



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 07:21 PM UTC

PDB ID : 6PPD / pdb_00006ppd
EMDB ID : EMD-20433
Title : Kaposi's sarcoma-associated herpesvirus (KSHV), C1 penton vertex register, CATC-absent structure
Authors : Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on : 2019-07-06
Resolution : 3.70 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:

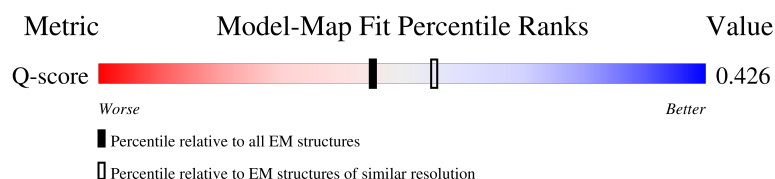
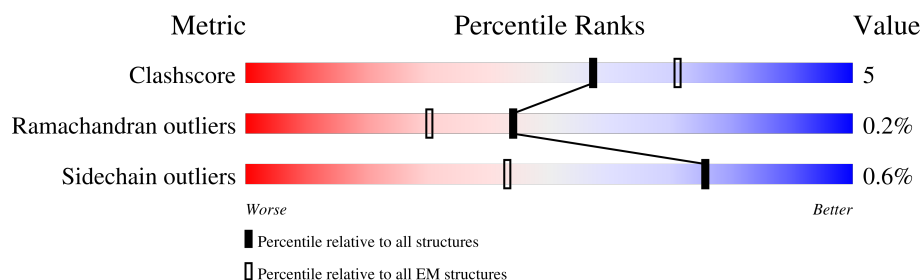
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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	11569 (3.20 - 4.20)

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	0	170	37% 39% 7% 54%
1	1	170	20% 41% 5% 54%
1	2	170	18% 39% 6% 54%
1	3	170	19% 39% 6% 54%

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Mol	Chain	Length	Quality of chain
1	A	170	
2	4	1376	
2	S	1376	
2	T	1376	
2	W	1376	
2	X	1376	
3	5	331	
3	b	331	
4	6	305	
4	7	305	
4	c	305	
4	d	305	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 68769 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 Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
1	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
1	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
1	A	44	Total	C	N	O	S	0	0
			380	244	72	62	2		
1	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

- Molecule 2 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	W	1354	Total	C	N	O	S	0	0
			10622	6748	1842	1960	72		
2	S	1281	Total	C	N	O	S	0	0
			10061	6401	1739	1852	69		
2	T	1360	Total	C	N	O	S	0	0
			10667	6776	1851	1967	73		
2	4	1222	Total	C	N	O	S	0	0
			9634	6133	1673	1757	71		
2	X	1341	Total	C	N	O	S	0	0
			10519	6685	1824	1939	71		

- Molecule 3 is a protein called Triplex capsid protein 1.

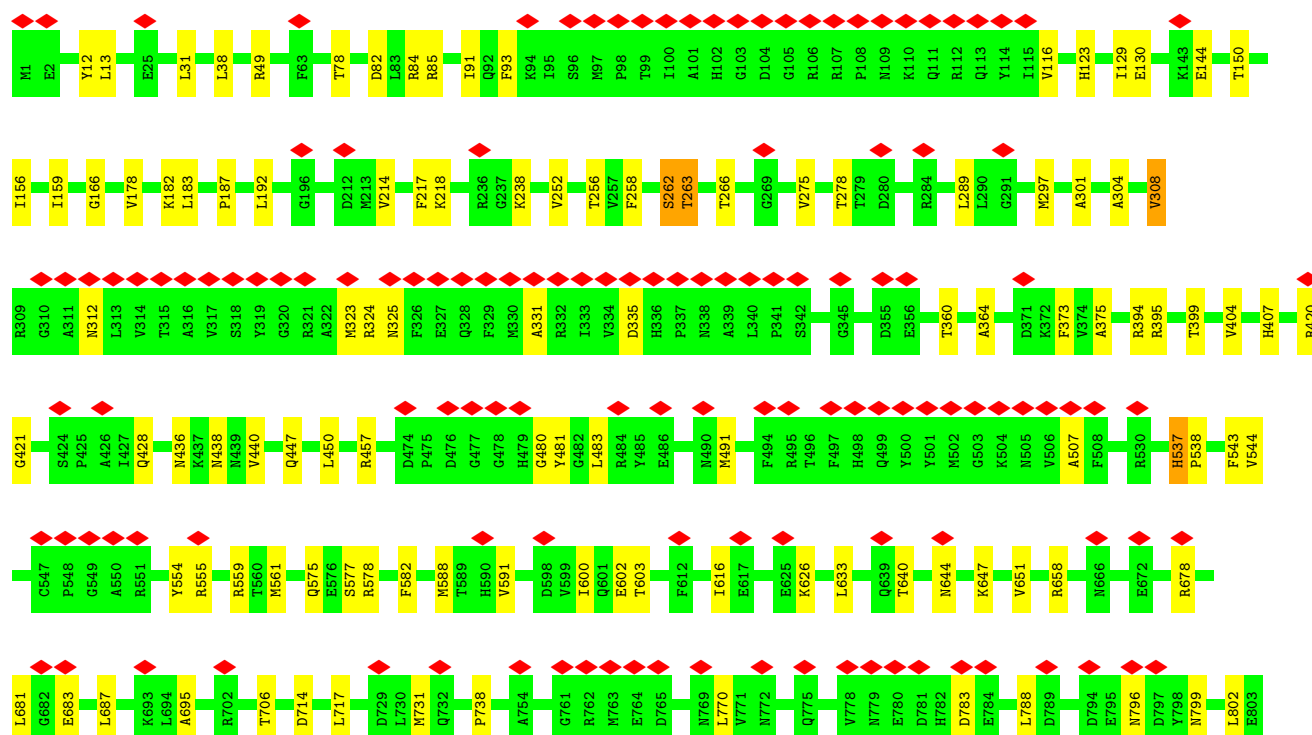
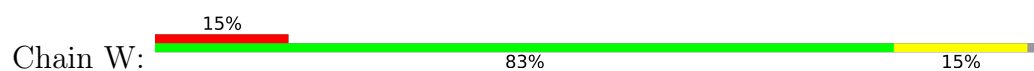
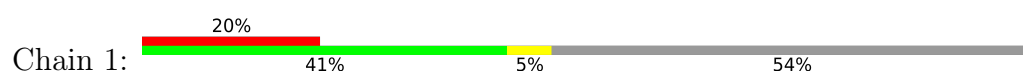
Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	314	Total	C	N	O	S	0	0
			2425	1554	416	441	14		
3	b	321	Total	C	N	O	S	0	0
			2478	1586	424	453	15		

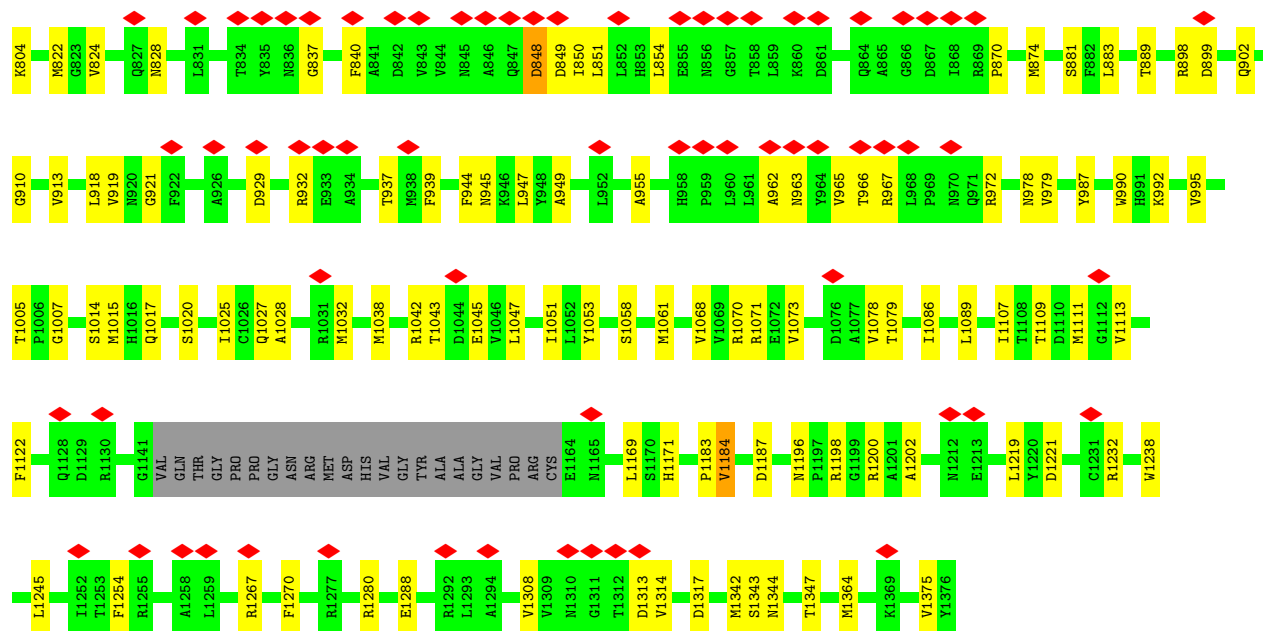
- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
4	7	291	Total	C	N	O	S	0	0
			2294	1465	388	426	15		
4	c	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
4	d	300	Total	C	N	O	S	0	0
			2365	1505	401	444	15		

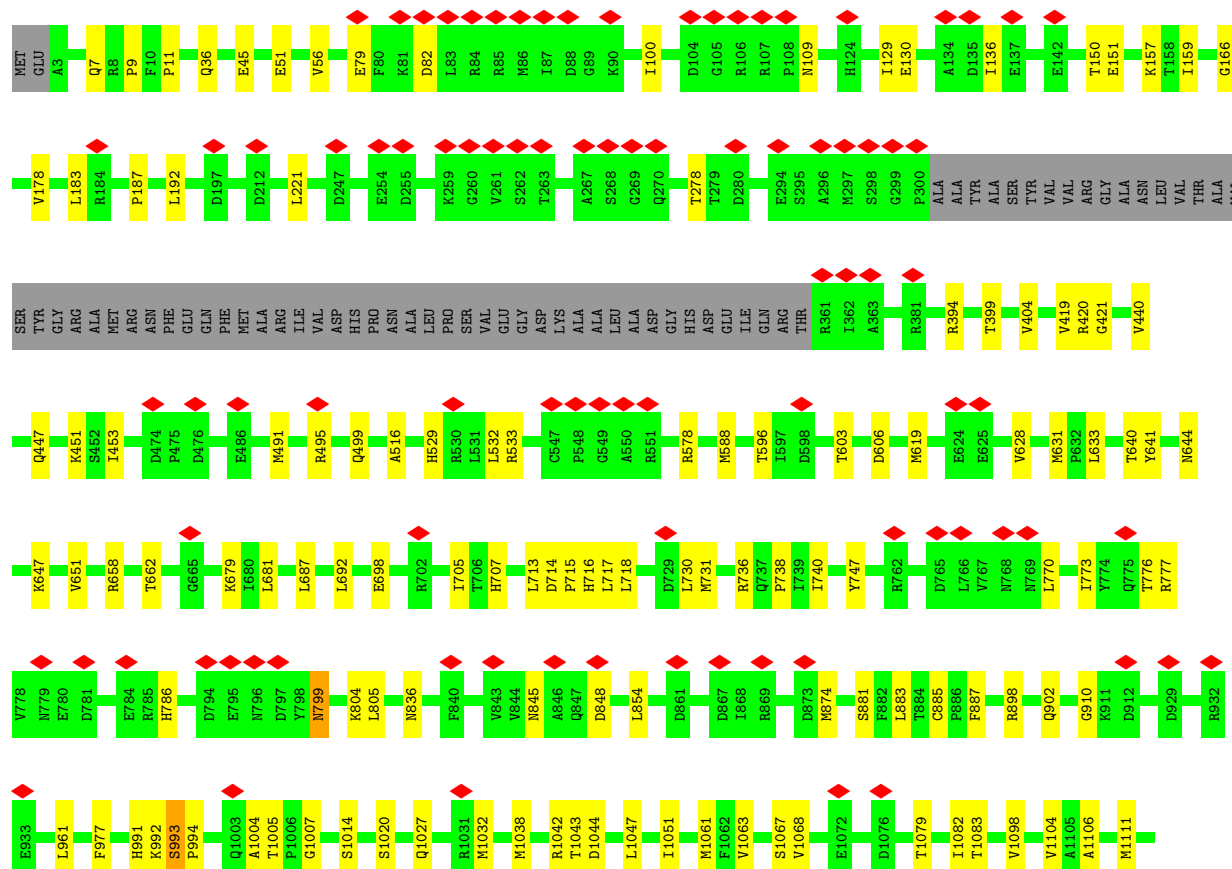
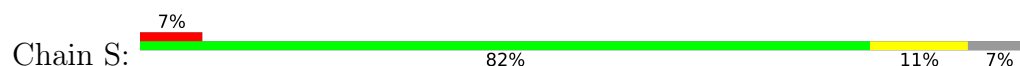


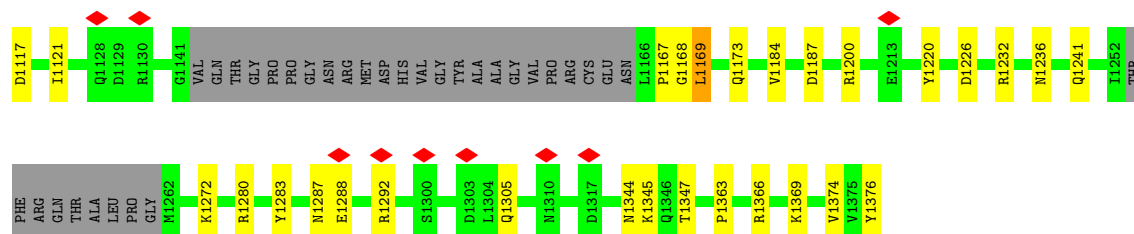
- Chain A:  25% 21% 5%



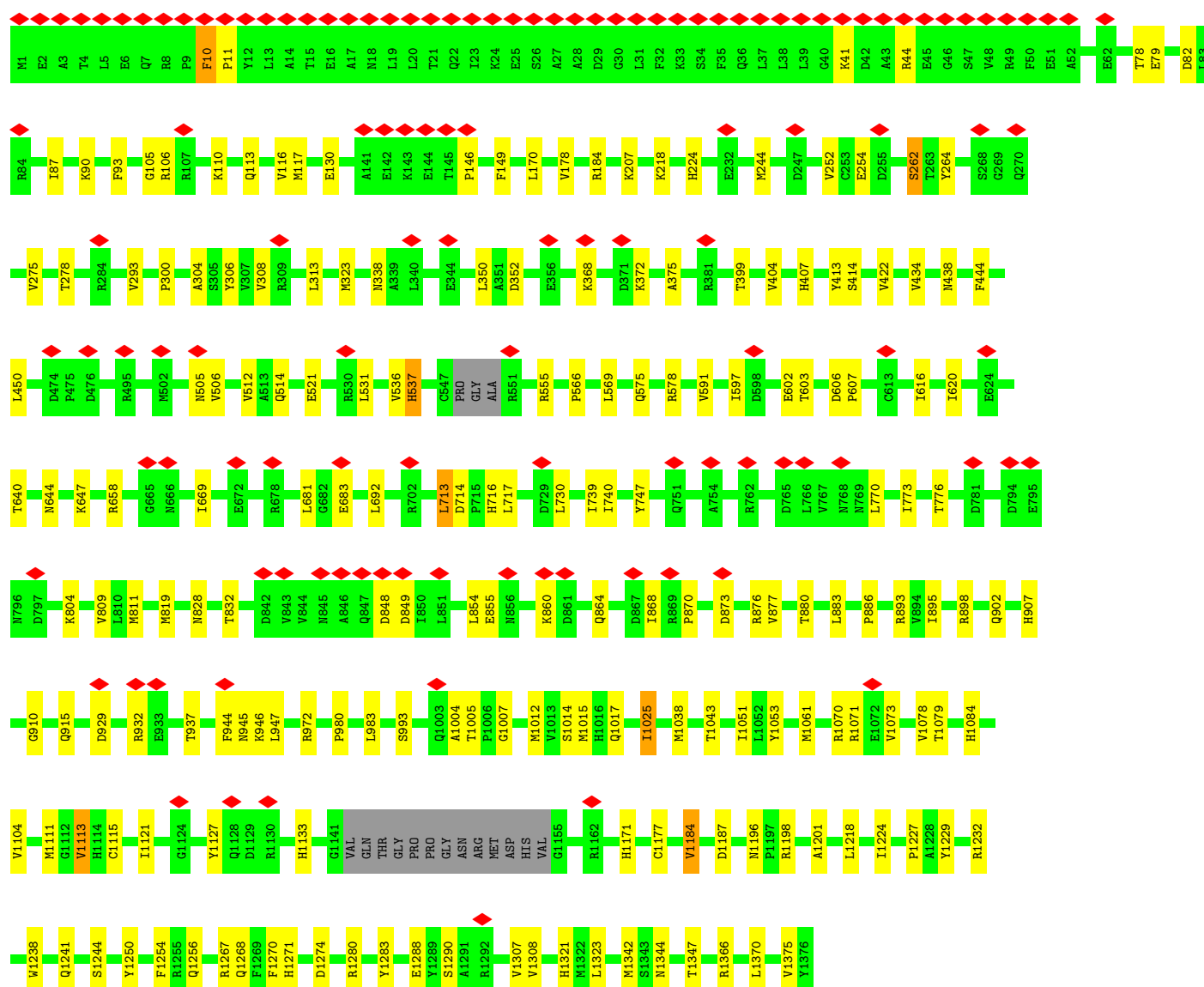
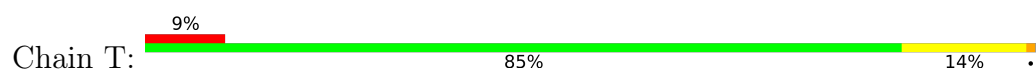


