



Full wwPDB EM Validation Report ⓘ

Dec 15, 2022 – 02:28 PM EST

PDB ID : 8F5P
EMDB ID : EMD-28867
Title : Structure of Leishmania tarentolae IFT-A (state 2)
Authors : Zhou, H.; Brown, A.
Deposited on : 2022-11-14
Resolution : 3.40 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
MolProbity : 4.02b-467
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

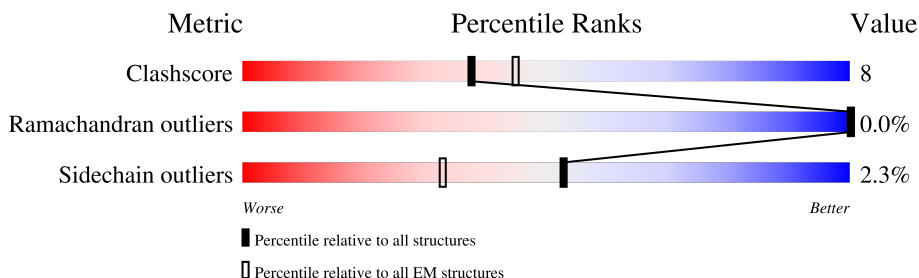
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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	368	
2	B	1247	
3	C	1292	
4	D	1642	
5	E	1654	
6	F	1376	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 39437 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 NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	75	Total	C	N	O	S	0	0
			585	361	97	120	7		

- Molecule 2 is a protein called Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1128	Total	C	N	O	S	0	0
			8917	5645	1557	1652	63		

- Molecule 3 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1176	Total	C	N	O	S	0	0
			9337	5918	1619	1732	68		

- Molecule 4 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	612	Total	C	N	O	S	0	0
			4826	3026	862	912	26		

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

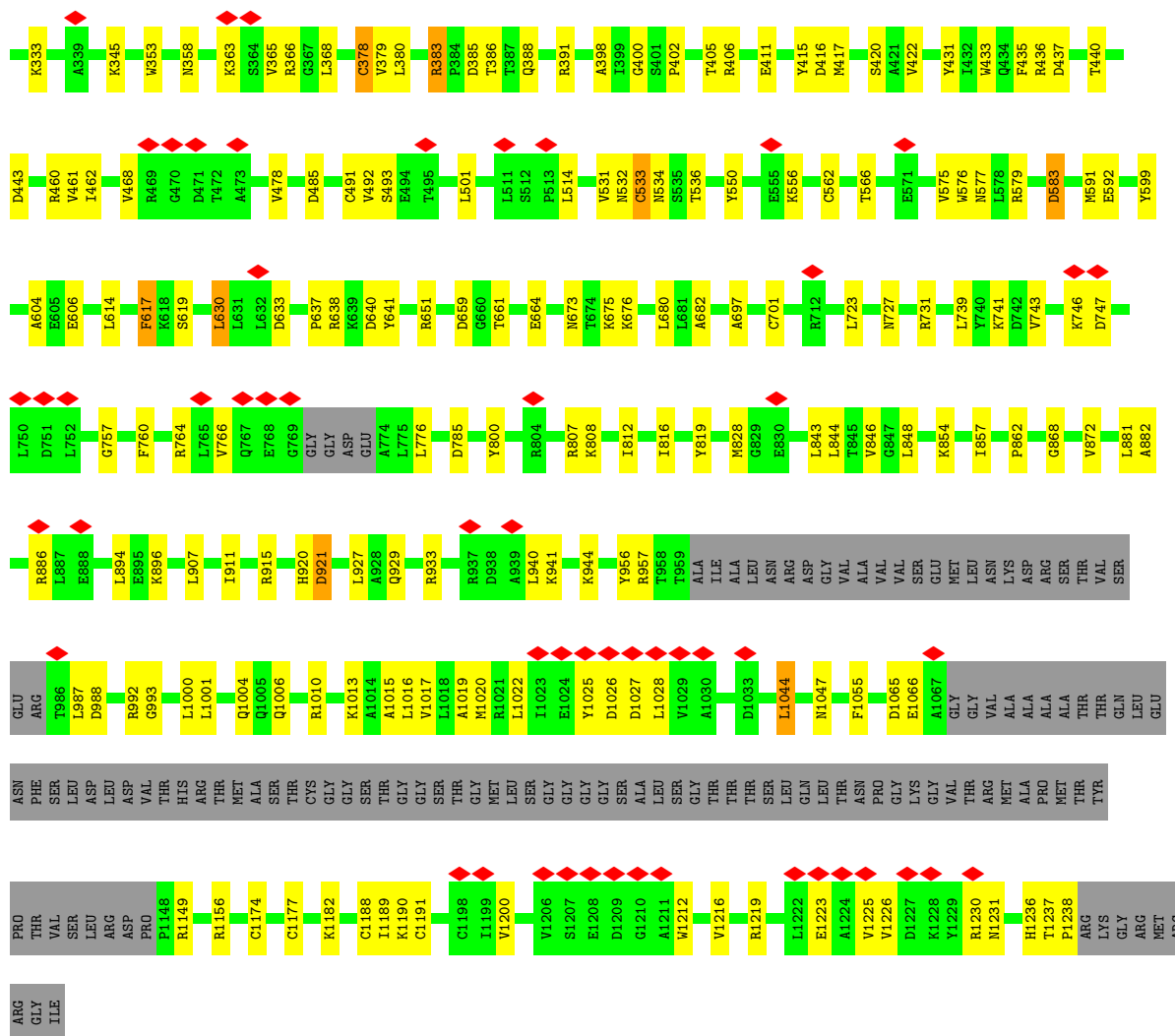
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	1057	Total	C	N	O	S	0	0
			8269	5228	1430	1561	50		

- Molecule 6 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	970	Total	C	N	O	S	0	0
			7499	4713	1315	1436	35		

