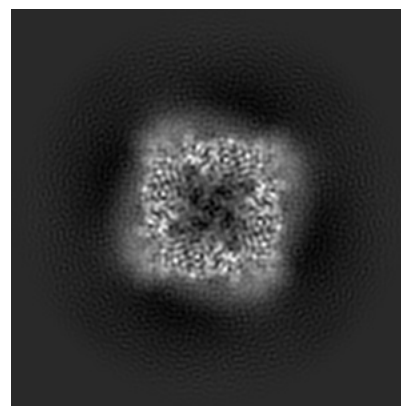
6.1.1 Primary map



X

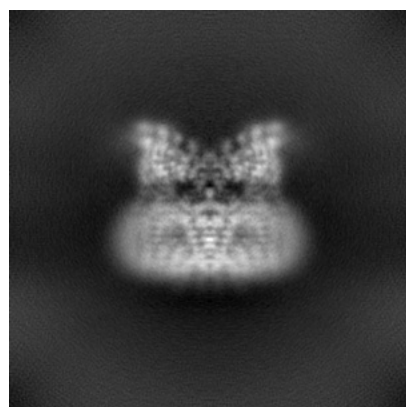


Y

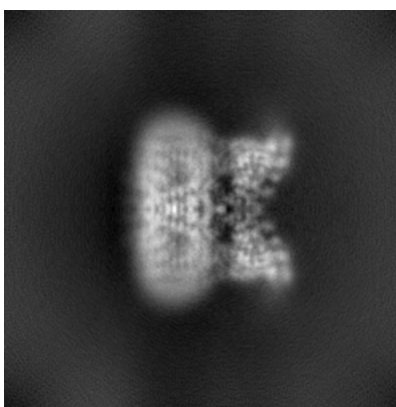


Z

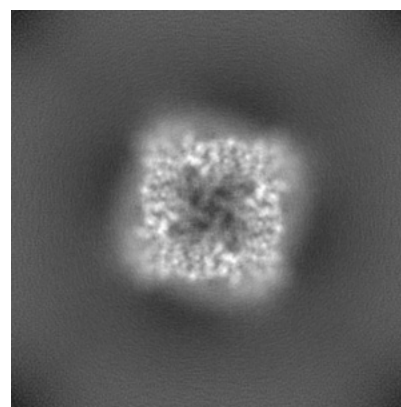
6.1.2 Raw map



X



Y

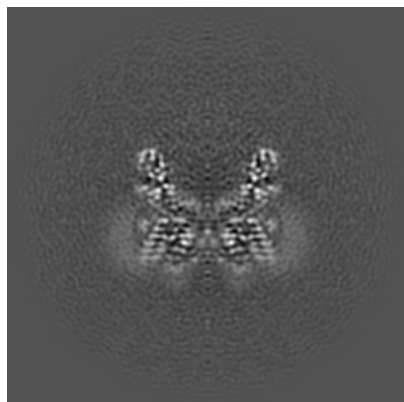


Z

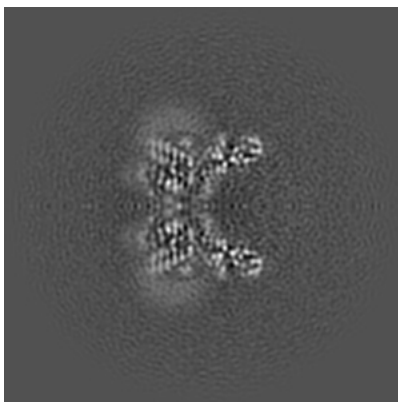
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