• Molecule 2: Major capsid protein

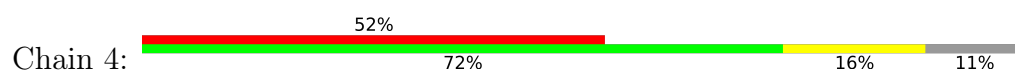




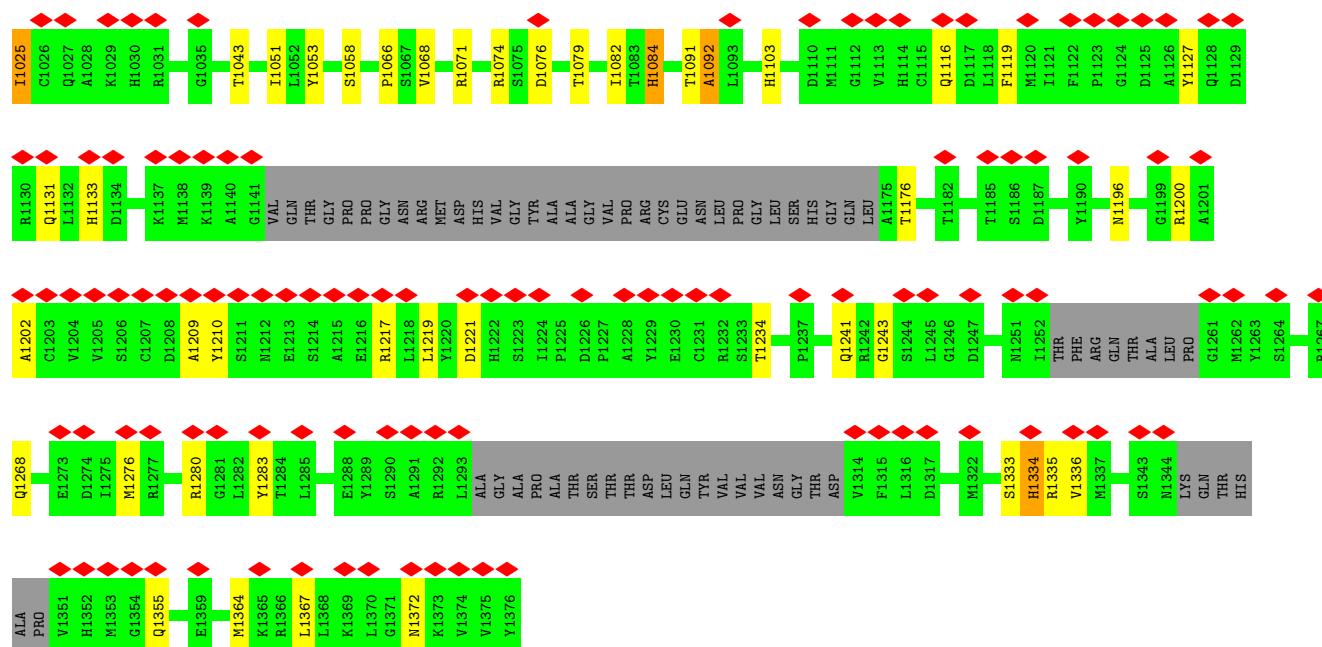
• Molecule 2: Major capsid protein



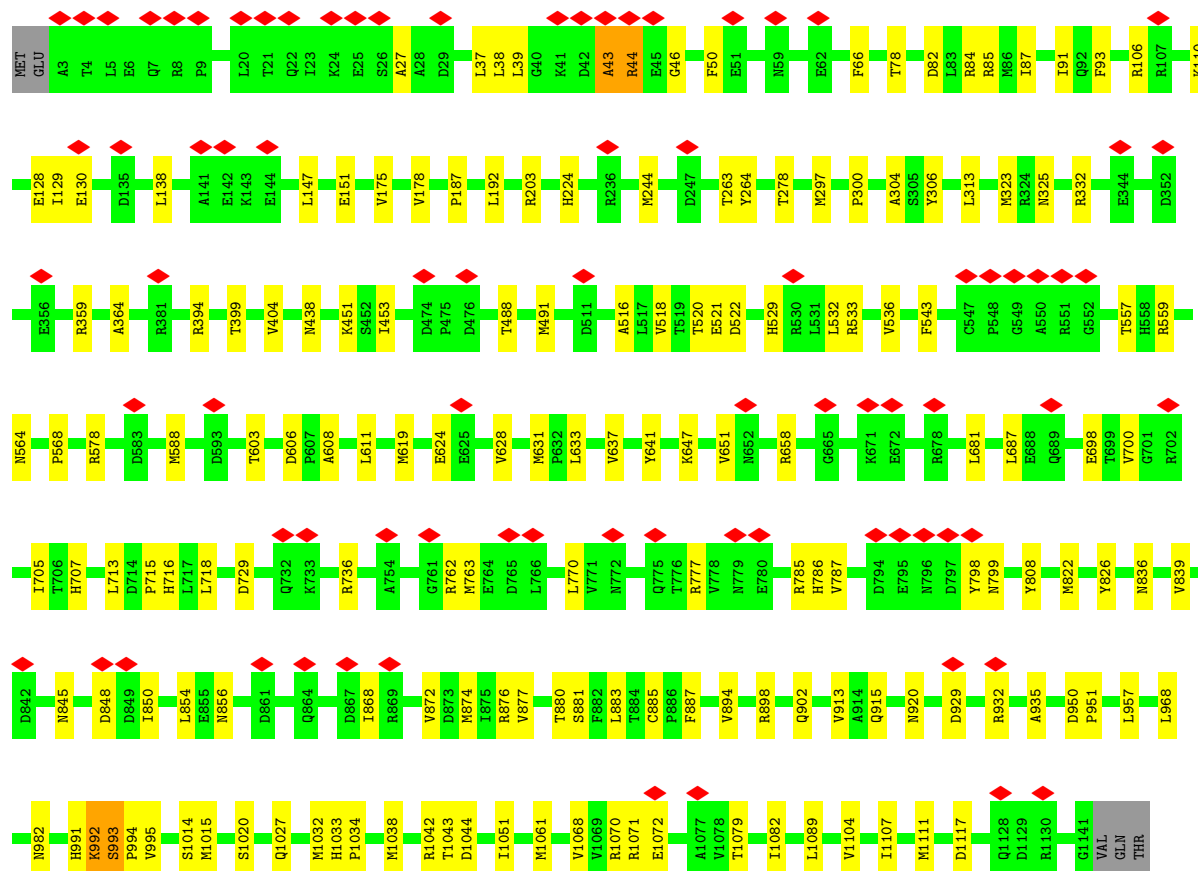
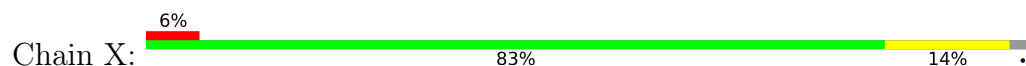
• Molecule 2: Major capsid protein

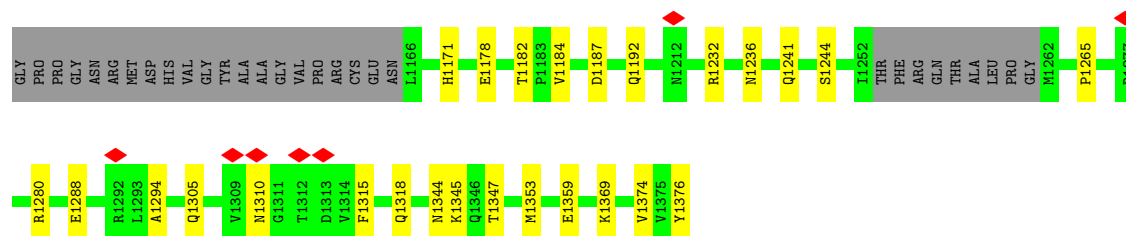


V965	T966	R967	L968	P969	N970	Q971	R972	N973	A974	Q915	T916	V917	L918	V919	P980	S981	L982	L983	M984	A985	E986	Y987	E988	E989	W990	H991	K992	S993	P994	V995	A996	A997	Y998	A999	A1000	S1001	C1002	Q1003	A1004	T1005	P1006	G1007	I1009	S1010	A1011	M1012	V1013	S1014	M1015	H1016	Q1017	K1018	L1019	S1020	P1022	S1023	F1024				
G680	Y481	G482	L483	R484	Y485	E486	Q487	T488	P489	N490	M491	N492	L493	F494	A495	T496	F497	H498	Q499	Y500	Y501	M502	G503	K504	N505	Y506	A507	F508	Y509	P510	D511	V512	A513	Q514	K515	A516	L517	V518	T519	T520	E521	D522	L523	L524	H525	P526	T527	S528	H529	R530	L531	L532	R533	L534	E535	V536	H537	P538			
F542	F543	V544	H545	P546	C547	P548	G549	A550	R551	G552	S553	Y554	R555	R559	T560	M561	N564	T566	P566	Q567	P568	L569	A570	P571	R572	E573	F574	Q575	E576	S577	R578	G579	A580	Q581	F582	D583	A584	V585	T586	N587	M588	T589	H590	V591	I592	D593	Q594	L595	T596	I597	D598	V599	I600	Q601	E602	T603	A604				
F605	D606	P607	A608	Y609	P610	L611	F612	C613	Y614	V615	L616	E617	A618	H619	I620	H621	G622	Q623	E624	E625	K626	F627	V628	H629	N630	H631	P632	L633	I634	A635	L636	V637	I638	Q639	T640	Y641	W642	V643	H644	S645	G646	K647	L648	A649	F650	V651	H652	Q653	Y654	H655	L656	H657	R658	F659	I660	C661	T662	H663	M664		
G665	H666	G667	S668	I669	P670	K671	E672	A673	H674	G675	H676	V677	R678	K679	I680	L681	G682	E683	L684	I685	A686	L687	E688	V689	A690	L691	L692	K693	L694	A695	G696	H697	E698	L699	T699	V700	G701	R702	T703	P704	T705	T706	H707	L708	V709	S710	A711	L712	L713	D714	P715	H716	L717	P718	P719	E720	F721	A722	Y723	H724	
D725	V726	F727	T728	D729	L730	M731	Q732	K733	S734	S735	R736	Q737	P738	T739	P800	V801	L802	G803	K804	L805	F806	Y807	V808	V809	L810	Q751	R752	K753	A754	T755	F756	I757	N758	L759	R760	G761	R762	M763	E764	D765	L766	Y826	Q827	N768	V829	A830	L831	T832	L833	T834	Y835	N836	G837	P838	V839	E790	D781	H782	D783	E784	
R785	H786	V787	L788	D789	V790	A791	L792	L793	D794	E795	N796	D797	Y798	N799	P800	V801	L802	G803	K804	L805	F806	Y807	V808	V809	L810	Q751	R752	K753	A754	T755	F756	I757	N758	L759	R760	G761	R762	M763	E764	D765	L766	Y826	Q827	N768	V829	A830	L831	T832	L833	T834	Y835	N836	G837	P838	V839	E790	D781	H782	D783	E784	
H845	A846	Q847	D848	D849	I850	L851	L852	H853	L854	E855	N856	G857	T858	L859	K860	D861	L862	L863	Q864	A865	G866	D867	I868	R869	P870	T871	H872	D873	M874	I875	R876	V877	L878	C879	T880	S881	R882	L883	T884	C885	P886	F887	V888	T889	Q890	A891	A892	R893	V894	I895	T896	K897	H898	D899	P900	L960	L961	Q902	S903	F904	
A905	T906	H907	E908	Y909	Q910	K911	D912	V913	A914	Q915	T916	V917	L918	V919	P920	G921	F922	G923	A924	F925	A926	V927	A928	D929	R930	S931	R932	E933	A934	A935	E936	R937	N938	P939	Y940	C820	C821	M822	C823	E824	D825	Y826	Q827	N768	V829	A830	L831	T832	L833	T834	Y835	N836	G837	P838	V839	E790	D781	H782	D783	E784	
R965	T966	R967	L968	P969	N970	Q971	R972	N973	A974	Q915	T916	V917	L918	V919	P980	S981	L982	L983	M984	A985	E986	Y987	E988	E989	W990	H991	K992	S993	P994	V995	A996	A997	Y998	A999	A1000	S1001	C1002	Q1003	A1004	T1005	P1006	G1007	I1009	S1010	A1011	M1012	V1013	S1014	M1015	H1016	Q1017	K1018	L1019	S1020	P1022	S1023	F1024				
MET	GLU	ALA	THR	LEU	GLN	ARG	PRO	PHE	PRO	TYR	LEU	ALA	THR	GLU	ALA	ASN	LEU	THR	GLN	ILE	LYS	GLU	SER	ALA	ASP	GLY	PHE	LYS	SER	PHE	GLN	LEU	LEU	LEU	GLY	LYS	ASP	ALA	ARG	GLU	GLY	S47	V48	E62	A70	E79	D82	L83	R84	R85	M86										

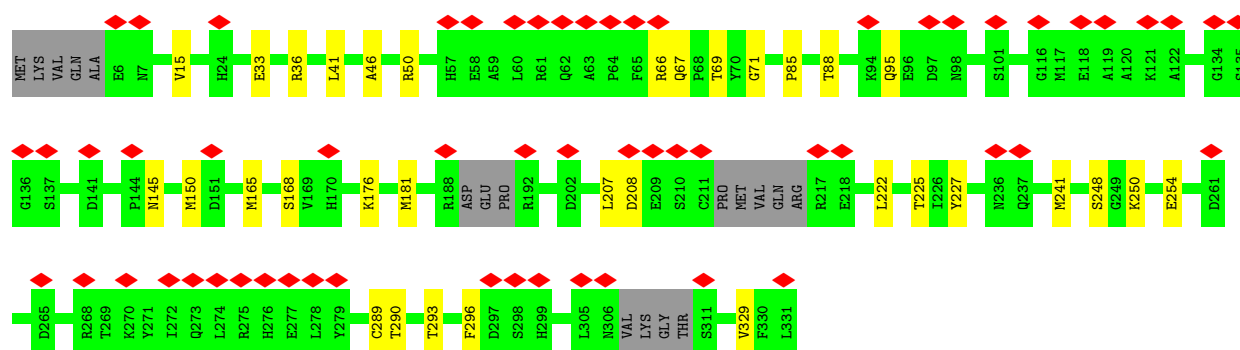
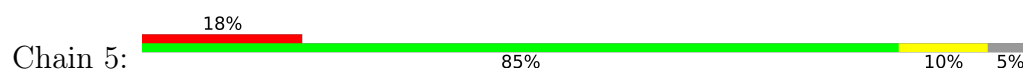


• Molecule 2: Major capsid protein

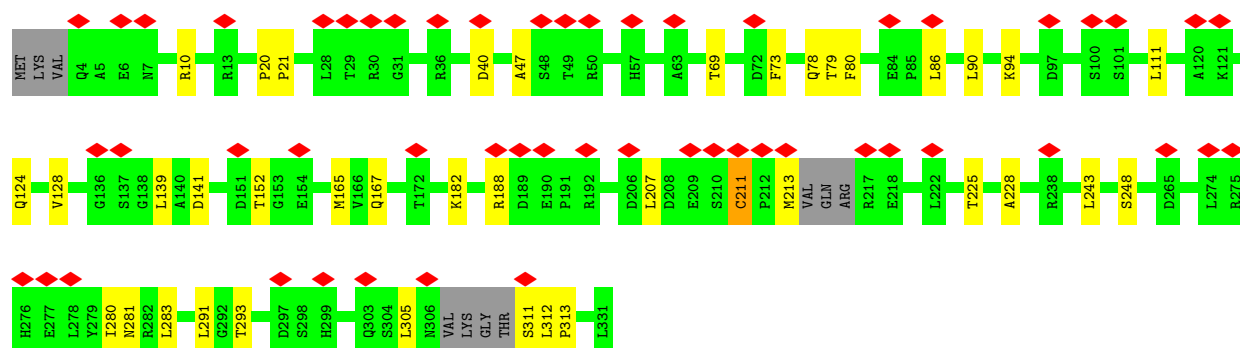
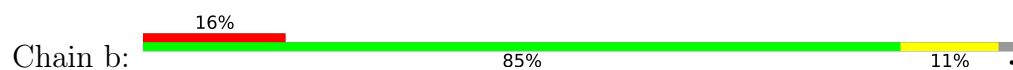




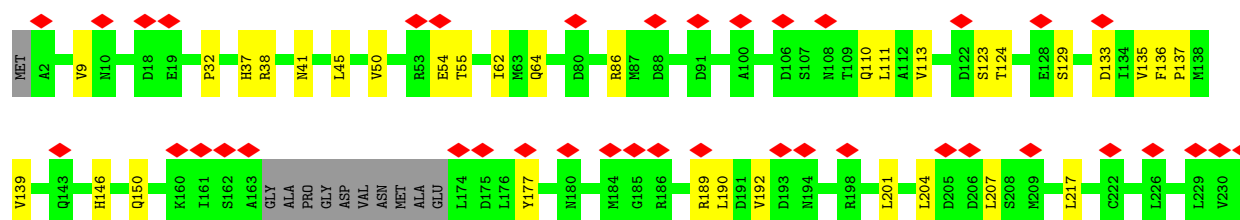
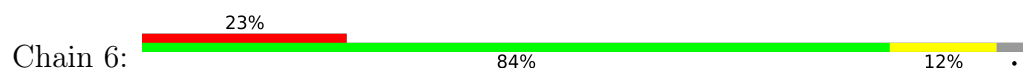
• Molecule 3: Triplex capsid protein 1