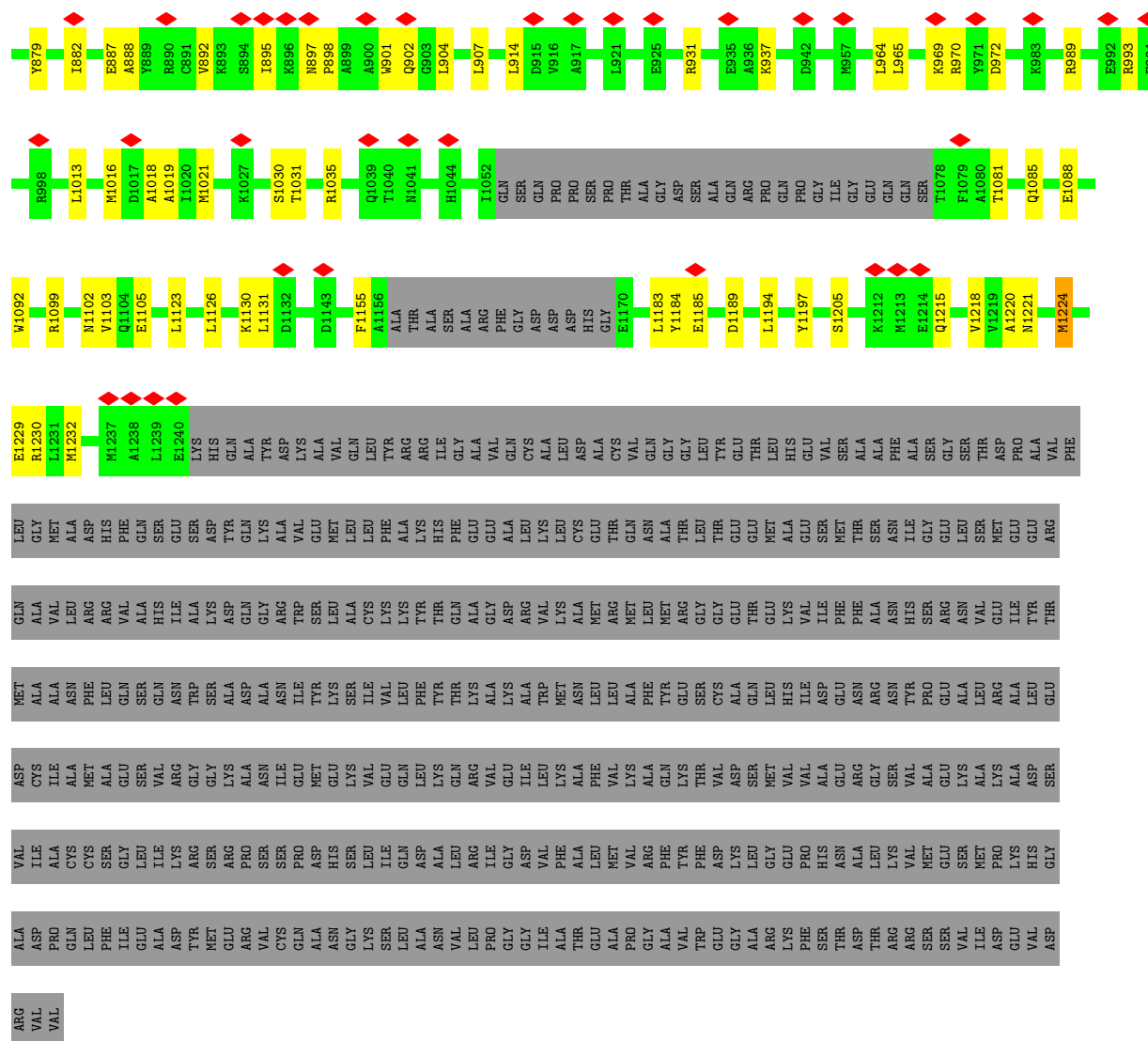
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	B	2	Total 2	Zn 2	0
7	C	2	Total 2	Zn 2	0