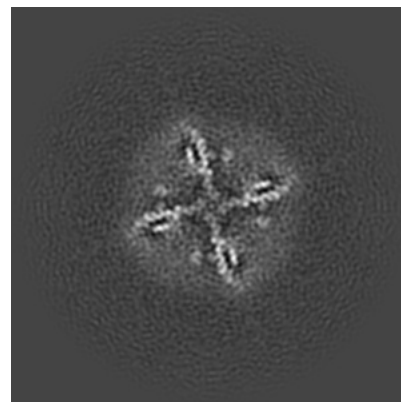
6.2.1 Primary map



X Index: 128

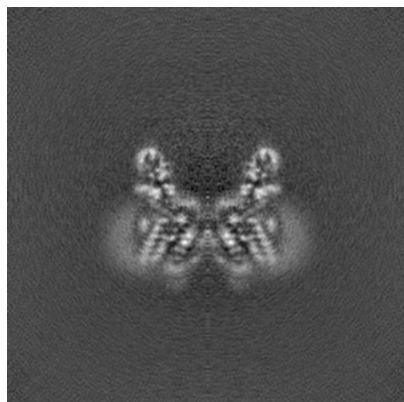


Y Index: 128

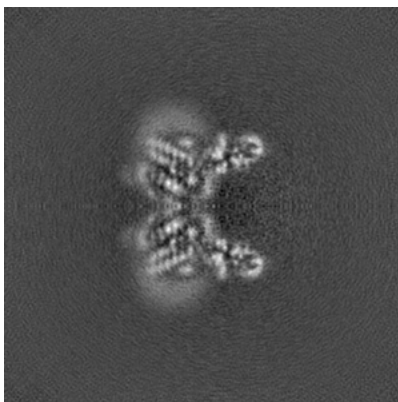


Z Index: 128

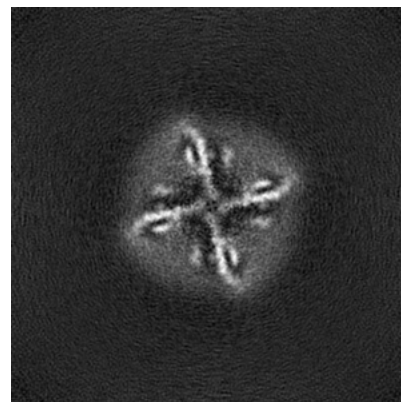
6.2.2 Raw map



X Index: 128



Y Index: 128

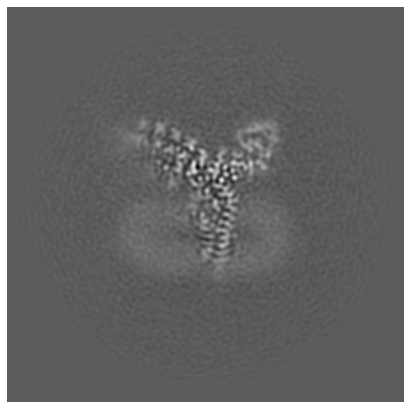


Z Index: 128

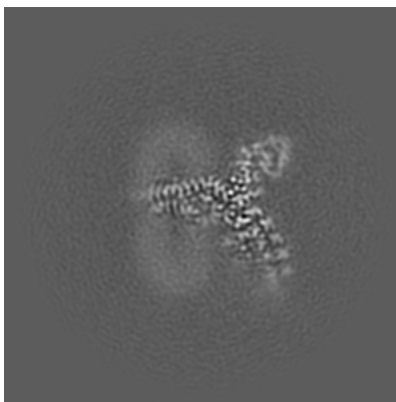
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