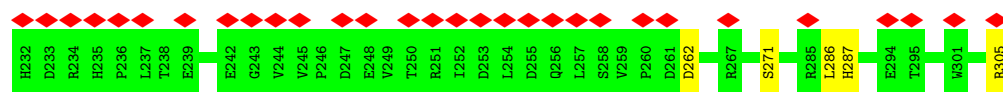


• Molecule 3: Triplex capsid protein 1



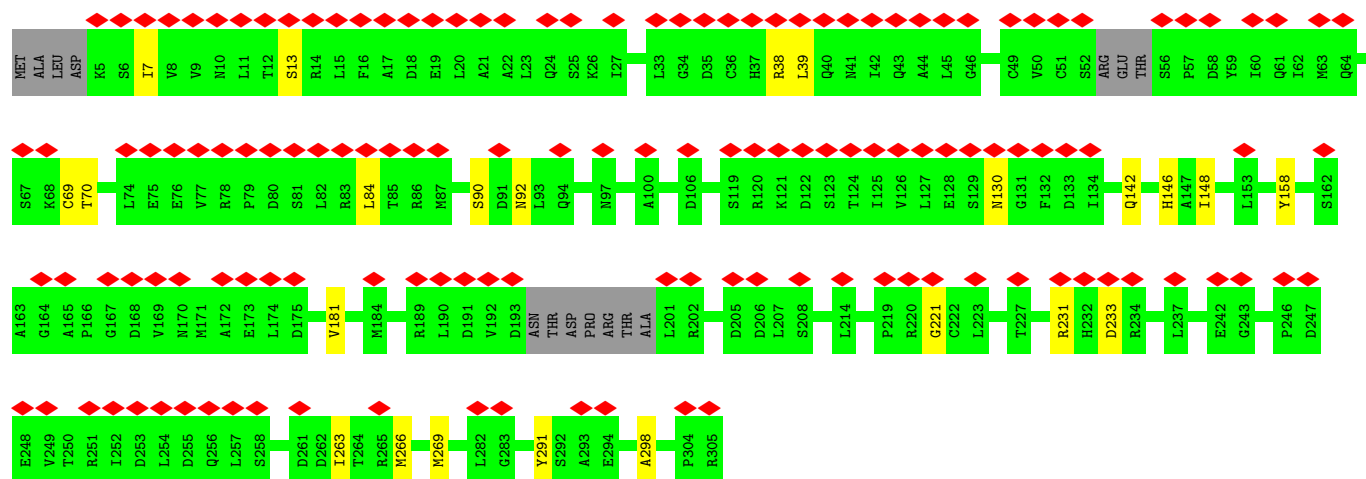
• Molecule 4: Triplex capsid protein 2





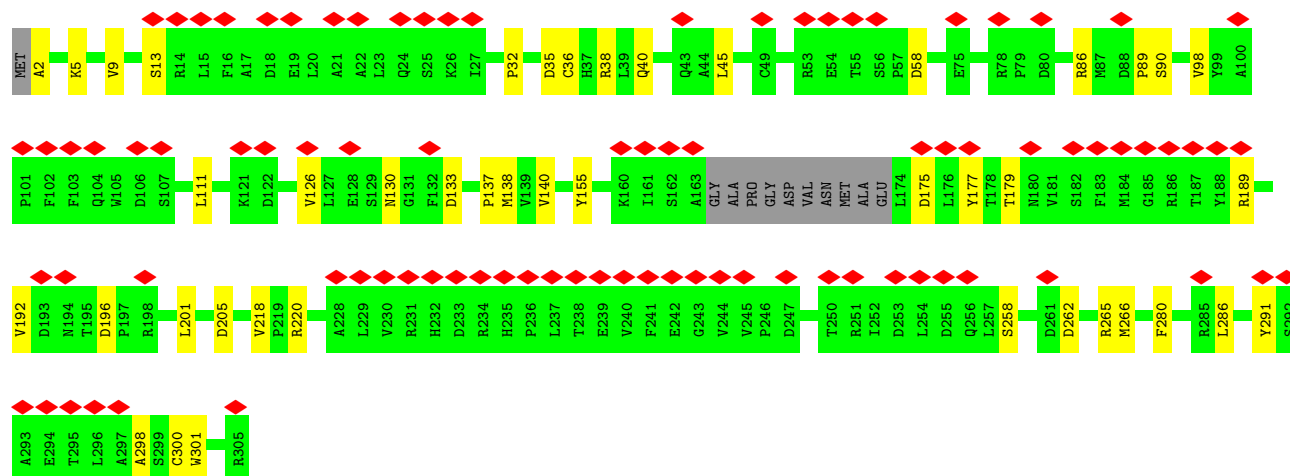
• Molecule 4: Triplex capsid protein 2

Chain 7: 46% 88% 8% 5%



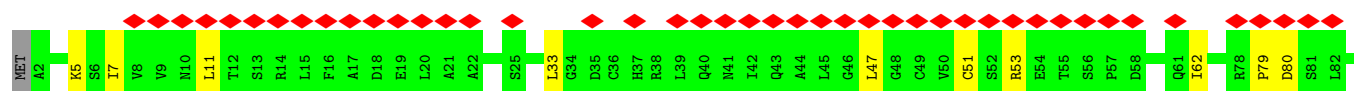
• Molecule 4: Triplex capsid protein 2

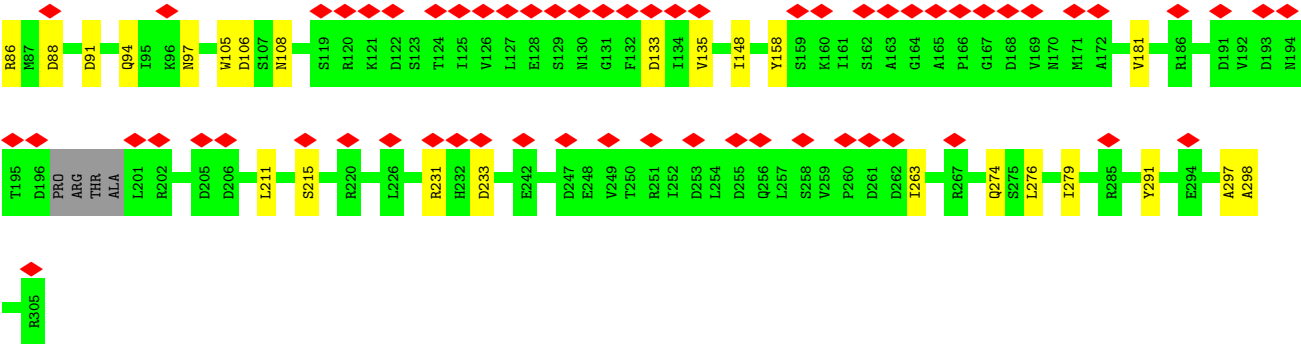
Chain c: 29% 82% 14% •



• Molecule 4: Triplex capsid protein 2

Chain d: 34% 87% 11% •





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1521505	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 ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0	0.24	0/682	0.58	2/919 (0.2%)
1	1	0.24	0/682	0.59	2/919 (0.2%)
1	2	0.24	0/682	0.58	2/919 (0.2%)
1	3	0.24	0/682	0.59	2/919 (0.2%)
1	A	0.18	0/391	0.46	0/528
2	4	0.30	0/9861	0.69	9/13391 (0.1%)
2	S	0.34	0/10300	0.59	3/13998 (0.0%)
2	T	0.37	0/10919	0.69	6/14839 (0.0%)
2	W	0.35	0/10874	0.68	8/14780 (0.1%)
2	X	0.33	0/10768	0.59	5/14635 (0.0%)
3	5	0.27	0/2484	0.51	2/3373 (0.1%)
3	b	0.31	0/2540	0.63	2/3452 (0.1%)
4	6	0.29	0/2376	0.57	0/3234
4	7	0.23	0/2339	0.52	0/3181
4	c	0.29	0/2376	0.63	2/3234 (0.1%)
4	d	0.29	0/2411	0.58	0/3281
All	All	0.33	0/70367	0.63	45/95602 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	4	0	12
2	S	0	1
2	T	0	7
2	W	0	5
2	X	0	2
All	All	0	27

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	W	421	GLY	N-CA-C	8.29	122.12	112.50
2	4	798	TYR	CA-C-N	7.26	134.77	121.70
2	4	798	TYR	C-N-CA	7.26	134.77	121.70
2	T	1113	VAL	N-CA-CB	-7.13	103.84	112.33
2	T	1113	VAL	CB-CA-C	7.07	118.25	110.62
2	T	848	ASP	CA-C-N	7.01	131.75	121.31
2	T	848	ASP	C-N-CA	7.01	131.75	121.31
1	3	20	ALA	CA-C-N	6.76	133.86	121.70
1	3	20	ALA	C-N-CA	6.76	133.86	121.70
1	0	20	ALA	CA-C-N	6.75	133.85	121.70
1	0	20	ALA	C-N-CA	6.75	133.85	121.70
1	1	20	ALA	CA-C-N	6.75	133.85	121.70
1	1	20	ALA	C-N-CA	6.75	133.85	121.70
1	2	20	ALA	CA-C-N	6.74	133.82	121.70
1	2	20	ALA	C-N-CA	6.74	133.82	121.70
2	W	262	SER	CA-C-N	6.53	134.01	121.54
2	W	262	SER	C-N-CA	6.53	134.01	121.54
2	S	1004	ALA	CA-C-N	6.29	145.49	121.95
2	S	1004	ALA	C-N-CA	6.29	145.49	121.95
2	X	993	SER	N-CA-C	6.10	123.28	109.81
2	4	103	GLY	CA-C-N	6.00	131.33	122.82
2	4	103	GLY	C-N-CA	6.00	131.33	122.82
2	W	308	VAL	N-CA-C	-5.94	106.63	111.91
2	S	993	SER	N-CA-C	5.93	122.93	109.81
3	5	296	PHE	CA-C-N	5.61	132.26	121.54
3	5	296	PHE	C-N-CA	5.61	132.26	121.54
2	4	888	VAL	N-CA-C	-5.44	101.89	108.53
2	W	837	GLY	N-CA-C	5.40	123.35	112.34
4	c	258	SER	CA-C-N	5.31	124.58	120.33
4	c	258	SER	C-N-CA	5.31	124.58	120.33
2	X	1070	ARG	CA-C-N	-5.31	112.91	122.46
2	X	1070	ARG	C-N-CA	-5.31	112.91	122.46
2	W	262	SER	N-CA-C	5.27	119.34	113.01
2	W	848	ASP	CA-C-N	5.26	131.59	121.54
2	W	848	ASP	C-N-CA	5.26	131.59	121.54
2	4	848	ASP	CA-C-N	5.25	131.57	121.54
2	4	848	ASP	C-N-CA	5.25	131.57	121.54
3	b	211	CYS	CA-C-N	5.17	139.42	127.00
3	b	211	CYS	C-N-CA	5.17	139.42	127.00
2	X	992	LYS	CA-C-N	5.04	134.10	121.80
2	X	992	LYS	C-N-CA	5.04	134.10	121.80
2	4	1209	ALA	CA-C-N	5.03	128.80	121.31
2	4	1209	ALA	C-N-CA	5.03	128.80	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	262	SER	CA-C-N	5.01	129.16	121.19
2	T	262	SER	C-N-CA	5.01	129.16	121.19

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	4	1084	HIS	Peptide
2	4	1091	THR	Peptide
2	4	1092	ALA	Peptide
2	4	110	LYS	Peptide
2	4	1334	HIS	Peptide
2	4	292	GLN	Peptide
2	4	313	LEU	Peptide
2	4	506	VAL	Peptide
2	4	842	ASP	Peptide
2	4	850	ILE	Peptide
2	4	886	PRO	Peptide
2	4	899	ASP	Peptide
2	S	991	HIS	Peptide
2	T	10	PHE	Peptide
2	T	262	SER	Peptide
2	T	505	ASN	Peptide
2	T	537	HIS	Peptide
2	T	849	ASP	Peptide
2	T	886	PRO	Peptide
2	T	944	PHE	Peptide
2	W	262	SER	Peptide
2	W	263	THR	Mainchain
2	W	537	HIS	Peptide
2	W	848	ASP	Peptide
2	W	849	ASP	Peptide
2	X	43	ALA	Peptide
2	X	991	HIS	Peptide

5.2 Too-close contacts ⓘ

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	0	666	0	647	7	0
1	1	666	0	647	4	0
1	2	666	0	647	7	0
1	3	666	0	647	6	0
1	A	380	0	369	7	0
2	4	9634	0	9527	126	0
2	S	10061	0	9956	90	0
2	T	10667	0	10543	108	0
2	W	10622	0	10500	129	0
2	X	10519	0	10399	114	0
3	5	2425	0	2419	22	0
3	b	2478	0	2466	25	0
4	6	2330	0	2354	24	0
4	7	2294	0	2315	16	0
4	c	2330	0	2354	29	0
4	d	2365	0	2379	24	0
All	All	68769	0	68169	661	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 5.