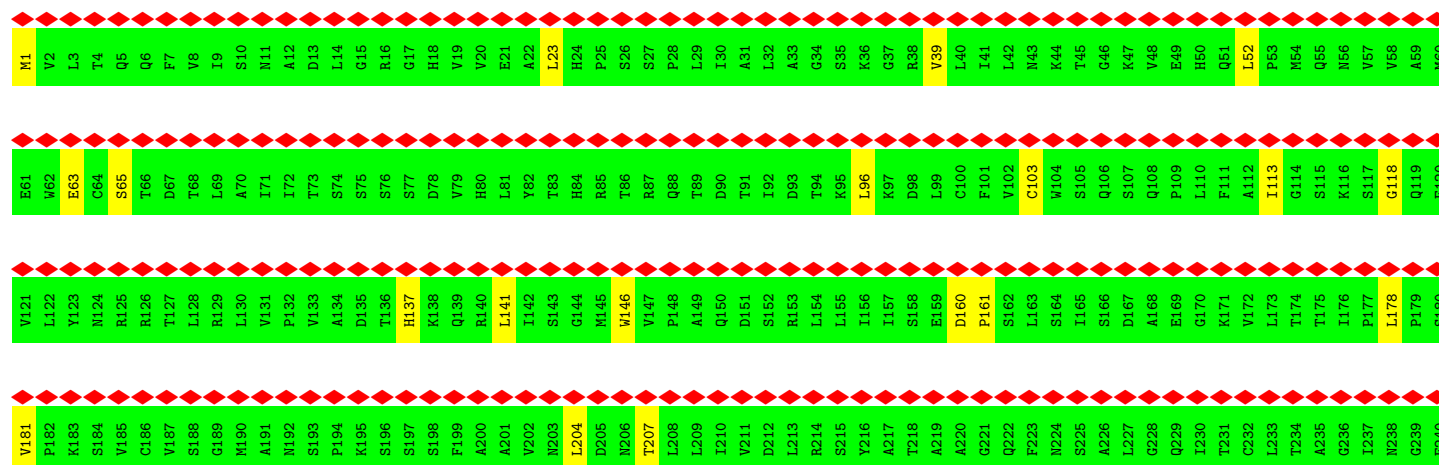








● Molecule 6: WD_REPEATS_REGION domain-containing protein



ALA	GLU	ASP	PRO	ALA	GLU	V939	H879	G812	V718	P625	H526	T441	I367	D301	F241
THR	PHE	LEU	LYS	GLY	PHE	E940	Q880	L813	L721	G626	L529	V442	G368	G302	L242
GLY	ARG	ARG	PRO	ALA	VAL	A941	R881	R814	E722	Y627	F533	Y444	N371	I303	A243
LEU	LEU	ALA	SER	GLY	LEU	E942	H882	H819	K723	T631	A532	P445	L372	A304	G244
ASP	LEU	ASP	TYR	MET	ALA	F943	E883	H820	I724	L632	F533	S446	Q373	P305	F245
GLY	SER	LEU	ILE	TYR	LYS	A944	E884	H820	I727	L632	A534	P447	Q374	T306	A246
ALA	LEU	LEU	PHE	TYR	LYS	F945	A885	T823	I727	F633	A534	P448	D374	G307	S247
GLY	LEU	LEU	LEU	LEU	LEU	A946	A886	E824	K730	R634	T539	T449	N375	D308	G248
CYS	ASP	HIS	TYR	SER	GLU	Q947	Q887	E824	H731	G635	Y643	W456	R376	E309	T249
ASN	ALA	THR	ALA	GLY	ALA	A948	Q887	E824	L732	G635	Y643	W457	T380	A310	T249
THR	PHE	ILE	ALA	HIS	PHE	E949	Y889	V827	L733	Q639	S548	Y461	T380	S311	A251
PRO	GLN	VAL	GLY	TYR	GLU	D950	E890	T828	L734	Q640	F549	Y462	V381	L312	L252
PHE	ASN	VAL	GLY	TYR	LEU	W951	E891	Q830	W738	T641	L550	D463	V383	E313	L253
CYS	GLU	ASP	TYR	LYS	ALA	D952	R891	Q830	H739	P642	V553	G464	V383	D254	L254
ILE	LEU	LEU	GLY	LEU	LYS	W953	A892	E831	Q748	W643	V553	G464	D386	E314	L255
VAL	HIS	LYS	LYS	ASN	HIS	A954	G893	E834	Q748	T645	A560	R465	P387	E315	L255
THR	ASP	LYS	ALA	LYS	ASP	E955	D894	R834	W753	L646	A560	R466	A388	R316	A256
GLY	CYS	LYS	ALA	LYS	CYS	W955	I895	E837	L761	L646	G565	Q467	F389	G317	A257
HIS	LYS	LEU	THR	LYS	PHE	R956	E896	Q838	L761	E647	Y566	Q467	I390	V318	S258
ILE	THR	ILE	THR	GLY	ASN	L957	R897	C839	W761	T648	Y566	Q467	S591	P319	E259
VAL	GLY	ASP	VAL	GLY	PHE	R958	A898	C839	R764	W649	P568	D473	K394	D320	V260
LYS	GLU	ASP	ILE	GLN	GLU	E959	A899	R840	R765	W649	P568	D473	K394	L321	R261
SER	ARG	THR	ILE	GLN	GLU	E960	T900	Q841	D766	W653	Q570	T474	A395	L322	L262
THR	LYS	CYS	ALA	ASP	LEU	R961	R901	Q842	W767	Q652	V573	P475	G400	A323	R263
ILE	ASN	ARG	LYS	ILE	LEU	L962	Y902	A843	W768	T653	L574	E476	W401	W324	G264
GLU	GLN	LEU	GLY	GLU	ASN	N963	Y903	A844	Q769	H654	W575	A477	M402	S225	S265
GLY	GLN	LEU	GLY	GLU	GLN	D964	E904	R845	E778	I657	A578	A479	V405	R326	L266
ILE	VAL	ARG	ILE	VAL	VAL	L965	R905	R846	E778	I657	A578	A479	V405	D327	R267
CYS	VAL	ILE	ILE	VAL	GLU	E966	E906	Q847	E778	I657	A578	A479	V405	G328	L268
VAL	VAL	ARG	THR	VAL	LEU	R967	R907	R848	A781	F658	I584	F483	E409	Q329	L269
ARG	ASP	SER	TYR	VAL	ASP	G967	R908	R849	P782	L659	T585	P484	I412	Q330	K270
ASN	GLY	ASN	LYS	GLY	GLY	A968	L909	R850	E783	R660	Y586	E485	L331	L331	N271
GLN	ILE	ILE	ALA	ALA	ILE	E969	L909	R851	E784	T661	S588	S486	F332	F332	A272
ASP	PRO	PHE	LYS	HIS	PRO	W970	R910	R852	I788	P662	E589	G487	V333	V333	V273
ALA	LEU	THR	LYS	LYS	LEU	Y971	A911	R853	S789	G663	K590	D483	G334	G334	E274
ALA	LEU	THR	LYS	LYS	LEU	Y972	A912	R854	Y792	A664	C591	T489	T335	T335	M275
VAL	ASN	VAL	LEU	LEU	SER	R973	A913	R855	A793	E665	F594	R490	N336	N336	V276
ASP	GLN	HIS	VAL	VAL	ASN	Q974	E913	R856	L796	E665	F594	R490	N336	N336	M276
PRO	ALA	ILE	GLU	GLU	GLN	T975	R914	R857	L796	E665	F594	R490	N336	N336	V277
THR	THR	THR	THR	THR	THR	T976	R915	R858	E797	S679	R601	S497	ASP	ASP	N277
VAL	MET	VAL	ARG	PHE	THR	S977	F917	R859	Y798	S679	R601	S497	ASP	ASP	F278
THR	ILE	THR	ILE	ILE	ILE	A978	F918	R860	R799	S679	R601	S497	ASP	ASP	G279
PRO	ALA	THR	GLN	THR	ALA	E979	R919	R861	R799	S679	R601	S497	ASP	ASP	E280
CYS	GLY	THR	GLN	GLY	GLU	A980	R920	R862	Y801	N681	R601	S497	ASP	ASP	G281
TYR	GLY	VAL	GLN	GLY	THR	E981	R921	R863	Y802	N681	R601	S497	ASP	ASP	G282
ASN	ASP	GLN	ASN	ASN	ASN	A982	R922	R864	Y802	N681	R601	S497	ASP	ASP	G283
ASP	GLY	CYS	THR	THR	THR	L983	R923	R865	Y802	N681	R601	S497	ASP	ASP	V284
ALA	GLY	VAL	VAL	VAL	VAL	W984	R924	R866	Y802	N681	R601	S497	ASP	ASP	V285
PRO	ALA	VAL	VAL	VAL	VAL	A985	R925	R867	Y802	N681	R601	S497	ASP	ASP	A286
THR	THR	THR	THR	THR	THR	K986	R926	R868	Y802	N681	R601	S497	ASP	ASP	A287
GLY	GLY	GLY	GLY	GLY	GLY	K987	R927	R869	Y802	N681	R601	S497	ASP	ASP	V288
VAL	VAL	VAL	VAL	VAL	VAL	C988	R928	R870	Y802	N681	R601	S497	ASP	ASP	A289
						T989	R929	R871	Y802	N681	R601	S497	ASP	ASP	D290
						A990	R930	R872	Y802	N681	R601	S497	ASP	ASP	N291
						Q991	R931	R873	Y802	N681	R601	S497	ASP	ASP	R292
						L992	R932	R874	Y802	N681	R601	S497	ASP	ASP	V293
						GLY	R933	L875	Y802	N681	R601	S497	ASP	ASP	G294
						THR	R934	C876	Y802	N681	R601	S497	ASP	ASP	L295
						ALA	R935	E877	Y802	N681	R601	S497	ASP	ASP	L296
						VAL	R936	E878	Y802	N681	R601	S497	ASP	ASP	R297
							R937		Y802	N681	R601	S497	ASP	ASP	I298
							F938		Y802	N681	R601	S497	ASP	ASP	T299
									Y802	N681	R601	S497	ASP	ASP	E300

ILE
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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	563466	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 ($e^-/\text{\AA}^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	74.154	Depositor
Minimum map value	-32.225	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.778	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/592	0.47	0/800
2	B	0.28	0/9108	0.50	0/12341
3	C	0.26	0/9531	0.50	0/12900
4	D	0.26	0/4905	0.51	0/6650
5	E	0.25	0/8429	0.50	0/11438
6	F	0.24	0/7633	0.49	0/10368
All	All	0.26	0/40198	0.50	0/54497

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	585	0	565	22	0
2	B	8917	0	8815	162	0
3	C	9337	0	9275	168	0
4	D	4826	0	4799	105	0
5	E	8269	0	8212	125	0
6	F	7499	0	7503	91	0
7	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	2	0	0	0	0
All	All	39437	0	39169	636	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 8.