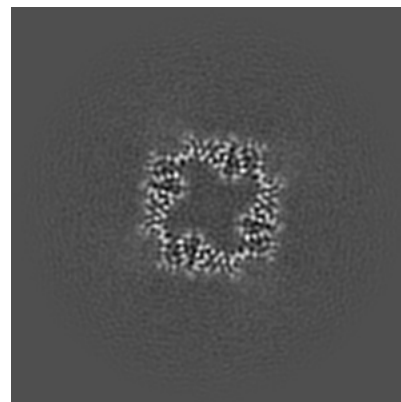
6.3.1 Primary map



X Index: 159

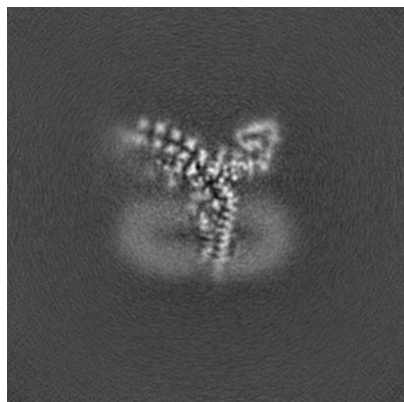


Y Index: 97

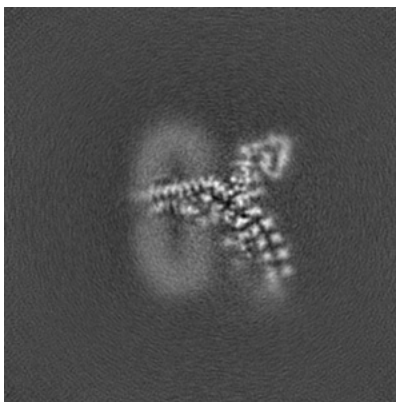


Z Index: 155

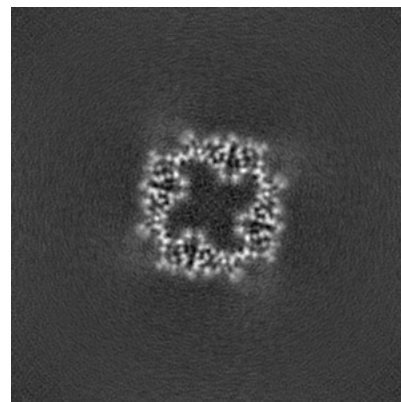
6.3.2 Raw map



X Index: 159



Y Index: 97

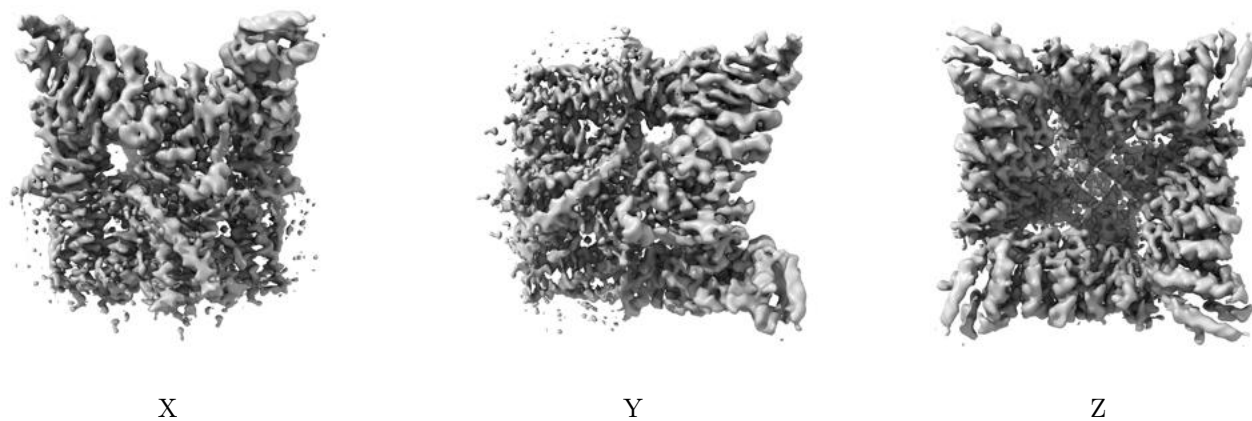


Z Index: 155

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

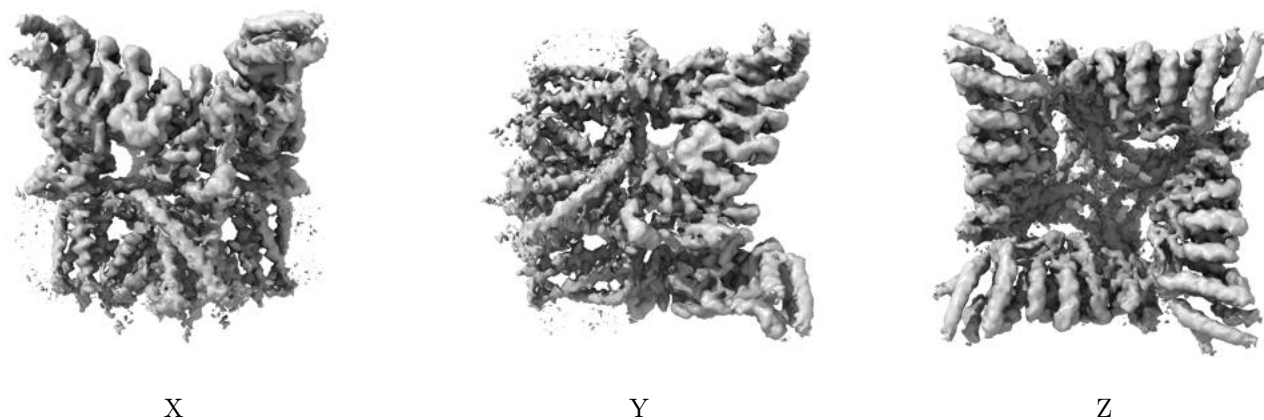
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