All (661) 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)
2:T:536:VAL:HG13	2:T:1244:SER:HA	1.72	0.72
2:X:178:VAL:HG22	2:X:1061:MET:HE2	1.73	0.70
1:2:70:ARG:NH2	1:3:12:GLN:O	2.26	0.68
2:S:770:LEU:HD21	2:S:883:LEU:HD22	1.75	0.67
1:1:55:HIS:HD2	2:X:770:LEU:HD22	1.59	0.67
4:d:97:ASN:HD22	4:d:105:TRP:HD1	1.41	0.66
2:W:799:ASN:HD21	2:W:802:LEU:HD12	1.61	0.66
2:T:1254:PHE:H	2:T:1267:ARG:HH21	1.44	0.66
2:4:566:PRO:HB2	2:4:568:PRO:HD2	1.77	0.65
2:4:893:ARG:NH2	2:4:984:MET:SD	2.69	0.65
2:W:38:LEU:HB2	2:T:113:GLN:HB3	1.79	0.65
2:4:130:GLU:HG2	2:4:1079:THR:HG22	1.78	0.65
2:X:399:THR:HG22	2:X:1043:THR:HG22	1.79	0.64
4:6:111:LEU:HB2	4:6:286:LEU:HB2	1.77	0.64
2:T:1201:ALA:HB3	2:T:1227:PRO:HG2	1.78	0.64
2:W:420:ARG:HH11	2:X:1353:MET:HE1	1.62	0.64
2:4:838:PRO:HD2	2:4:854:LEU:HA	1.79	0.63
2:4:1074:ARG:HG2	2:4:1076:ASP:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:575:GLN:NE2	2:W:1015:MET:SD	2.70	0.63
1:2:55:HIS:HD2	2:S:770:LEU:HD22	1.63	0.63
2:4:916:THR:HG23	2:4:984:MET:HG2	1.81	0.63
2:4:1333:SER:HB2	2:4:1355:GLN:HB2	1.81	0.63
2:W:278:THR:HG22	2:W:1051:ILE:HG12	1.78	0.63
2:4:875:ILE:HG23	2:4:878:LEU:HD12	1.81	0.63
2:S:845:ASN:HB3	2:S:848:ASP:HB2	1.81	0.63
2:T:717:LEU:HA	2:T:915:GLN:HE22	1.64	0.63
2:4:128:GLU:OE2	2:4:1071:ARG:NH2	2.32	0.62
2:W:561:MET:HE3	2:W:990:TRP:HB3	1.80	0.62
2:T:566:PRO:HG2	2:T:569:LEU:HD12	1.81	0.62
2:X:37:LEU:HB2	2:X:50:PHE:HB2	1.81	0.62
2:4:698:GLU:HG3	2:4:705:ILE:HD12	1.81	0.62
2:W:602:GLU:HB3	2:W:647:LYS:HE2	1.82	0.62
2:T:1280:ARG:NH2	2:T:1288:GLU:OE1	2.33	0.61
2:S:692:LEU:HD13	2:T:972:ARG:HG2	1.82	0.61
2:T:770:LEU:HD21	2:T:883:LEU:HD22	1.82	0.61
2:4:864:GLN:HB2	2:4:930:ARG:HH22	1.66	0.61
2:S:578:ARG:NH1	2:S:1014:SER:O	2.34	0.61
2:S:1068:VAL:HG22	2:S:1082:ILE:HG12	1.82	0.61
2:W:130:GLU:HG2	2:W:1079:THR:HG22	1.83	0.61
2:4:777:ARG:NH2	2:4:885:CYS:O	2.34	0.61
2:W:1070:ARG:NH1	4:c:2:ALA:O	2.34	0.60
2:W:591:VAL:HB	2:W:683:GLU:HB2	1.83	0.60
2:W:929:ASP:OD1	2:W:932:ARG:NH2	2.34	0.60
3:5:254:GLU:HG2	4:6:64:GLN:HE21	1.67	0.60
2:W:1200:ARG:NH1	2:W:1221:ASP:O	2.35	0.60
2:X:1187:ASP:OD2	2:X:1232:ARG:NH2	2.35	0.60
4:6:9:VAL:HG21	4:6:45:LEU:HD13	1.83	0.60
2:W:238:LYS:HG2	2:W:289:LEU:HD22	1.84	0.60
2:W:1187:ASP:OD2	2:W:1232:ARG:NH1	2.35	0.60
2:T:740:ILE:HB	2:T:747:TYR:HB3	1.84	0.59
2:T:1256:GLN:NE2	3:b:78:GLN:OE1	2.31	0.59
2:W:678:ARG:NH1	2:X:606:ASP:OD1	2.34	0.59
2:X:297:MET:HE3	2:X:364:ALA:HB3	1.84	0.59
3:5:289:CYS:SG	3:5:290:THR:N	2.75	0.59
2:S:150:THR:HG21	2:X:313:LEU:HD21	1.84	0.59
2:T:178:VAL:HG22	2:T:1061:MET:HE2	1.85	0.59
2:X:588:MET:HE1	2:X:687:LEU:HD12	1.84	0.59
2:T:1241:GLN:HB3	2:T:1244:SER:HB3	1.84	0.59
2:4:309:ARG:HD3	2:X:38:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:603:THR:HG22	2:X:647:LYS:HB3	1.85	0.59
2:T:578:ARG:NH2	2:T:1017:GLN:OE1	2.35	0.59
4:c:5:LYS:HB2	4:c:86:ARG:HB3	1.83	0.59
2:W:1280:ARG:NH2	2:W:1288:GLU:OE1	2.36	0.58
2:S:399:THR:HG22	2:S:1043:THR:HG22	1.85	0.58
2:S:1111:MET:SD	2:S:1366:ARG:NH2	2.73	0.58
2:W:144:GLU:OE1	3:b:10:ARG:NH1	2.36	0.58
2:4:535:GLU:OE2	2:4:559:ARG:NH2	2.37	0.58
3:5:66:ARG:NH1	4:7:90:SER:O	2.36	0.58
2:X:770:LEU:HD21	2:X:883:LEU:HD22	1.86	0.58
2:4:611:LEU:HD22	2:4:862:ILE:HD13	1.84	0.58
4:7:69:CYS:SG	4:7:70:THR:N	2.76	0.58
1:0:66:GLY:O	2:X:856:ASN:ND2	2.37	0.58
2:W:481:TYR:OH	2:W:979:VAL:O	2.20	0.58
2:S:633:LEU:HD12	2:S:874:MET:HB3	1.86	0.58
2:S:453:ILE:HD11	2:S:1038:MET:HE1	1.86	0.58
2:X:488:THR:OG1	2:X:982:ASN:ND2	2.34	0.58
2:T:929:ASP:OD1	2:T:932:ARG:NH2	2.37	0.57
4:d:7:ILE:HG21	4:d:33:LEU:HD21	1.86	0.57
2:W:965:VAL:HG13	2:W:972:ARG:HG2	1.86	0.57
4:6:201:LEU:HD13	4:7:231:ARG:HH12	1.69	0.57
3:b:90:LEU:HD11	3:b:165:MET:HG3	1.86	0.57
3:b:128:VAL:HG11	3:b:312:LEU:HD22	1.86	0.57
2:S:1200:ARG:HG2	2:S:1226:ASP:HB3	1.85	0.57
3:5:329:VAL:HG21	4:6:271:SER:HB2	1.86	0.57
2:W:399:THR:HG22	2:W:1043:THR:HG22	1.85	0.57
2:4:594:GLN:HB2	2:4:1006:PRO:HD3	1.87	0.57
3:5:222:LEU:HD22	4:6:86:ARG:HH22	1.68	0.57
4:c:179:THR:OG1	4:c:189:ARG:NH1	2.38	0.57
2:W:543:PHE:HZ	2:W:555:ARG:HH11	1.53	0.57
2:S:658:ARG:HA	2:S:681:LEU:HD11	1.85	0.57
2:W:183:LEU:HD13	2:W:394:ARG:HH21	1.70	0.57
4:6:189:ARG:NH1	4:6:190:LEU:O	2.37	0.57
2:X:658:ARG:HA	2:X:681:LEU:HD11	1.85	0.57
4:6:124:THR:HG22	4:6:135:VAL:HG22	1.87	0.57
2:T:811:MET:HB3	2:T:819:MET:HE1	1.86	0.56
2:T:1070:ARG:HH21	2:T:1073:VAL:HG21	1.70	0.56
2:S:714:ASP:OD1	2:S:736:ARG:NH2	2.38	0.56
2:T:640:THR:O	2:T:644:ASN:ND2	2.38	0.56
1:A:28:MET:HE3	1:A:45:LYS:HE2	1.87	0.56
2:X:1344:ASN:ND2	2:X:1347:THR:OG1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:1045:GLU:N	2:W:1109:THR:OG1	2.34	0.56
4:c:13:SER:OG	4:c:130:ASN:ND2	2.39	0.56
2:T:658:ARG:HA	2:T:681:LEU:HD11	1.87	0.56
2:4:1068:VAL:HG11	3:5:41:LEU:HD21	1.87	0.56
4:d:94:GLN:HE21	4:d:297:ALA:HB1	1.70	0.56
2:4:567:GLN:HE21	2:4:998:TYR:HA	1.71	0.56
2:X:729:ASP:OD2	2:X:798:TYR:OH	2.24	0.56
2:S:603:THR:HG22	2:S:647:LYS:HB3	1.86	0.56
2:S:633:LEU:HA	2:S:874:MET:HE3	1.88	0.56
2:4:700:VAL:O	2:4:1131:GLN:NE2	2.39	0.56
2:W:1313:ASP:OD2	2:X:203:ARG:NH1	2.38	0.56
2:4:450:LEU:HD11	2:4:1025:ILE:HA	1.87	0.56
2:W:1005:THR:HG22	2:W:1007:GLY:H	1.70	0.55
1:3:13:GLU:OE1	1:3:46:ARG:NH2	2.38	0.55
2:4:495:ARG:O	2:4:499:GLN:N	2.39	0.55
2:X:1280:ARG:NH2	2:X:1288:GLU:OE1	2.39	0.55
4:c:177:TYR:HB3	4:d:263:ILE:HG21	1.86	0.55
2:S:1042:ARG:NH1	2:S:1044:ASP:OD2	2.40	0.55
2:W:31:LEU:HB2	2:T:1283:TYR:HD2	1.72	0.55
2:W:850:ILE:HD12	2:W:870:PRO:HG2	1.88	0.55
2:W:578:ARG:NH2	2:W:1017:GLN:OE1	2.38	0.55
2:W:918:LEU:HD22	2:W:944:PHE:HZ	1.71	0.55
2:W:447:GLN:HB3	2:W:1028:ALA:HB1	1.88	0.55
2:4:399:THR:HG21	2:4:1268:GLN:HE22	1.71	0.55
3:5:176:LYS:NZ	2:X:1310:ASN:OD1	2.39	0.55
2:W:182:LYS:NZ	2:W:1058:SER:OG	2.40	0.54
2:T:575:GLN:NE2	2:T:1015:MET:SD	2.81	0.54
2:T:1344:ASN:ND2	2:T:1347:THR:OG1	2.40	0.54
2:4:846:ALA:HA	2:4:872:VAL:HB	1.89	0.54
3:5:207:LEU:HB2	3:5:248:SER:HB3	1.88	0.54
3:b:167:GLN:HB2	3:b:188:ARG:HG3	1.89	0.54
2:X:491:MET:HE3	2:X:786:HIS:HA	1.89	0.54
2:4:298:SER:HB3	2:4:359:ARG:HD2	1.88	0.54
4:c:291:TYR:HD1	4:c:298:ALA:HB2	1.73	0.54
2:W:1344:ASN:ND2	2:W:1347:THR:OG1	2.40	0.54
2:S:491:MET:HE3	2:S:786:HIS:HA	1.89	0.54
2:4:963:ASN:HA	2:4:966:THR:HG22	1.89	0.54
2:W:537:HIS:HA	2:W:1238:TRP:CD1	2.42	0.54
2:S:187:PRO:HG2	2:S:192:LEU:HD12	1.90	0.54
2:T:1071:ARG:O	2:T:1079:THR:OG1	2.22	0.54
2:S:1083:THR:HG22	4:6:38:ARG:HH22	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:811:MET:O	2:4:815:SER:N	2.39	0.54
2:W:828:ASN:ND2	2:W:937:THR:O	2.40	0.54
2:4:1071:ARG:O	2:4:1079:THR:OG1	2.24	0.54
3:5:225:THR:HG22	3:5:293:THR:HG22	1.90	0.54
1:1:13:GLU:OE1	1:1:46:ARG:NH2	2.38	0.54
2:W:658:ARG:HA	2:W:681:LEU:HD11	1.90	0.54
2:S:278:THR:HG22	2:S:1051:ILE:HG12	1.89	0.54
2:4:935:ALA:HA	2:4:938:MET:HB2	1.89	0.53
2:X:785:ARG:NH1	2:X:787:VAL:O	2.41	0.53
2:X:1042:ARG:NH1	2:X:1044:ASP:OD2	2.41	0.53
2:S:640:THR:O	2:S:644:ASN:ND2	2.42	0.53
2:S:1344:ASN:ND2	2:S:1347:THR:OG1	2.40	0.53
2:4:399:THR:HG22	2:4:1043:THR:HG22	1.91	0.53
2:T:537:HIS:HA	2:T:1238:TRP:CD1	2.44	0.53
2:T:1250:TYR:HB2	2:T:1270:PHE:HD2	1.73	0.53
2:4:861:ASP:O	2:4:930:ARG:NH2	2.41	0.53
2:W:851:LEU:HD23	2:W:854:LEU:HD12	1.90	0.53
2:W:899:ASP:OD1	2:W:899:ASP:N	2.40	0.53
2:T:716:HIS:HA	2:T:730:LEU:HD11	1.90	0.53
2:4:619:MET:SD	2:4:630:ASN:ND2	2.77	0.53
2:X:559:ARG:O	2:X:564:ASN:ND2	2.30	0.53
2:T:1073:VAL:HG22	2:T:1078:VAL:HG13	1.91	0.53
2:X:578:ARG:NH1	2:X:1014:SER:O	2.41	0.53
2:X:1345:LYS:NZ	2:X:1376:TYR:OXT	2.38	0.53
2:W:13:LEU:HD23	2:T:350:LEU:HD12	1.90	0.53
2:T:828:ASN:ND2	2:T:937:THR:O	2.42	0.53
3:b:152:THR:HA	3:b:281:ASN:HB3	1.90	0.53
4:c:280:PHE:O	4:d:274:GLN:NE2	2.41	0.53
2:W:902:GLN:NE2	2:W:1020:SER:OG	2.41	0.53
2:4:1127:TYR:HB2	2:4:1133:HIS:HB2	1.91	0.53
2:W:1068:VAL:HG23	3:b:47:ALA:HB2	1.91	0.53
2:S:1292:ARG:NH2	4:6:129:SER:O	2.41	0.53
2:4:724:HIS:HB3	2:4:793:LEU:HB2	1.90	0.53
2:4:731:MET:HG2	2:4:738:PRO:HG2	1.90	0.53
2:W:491:MET:HB2	2:W:783:ASP:HA	1.91	0.53
3:5:46:ALA:O	3:5:50:ARG:NH1	2.42	0.53
2:W:1308:VAL:HG21	2:W:1314:VAL:HG21	1.91	0.53
4:7:148:ILE:HD12	4:7:181:VAL:HG21	1.91	0.53
2:X:777:ARG:HG2	2:X:887:PHE:HE1	1.74	0.53
2:W:678:ARG:HH22	2:X:608:ALA:HB3	1.74	0.52
2:S:902:GLN:NE2	2:S:1020:SER:OG	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:399:THR:HG22	2:T:1043:THR:HG22	1.91	0.52
3:b:40:ASP:O	4:c:2:ALA:N	2.43	0.52
2:X:278:THR:HG22	2:X:1051:ILE:HG12	1.91	0.52
2:W:963:ASN:HA	2:W:966:THR:HG22	1.91	0.52
2:S:1187:ASP:OD2	2:S:1232:ARG:NH2	2.42	0.52
3:b:124:GLN:NE2	3:b:311:SER:O	2.42	0.52
4:d:97:ASN:HD22	4:d:105:TRP:CD1	2.24	0.52
2:X:91:ILE:HD11	2:X:1089:LEU:HD22	1.90	0.52
2:W:987:TYR:O	2:W:992:LYS:NZ	2.42	0.52
2:S:7:GLN:NE2	2:S:36:GLN:OE1	2.41	0.52
2:S:1047:LEU:HD12	2:S:1106:ALA:HB3	1.91	0.52
2:W:275:VAL:HG22	2:W:375:ALA:HB3	1.92	0.52
2:W:714:ASP:O	2:W:804:LYS:NZ	2.43	0.52
2:T:946:LYS:HE2	2:T:993:SER:HA	1.90	0.52
4:c:9:VAL:HG21	4:c:45:LEU:HD21	1.91	0.52
2:W:1071:ARG:HH22	4:c:38:ARG:H	1.55	0.52
2:4:140:PHE:O	3:5:50:ARG:NH2	2.42	0.52
2:S:731:MET:HG2	2:S:738:PRO:HG2	1.91	0.52
2:4:756:PHE:O	2:4:788:LEU:N	2.43	0.52
2:T:293:VAL:HG21	2:T:368:LYS:HE3	1.92	0.52
2:4:428:GLN:NE2	2:4:577:SER:OG	2.34	0.52
2:W:1107:ILE:HD11	2:W:1364:MET:HE1	1.91	0.52
2:S:157:LYS:HD2	2:T:338:ASN:HA	1.91	0.52
3:b:94:LYS:NZ	4:d:106:ASP:OD2	2.39	0.52
2:X:44:ARG:HB3	2:X:46:GLY:H	1.75	0.52
2:W:93:PHE:HB2	2:W:116:VAL:HB	1.91	0.51
2:W:150:THR:HG21	2:T:313:LEU:HD21	1.93	0.51
1:2:13:GLU:OE1	1:2:46:ARG:NH2	2.38	0.51
2:T:854:LEU:HD13	2:T:860:LYS:HG2	1.92	0.51
4:6:133:ASP:OD1	4:6:133:ASP:N	2.40	0.51
2:T:224:HIS:HD2	2:T:244:MET:HE1	1.75	0.51
3:5:69:THR:HG21	4:7:92:ASN:HD21	1.74	0.51
2:W:214:VAL:HG12	2:W:218:LYS:HE2	1.93	0.51
2:S:777:ARG:NH2	2:S:885:CYS:O	2.43	0.51
2:4:183:LEU:HD13	2:4:394:ARG:HH21	1.76	0.51
2:4:597:ILE:HA	2:4:600:ILE:HB	1.93	0.51
2:X:1182:THR:HG23	2:X:1236:ASN:HB3	1.93	0.51
2:S:421:GLY:HA3	2:T:413:TYR:HA	1.92	0.51
2:T:450:LEU:HD11	2:T:1025:ILE:HA	1.93	0.51
2:4:182:LYS:NZ	2:4:1058:SER:OG	2.44	0.51
2:4:676:HIS:HA	2:4:679:LYS:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:839:VAL:HG23	2:4:854:LEU:HD21	1.93	0.51
2:4:973:ASN:HB3	2:4:976:VAL:HG23	1.92	0.51
2:T:306:TYR:OH	2:T:323:MET:O	2.29	0.51
2:4:620:ILE:HG22	2:4:622:GLY:H	1.75	0.51
3:5:67:GLN:NE2	2:X:1071:ARG:O	2.44	0.51
3:b:207:LEU:HB3	3:b:248:SER:HB3	1.92	0.51
4:d:53:ARG:NH2	4:d:133:ASP:OD2	2.44	0.51
2:W:12:TYR:HA	2:S:56:VAL:HG12	1.93	0.51
2:W:898:ARG:HE	2:W:913:VAL:HG23	1.74	0.51
2:W:78:THR:HG22	2:W:304:ALA:HB3	1.91	0.51
2:S:1283:TYR:O	2:S:1287:ASN:ND2	2.44	0.51
2:X:536:VAL:HG13	2:X:1244:SER:HA	1.93	0.51
2:W:1071:ARG:O	2:W:1079:THR:OG1	2.27	0.51
2:T:275:VAL:HG22	2:T:375:ALA:HB3	1.93	0.51
2:4:206:LYS:HG3	2:4:208:ALA:H	1.76	0.51
2:W:538:PRO:O	2:W:559:ARG:NH1	2.44	0.50
2:W:626:LYS:NZ	2:W:881:SER:O	2.43	0.50
4:7:7:ILE:HG23	4:7:38:ARG:HA	1.92	0.50
2:W:582:PHE:HA	2:W:1032:MET:HE1	1.92	0.50
2:S:1345:LYS:NZ	2:S:1376:TYR:OXT	2.33	0.50
4:d:5:LYS:HB2	4:d:86:ARG:HB3	1.94	0.50
2:X:633:LEU:HA	2:X:874:MET:HE3	1.93	0.50
2:X:777:ARG:NH2	2:X:885:CYS:O	2.44	0.50
2:W:394:ARG:NH1	2:W:1317:ASP:OD2	2.44	0.50
2:S:495:ARG:HE	2:S:499:GLN:HE21	1.58	0.50
2:T:555:ARG:HE	2:T:907:HIS:CD2	2.29	0.50
2:4:82:ASP:N	2:4:82:ASP:OD1	2.42	0.50
2:W:256:THR:HG22	2:W:258:PHE:H	1.76	0.50
2:W:324:ARG:NH1	2:W:325:ASN:OD1	2.45	0.50
2:W:603:THR:HG22	2:W:647:LYS:HB3	1.94	0.50
2:S:451:LYS:HB3	2:S:1117:ASP:HB3	1.94	0.50
4:c:58:ASP:OD1	4:c:58:ASP:N	2.42	0.50
1:0:13:GLU:OE1	1:0:46:ARG:NH2	2.38	0.50
2:W:266:THR:HG21	2:W:373:PHE:HD2	1.77	0.50
2:T:809:VAL:HG13	2:T:1012:MET:HB2	1.94	0.50
2:4:560:THR:H	2:4:564:ASN:HD22	1.60	0.50
2:W:84:ARG:HH22	2:W:85:ARG:HH21	1.60	0.50
2:T:602:GLU:HB3	2:T:647:LYS:HE2	1.93	0.50
2:W:588:MET:HE1	2:W:687:LEU:HD12	1.94	0.50
2:W:824:VAL:H	2:W:889:THR:HG21	1.76	0.50
2:W:1342:MET:HA	2:W:1375:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:707:HIS:HD2	2:S:715:PRO:HD3	1.77	0.50
2:4:840:PHE:CG	1:A:53:ILE:HG12	2.47	0.50
4:7:231:ARG:HG2	4:7:233:ASP:H	1.76	0.50
2:W:633:LEU:HD12	2:W:874:MET:HB3	1.94	0.49
2:4:102:HIS:O	2:4:106:ARG:NH1	2.44	0.49
2:X:128:GLU:OE2	2:X:1071:ARG:NH2	2.45	0.49
2:X:877:VAL:O	2:X:880:THR:OG1	2.28	0.49
2:T:980:PRO:HD2	2:T:983:LEU:HD12	1.94	0.49
3:b:79:THR:HA	3:b:139:LEU:HD21	1.94	0.49
4:c:300:CYS:SG	4:c:301:TRP:N	2.85	0.49
2:X:264:TYR:CE1	2:X:300:PRO:HD2	2.47	0.49
2:4:85:ARG:HH21	2:X:151:GLU:HG2	1.77	0.49
2:S:100:ILE:O	2:S:109:ASN:ND2	2.45	0.49
2:X:698:GLU:HG3	2:X:705:ILE:HD12	1.93	0.49
2:X:1068:VAL:HG22	2:X:1082:ILE:HG12	1.95	0.49
2:X:1369:LYS:HG2	2:X:1374:VAL:HG22	1.93	0.49
1:2:70:ARG:HE	2:T:855:GLU:HG2	1.76	0.49
2:T:1342:MET:HA	2:T:1375:VAL:HG21	1.95	0.49
2:4:578:ARG:NH2	2:4:1017:GLN:OE1	2.46	0.49
2:W:963:ASN:O	2:W:967:ARG:N	2.44	0.49
2:S:130:GLU:HG2	2:S:1079:THR:HG22	1.94	0.49
2:S:1005:THR:HG22	2:S:1007:GLY:H	1.77	0.49
2:S:1167:PRO:HD3	2:T:1224:ILE:HD13	1.95	0.49
2:T:278:THR:HG22	2:T:1051:ILE:HG12	1.95	0.49
2:4:633:LEU:HD11	2:4:874:MET:HA	1.94	0.49
3:b:225:THR:HG22	3:b:293:THR:HG22	1.93	0.49
2:X:453:ILE:HD11	2:X:1038:MET:HE1	1.94	0.49
2:W:947:LEU:HD21	2:W:995:VAL:HG12	1.95	0.49
2:S:716:HIS:HD2	2:S:736:ARG:HH21	1.60	0.49
2:W:178:VAL:HG22	2:W:1061:MET:HE2	1.94	0.49
2:4:90:LYS:HE2	2:X:27:ALA:HB3	1.95	0.49
4:6:262:ASP:OD2	4:7:158:TYR:OH	2.31	0.49
2:X:520:THR:HG22	2:X:568:PRO:HA	1.94	0.49
2:X:929:ASP:HA	2:X:932:ARG:HG3	1.95	0.49
2:4:842:ASP:O	2:4:844:VAL:N	2.46	0.49
2:T:898:ARG:HD3	2:T:902:GLN:HG3	1.94	0.48
4:c:218:VAL:HG13	4:d:215:SER:HB2	1.94	0.48
2:X:130:GLU:HG2	2:X:1079:THR:HG22	1.94	0.48
2:W:770:LEU:HD21	2:W:883:LEU:HD22	1.94	0.48
2:S:1117:ASP:OD1	2:S:1117:ASP:N	2.46	0.48
2:T:407:HIS:HB2	2:T:1184:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:868:ILE:HG22	2:T:870:PRO:HD3	1.94	0.48
4:6:50:VAL:HG13	4:6:62:ILE:HG12	1.95	0.48
2:S:151:GLU:HG2	2:X:85:ARG:HH22	1.78	0.48
2:T:603:THR:HG22	2:T:647:LYS:HB3	1.93	0.48
1:3:36:MET:HE3	1:3:40:GLU:HB3	1.95	0.48
3:5:165:MET:SD	3:5:168:SER:OG	2.71	0.48
2:X:619:MET:SD	2:X:881:SER:OG	2.68	0.48
2:S:687:LEU:HD23	2:S:805:LEU:HD22	1.95	0.48
2:S:799:ASN:N	2:S:799:ASN:OD1	2.46	0.48
2:4:623:GLN:NE2	2:4:761:GLY:O	2.37	0.48
1:1:36:MET:HE3	1:1:40:GLU:HB3	1.95	0.48
2:W:438:ASN:HB2	2:W:1171:HIS:HD2	1.78	0.48
2:W:717:LEU:HD23	2:W:804:LYS:HD3	1.96	0.48
2:W:1196:ASN:HD21	2:W:1202:ALA:H	1.61	0.48
2:4:1334:HIS:O	2:4:1336:VAL:N	2.47	0.48
4:6:54:GLU:HG3	4:6:55:THR:HG23	1.96	0.48
2:W:428:GLN:NE2	2:W:577:SER:OG	2.42	0.48
2:X:1294:ALA:HB3	2:X:1318:GLN:HE21	1.79	0.48
2:4:839:VAL:HG13	2:4:872:VAL:HG13	1.96	0.48
2:X:263:THR:O	2:X:359:ARG:NH1	2.47	0.48
2:S:898:ARG:NH1	2:S:910:GLY:O	2.47	0.48
2:T:444:PHE:HD1	2:T:1113:VAL:HG13	1.79	0.48
2:4:684:LEU:HD11	2:4:805:LEU:HB2	1.96	0.48
2:X:700:VAL:HG23	2:X:705:ILE:HG12	1.96	0.48
2:4:278:THR:HG22	2:4:1051:ILE:HG12	1.96	0.48
3:b:79:THR:OG1	3:b:80:PHE:N	2.46	0.48
3:b:228:ALA:HB2	3:b:291:LEU:HD11	1.95	0.48
3:b:280:ILE:HA	3:b:283:LEU:HD13	1.96	0.48
4:c:111:LEU:HB2	4:c:286:LEU:HB2	1.95	0.48
2:T:832:THR:HG22	1:3:11:ILE:HD11	1.95	0.47
2:W:640:THR:O	2:W:644:ASN:ND2	2.47	0.47
1:2:36:MET:HE3	1:2:40:GLU:HB3	1.95	0.47
2:X:707:HIS:HD2	2:X:715:PRO:HD3	1.78	0.47
1:0:36:MET:HE3	1:0:40:GLU:HB3	1.95	0.47
2:W:1343:SER:HB2	2:X:1347:THR:HA	1.95	0.47