All (636) 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)
5:E:539:GLY:HA3	5:E:551:GLU:O	1.71	0.91
3:C:1061:CYS:HB3	3:C:1064:CYS:SG	2.19	0.82
3:C:62:ILE:HA	3:C:78:GLY:HA2	1.66	0.76
5:E:656:LEU:HB2	5:E:671:TRP:HB2	1.68	0.76
2:B:1174:CYS:HB3	2:B:1177:CYS:SG	2.26	0.75
2:B:920:HIS:HB2	2:B:956:TYR:HB2	1.69	0.74
4:D:1221:ASN:HD22	4:D:1587:VAL:HG13	1.52	0.74
6:F:589:GLU:HG3	6:F:590:LYS:HG3	1.67	0.74
3:C:441:MET:HG2	3:C:452:LEU:HA	1.71	0.72
6:F:730:LYS:O	6:F:734:LEU:HB2	1.89	0.72
5:E:804:THR:HG22	5:E:806:ASP:H	1.55	0.72
3:C:964:ALA:HA	3:C:985:ILE:HD11	1.71	0.71
2:B:988:ASP:HB2	2:B:1219:ARG:HH22	1.56	0.71
6:F:601:ARG:HA	6:F:734:LEU:HD21	1.74	0.70
2:B:402:PRO:HG2	3:C:561:PRO:HG3	1.75	0.69
2:B:846:VAL:HA	3:C:430:ILE:HD11	1.75	0.69
3:C:1180:ARG:HE	3:C:1181:PRO:HD2	1.58	0.69
4:D:1587:VAL:HG12	4:D:1590:ALA:H	1.59	0.68
2:B:872:VAL:O	3:C:447:ASN:ND2	2.25	0.68
5:E:33:TRP:O	5:E:37:PRO:HA	1.94	0.68
3:C:152:THR:HG21	3:C:211:LEU:HD21	1.78	0.66
5:E:17:GLU:HG3	5:E:427:ASP:HB3	1.78	0.66
4:D:1012:ARG:O	4:D:1016:HIS:ND1	2.29	0.66
5:E:1220:ALA:O	5:E:1221:ASN:ND2	2.28	0.66
3:C:414:SER:HB2	3:C:435:LEU:HB3	1.77	0.65
6:F:161:PRO:HB2	6:F:178:LEU:HB2	1.78	0.65
4:D:1223:ASN:ND2	4:D:1256:PRO:O	2.30	0.65
6:F:727:ILE:HG12	6:F:732:LEU:HD22	1.77	0.65
5:E:365:THR:HA	5:E:378:PHE:O	1.96	0.64
4:D:1027:ILE:O	4:D:1031:ARG:NH1	2.30	0.64
2:B:757:GLY:HA3	3:C:612:THR:HG23	1.79	0.64
2:B:125:CYS:SG	2:B:157:TRP:NE1	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:829:PRO:O	5:E:854:ARG:NH1	2.31	0.64
4:D:1155:ARG:NH1	4:D:1184:GLN:OE1	2.31	0.64
4:D:1592:PRO:HD3	4:D:1622:HIS:HD2	1.61	0.64
3:C:545:ASN:OD1	3:C:562:HIS:NE2	2.29	0.64
3:C:354:VAL:HB	3:C:371:ALA:HB3	1.80	0.63
5:E:441:CYS:O	5:E:445:GLU:HB3	1.98	0.63
6:F:39:VAL:HB	6:F:52:LEU:HB2	1.81	0.63
6:F:570:GLN:HA	6:F:587:ASP:HB3	1.80	0.63
1:A:188:ASP:HB2	2:B:1001:LEU:HD13	1.81	0.63
2:B:485:ASP:HB3	2:B:501:LEU:HD23	1.81	0.63
6:F:573:VAL:HG22	6:F:585:THR:HG22	1.80	0.63
4:D:1117:CYS:SG	4:D:1118:GLU:N	2.72	0.62
3:C:422:VAL:O	3:C:469:ARG:NH1	2.32	0.62
4:D:1311:ILE:HD12	4:D:1339:THR:HG22	1.80	0.62
2:B:146:ARG:NH2	2:B:180:SER:O	2.32	0.62
4:D:1236:PRO:O	4:D:1239:ASN:ND2	2.30	0.62
5:E:18:GLN:OE1	5:E:428:ARG:NH1	2.32	0.62
1:A:171:ARG:NH1	4:D:1320:LEU:O	2.33	0.62
2:B:462:ILE:HD13	2:B:514:LEU:HD21	1.80	0.62
4:D:1541:ASP:N	4:D:1541:ASP:OD1	2.33	0.62
3:C:309:ARG:HE	3:C:312:MET:HA	1.65	0.62
5:E:149:LEU:HB3	5:E:161:TRP:HB2	1.82	0.61
2:B:91:VAL:HG13	2:B:102:GLU:HB3	1.82	0.61
2:B:227:LYS:NZ	2:B:243:ASP:OD2	2.33	0.61
2:B:619:SER:HB3	2:B:676:LYS:HD3	1.82	0.61
3:C:379:CYS:HA	3:C:393:ASN:HB2	1.82	0.61
6:F:331:LEU:HD23	6:F:343:PHE:HB2	1.83	0.61
4:D:1338:ALA:O	4:D:1340:ARG:NH1	2.34	0.61
5:E:672:VAL:HG21	5:E:808:LEU:HD21	1.82	0.61
3:C:524:LYS:NZ	3:C:528:LEU:O	2.34	0.61
6:F:806:LEU:HD11	6:F:847:GLN:HG3	1.82	0.61
4:D:1309:ASP:O	4:D:1313:HIS:ND1	2.33	0.61
2:B:921:ASP:OD1	2:B:921:ASP:N	2.33	0.61
3:C:224:PHE:HB3	3:C:244:ASP:HB2	1.81	0.61
3:C:375:ARG:NH1	3:C:404:GLY:O	2.34	0.61
3:C:866:GLU:OE1	3:C:869:ARG:NH1	2.33	0.60
5:E:1224:MET:SD	5:E:1224:MET:N	2.68	0.60
2:B:723:LEU:O	2:B:727:ASN:ND2	2.33	0.60
3:C:795:ALA:HA	3:C:798:PHE:HD2	1.67	0.60
3:C:799:ARG:NH2	3:C:811:TYR:OH	2.33	0.60
3:C:951:GLN:NE2	5:E:1031:THR:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1460:ARG:NH2	4:D:1536:GLU:OE2	2.34	0.60
6:F:350:VAL:HG12	6:F:390:ILE:HG12	1.84	0.60
4:D:1063:LYS:HE3	4:D:1067:ALA:HB2	1.83	0.60
6:F:876:CYS:HB2	6:F:885:ALA:HB2	1.82	0.60
2:B:191:CYS:HB2	2:B:227:LYS:HE3	1.84	0.60
3:C:1043:ARG:NH2	3:C:1048:ASN:OD1	2.34	0.60
5:E:1229:GLU:OE1	5:E:1230:ARG:NH2	2.35	0.60
5:E:931:ARG:NH1	6:F:739:MET:SD	2.75	0.60
6:F:466:VAL:HG21	6:F:494:ILE:HG21	1.82	0.60
2:B:209:TRP:HD1	2:B:218:THR:HG21	1.68	0.59
3:C:621:GLU:HA	3:C:624:LYS:HG2	1.83	0.59
1:A:169:MET:HE1	2:B:1010:ARG:HE	1.67	0.59
3:C:575:PHE:HB2	3:C:603:ARG:HE	1.66	0.59
1:A:158:ASP:OD2	4:D:1231:ASN:ND2	2.36	0.59
2:B:69:ASP:HB3	2:B:70:LEU:HD12	1.84	0.59
4:D:1437:VAL:HG11	4:D:1466:LEU:HA	1.84	0.59
4:D:1050:PRO:HG3	4:D:1079:ARG:HH11	1.68	0.59
5:E:194:VAL:O	5:E:225:SER:OG	2.21	0.59
5:E:186:GLU:HB2	5:E:230:ASP:HB2	1.84	0.59