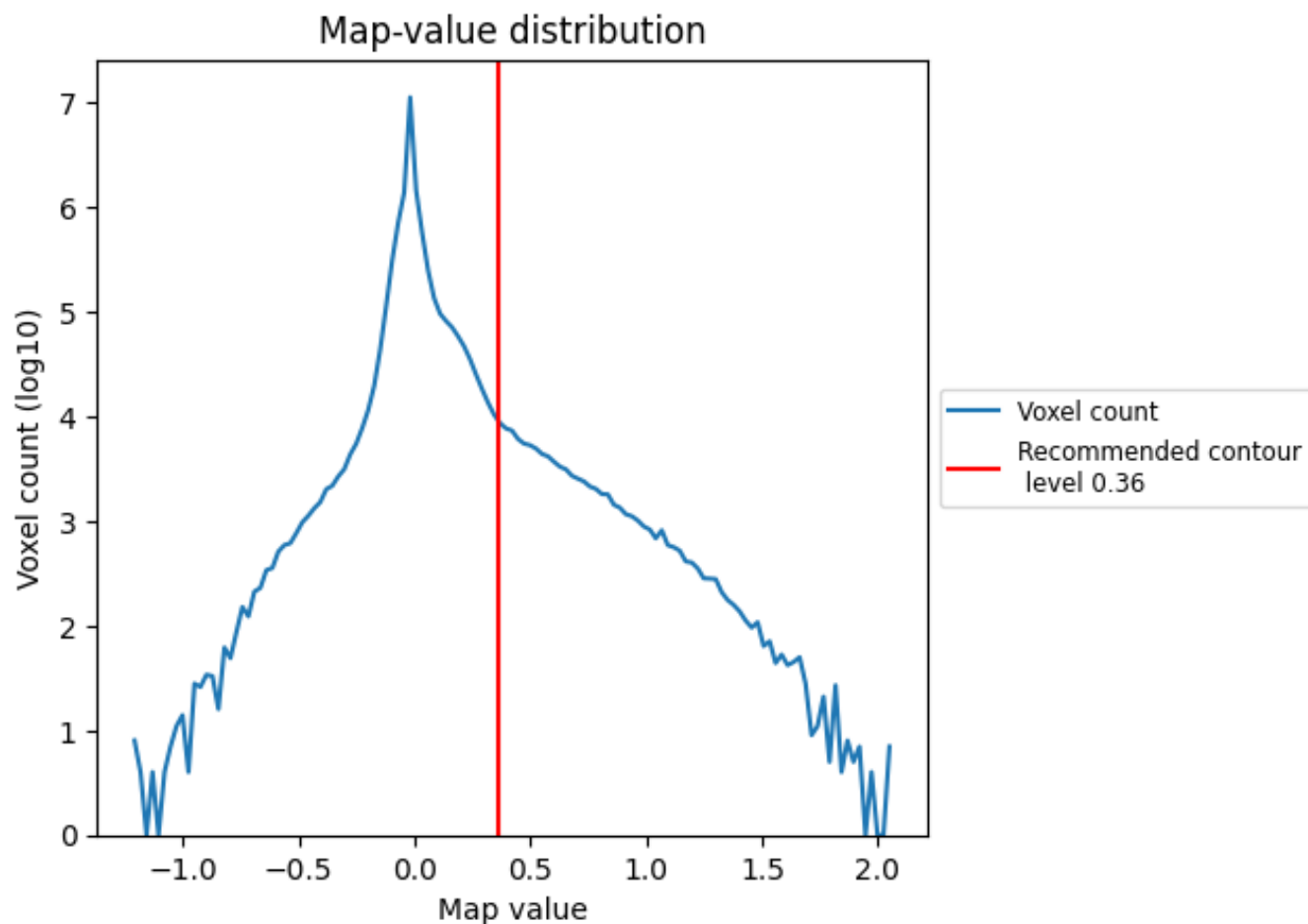
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

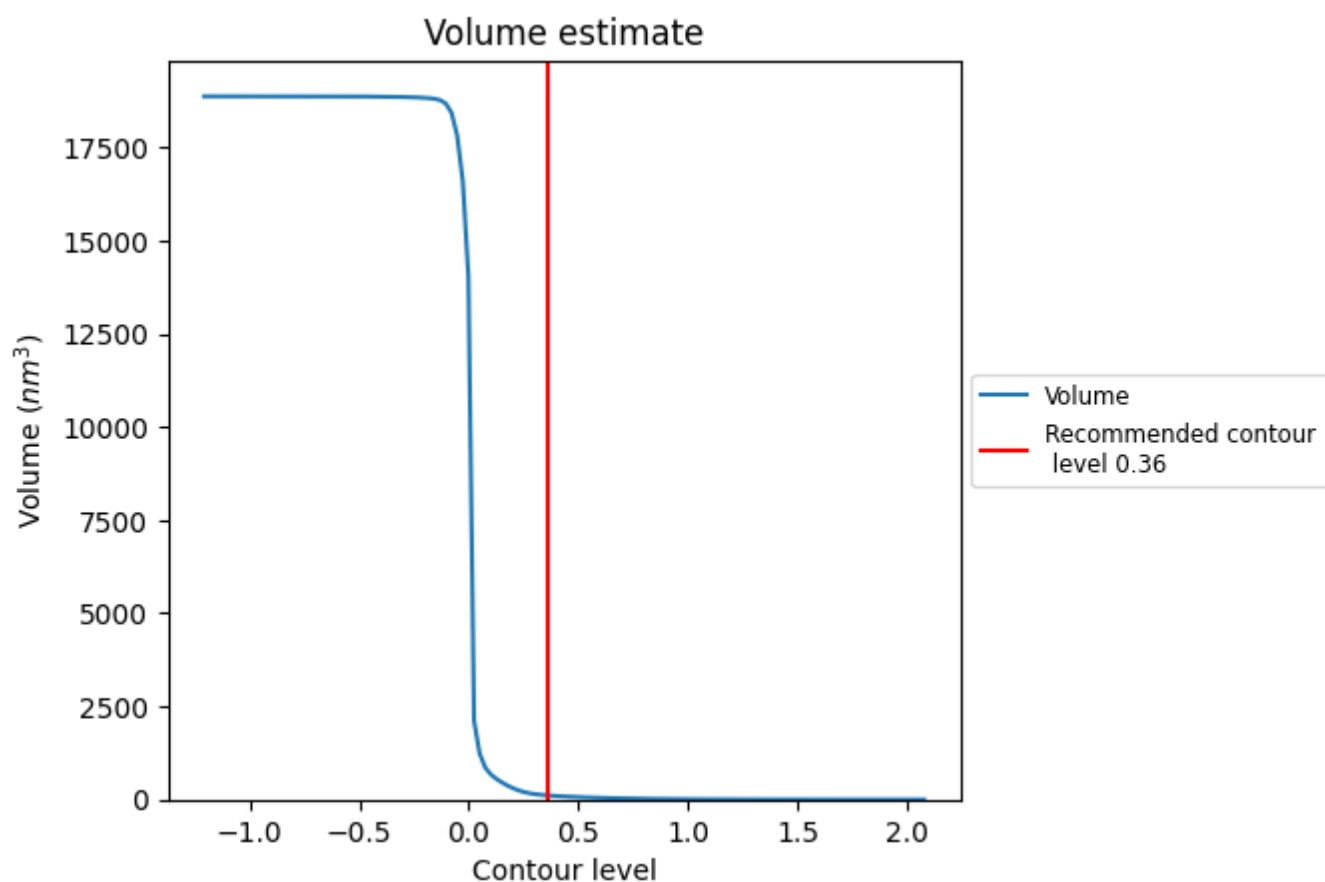
This section contains the results of statistical analysis of the map.