2:T:146:PRO:HA	2:T:149:PHE:HD2	1.79	0.47
2:X:39:LEU:HB3	2:X:43:ALA:HB1	1.96	0.47
2:X:902:GLN:NE2	2:X:1020:SER:OG	2.37	0.47
2:W:447:GLN:NE2	2:X:521:GLU:OE1	2.47	0.47
2:S:1027:GLN:HB3	2:S:1032:MET:HB2	1.95	0.47
2:S:1369:LYS:HG2	2:S:1374:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1005:THR:HG22	2:T:1007:GLY:H	1.79	0.47
2:T:1196:ASN:HD22	2:T:1201:ALA:HA	1.80	0.47
2:4:835:TYR:HB2	1:A:46:ARG:HD3	1.95	0.47
2:4:902:GLN:NE2	2:4:1020:SER:OG	2.35	0.47
2:X:1192:GLN:NE2	2:X:1359:GLU:O	2.36	0.47
2:S:129:ILE:HD11	2:S:166:GLY:HA3	1.96	0.47
2:4:725:ASP:HB2	2:4:790:VAL:HG11	1.95	0.47
4:c:126:VAL:HG23	4:c:133:ASP:HB3	1.97	0.47
1:0:55:HIS:HD2	2:W:770:LEU:HD22	1.79	0.47
2:4:699:THR:HA	2:4:704:PRO:HA	1.96	0.47
2:4:712:LEU:HD23	2:4:804:LYS:HD2	1.97	0.47
4:d:11:LEU:HD12	4:d:80:ASP:HB2	1.96	0.47
2:T:512:VAL:HG12	2:T:993:SER:HB3	1.95	0.47
2:4:278:THR:HB	2:4:282:VAL:HB	1.97	0.47
4:7:291:TYR:HD1	4:7:298:ALA:HB2	1.78	0.47
2:X:716:HIS:HD2	2:X:736:ARG:HH21	1.63	0.47
2:S:773:ILE:O	2:S:776:THR:OG1	2.32	0.47
2:4:214:VAL:HG12	2:4:218:LYS:HE2	1.97	0.47
2:4:228:LEU:HD21	2:4:285:ARG:HG3	1.97	0.47
2:4:561:MET:H	2:4:564:ASN:ND2	2.13	0.47
4:c:89:PRO:HA	4:c:90:SER:HA	1.59	0.47
4:c:138:MET:HE2	4:c:140:VAL:HG22	1.97	0.47
2:W:898:ARG:NH1	2:W:910:GLY:O	2.48	0.46
2:S:1220:TYR:HE2	2:S:1272:LYS:HD3	1.80	0.46
2:4:1066:PRO:HB3	2:4:1084:HIS:HA	1.95	0.46
3:5:208:ASP:OD1	3:5:250:LYS:NZ	2.48	0.46
2:X:543:PHE:HE1	2:X:557:THR:HG23	1.80	0.46
4:7:266:MET:HA	4:7:269:MET:HB3	1.98	0.46
2:X:93:PHE:HB2	2:X:116:VAL:HB	1.96	0.46
2:X:611:LEU:HD11	2:X:935:ALA:HB2	1.98	0.46
2:X:1117:ASP:OD1	2:X:1117:ASP:N	2.48	0.46
2:S:136:ILE:HG12	2:S:159:ILE:HD11	1.98	0.46
2:S:532:LEU:O	2:S:1241:GLN:NE2	2.47	0.46
2:T:907:HIS:HB2	2:T:910:GLY:N	2.31	0.46
1:3:27:ARG:O	1:3:30:THR:OG1	2.31	0.46
2:4:1068:VAL:HG22	2:4:1082:ILE:HG12	1.97	0.46
2:T:130:GLU:HG2	2:T:1079:THR:HG22	1.96	0.46
3:b:141:ASP:N	3:b:141:ASP:OD1	2.47	0.46
4:c:35:ASP:HB2	4:c:40:GLN:HE22	1.80	0.46
2:S:420:ARG:NH2	2:T:414:SER:OG	2.49	0.46
2:S:447:GLN:NE2	2:T:521:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:15:VAL:HG22	2:X:1068:VAL:HG11	1.98	0.46
2:W:600:ILE:HG23	2:W:651:VAL:HG11	1.97	0.46
2:S:11:PRO:HB2	2:X:332:ARG:HD2	1.97	0.46
2:S:628:VAL:HA	2:S:631:MET:HE3	1.98	0.46
2:4:1210:TYR:HB3	2:4:1283:TYR:HE2	1.80	0.46
2:T:41:LYS:O	2:T:44:ARG:NH1	2.47	0.46
4:6:113:VAL:HG22	4:6:139:VAL:HG12	1.98	0.46
4:7:7:ILE:HB	4:7:84:LEU:HB2	1.98	0.46
4:c:262:ASP:OD2	4:d:158:TYR:OH	2.32	0.46
2:X:1107:ILE:HG21	2:X:1111:MET:HE3	1.98	0.46
1:0:53:ILE:HD13	2:W:840:PHE:CE1	2.51	0.46
2:S:82:ASP:OD1	2:S:82:ASP:N	2.48	0.46
2:S:606:ASP:OD2	2:S:641:TYR:OH	2.26	0.46
3:b:305:LEU:O	3:b:312:LEU:N	2.46	0.46
2:W:82:ASP:OD1	2:W:82:ASP:N	2.50	0.45
2:T:352:ASP:N	2:T:352:ASP:OD1	2.43	0.45
2:4:592:ILE:HG13	2:4:683:GLU:HG2	1.98	0.45
2:X:606:ASP:OD2	2:X:641:TYR:OH	2.28	0.45
2:W:1183:PRO:HB3	2:W:1238:TRP:HZ3	1.81	0.45
2:W:537:HIS:HB2	2:W:1245:LEU:HB2	1.98	0.45
2:S:619:MET:SD	2:S:881:SER:OG	2.70	0.45
2:4:950:ASP:HB2	2:4:954:ALA:H	1.81	0.45
2:W:407:HIS:HB2	2:W:1184:VAL:HG12	1.98	0.45
2:W:731:MET:HG2	2:W:738:PRO:HG2	1.98	0.45
2:T:90:LYS:HG3	2:T:117:MET:SD	2.57	0.45
2:4:206:LYS:HB3	2:4:209:VAL:HG23	1.98	0.45
4:7:13:SER:OG	4:7:130:ASN:OD1	2.32	0.45
2:X:826:TYR:OH	2:X:920:ASN:O	2.35	0.45
2:4:129:ILE:HD13	2:4:163:LEU:HD23	1.99	0.45
3:b:111:LEU:HD23	3:b:243:LEU:HD13	1.99	0.45
2:W:123:HIS:HB2	2:W:1086:ILE:HB	1.98	0.45
2:W:507:ALA:HB1	2:W:978:ASN:HD22	1.80	0.45
2:W:955:ALA:HB1	2:W:962:ALA:HA	1.98	0.45
2:S:1280:ARG:NH2	2:S:1288:GLU:OE1	2.50	0.45
2:4:689:GLN:HE21	2:4:693:LYS:NZ	2.15	0.45
2:W:438:ASN:HD22	2:W:1171:HIS:CD2	2.35	0.45
2:S:79:GLU:HG2	2:S:1063:VAL:HB	1.99	0.45
2:T:1111:MET:SD	2:T:1366:ARG:NH2	2.90	0.45
2:4:340:LEU:HD12	2:4:341:PRO:HD2	1.99	0.45
2:4:913:VAL:HG12	2:4:990:TRP:HD1	1.81	0.45
2:W:331:ALA:HA	2:W:335:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:796:ASN:HB3	2:X:932:ARG:HH12	1.82	0.45
2:S:178:VAL:HG22	2:S:1061:MET:HE2	1.98	0.45
2:S:718:LEU:HD21	2:S:730:LEU:HD12	1.99	0.45
2:T:873:ASP:HA	2:T:876:ARG:HD2	1.99	0.45
2:4:838:PRO:HA	2:4:841:ALA:HB3	1.97	0.45
4:d:47:LEU:HB2	4:d:135:VAL:HB	1.99	0.45
2:X:187:PRO:HG2	2:X:192:LEU:HD12	1.99	0.45
2:W:91:ILE:HD12	2:W:1089:LEU:HD22	1.99	0.44
2:W:297:MET:HE3	2:W:364:ALA:HB3	1.99	0.44
2:T:254:GLU:OE2	2:T:372:LYS:NZ	2.48	0.44
2:T:578:ARG:NH1	2:T:1014:SER:O	2.46	0.44
2:T:606:ASP:OD1	2:T:647:LYS:NZ	2.36	0.44
2:X:1043:THR:OG1	2:X:1305:GLN:NE2	2.50	0.44
1:0:27:ARG:O	1:0:30:THR:OG1	2.31	0.44
2:W:312:ASN:ND2	2:W:323:MET:O	2.49	0.44
2:W:1254:PHE:HB2	2:W:1267:ARG:HH22	1.83	0.44
2:T:264:TYR:HE1	2:T:300:PRO:HD2	1.81	0.44
2:T:404:VAL:HG13	2:T:1038:MET:HG3	1.98	0.44
2:4:639:GLN:HA	2:4:670:PRO:HG3	1.99	0.44
2:4:684:LEU:HD21	2:4:805:LEU:HD12	1.99	0.44
4:c:220:ARG:HG2	4:c:265:ARG:HH12	1.81	0.44
2:X:306:TYR:OH	2:X:323:MET:O	2.34	0.44
1:2:27:ARG:O	1:2:30:THR:OG1	2.31	0.44
2:4:275:VAL:HG22	2:4:375:ALA:HB3	1.98	0.44
2:4:455:HIS:HD2	2:4:1119:PHE:HD1	1.64	0.44
2:4:709:VAL:O	2:4:1018:LYS:HB2	2.17	0.44
2:4:834:THR:HG22	1:A:53:ILE:HD12	1.99	0.44
3:5:71:GLY:HA3	3:5:181:MET:HE3	1.99	0.44
2:S:740:ILE:HB	2:S:747:TYR:HB3	2.00	0.44
2:T:591:VAL:HB	2:T:683:GLU:HB2	1.99	0.44
2:T:714:ASP:O	2:T:804:LYS:NZ	2.50	0.44
2:T:1271:HIS:ND1	2:T:1274:ASP:OD2	2.47	0.44
2:X:66:PHE:HD1	2:X:175:VAL:HG22	1.83	0.44
2:S:596:THR:HG21	2:S:679:LYS:HD2	2.00	0.44
2:4:833:LEU:HD22	2:4:878:LEU:HB3	1.98	0.44
2:X:532:LEU:O	2:X:1241:GLN:NE2	2.43	0.44
3:5:85:PRO:O	3:5:88:THR:OG1	2.29	0.44
2:X:78:THR:HG22	2:X:304:ALA:HB3	1.99	0.44
2:W:537:HIS:HA	2:W:1238:TRP:NE1	2.33	0.44
2:T:877:VAL:O	2:T:880:THR:OG1	2.34	0.44
2:T:1073:VAL:HG13	2:T:1078:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:727:PHE:HB3	2:4:731:MET:HE3	1.99	0.44
1:2:28:MET:HE2	1:2:45:LYS:HG2	2.00	0.44
2:4:743:GLY:O	2:4:746:ASN:ND2	2.51	0.44
2:4:1116:GLN:HB2	2:4:1176:THR:HB	2.00	0.44
2:X:82:ASP:OD1	2:X:82:ASP:N	2.40	0.44
2:X:394:ARG:HD3	2:X:1315:PHE:HB3	1.99	0.44
2:X:995:VAL:HG22	2:X:1015:MET:HE3	2.00	0.44
2:S:51:GLU:HB3	2:T:87:ILE:HB	2.00	0.43
2:S:662:THR:HG22	2:T:607:PRO:HB2	2.00	0.43
2:T:692:LEU:HD23	2:T:713:LEU:HD11	2.00	0.43
2:X:718:LEU:HD12	2:X:894:VAL:HG21	1.99	0.43
2:4:880:THR:HG22	1:A:54:ALA:HA	1.99	0.43
2:4:1276:MET:HE3	2:4:1280:ARG:HD2	2.00	0.43
4:c:58:ASP:HB3	4:c:196:ASP:HB3	1.99	0.43
2:X:628:VAL:HA	2:X:631:MET:HE3	2.01	0.43
2:X:1236:ASN:OD1	2:X:1236:ASN:N	2.48	0.43
2:S:836:ASN:HD21	2:S:854:LEU:HD12	1.82	0.43
2:4:456:PRO:HA	2:4:459:HIS:HB2	2.00	0.43
3:5:227:TYR:OH	4:6:305:ARG:NH1	2.51	0.43
2:W:436:ASN:HB2	2:W:440:VAL:O	2.18	0.43
2:W:438:ASN:HD22	2:W:1171:HIS:HD2	1.66	0.43
2:W:913:VAL:HG21	2:W:990:TRP:HE1	1.84	0.43
2:T:860:LYS:O	2:T:864:GLN:N	2.45	0.43
2:4:743:GLY:HA3	2:4:786:HIS:CE1	2.53	0.43
4:6:123:SER:OG	4:6:136:PHE:O	2.34	0.43
2:W:944:PHE:H	2:W:949:ALA:HB2	1.83	0.43
2:W:1073:VAL:HG13	2:W:1078:VAL:HG22	2.01	0.43
2:T:1127:TYR:HB2	2:T:1133:HIS:HB2	1.99	0.43
4:d:51:CYS:HB2	4:d:62:ILE:HD11	1.99	0.43
2:T:79:GLU:N	2:T:304:ALA:O	2.49	0.43
2:T:1115:CYS:HA	2:T:1177:CYS:HB2	2.00	0.43
2:4:306:TYR:HE1	2:X:39:LEU:HD23	1.83	0.43
3:b:211:CYS:HB2	3:b:213:MET:HB2	2.01	0.43
2:X:516:ALA:HB2	2:X:994:PRO:HG3	1.99	0.43
2:X:716:HIS:CD2	2:X:736:ARG:HH21	2.36	0.43
2:X:822:MET:HE2	2:X:957:LEU:HD21	2.01	0.43
2:X:1033:HIS:ND1	2:X:1034:PRO:O	2.51	0.43
2:T:105:GLY:HA3	4:6:41:ASN:HB2	2.01	0.43
2:4:685:ILE:HA	2:4:688:GLU:HG2	2.00	0.43
2:4:1241:GLN:HG3	2:4:1243:GLY:H	1.83	0.43
3:b:86:LEU:HA	3:b:165:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:252:VAL:HG21	2:W:1053:TYR:HD2	1.83	0.43
2:W:822:MET:SD	2:W:939:PHE:HB3	2.58	0.43
2:S:961:LEU:HD11	2:S:977:PHE:HZ	1.83	0.43
2:T:184:ARG:O	2:T:1290:SER:OG	2.37	0.43
2:W:695:ALA:HB1	2:W:706:THR:HG22	2.01	0.43
4:c:175:ASP:HB3	4:c:189:ARG:HH12	1.84	0.43
4:d:291:TYR:HD1	4:d:298:ALA:HB2	1.84	0.43
2:4:226:PHE:CD2	2:4:1364:MET:HB3	2.54	0.43
2:4:561:MET:H	2:4:564:ASN:HD22	1.67	0.43
2:X:84:ARG:HH22	2:X:85:ARG:HH21	1.66	0.43
2:W:49:ARG:HD3	2:X:87:ILE:HD11	2.01	0.42
2:W:1198:ARG:NH2	2:W:1219:LEU:O	2.48	0.42
2:S:221:LEU:HD23	2:S:1363:PRO:HB3	2.01	0.42
2:T:1342:MET:HE1	2:T:1370:LEU:H	1.84	0.42
2:4:1200:ARG:HG3	2:4:1234:THR:HG23	2.00	0.42
4:6:177:TYR:HB3	4:7:263:ILE:HG21	2.00	0.42
4:7:38:ARG:HE	4:7:39:LEU:HG	1.84	0.42
2:X:224:HIS:CD2	2:X:244:MET:HE1	2.53	0.42
2:S:9:PRO:HB3	2:S:45:GLU:HB3	2.01	0.42
2:S:698:GLU:HG3	2:S:705:ILE:HD12	2.02	0.42
4:c:32:PRO:HD3	4:c:137:PRO:HG3	2.01	0.42
2:X:637:VAL:HG22	2:X:868:ILE:HD13	2.01	0.42
2:X:1027:GLN:HB3	2:X:1032:MET:HB2	2.01	0.42
4:d:88:ASP:HB2	4:d:91:ASP:HB2	2.01	0.42
1:1:28:MET:HE2	1:1:45:LYS:HG2	2.00	0.42
2:X:451:LYS:HB3	2:X:1117:ASP:HB3	2.00	0.42
2:W:578:ARG:NH1	2:W:1014:SER:O	2.51	0.42
1:3:28:MET:HE2	1:3:45:LYS:HG2	2.00	0.42
2:4:686:ALA:HA	2:4:689:GLN:HG2	2.00	0.42
2:4:1200:ARG:NE	2:4:1219:LEU:O	2.49	0.42
2:4:1217:ARG:HG3	2:4:1221:ASP:HB2	2.00	0.42
1:0:28:MET:HE2	1:0:45:LYS:HG2	2.00	0.42
2:W:187:PRO:HG2	2:W:192:LEU:HD12	2.00	0.42
2:W:918:LEU:HD23	2:W:921:GLY:HA3	2.00	0.42
2:W:1027:GLN:HB3	2:W:1032:MET:HB2	2.01	0.42
4:7:142:GLN:HG3	4:7:146:HIS:HE1	1.85	0.42
4:d:148:ILE:HD12	4:d:181:VAL:HG21	2.02	0.42
2:X:624:GLU:HB3	2:X:762:ARG:HH12	1.84	0.42
2:X:1071:ARG:HG3	2:X:1072:GLU:HG3	2.02	0.42
2:W:788:LEU:HD11	2:W:919:VAL:HG21	2.02	0.42
2:4:85:ARG:NH2	2:X:138:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:150:MET:HE2	3:5:241:MET:HE3	2.02	0.42
4:6:110:GLN:HE22	4:6:287:HIS:CE1	2.37	0.42
2:W:130:GLU:HG3	2:X:110:LYS:HD2	2.01	0.42
2:S:777:ARG:HG2	2:S:887:PHE:HE1	1.85	0.42
2:S:1169:LEU:H	2:S:1169:LEU:HG	1.48	0.42
4:6:204:LEU:HD23	4:6:207:LEU:HD12	2.01	0.42
2:X:950:ASP:HA	2:X:951:PRO:HD3	1.90	0.42
2:T:739:ILE:HB	2:T:895:ILE:HB	2.02	0.42
2:4:88:ASP:OD1	2:4:88:ASP:N	2.53	0.42
2:4:224:HIS:HD2	2:4:244:MET:HE1	1.84	0.42
2:X:763:MET:HE1	2:X:881:SER:HA	2.00	0.42
2:X:839:VAL:HG13	2:X:876:ARG:HG2	2.00	0.42
2:W:480:GLY:HA3	2:W:483:LEU:HD11	2.00	0.42
2:S:1168:GLY:HA2	2:T:207:LYS:HD3	2.02	0.42
2:T:773:ILE:O	2:T:776:THR:OG1	2.35	0.42
2:4:680:ILE:O	2:4:684:LEU:HB2	2.20	0.42
2:4:708:LEU:HD22	2:4:1022:PRO:HG3	2.01	0.42
2:X:808:TYR:OH	2:X:915:GLN:NE2	2.53	0.42
2:W:214:VAL:HA	2:W:217:PHE:HD2	1.84	0.42
2:S:192:LEU:HD13	2:S:1098:VAL:HG22	2.01	0.42
2:T:106:ARG:O	4:6:37:HIS:NE2	2.53	0.42
2:T:438:ASN:HD22	2:T:1171:HIS:CD2	2.38	0.42
2:4:70:ALA:N	2:4:377:GLU:OE2	2.50	0.42
2:S:130:GLU:HG3	2:T:110:LYS:HD2	2.02	0.41
2:T:450:LEU:HD21	2:T:1025:ILE:HG13	2.02	0.41
2:T:514:GLN:HG2	2:T:531:LEU:HD21	2.01	0.41
2:4:228:LEU:HD22	2:4:1103:HIS:HB2	2.02	0.41
3:b:124:GLN:HG2	3:b:313:PRO:HD2	2.01	0.41
2:W:395:ARG:HH21	2:W:1047:LEU:HD21	1.84	0.41
2:S:1173:GLN:HE21	2:S:1305:GLN:HA	1.84	0.41
2:T:1187:ASP:OD2	2:T:1232:ARG:NH2	2.53	0.41
2:X:529:HIS:O	2:X:533:ARG:N	2.51	0.41
2:W:129:ILE:HD11	2:W:166:GLY:HA3	2.02	0.41
2:W:1042:ARG:NH2	2:W:1111:MET:O	2.54	0.41
2:S:440:VAL:HG11	2:T:1229:TYR:HE1	1.86	0.41
2:S:1226:ASP:N	2:S:1226:ASP:OD1	2.53	0.41
2:T:893:ARG:HG3	2:T:915:GLN:O	2.20	0.41
2:4:226:PHE:HD2	2:4:1364:MET:HB3	1.85	0.41
2:4:276:LEU:HA	2:4:1053:TYR:HA	2.02	0.41
2:4:566:PRO:HD2	2:4:569:LEU:HD12	2.01	0.41
2:4:777:ARG:HH22	2:4:885:CYS:H	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:518:VAL:HG13	2:X:522:ASP:HB3	2.01	0.41
2:X:902:GLN:HE21	2:X:1020:SER:HG	1.61	0.41
2:W:457:ARG:HG3	2:W:1122:PHE:CD2	2.55	0.41
2:S:516:ALA:HB2	2:S:994:PRO:HG3	2.03	0.41
2:T:1218:LEU:HD11	2:T:1227:PRO:HG3	2.01	0.41
2:4:47:SER:OG	2:4:48:VAL:N	2.52	0.41
4:c:133:ASP:OD1	4:c:133:ASP:N	2.52	0.41
4:c:266:MET:HE1	4:d:211:LEU:HD13	2.03	0.41
2:X:850:ILE:HD11	2:X:872:VAL:HA	2.02	0.41
2:T:252:VAL:HG21	2:T:1053:TYR:HD2	1.85	0.41
2:4:543:PHE:CZ	2:4:555:ARG:HD3	2.56	0.41
4:c:36:CYS:SG	4:c:86:ARG:NH2	2.85	0.41
2:S:717:LEU:HD23	2:S:804:LYS:HD3	2.02	0.41
2:S:1236:ASN:OD1	2:S:1236:ASN:N	2.49	0.41
2:T:78:THR:HG22	2:T:304:ALA:HB3	2.01	0.41
1:A:44:GLN:HA	1:A:47:HIS:HB2	2.03	0.41
4:c:201:LEU:O	4:c:205:ASP:N	2.53	0.41
2:T:93:PHE:HB2	2:T:116:VAL:HB	2.02	0.41
4:6:32:PRO:HD3	4:6:137:PRO:HG3	2.03	0.41
3:b:73:PHE:HE1	4:d:108:ASN:HD21	1.68	0.41
4:6:146:HIS:O	4:6:150:GLN:HG2	2.21	0.41
2:4:368:LYS:HD3	2:4:373:PHE:HE1	1.86	0.41
2:4:525:HIS:CD2	2:4:527:THR:HG22	2.56	0.41
2:4:955:ALA:HB1	2:4:962:ALA:HA	2.02	0.41
2:4:1196:ASN:HD22	2:4:1202:ALA:H	1.67	0.41
1:A:22:HIS:NE2	1:A:24:LEU:HB2	2.36	0.41
3:5:95:GLN:HE22	3:5:145:ASN:HD22	1.69	0.41
4:c:155:TYR:CE2	4:c:192:VAL:HG11	2.56	0.41
4:c:201:LEU:HD22	4:d:231:ARG:HH21	1.86	0.41
2:W:156:ILE:HA	2:W:159:ILE:HG22	2.03	0.41
2:W:301:ALA:HB2	2:W:360:THR:HB	2.03	0.41
2:W:404:VAL:HG13	2:W:1038:MET:HG3	2.03	0.41
2:T:1198:ARG:HB3	2:T:1270:PHE:CE1	2.56	0.41
2:4:804:LYS:HE3	2:4:804:LYS:HB2	1.88	0.41
3:b:20:PRO:HA	3:b:21:PRO:HD3	1.95	0.41
3:b:69:THR:HG23	3:b:182:LYS:HD2	2.03	0.41
2:X:438:ASN:HD22	2:X:1171:HIS:CD2	2.39	0.41
2:X:799:ASN:OD1	2:X:799:ASN:N	2.54	0.41
2:S:183:LEU:HD13	2:S:394:ARG:HH21	1.85	0.40
2:S:588:MET:HE1	2:S:687:LEU:HD12	2.03	0.40
2:T:82:ASP:OD1	2:T:82:ASP:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:170:LEU:HD11	2:T:1084:HIS:HB2	2.03	0.40
2:T:218:LYS:NZ	2:T:1323:LEU:O	2.54	0.40
2:T:1268:GLN:HG2	2:T:1321:HIS:CD2	2.56	0.40
2:4:712:LEU:HD11	2:4:805:LEU:HD21	2.03	0.40
3:5:33:GLU:OE2	3:5:36:ARG:NH2	2.53	0.40
2:X:37:LEU:HD21	2:X:147:LEU:HD13	2.03	0.40
2:X:633:LEU:HD12	2:X:874:MET:HB3	2.03	0.40
2:X:1178:GLU:CD	2:X:1265:PRO:HD2	2.45	0.40
2:W:544:VAL:HG22	2:W:554:TYR:HE1	1.86	0.40
2:S:529:HIS:O	2:S:533:ARG:N	2.52	0.40
2:4:233:LEU:HD11	2:4:1367:LEU:HD21	2.03	0.40
4:7:221:GLY:HA3	4:7:269:MET:HE1	2.03	0.40
4:d:276:LEU:HD12	4:d:279:ILE:HD11	2.03	0.40
2:X:836:ASN:HD21	2:X:854:LEU:HD12	1.86	0.40
2:X:845:ASN:HB3	2:X:848:ASP:HB2	2.03	0.40
2:X:898:ARG:HE	2:X:913:VAL:HB	1.84	0.40
2:W:1198:ARG:HG2	2:W:1270:PHE:HE1	1.86	0.40
2:W:1364:MET:HE3	2:W:1364:MET:HB2	1.91	0.40
2:T:597:ILE:HG21	2:T:1004:ALA:HB1	2.04	0.40
2:4:439:ASN:ND2	2:4:1372:ASN:O	2.48	0.40
4:d:97:ASN:OD1	4:d:97:ASN:N	2.48	0.40
2:W:447:GLN:HA	2:W:450:LEU:HB2	2.02	0.40
2:4:600:ILE:O	2:4:603:THR:OG1	2.39	0.40
2:4:605:PHE:HZ	2:4:816:ASN:HB2	1.87	0.40
2:S:1067:SER:OG	2:S:1083:THR:OG1	2.30	0.40
2:4:476:ASP:H	2:4:544:VAL:HG11	1.87	0.40
4:d:79:PRO:HA	4:d:80:ASP:HA	1.59	0.40
4:d:231:ARG:HB3	4:d:233:ASP:H	1.85	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	0	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	1	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	2	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	3	76/170 (45%)	74 (97%)	2 (3%)	0	100	100
1	A	42/170 (25%)	42 (100%)	0	0	100	100
2	4	1206/1376 (88%)	1120 (93%)	80 (7%)	6 (0%)	24	56
2	S	1273/1376 (92%)	1188 (93%)	83 (6%)	2 (0%)	43	72
2	T	1354/1376 (98%)	1276 (94%)	74 (6%)	4 (0%)	36	65
2	W	1350/1376 (98%)	1282 (95%)	66 (5%)	2 (0%)	48	78
2	X	1335/1376 (97%)	1246 (93%)	86 (6%)	3 (0%)	43	72
3	5	306/331 (92%)	293 (96%)	13 (4%)	0	100	100
3	b	315/331 (95%)	307 (98%)	8 (2%)	0	100	100
4	6	290/305 (95%)	273 (94%)	17 (6%)	0	100	100
4	7	285/305 (93%)	268 (94%)	17 (6%)	0	100	100
4	c	290/305 (95%)	277 (96%)	13 (4%)	0	100	100
4	d	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
All	All	8646/9612 (90%)	8160 (94%)	469 (5%)	17 (0%)	44	72