6:F:440:ARG:NH2	6:F:471:ILE:O	2.35	0.59
2:B:675:LYS:HE3	2:B:701:CYS:HB2	1.85	0.59
6:F:710:ARG:NH2	6:F:722:GLU:OE2	2.35	0.59
4:D:1179:LEU:HD12	4:D:1188:ALA:HB2	1.84	0.59
4:D:1323:VAL:HA	4:D:1328:ARG:HD2	1.85	0.58
6:F:802:TYR:OH	6:F:849:ARG:NH1	2.36	0.58
3:C:162:VAL:HB	3:C:175:ILE:HB	1.84	0.58
2:B:156:CYS:SG	2:B:157:TRP:N	2.77	0.58
2:B:177:ASP:HB3	2:B:181:GLY:H	1.69	0.58
2:B:1212:TRP:N	2:B:1223:GLU:OE2	2.36	0.58
3:C:507:ASP:HB2	3:C:544:ALA:HB2	1.85	0.58
3:C:629:ARG:O	3:C:629:ARG:NH1	2.30	0.58
2:B:127:THR:HG21	2:B:155:VAL:HG21	1.86	0.58
2:B:579:ARG:HH21	2:B:617:PHE:H	1.50	0.58
3:C:220:ARG:HG3	3:C:254:GLY:HA3	1.86	0.58
5:E:1102:ASN:ND2	5:E:1105:GLU:OE1	2.37	0.58
1:A:191:VAL:O	2:B:1236:HIS:ND1	2.30	0.58
6:F:591:CYS:SG	6:F:621:THR:OG1	2.62	0.58
3:C:505:ASN:ND2	3:C:543:LYS:O	2.37	0.58
5:E:1081:THR:O	5:E:1085:GLN:NE2	2.37	0.58
2:B:151:LYS:O	2:B:169:ALA:N	2.37	0.57
2:B:731:ARG:NH2	3:C:615:GLN:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1224:ARG:NH2	3:C:1226:ASP:OD2	2.37	0.57
3:C:788:VAL:O	3:C:791:ILE:HB	2.03	0.57
2:B:229:GLN:HE21	2:B:239:PRO:HG3	1.69	0.57
5:E:319:SER:HB2	5:E:322:VAL:HB	1.86	0.57
3:C:951:GLN:OE1	5:E:1092:TRP:NE1	2.32	0.57
4:D:1009:LEU:O	4:D:1011:ARG:N	2.38	0.57
2:B:843:LEU:HA	2:B:846:VAL:HG12	1.86	0.57
2:B:142:ARG:HH21	2:B:145:GLY:HA3	1.69	0.56
5:E:892:VAL:HG21	5:E:904:LEU:HD22	1.87	0.56
2:B:383:ARG:NH1	2:B:386:THR:O	2.38	0.56
6:F:590:LYS:HD2	6:F:620:TYR:HB3	1.88	0.56
5:E:20:ILE:HB	5:E:430:VAL:HG21	1.87	0.56
5:E:551:GLU:HG2	5:E:557:PRO:HA	1.87	0.56
5:E:721:GLN:O	5:E:794:ARG:NH1	2.38	0.56
2:B:661:THR:HG23	2:B:664:GLU:H	1.70	0.56
4:D:1326:GLU:OE1	4:D:1329:ARG:NH2	2.37	0.56
6:F:491:LEU:HD23	6:F:505:THR:HG22	1.87	0.56
3:C:685:LEU:HD22	3:C:690:LYS:HB2	1.87	0.56
1:A:181:SER:OG	4:D:1237:ALA:O	2.23	0.56
1:A:211:GLU:HA	1:A:214:LYS:HB2	1.88	0.56
3:C:57:GLY:HA3	3:C:86:TRP:HH2	1.71	0.56
2:B:200:LEU:HA	2:B:223:TYR:HA	1.88	0.55
4:D:1584:TRP:NE1	4:D:1589:GLU:HG3	2.22	0.55
5:E:653:ARG:NH1	5:E:803:ALA:O	2.40	0.55
5:E:1013:LEU:HD13	6:F:707:ARG:HE	1.70	0.55
1:A:171:ARG:NH2	1:A:177:SER:OG	2.39	0.55
6:F:958:ARG:HG2	6:F:962:LEU:HD12	1.87	0.55
2:B:310:VAL:HG13	2:B:321:ALA:HB3	1.88	0.55
2:B:63:GLY:O	2:B:88:ARG:NH1	2.40	0.55
2:B:812:ILE:O	2:B:816:ILE:HG13	2.06	0.55
3:C:831:ARG:HD2	5:E:1155:PHE:HE1	1.72	0.55
5:E:456:ARG:HB2	5:E:824:VAL:HG23	1.88	0.55
2:B:214:GLU:OE2	2:B:366:ARG:NH2	2.39	0.55
2:B:237:GLU:OE2	3:C:275:ARG:NH1	2.40	0.55
5:E:831:PHE:HB2	5:E:853:LYS:HG3	1.89	0.55
5:E:1184:TYR:HB3	5:E:1189:ASP:HB2	1.88	0.55
3:C:210:ASN:HD21	3:C:214:THR:HB	1.72	0.54
6:F:96:LEU:HD12	6:F:113:ILE:HG13	1.89	0.54
6:F:299:THR:OG1	6:F:302:GLY:O	2.25	0.54
6:F:492:VAL:HG21	6:F:529:LEU:HG	1.87	0.54
3:C:332:GLU:HB2	3:C:348:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:940:LEU:HG	2:B:944:LYS:HE2	1.90	0.54
3:C:44:TYR:HB3	3:C:49:GLY:HA2	1.89	0.54
3:C:40:ARG:NH1	3:C:54:SER:OG	2.41	0.54
3:C:861:PHE:HA	3:C:864:ALA:HB3	1.89	0.54
2:B:72:THR:HG22	2:B:81:THR:HB	1.89	0.54
6:F:271:ASN:ND2	6:F:290:ASP:OD2	2.33	0.54
3:C:183:ALA:HB1	3:C:229:VAL:HG22	1.89	0.54
2:B:245:ASP:OD1	2:B:245:ASP:N	2.41	0.54
3:C:27:SER:HB3	3:C:32:TYR:HB2	1.90	0.54
3:C:767:MET:HE2	3:C:772:GLN:HB2	1.90	0.54
3:C:6:ARG:NH1	3:C:47:SER:O	2.40	0.54
3:C:576:ASP:OD1	3:C:603:ARG:NH2	2.41	0.53
3:C:907:GLU:HG3	3:C:910:ARG:HD2	1.89	0.53
1:A:167:LEU:HD11	1:A:180:THR:HG21	1.90	0.53
2:B:957:ARG:NH2	2:B:987:LEU:O	2.30	0.53
3:C:67:TYR:HE1	3:C:71:GLY:HA2	1.73	0.53
3:C:711:TYR:HB3	3:C:720:ALA:HB2	1.91	0.53
4:D:1155:ARG:O	4:D:1159:GLU:HG2	2.09	0.53
5:E:381:HIS:ND1	5:E:413:GLN:O	2.41	0.53
4:D:1341:ARG:HD2	4:D:1344:GLU:HG3	1.90	0.53
2:B:992:ARG:HD3	2:B:1025:TYR:HE1	1.74	0.53
4:D:1312:ARG:HG2	4:D:1316:GLN:HE21	1.73	0.53
2:B:583:ASP:OD1	2:B:583:ASP:N	2.38	0.53
5:E:543:VAL:HG22	5:E:548:ILE:HG22	1.91	0.53
3:C:238:ILE:HG23	3:C:250:PHE:HB2	1.89	0.53
5:E:879:TYR:HA	5:E:882:ILE:HG12	1.90	0.53
6:F:706:ILE:HG23	6:F:718:VAL:HG13	1.91	0.53
5:E:190:ARG:NH1	5:E:257:VAL:O	2.41	0.53
5:E:989:ARG:HB3	5:E:993:ARG:HH12	1.74	0.53
2:B:83:SER:OG	2:B:84:ASP:N	2.42	0.53
2:B:276:ILE:HD12	2:B:314:VAL:HG22	1.91	0.53