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.

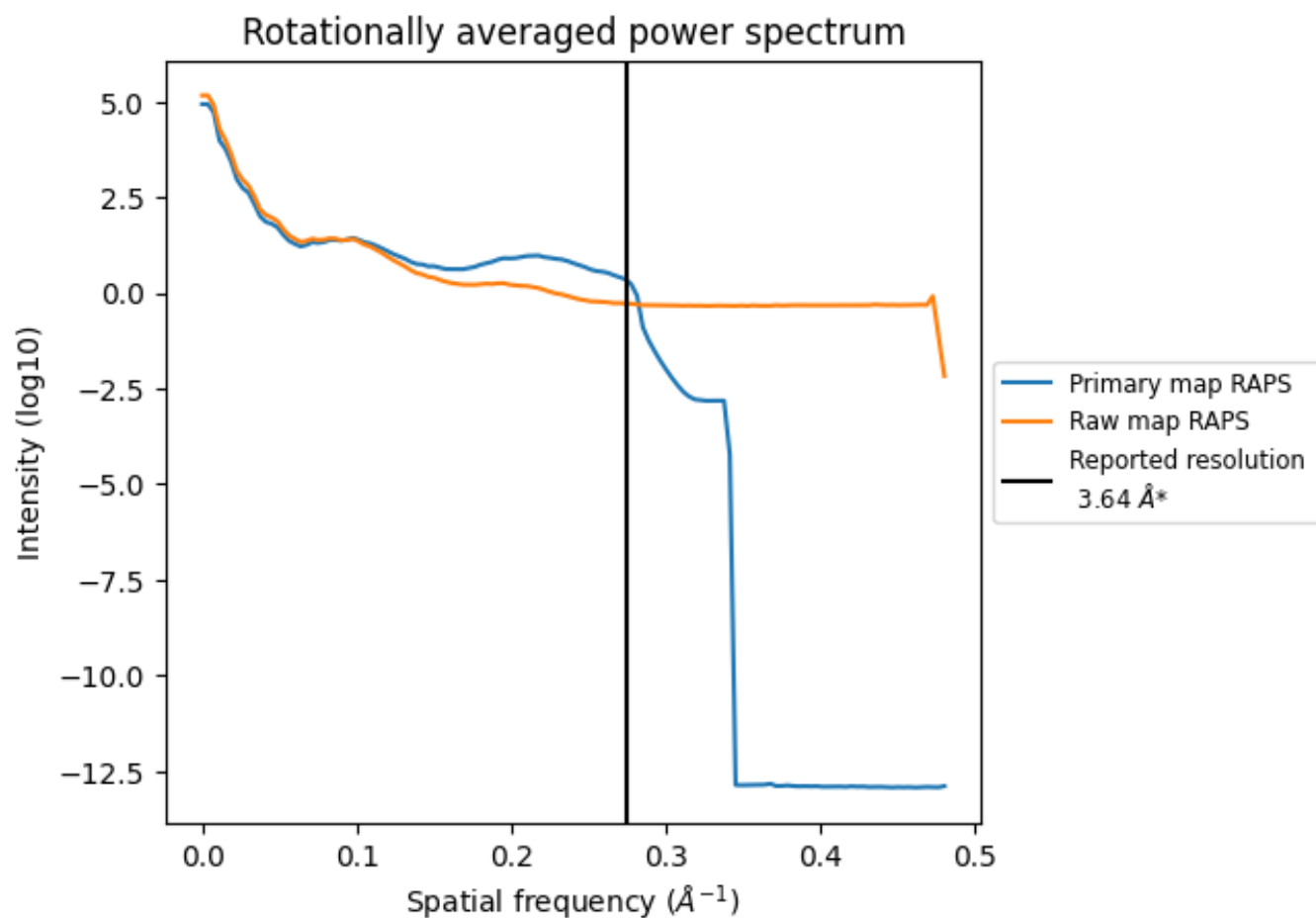
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm³; this corresponds to an approximate mass of 99 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 ⓘ