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	W	263	THR
2	4	843	VAL
2	S	992	LYS
2	T	10	PHE
2	X	992	LYS
2	T	945	ASN
2	4	293	VAL
2	S	993	SER
2	4	842	ASP
2	4	1092	ALA
2	X	44	ARG
2	X	993	SER
2	W	945	ASN
2	4	1335	ARG
2	T	11	PRO
2	T	506	VAL

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Mol	Chain	Res	Type
2	4	314	VAL

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	0	70/141 (50%)	70 (100%)	0	100	100
1	1	70/141 (50%)	70 (100%)	0	100	100
1	2	70/141 (50%)	70 (100%)	0	100	100
1	3	70/141 (50%)	70 (100%)	0	100	100
1	A	39/141 (28%)	39 (100%)	0	100	100
2	4	1044/1166 (90%)	1037 (99%)	7 (1%)	76	77
2	S	1094/1166 (94%)	1085 (99%)	9 (1%)	73	76
2	T	1154/1166 (99%)	1140 (99%)	14 (1%)	63	72
2	W	1150/1166 (99%)	1144 (100%)	6 (0%)	81	80
2	X	1139/1166 (98%)	1130 (99%)	9 (1%)	73	76
3	5	266/281 (95%)	266 (100%)	0	100	100
3	b	272/281 (97%)	272 (100%)	0	100	100
4	6	267/274 (97%)	265 (99%)	2 (1%)	76	77
4	7	262/274 (96%)	262 (100%)	0	100	100
4	c	267/274 (97%)	266 (100%)	1 (0%)	84	81
4	d	270/274 (98%)	270 (100%)	0	100	100
All	All	7504/8193 (92%)	7456 (99%)	48 (1%)	76	79

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	W	308	VAL
2	W	616	ILE
2	W	1025	ILE

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Mol	Chain	Res	Type
2	W	1113	VAL
2	W	1169	LEU
2	W	1184	VAL
2	S	404	VAL
2	S	419	VAL
2	S	651	VAL
2	S	713	LEU
2	S	799	ASN
2	S	1104	VAL
2	S	1121	ILE
2	S	1169	LEU
2	S	1184	VAL
2	T	308	VAL
2	T	422	VAL
2	T	434	VAL
2	T	616	ILE
2	T	620	ILE
2	T	669	ILE
2	T	713	LEU
2	T	947	LEU
2	T	1025	ILE
2	T	1104	VAL
2	T	1121	ILE
2	T	1184	VAL
2	T	1307	VAL
2	T	1308	VAL
2	4	434	VAL
2	4	620	ILE
2	4	713	LEU
2	4	895	ILE
2	4	916	THR
2	4	947	LEU
2	4	1025	ILE
4	6	192	VAL
4	6	217	LEU
4	c	98	VAL
2	X	106	ARG
2	X	129	ILE
2	X	325	ASN
2	X	404	VAL
2	X	651	VAL
2	X	713	LEU

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Mol	Chain	Res	Type
2	X	968	LEU
2	X	1104	VAL
2	X	1184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	17	HIS
1	0	44	GLN
1	0	55	HIS
1	0	73	HIS
1	0	75	GLN
2	W	92	GLN
2	W	102	HIS
2	W	113	GLN
2	W	123	HIS
2	W	312	ASN
2	W	380	GLN
2	W	479	HIS
2	W	498	HIS
2	W	537	HIS
2	W	623	GLN
2	W	674	HIS
2	W	746	ASN
2	W	799	ASN
2	W	902	GLN
2	W	907	HIS
2	W	958	HIS
2	W	978	ASN
2	W	982	ASN
2	W	1116	GLN
2	W	1133	HIS
2	W	1171	HIS
2	W	1334	HIS
2	W	1344	ASN
1	2	17	HIS
1	2	44	GLN
1	2	55	HIS
1	2	73	HIS
1	2	75	GLN
2	S	123	HIS
2	S	124	HIS

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Mol	Chain	Res	Type
2	S	292	GLN
2	S	387	GLN
2	S	407	HIS
2	S	499	GLN
2	S	575	GLN
2	S	623	GLN
2	S	630	ASN
2	S	652	ASN
2	S	697	HIS
2	S	707	HIS
2	S	716	HIS
2	S	746	ASN
2	S	818	HIS
2	S	902	GLN
2	S	982	ASN
2	S	1017	GLN
2	S	1030	HIS
2	S	1114	HIS
2	S	1171	HIS
2	S	1235	ASN
2	S	1318	GLN
2	S	1324	GLN
2	S	1344	ASN
2	T	36	GLN
2	T	113	GLN
2	T	224	HIS
2	T	312	ASN
2	T	354	HIS
2	T	498	HIS
2	T	623	GLN
2	T	663	HIS
2	T	697	HIS
2	T	724	HIS
2	T	782	HIS
2	T	818	HIS
2	T	907	HIS
2	T	915	GLN
2	T	978	ASN
2	T	1050	HIS
2	T	1116	GLN
2	T	1133	HIS
2	T	1171	HIS

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Mol	Chain	Res	Type
2	T	1196	ASN
2	T	1241	GLN
2	T	1321	HIS
2	T	1344	ASN
1	3	17	HIS
1	3	44	GLN
1	3	75	GLN
2	4	428	GLN
2	4	498	HIS
2	4	564	ASN
2	4	567	GLN
2	4	575	GLN
2	4	590	HIS
2	4	601	GLN
2	4	652	ASN
2	4	663	HIS
2	4	689	GLN
2	4	1133	HIS
2	4	1196	ASN
1	A	38	GLN
1	A	44	GLN
3	5	24	HIS
3	5	145	ASN
4	6	64	GLN
4	6	110	GLN
4	6	130	ASN
4	6	150	GLN
4	6	151	GLN
4	6	235	HIS
4	7	37	HIS
4	7	40	GLN
4	7	92	ASN
4	7	110	GLN
3	b	124	GLN
3	b	126	HIS
3	b	194	HIS
3	b	262	HIS
4	c	40	GLN
4	c	110	GLN
4	c	130	ASN
4	c	151	GLN
4	d	94	GLN

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Mol	Chain	Res	Type
4	d	108	ASN
4	d	150	GLN
4	d	156	HIS
4	d	194	ASN
4	d	274	GLN
1	1	17	HIS
1	1	44	GLN
1	1	55	HIS
1	1	75	GLN
2	X	113	GLN
2	X	123	HIS
2	X	224	HIS
2	X	312	ASN
2	X	325	ASN
2	X	336	HIS
2	X	387	GLN
2	X	479	HIS
2	X	575	GLN
2	X	630	ASN
2	X	707	HIS
2	X	716	HIS
2	X	786	HIS
2	X	982	ASN
2	X	991	HIS
2	X	1017	GLN
2	X	1084	HIS
2	X	1114	HIS
2	X	1171	HIS
2	X	1235	ASN
2	X	1318	GLN
2	X	1344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

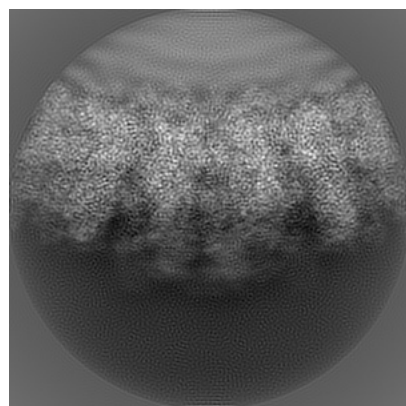
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20433. These allow visual inspection of the internal detail of the map and identification of artifacts.

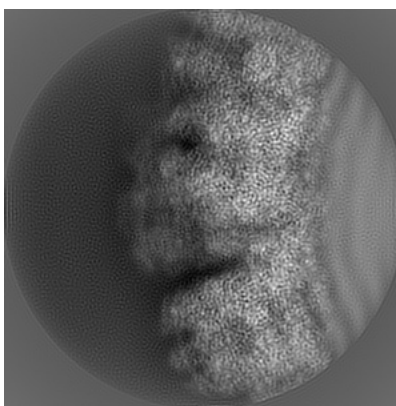
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

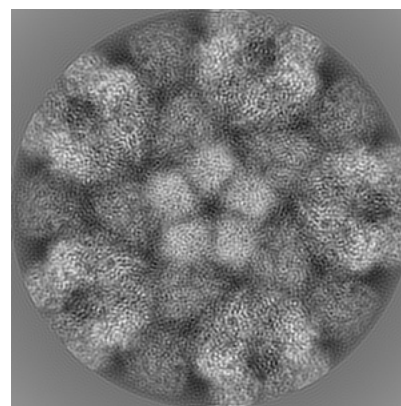
6.1.1 Primary map



X

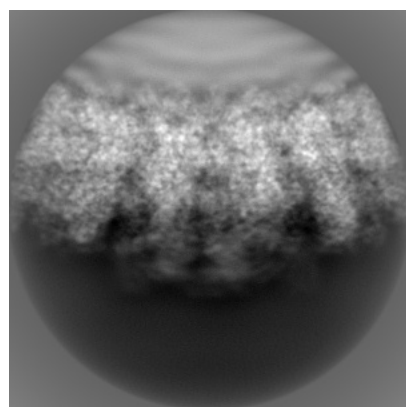


Y

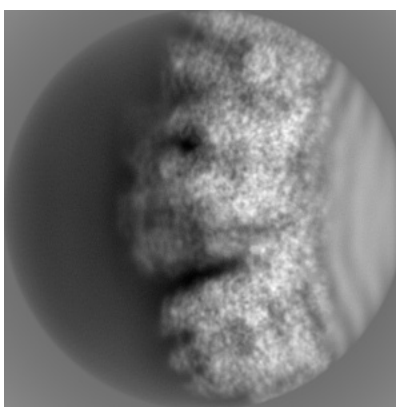


Z

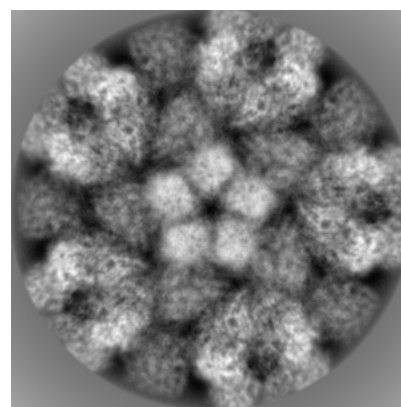
6.1.2 Raw map



X



Y

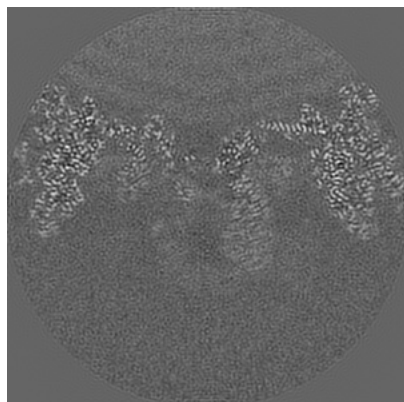


Z

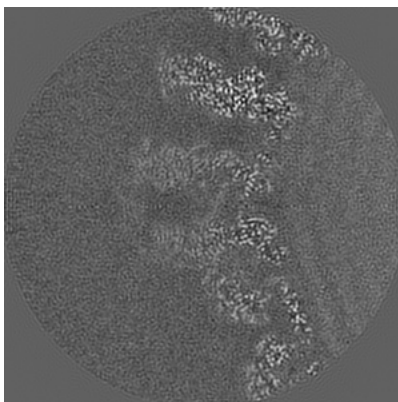
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