2:B:556:LYS:NZ	2:B:562:CYS:SG	2.82	0.53
5:E:484:LEU:HG	5:E:520:ILE:HD13	1.90	0.53
2:B:630:LEU:HG	2:B:641:TYR:HD2	1.74	0.52
4:D:1030:GLN:OE1	4:D:1031:ARG:NH1	2.43	0.52
4:D:1254:LEU:HD12	4:D:1261:LEU:HD11	1.90	0.52
4:D:1353:LEU:HD13	4:D:1428:THR:HB	1.91	0.52
2:B:326:ASN:OD1	2:B:326:ASN:N	2.41	0.52
4:D:1523:GLU:OE1	4:D:1523:GLU:N	2.39	0.52
3:C:1069:VAL:HG21	3:C:1080:LEU:HB2	1.91	0.52
1:A:151:LEU:HD11	4:D:1256:PRO:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:20:ILE:HD11	5:E:440:CYS:HB2	1.91	0.52
3:C:455:LYS:NZ	3:C:456:GLY:O	2.42	0.52
2:B:156:CYS:HB2	2:B:203:LEU:HG	1.91	0.52
3:C:754:TYR:O	3:C:758:GLY:N	2.41	0.52
2:B:437:ASP:O	2:B:440:THR:OG1	2.28	0.52
2:B:606:GLU:OE2	2:B:651:ARG:NH2	2.43	0.52
2:B:244:ARG:HH21	2:B:279:GLN:HG3	1.76	0.51
5:E:570:PRO:HA	5:E:584:SER:HA	1.92	0.51
5:E:1103:VAL:HG11	5:E:1126:LEU:HD21	1.92	0.51
5:E:1185:GLU:OE1	5:E:1197:TYR:OH	2.24	0.51
2:B:146:ARG:HH12	2:B:182:GLU:HA	1.74	0.51
5:E:22:ALA:HB1	5:E:432:THR:HA	1.92	0.51
3:C:760:TYR:HA	3:C:763:ALA:HB3	1.93	0.51
5:E:237:ALA:HB2	5:E:247:CYS:HB2	1.92	0.51
5:E:377:VAL:HB	5:E:418:THR:HG22	1.91	0.51
6:F:793:ALA:HA	6:F:796:LEU:HD12	1.92	0.51
3:C:232:PHE:HB3	3:C:237:TYR:HB2	1.92	0.51
3:C:349:GLN:O	3:C:376:ARG:NH1	2.43	0.51
4:D:1006:ALA:HB1	4:D:1034:MET:SD	2.51	0.51
2:B:324:ARG:HG3	2:B:576:TRP:CG	2.46	0.51
3:C:516:THR:OG1	3:C:518:ASP:OD1	2.22	0.51
5:E:273:SER:HB3	5:E:294:LEU:HB2	1.93	0.51
5:E:1131:LEU:HD12	5:E:1183:LEU:HD23	1.92	0.51
2:B:175:VAL:HG21	2:B:234:ILE:HG23	1.93	0.51
3:C:82:THR:HA	3:C:97:GLN:HA	1.92	0.51
5:E:375:LEU:HD21	5:E:439:LEU:HD21	1.93	0.51
5:E:898:PRO:HA	5:E:901:TRP:HD1	1.76	0.51
3:C:400:TYR:HE1	3:C:406:LYS:HE3	1.76	0.51
3:C:247:VAL:HG23	3:C:260:LEU:HB2	1.93	0.50
4:D:957:THR:O	4:D:961:ARG:HG3	2.11	0.50
2:B:15:VAL:HG13	2:B:34:GLU:HG2	1.93	0.50
2:B:461:VAL:HG11	2:B:478:VAL:HG12	1.92	0.50
2:B:114:ASP:OD1	2:B:115:PHE:N	2.45	0.50
2:B:577:ASN:HB3	2:B:591:MET:HB2	1.94	0.50
5:E:189:ALA:N	5:E:229:ALA:O	2.45	0.50
5:E:132:HIS:CD2	5:E:153:SER:HB2	2.47	0.50
5:E:815:PRO:HD2	5:E:856:ARG:HH22	1.76	0.50
5:E:837:LYS:HE2	5:E:847:ASP:HA	1.92	0.50
2:B:268:ALA:HB2	2:B:274:PRO:HG3	1.93	0.50
3:C:565:ALA:HB3	3:C:581:VAL:HG11	1.93	0.50
4:D:992:ASP:HA	4:D:1050:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:367:ILE:HG13	5:E:431:LEU:HD11	1.92	0.50
5:E:1030:SER:HB2	5:E:1088:GLU:HB3	1.94	0.50
4:D:1331:LEU:HD23	4:D:1334:TYR:HD2	1.77	0.50
3:C:735:ARG:NH2	3:C:754:TYR:OH	2.42	0.50
4:D:1334:TYR:HE1	4:D:1448:ILE:HD11	1.76	0.50
4:D:930:VAL:HG13	4:D:961:ARG:HG2	1.93	0.49
1:A:190:ASP:O	2:B:1230:ARG:NH2	2.45	0.49
3:C:1264:GLN:HB2	3:C:1267:ARG:HG3	1.94	0.49
5:E:357:LEU:HD21	5:E:368:VAL:HG22	1.94	0.49
5:E:445:GLU:OE2	5:E:447:GLN:NE2	2.45	0.49
5:E:914:LEU:HB3	5:E:937:LYS:HZ1	1.77	0.49
3:C:184:LEU:HD12	3:C:197:LEU:HD21	1.95	0.49
3:C:255:ASN:HD22	3:C:332:GLU:HG2	1.77	0.49
2:B:172:GLU:OE1	2:B:186:GLN:NE2	2.46	0.49
2:B:219:LEU:HD23	2:B:231:MET:HB2	1.95	0.49
3:C:303:ASP:HA	3:C:506:ILE:HD13	1.95	0.49
4:D:957:THR:O	4:D:960:GLU:HG2	2.12	0.49
4:D:1045:CYS:HB2	4:D:1083:ALA:HB2	1.93	0.49
5:E:587:ASN:ND2	5:E:608:LEU:O	2.45	0.49
5:E:876:PHE:HD1	5:E:888:ALA:HB1	1.77	0.49
3:C:84:ILE:HG12	3:C:95:LYS:HG3	1.94	0.49
3:C:163:MET:HB2	3:C:165:LEU:HD13	1.93	0.49
3:C:505:ASN:HB2	3:C:511:ASN:HB3	1.95	0.49
4:D:1044:ARG:O	4:D:1048:SER:OG	2.20	0.49
5:E:76:LEU:HD11	5:E:88:LEU:HD12	1.94	0.49
6:F:103:CYS:HG	6:F:146:TRP:HE1	1.60	0.49
2:B:74:ASN:HB2	2:B:117:TRP:CE2	2.47	0.49
6:F:848:ILE:HG22	6:F:875:LEU:HB2	1.95	0.49
2:B:882:ALA:O	2:B:886:ARG:NH1	2.46	0.49
3:C:99:THR:HG22	3:C:100:GLU:HG2	1.95	0.49
6:F:529:LEU:HD13	6:F:543:TYR:HB2	1.93	0.49
1:A:163:TRP:HH2	2:B:1004:GLN:HB3	1.78	0.49
6:F:389:PHE:HZ	6:F:448:VAL:HB	1.78	0.49
5:E:456:ARG:HG3	5:E:824:VAL:HA	1.95	0.49
5:E:1013:LEU:O	6:F:681:ASN:ND2	2.37	0.49
2:B:1006:GLN:NE2	2:B:1200:VAL:O	2.43	0.48
6:F:489:THR:OG1	6:F:490:ARG:N	2.45	0.48
6:F:972:VAL:HG21	6:F:984:VAL:HG21	1.95	0.48
2:B:175:VAL:HG11	2:B:234:ILE:HD13	1.95	0.48
3:C:1080:LEU:HA	3:C:1221:ARG:O	2.13	0.48
5:E:103:TYR:HB3	5:E:109:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:463:ALA:HB1	5:E:824:VAL:HG21	1.96	0.48