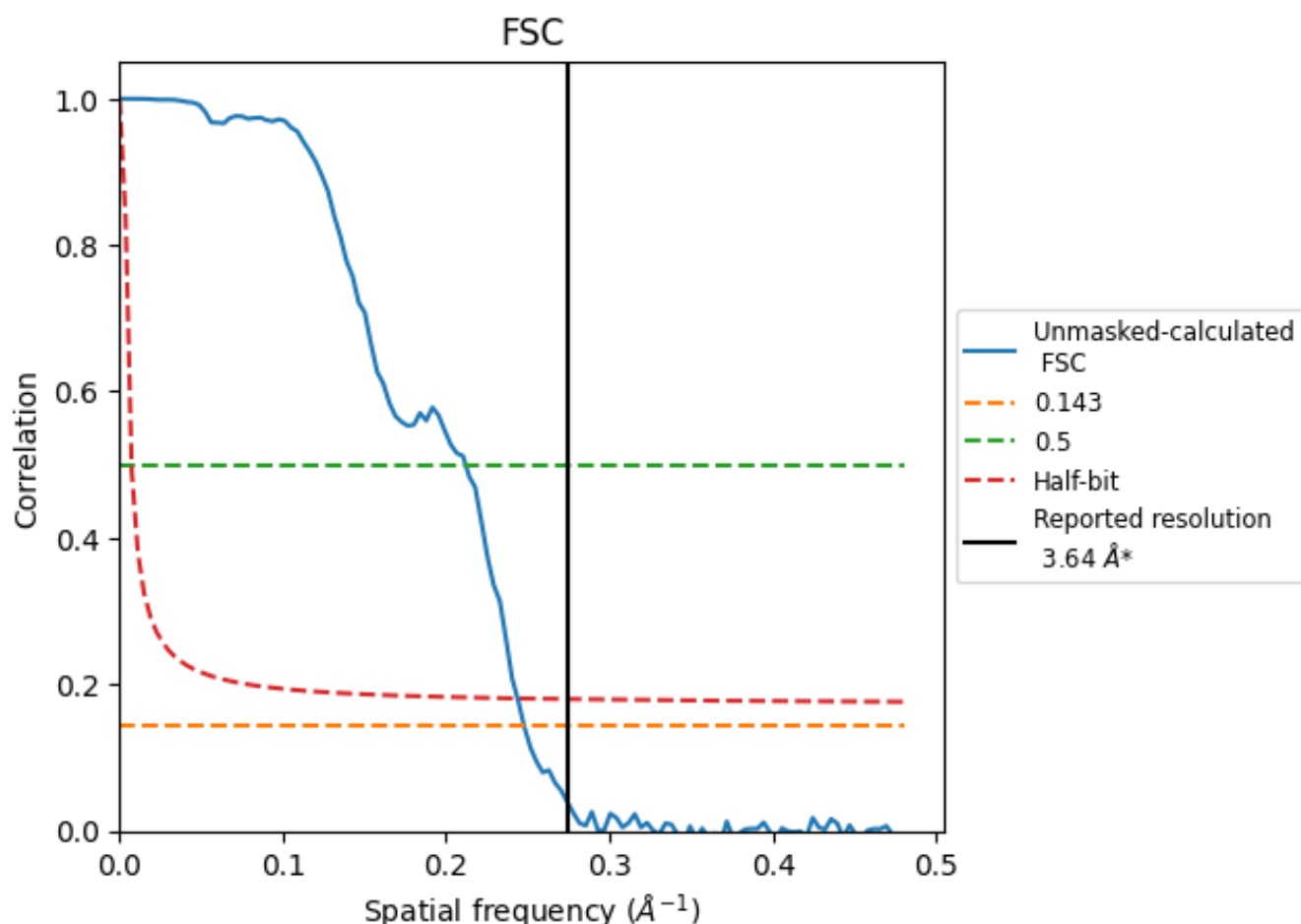


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 0.275 \AA^{-1}

8.2 Resolution estimates [i](#)

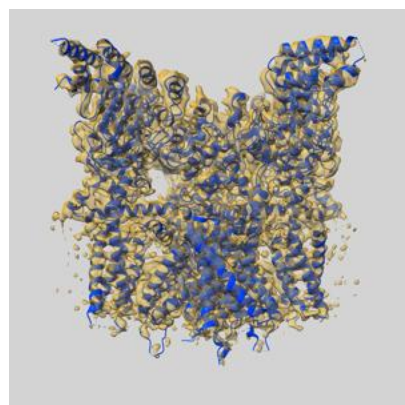
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	4.72	4.10