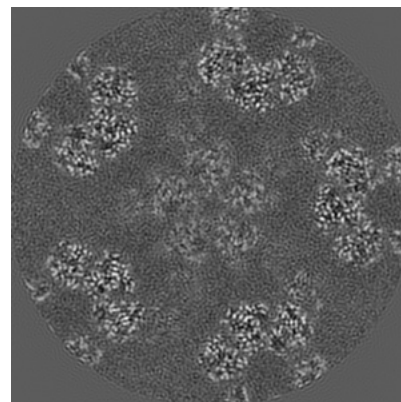
6.2.1 Primary map



X Index: 192

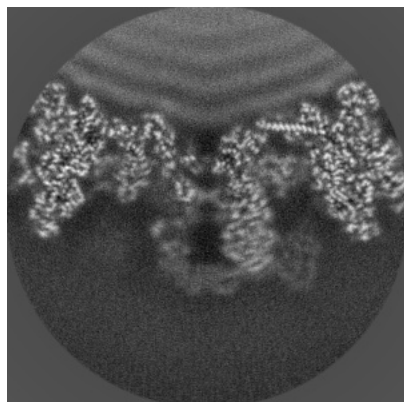


Y Index: 192

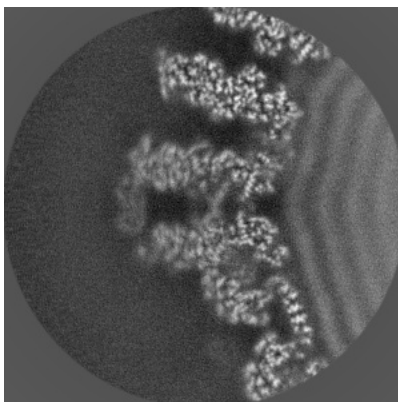


Z Index: 192

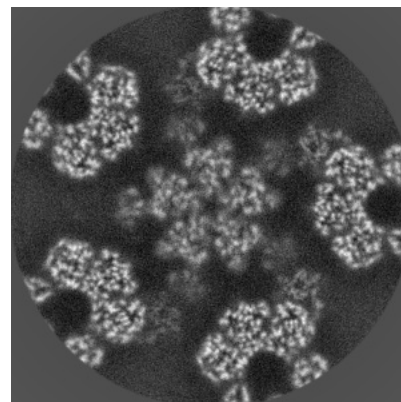
6.2.2 Raw map



X Index: 192



Y Index: 192

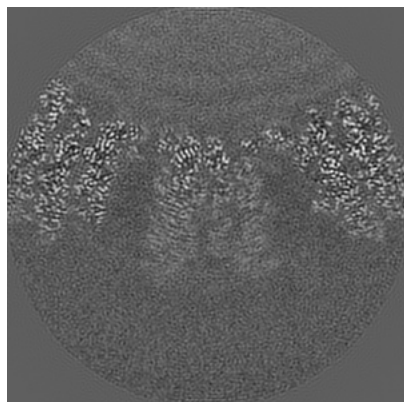


Z Index: 192

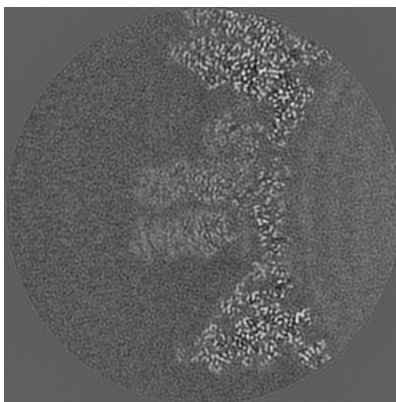
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

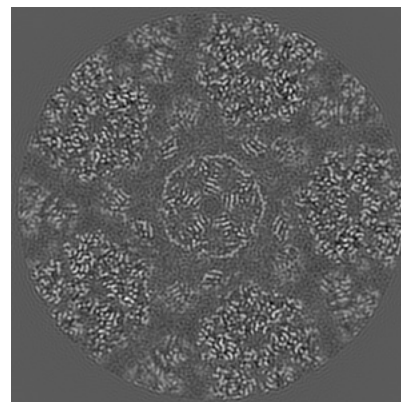
6.3.1 Primary map



X Index: 208

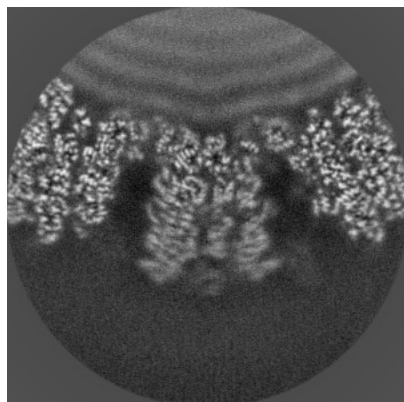


Y Index: 155

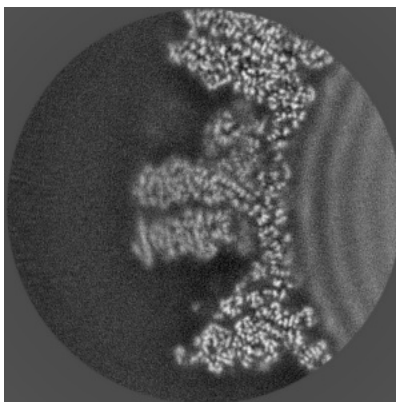


Z Index: 246

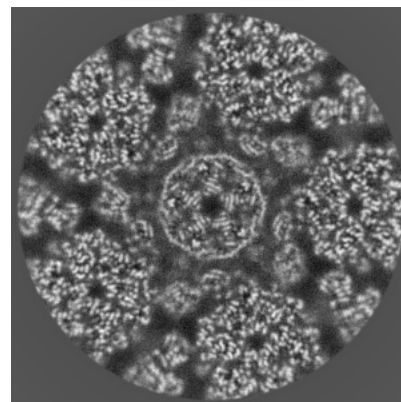
6.3.2 Raw map



X Index: 209



Y Index: 154

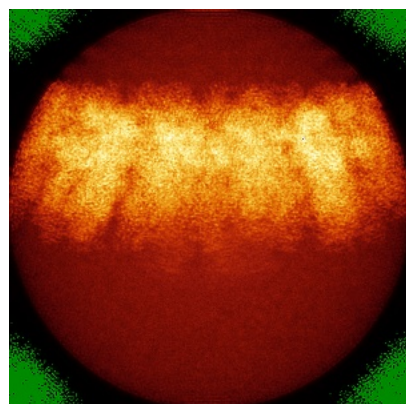


Z Index: 246

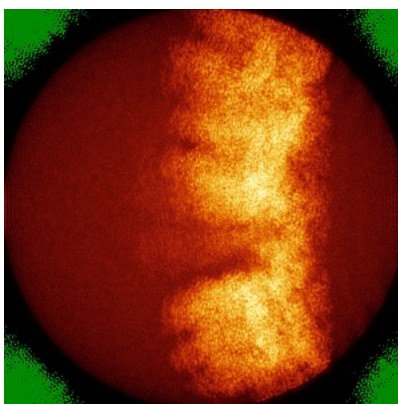
The images above show the largest variance slices of the map in three orthogonal directions.

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

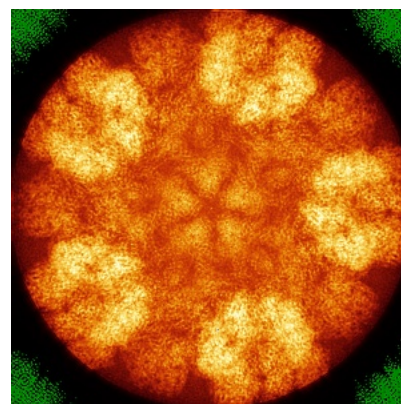
6.4.1 Primary map



X

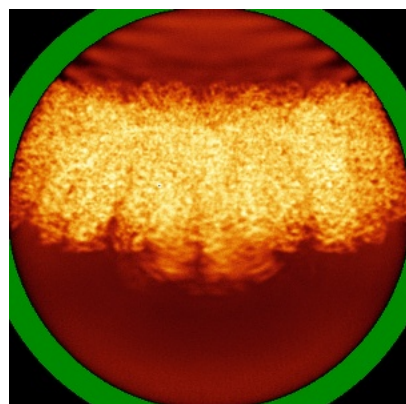


Y

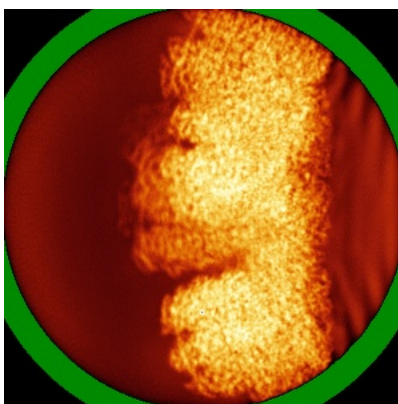


Z

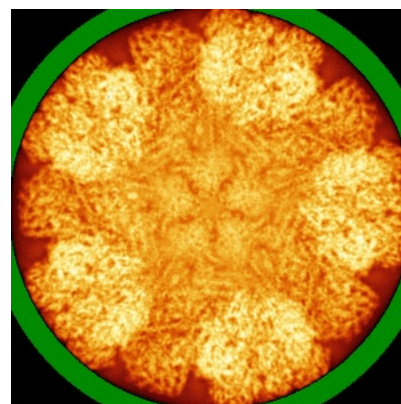
6.4.2 Raw map



X



Y

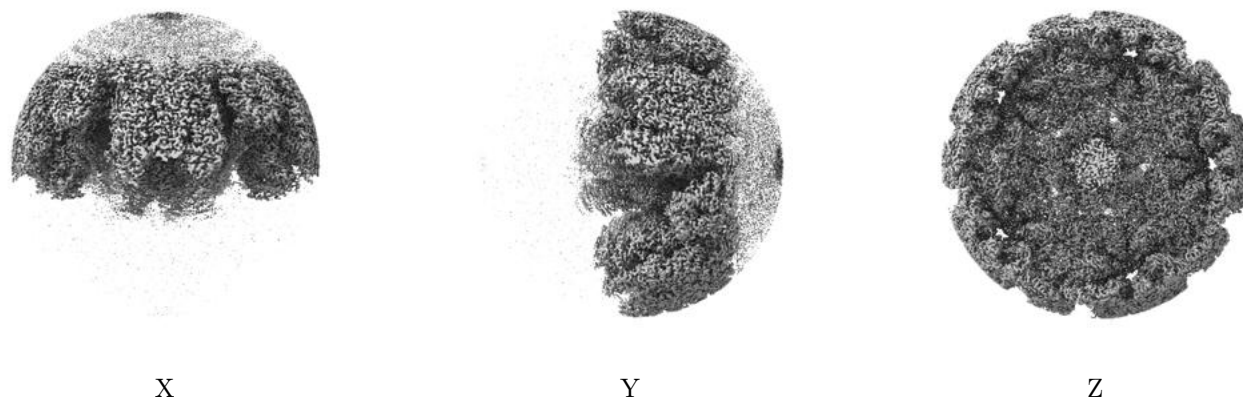


Z

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.

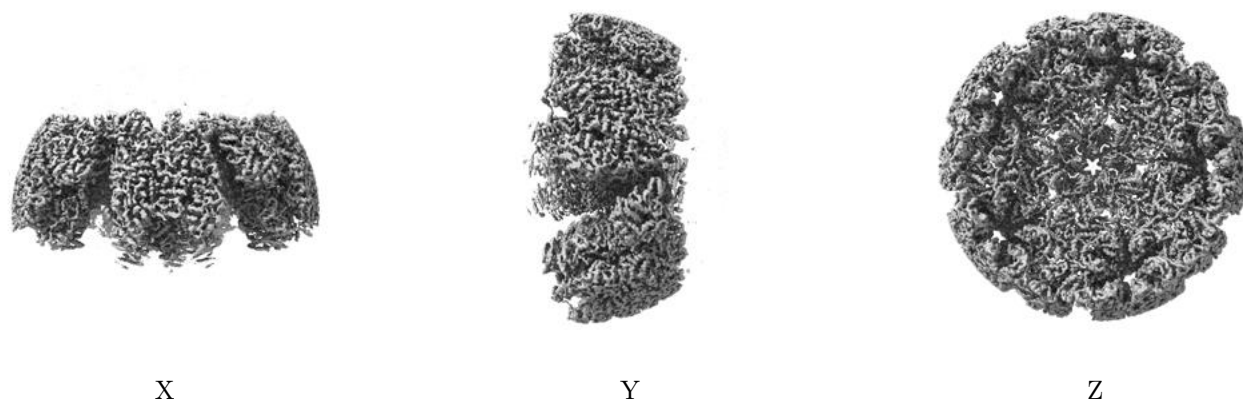
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

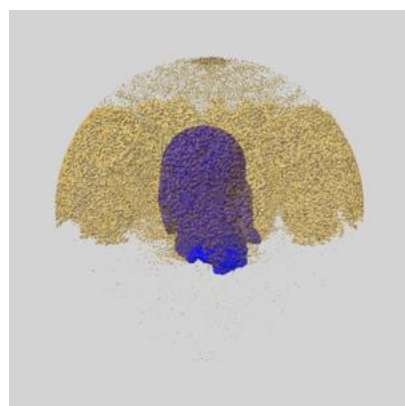
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

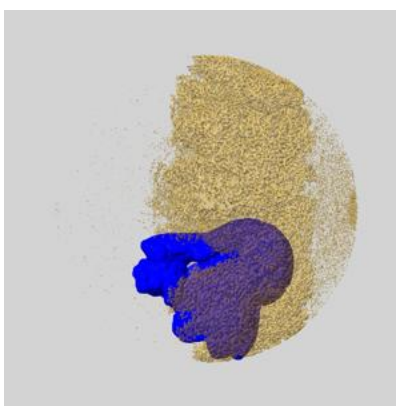
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

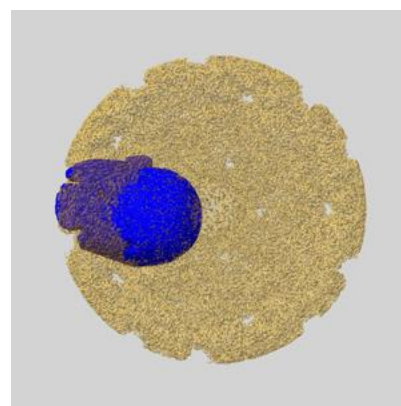
6.6.1 emd_20433_msk_1.map [i](#)



X



Y

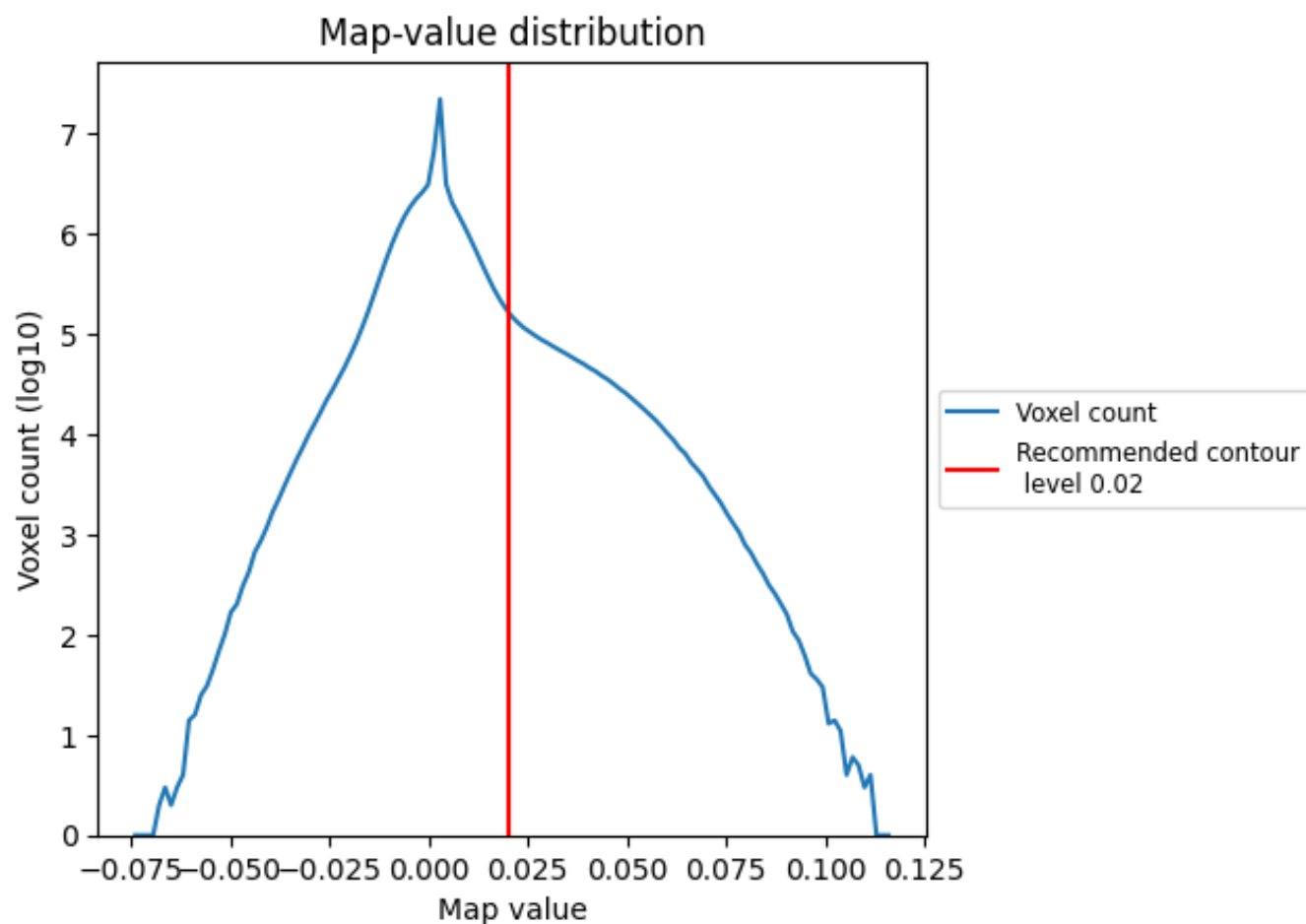


Z

7 Map analysis [i](#)

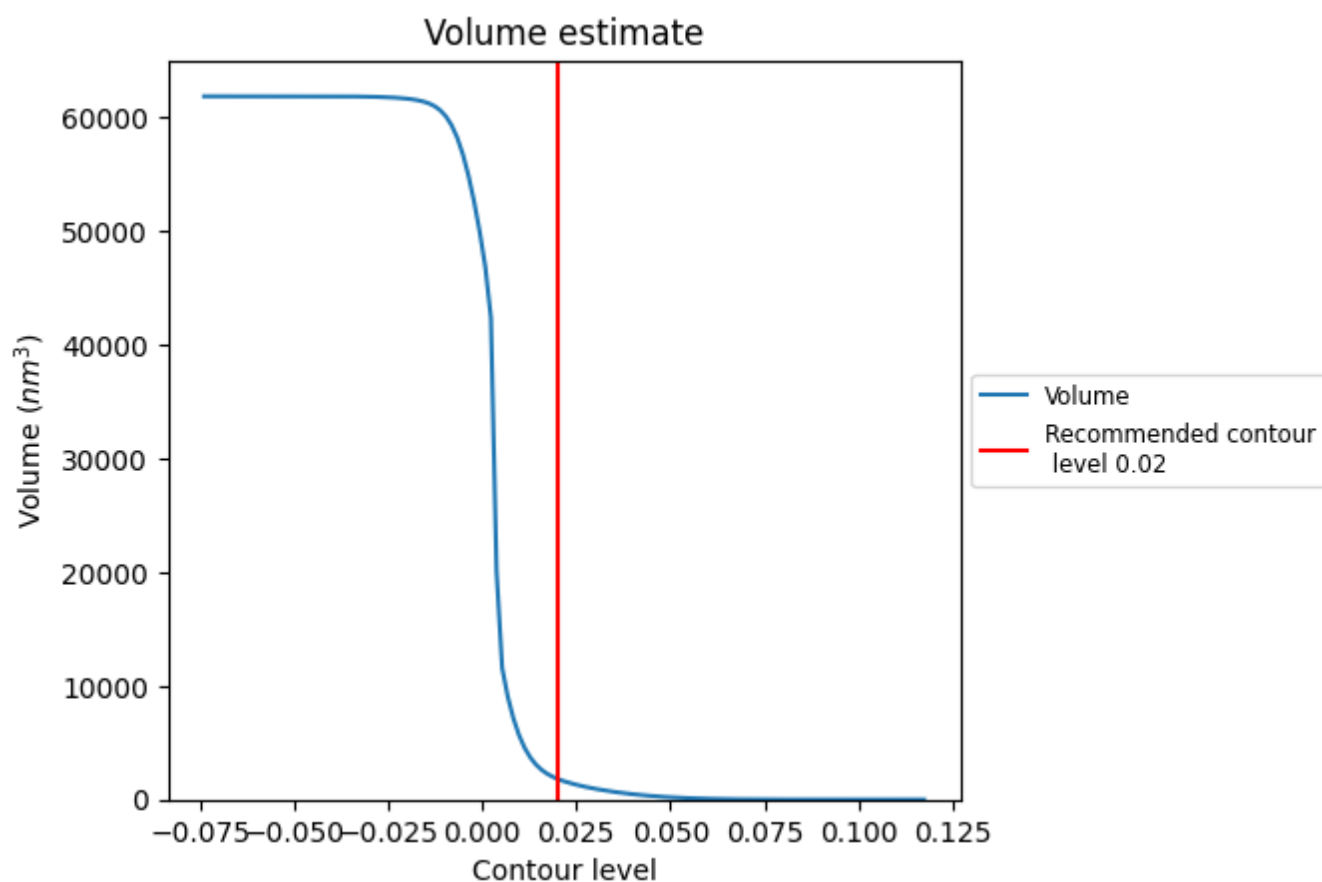
This section contains the results of statistical analysis of the map.