2:B:353:TRP:HE1	2:B:358:ASN:HA	1.79	0.48
2:B:1156:ARG:HH22	4:D:914:ARG:HH11	1.61	0.48
3:C:268:TRP:HH2	4:D:1640:LEU:HD21	1.78	0.48
3:C:951:GLN:HE21	5:E:1035:ARG:HB2	1.78	0.48
5:E:252:GLU:OE1	5:E:272:THR:OG1	2.30	0.48
5:E:572:ILE:HB	5:E:583:VAL:HB	1.95	0.48
5:E:674:ASP:O	5:E:678:ASP:N	2.47	0.48
6:F:473:ASP:OD1	6:F:473:ASP:N	2.46	0.48
3:C:717:TRP:CD2	3:C:737:GLN:HG2	2.49	0.48
6:F:653:THR:OG1	6:F:654:HIS:ND1	2.45	0.48
3:C:369:ASP:OD1	3:C:369:ASP:N	2.43	0.48
4:D:1591:ASP:HB3	4:D:1594:VAL:HG12	1.96	0.48
3:C:181:VAL:HG13	3:C:199:ILE:HG23	1.95	0.48
3:C:240:LEU:HD12	3:C:250:PHE:HE2	1.78	0.48
5:E:537:ARG:NH2	5:E:577:ASN:O	2.46	0.48
5:E:1194:LEU:HD21	5:E:1218:VAL:HG21	1.96	0.48
6:F:857:MET:HG3	6:F:884:GLU:HG2	1.96	0.48
2:B:550:TYR:HA	2:B:566:THR:HA	1.94	0.48
2:B:747:ASP:OD1	2:B:747:ASP:N	2.47	0.48
2:B:741:LYS:HG2	2:B:746:LYS:HD3	1.96	0.48
3:C:66:ASP:OD2	3:C:107:HIS:ND1	2.47	0.48
3:C:229:VAL:HG12	3:C:240:LEU:HD21	1.95	0.48
3:C:791:ILE:HA	3:C:794:CYS:HB3	1.96	0.48
4:D:1239:ASN:OD1	4:D:1242:CYS:N	2.46	0.48
2:B:785:ASP:OD1	2:B:800:TYR:OH	2.25	0.47
3:C:233:ASN:OD1	3:C:277:LYS:NZ	2.46	0.47
4:D:1087:LEU:HD12	4:D:1107:LEU:HD22	1.96	0.47
3:C:731:LYS:NZ	3:C:732:ASP:OD1	2.45	0.47
3:C:794:CYS:HA	3:C:797:PHE:HD1	1.79	0.47
3:C:951:GLN:HB3	3:C:953:LEU:HD23	1.95	0.47
4:D:1085:GLU:OE1	4:D:1088:ARG:NH1	2.47	0.47
4:D:1162:LEU:HD12	4:D:1175:TYR:HD2	1.78	0.47
6:F:619:LEU:HD11	6:F:653:THR:HG22	1.96	0.47
2:B:443:ASP:OD1	2:B:443:ASP:N	2.44	0.47
2:B:93:VAL:HG12	2:B:102:GLU:HB2	1.95	0.47
3:C:964:ALA:HB1	3:C:989:LEU:HB2	1.96	0.47
2:B:766:VAL:HG11	2:B:776:LEU:HB2	1.96	0.47
3:C:848:TYR:HB2	3:C:871:ALA:HB2	1.97	0.47
3:C:1190:ALA:HA	3:C:1194:ILE:HD12	1.95	0.47
4:D:1531:TYR:O	4:D:1534:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:972:ASP:N	5:E:972:ASP:OD1	2.46	0.47
2:B:118:ASN:OD1	2:B:121:GLY:N	2.48	0.47
3:C:117:VAL:HG21	3:C:144:ALA:HB2	1.96	0.47
3:C:593:MET:HG2	3:C:597:HIS:HD1	1.79	0.47
4:D:1124:VAL:HA	4:D:1127:MET:HB2	1.97	0.47
4:D:1177:ILE:HG13	4:D:1181:HIS:CE1	2.50	0.47
5:E:879:TYR:CD2	5:E:887:GLU:HB3	2.50	0.47
6:F:160:ASP:OD1	6:F:160:ASP:N	2.46	0.47
6:F:903:ILE:HD13	6:F:924:ILE:HG23	1.97	0.47
3:C:1081:VAL:O	3:C:1220:TYR:HA	2.15	0.47
4:D:1147:GLU:HA	4:D:1514:LEU:HD23	1.97	0.47
4:D:1159:GLU:OE2	4:D:1175:TYR:OH	2.26	0.47
5:E:895:ILE:HG22	5:E:897:ASN:H	1.79	0.47
2:B:760:PHE:O	2:B:764:ARG:HG2	2.15	0.47
6:F:63:GLU:OE2	6:F:65:SER:OG	2.33	0.47
6:F:387:PRO:HA	6:F:401:VAL:HG13	1.95	0.47
1:A:166:LEU:O	1:A:169:MET:HG2	2.15	0.47
1:A:168:ARG:HB3	4:D:1406:LEU:HD13	1.96	0.47
4:D:1099:ARG:O	4:D:1103:GLU:HG2	2.15	0.47
4:D:1574:LYS:O	4:D:1574:LYS:NZ	2.40	0.47
5:E:646:ARG:HB3	5:E:697:TRP:HD1	1.79	0.47
5:E:859:GLU:OE1	5:E:902:GLN:NE2	2.48	0.47
6:F:465:ARG:HA	6:F:491:LEU:HD12	1.96	0.47
2:B:808:LYS:O	2:B:812:ILE:HG12	2.15	0.46
2:B:854:LYS:HA	2:B:857:ILE:HG12	1.97	0.46
3:C:102:ILE:HA	3:C:118:SER:HA	1.97	0.46
3:C:316:VAL:HG22	3:C:327:VAL:HG22	1.97	0.46
5:E:415:GLU:HB3	5:E:794:ARG:HH21	1.80	0.46
1:A:153:ARG:HB3	1:A:156:GLU:HG3	1.97	0.46
2:B:177:ASP:OD2	2:B:180:SER:N	2.42	0.46
2:B:846:VAL:HG13	2:B:848:LEU:HG	1.97	0.46
6:F:533:PHE:CG	6:F:573:VAL:HB	2.50	0.46
3:C:246:LYS:HE2	3:C:262:SER:HB3	1.97	0.46
2:B:212:ARG:NH1	2:B:345:LYS:O	2.48	0.46
3:C:58:HIS:CE1	3:C:78:GLY:H	2.33	0.46
3:C:240:LEU:HD12	3:C:250:PHE:CE2	2.50	0.46
3:C:622:LEU:HD13	3:C:687:PHE:CG	2.50	0.46
3:C:953:LEU:HD13	3:C:954:PRO:HD2	1.97	0.46
4:D:1259:GLN:HB3	4:D:1263:VAL:HG11	1.97	0.46
4:D:1329:ARG:HG2	4:D:1355:CYS:SG	2.55	0.46
4:D:1446:LEU:O	4:D:1450:LEU:HG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1549:VAL:O	4:D:1553:ASN:N	2.47	0.46
2:B:84:ASP:OD1	2:B:85:VAL:N	2.49	0.46
2:B:993:GLY:HA2	2:B:1028:LEU:HD13	1.96	0.46
3:C:55:LEU:HD12	3:C:55:LEU:H	1.81	0.46
5:E:587:ASN:HD21	5:E:608:LEU:HB2	1.80	0.46
6:F:601:ARG:HB2	6:F:698:HIS:CE1	2.50	0.46
6:F:161:PRO:HD3	6:F:181:VAL:HG22	1.98	0.46
2:B:119:PRO:HG3	2:B:207:PRO:HG3	1.97	0.46
2:B:630:LEU:HD21	2:B:637:PRO:HB3	1.98	0.46
3:C:1004:ALA:O	3:C:1007:GLU:HG2	2.16	0.46
5:E:195:PRO:HG3	5:E:261:ALA:HB1	1.98	0.46
6:F:118:GLY:HA2	6:F:141:LEU:HD21	1.97	0.46