*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 4.04 differs from the reported value 3.64 by more than 10 %

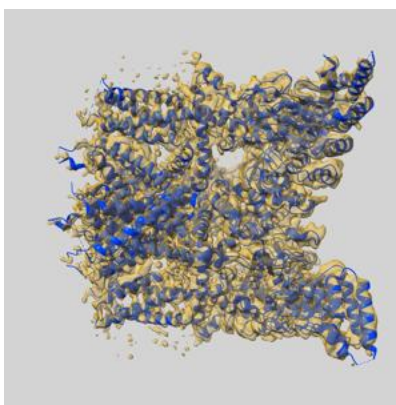
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33217 and PDB model 7XJ2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

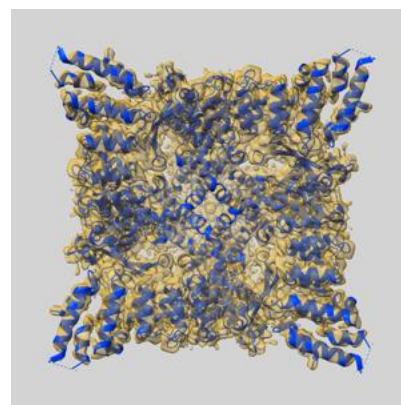
9.1 Map-model overlay [i](#)



X



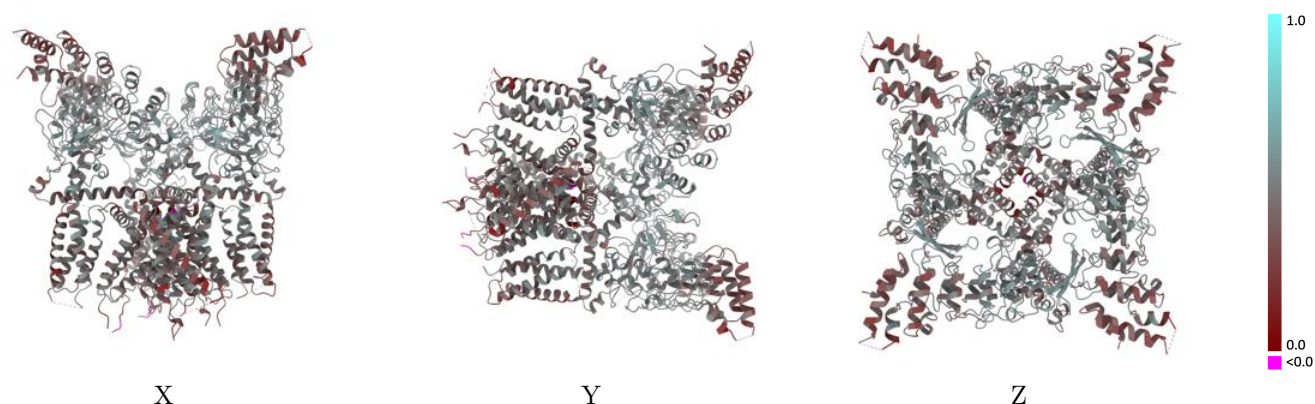
Y



Z

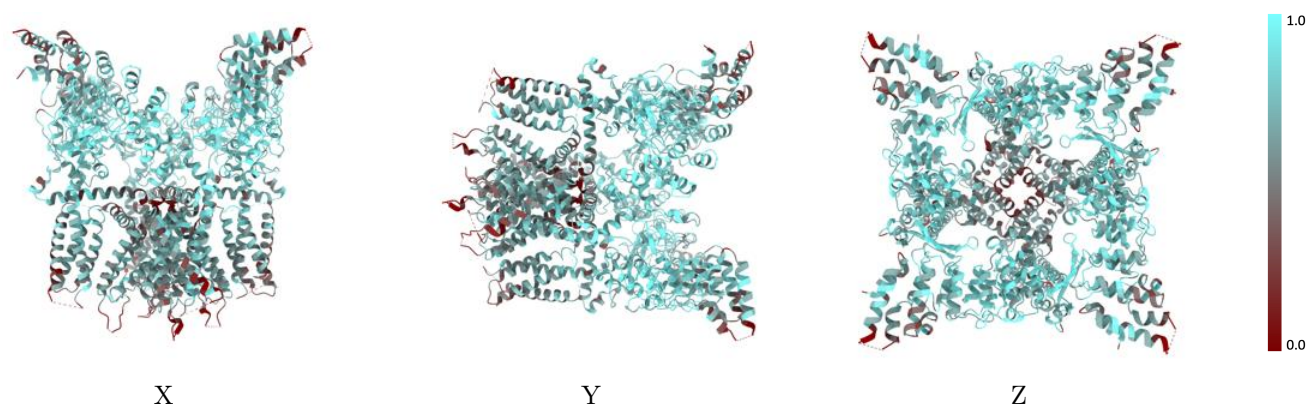
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