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.

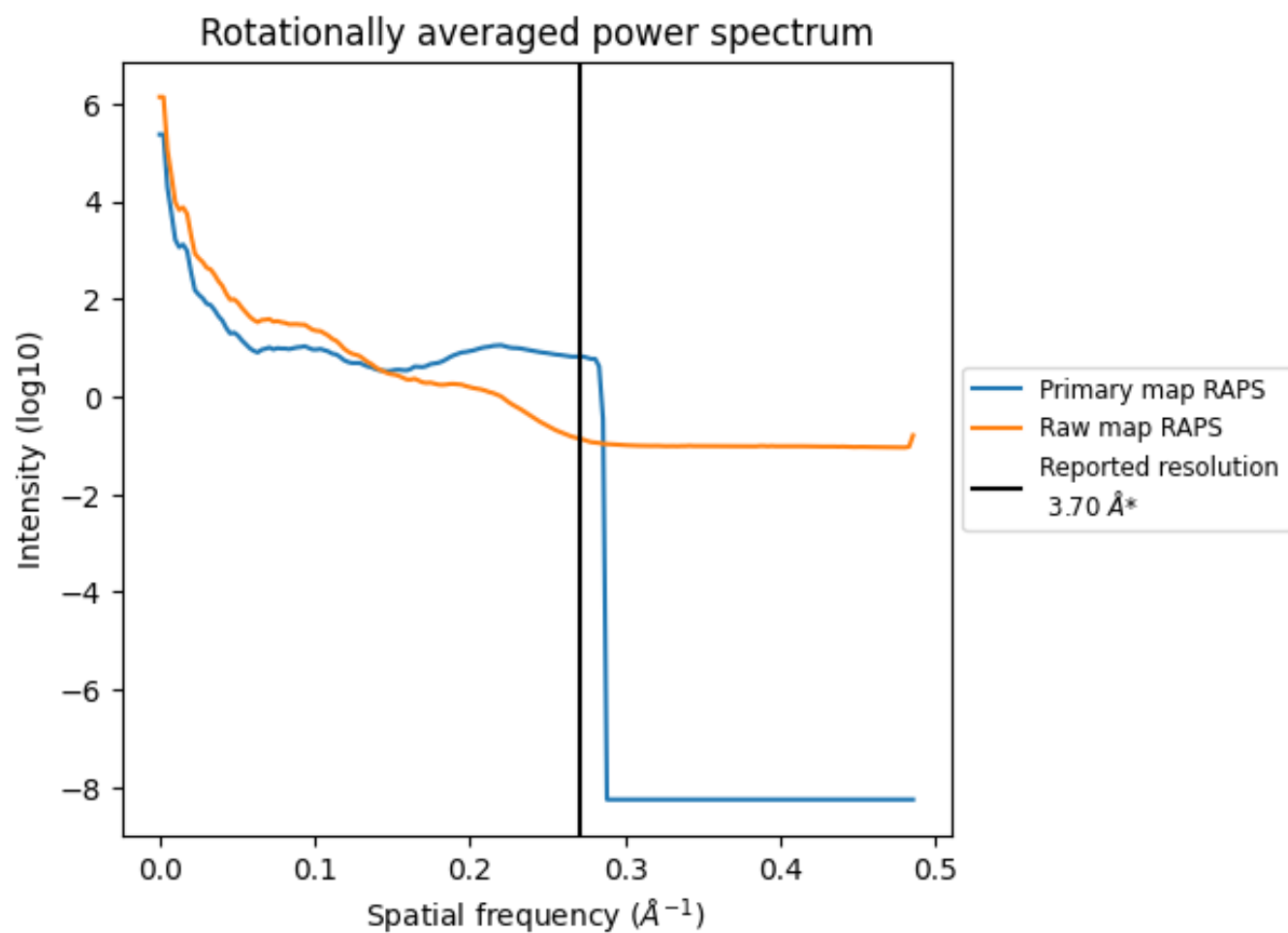
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1827 nm^3 ; this corresponds to an approximate mass of 1651 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 ⓘ

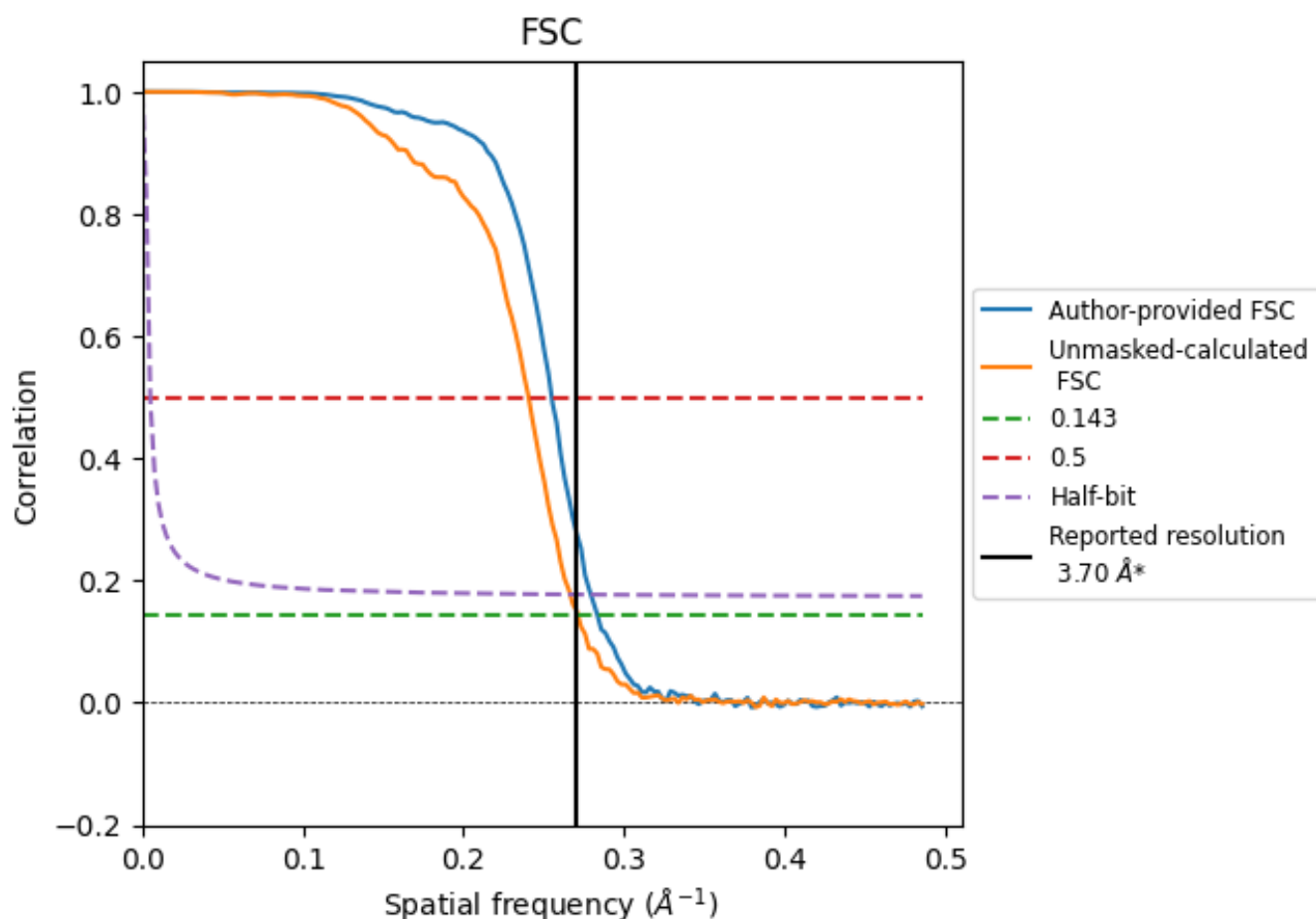


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

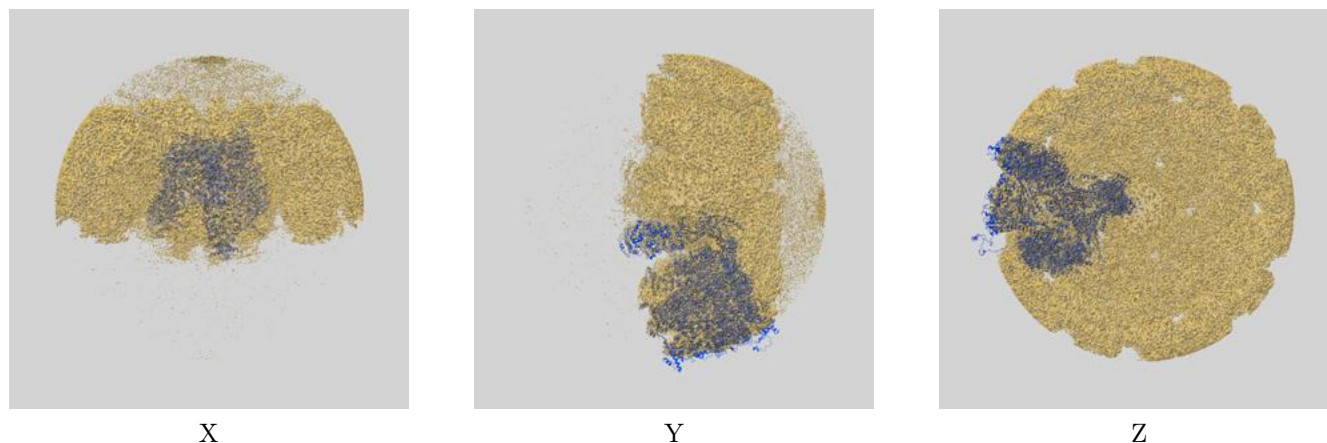
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.53	3.92	3.58
Unmasked-calculated*	3.69	4.16	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

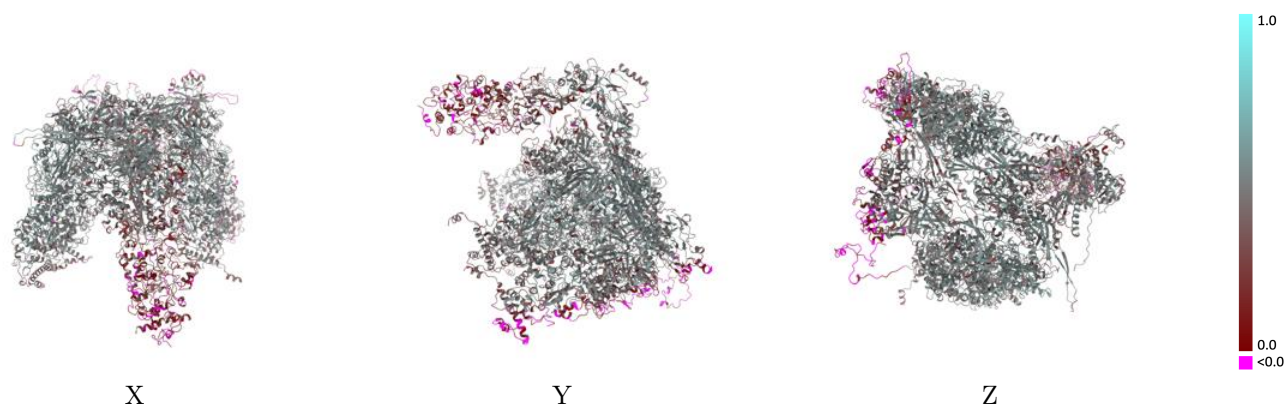
This section contains information regarding the fit between EMDB map EMD-20433 and PDB model 6PPD. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



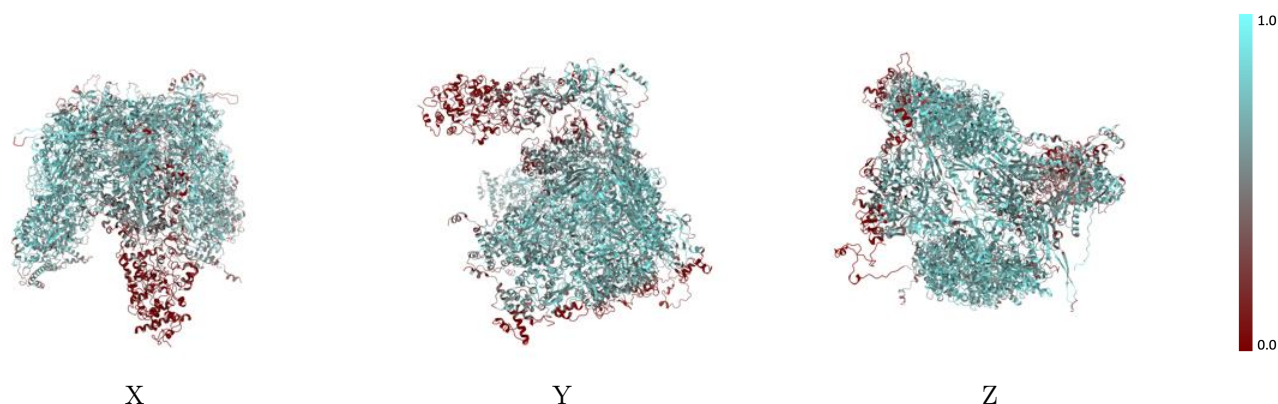
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



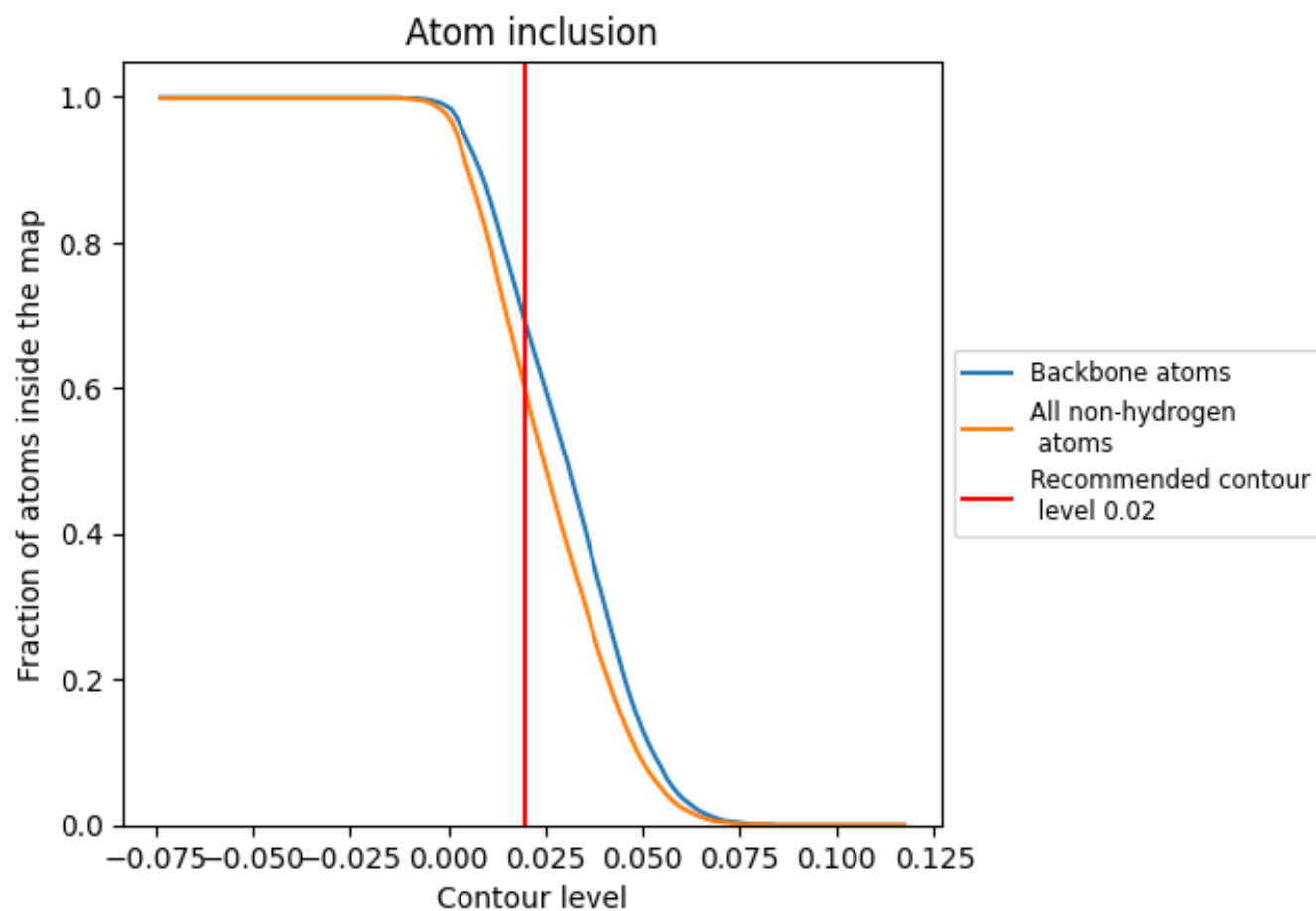
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5950	0.4260
0	0.1790	0.1420
1	0.4720	0.3820
2	0.5190	0.3700
3	0.4840	0.3680
4	0.3500	0.3030
5	0.5740	0.4690
6	0.5680	0.4580
7	0.4140	0.3970
A	0.0760	0.1380
S	0.7150	0.5000
T	0.6920	0.4580
W	0.6380	0.4310
X	0.7140	0.4930
b	0.6160	0.4330
c	0.5030	0.3550
d	0.4880	0.3290