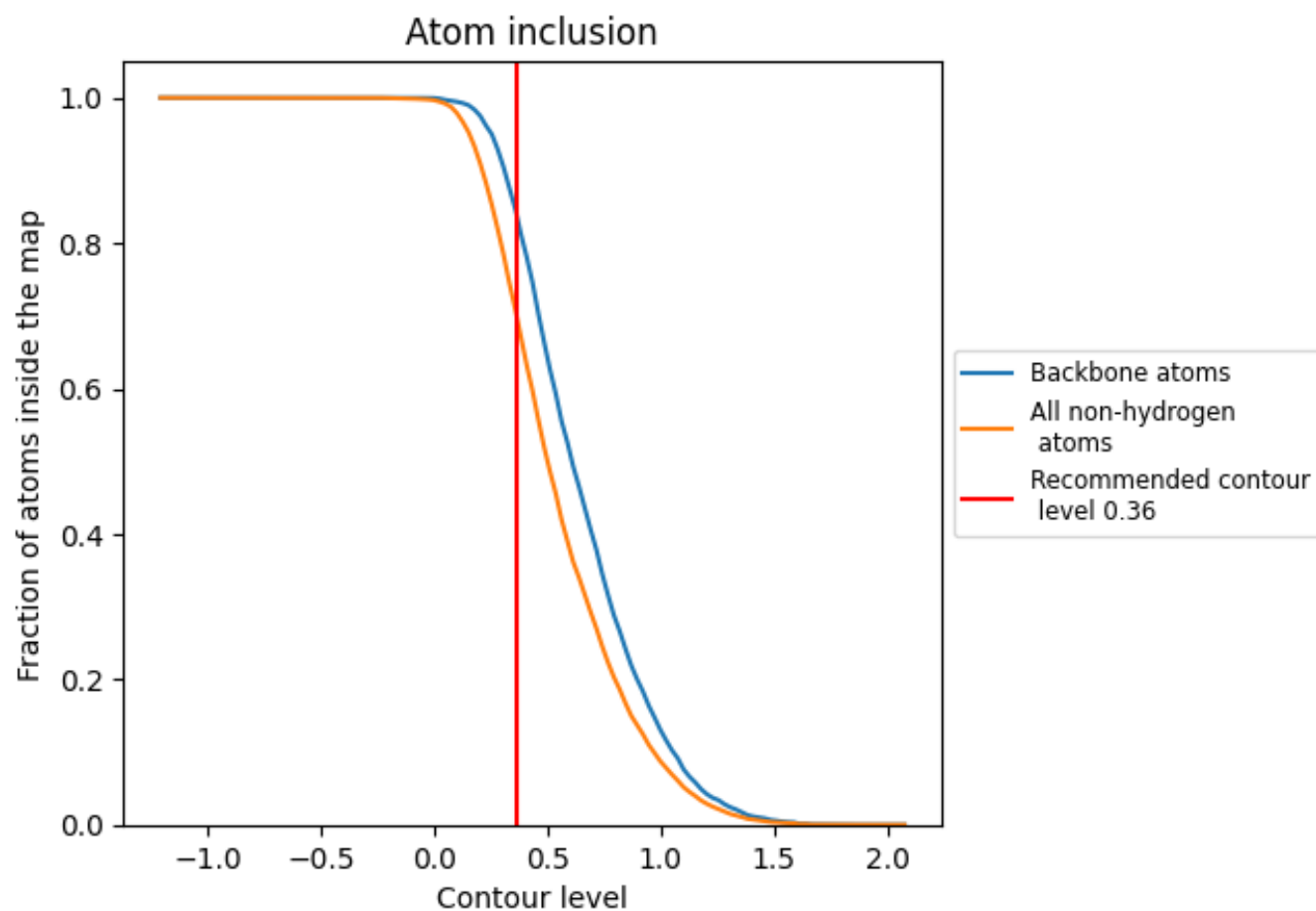
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 71% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7062	<div></div> 0.4470
A	<div></div> 0.7087	<div></div> 0.4490
B	<div></div> 0.7014	<div></div> 0.4440
C	<div></div> 0.7076	<div></div> 0.4460
D	<div></div> 0.7072	<div></div> 0.4480