3:C:250:PHE:HE1	3:C:256:ARG:HG3	1.79	0.46
1:A:148:GLN:HB2	4:D:1306:GLU:HG2	1.98	0.46
5:E:876:PHE:CD1	5:E:888:ALA:HB1	2.51	0.46
4:D:1085:GLU:HA	4:D:1088:ARG:HG2	1.98	0.46
5:E:553:MET:SD	5:E:553:MET:N	2.89	0.46
5:E:548:ILE:HG12	5:E:561:MET:HG2	1.98	0.45
2:B:5:LEU:HD11	2:B:293:VAL:HG12	1.98	0.45
3:C:796:ASN:HA	3:C:799:ARG:HH21	1.81	0.45
3:C:1028:LEU:HD11	6:F:499:VAL:HG21	1.99	0.45
4:D:1242:CYS:SG	4:D:1243:THR:N	2.89	0.45
2:B:249:HIS:CE1	2:B:265:ALA:H	2.34	0.45
2:B:1016:LEU:O	2:B:1020:MET:HG2	2.15	0.45
3:C:969:GLY:O	3:C:1058:GLY:N	2.49	0.45
4:D:879:VAL:HG11	4:D:911:LEU:HD21	1.99	0.45
4:D:1263:VAL:HG12	4:D:1531:TYR:HE2	1.80	0.45
4:D:1592:PRO:HD3	4:D:1622:HIS:CD2	2.44	0.45
5:E:6:VAL:HG22	5:E:449:LEU:HG	1.99	0.45
5:E:32:ALA:HB1	5:E:65:PRO:HG2	1.98	0.45
6:F:118:GLY:HA3	6:F:137:HIS:HB2	1.98	0.45
6:F:400:GLY:HA3	6:F:405:VAL:HG12	1.99	0.45
6:F:584:ILE:HD11	6:F:591:CYS:HB2	1.99	0.45
6:F:748:GLN:OE1	6:F:764:ARG:NH2	2.34	0.45
5:E:866:ASP:OD1	5:E:866:ASP:N	2.50	0.45
6:F:565:GLY:O	6:F:618:ASN:ND2	2.33	0.45
2:B:127:THR:HG22	2:B:133:VAL:HG13	1.97	0.45
3:C:764:ILE:HD12	3:C:790:LEU:HD22	1.99	0.45
5:E:165:LYS:HE3	5:E:174:PHE:HE1	1.82	0.45
2:B:940:LEU:HB3	2:B:941:LYS:HZ2	1.82	0.45
2:B:1231:ASN:HA	2:B:1238:PRO:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:973:GLU:HA	3:C:1057:ALA:HB1	1.98	0.45
4:D:1334:TYR:HA	4:D:1337:MET:HG2	1.99	0.45
6:F:446:SER:HB2	6:F:462:TYR:HB2	1.97	0.45
3:C:685:LEU:HD13	3:C:693:ASP:HB2	1.99	0.45
5:E:783:GLU:HG2	5:E:817:ARG:HD2	1.99	0.45
3:C:505:ASN:OD1	3:C:508:VAL:N	2.45	0.45
4:D:1318:LEU:HD21	4:D:1332:GLN:HG3	1.98	0.45
1:A:175:ASP:HB2	4:D:1322:PRO:HB3	1.99	0.45
2:B:577:ASN:ND2	2:B:614:LEU:H	2.15	0.45
2:B:630:LEU:HG	2:B:641:TYR:CD2	2.52	0.45
2:B:1188:CYS:SG	2:B:1191:CYS:N	2.87	0.45
3:C:1169:PHE:O	3:C:1172:LEU:HB3	2.17	0.45
5:E:158:VAL:HG21	5:E:228:LEU:HD13	1.98	0.45
6:F:853:ILE:HG13	6:F:881:LYS:HG3	1.99	0.45
2:B:93:VAL:HG13	2:B:95:HIS:CE1	2.52	0.45
2:B:819:TYR:CZ	2:B:846:VAL:HG21	2.52	0.45
2:B:929:GLN:OE1	2:B:933:ARG:NH2	2.50	0.45
4:D:1580:TYR:HB3	4:D:1598:LEU:HD13	1.99	0.45
5:E:194:VAL:HG22	5:E:259:TYR:CZ	2.52	0.45
5:E:600:GLN:N	5:E:600:GLN:OE1	2.50	0.45
6:F:457:LEU:HD23	6:F:468:LEU:HG	1.99	0.45
6:F:806:LEU:HD13	6:F:806:LEU:HA	1.81	0.45
2:B:1006:GLN:HB2	2:B:1015:ALA:HB2	1.99	0.44
3:C:233:ASN:HB2	3:C:236:GLU:HB3	1.99	0.44
3:C:1260:ARG:HE	3:C:1263:LYS:HE3	1.83	0.44
4:D:1584:TRP:CE2	4:D:1589:GLU:HG3	2.53	0.44
1:A:153:ARG:HG3	4:D:1313:HIS:NE2	2.32	0.44
4:D:1604:ARG:HD3	4:D:1604:ARG:HA	1.81	0.44
6:F:700:LEU:HD21	6:F:734:LEU:HG	1.99	0.44
2:B:391:ARG:HH22	2:B:411:GLU:HG3	1.81	0.44
5:E:260:ASP:HB2	5:E:317:TRP:CZ2	2.52	0.44
5:E:824:VAL:HG12	5:E:832:LEU:HB3	1.99	0.44
6:F:601:ARG:NH1	6:F:738:SER:OG	2.51	0.44
4:D:1513:ILE:HG23	4:D:1523:GLU:HG3	2.00	0.44
4:D:1568:GLU:OE1	4:D:1580:TYR:OH	2.30	0.44
6:F:529:LEU:HD21	6:F:532:ALA:HB2	2.00	0.44
2:B:7:LYS:HB3	2:B:320:PHE:HB2	2.00	0.44
3:C:736:GLN:OE1	3:C:739:ARG:NH2	2.44	0.44
4:D:1105:ALA:HB2	4:D:1127:MET:HE1	2.00	0.44
4:D:1520:ASP:OD1	4:D:1520:ASP:N	2.50	0.44
4:D:1561:ASN:HD22	4:D:1594:VAL:HB	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:440:ARG:HD2	6:F:442:VAL:HG22	2.00	0.44
2:B:532:ASN:ND2	2:B:536:THR:OG1	2.48	0.44
4:D:1619:LEU:HD21	4:D:1628:ILE:HG21	1.99	0.44
6:F:860:VAL:HG13	6:F:869:VAL:HG12	1.99	0.44
2:B:76:GLN:NE2	2:B:119:PRO:O	2.51	0.44
2:B:244:ARG:HD2	2:B:281:PHE:HZ	1.83	0.44
2:B:1013:LYS:O	2:B:1017:VAL:HG23	2.18	0.44
3:C:250:PHE:CD1	3:C:256:ARG:HA	2.53	0.44
3:C:458:ALA:HB3	3:C:476:ASP:HB3	2.00	0.44
3:C:726:ASP:O	3:C:729:VAL:HG12	2.17	0.44
3:C:792:THR:HG23	3:C:814:VAL:HG11	1.99	0.44
3:C:953:LEU:HD21	5:E:1092:TRP:NE1	2.32	0.44
3:C:954:PRO:HD3	5:E:1099:ARG:HB2	1.99	0.44
3:C:1064:CYS:SG	3:C:1066:HIS:HB3	2.58	0.44
4:D:1124:VAL:HA	4:D:1127:MET:HE2	1.99	0.44
4:D:1613:ASP:HA	4:D:1616:LYS:HD3	2.00	0.44
5:E:1018:ALA:HA	5:E:1021:MET:HG2	1.99	0.44
6:F:548:SER:HB3	6:F:568:PRO:HB3	2.00	0.44
6:F:765:ARG:NH2	6:F:784:GLU:OE1	2.48	0.44
2:B:579:ARG:HG3	2:B:614:LEU:HB3	2.00	0.44
2:B:599:TYR:CZ	2:B:604:ALA:HB2	2.53	0.44
3:C:998:MET:O	3:C:1002:ALA:N	2.43	0.44
4:D:1176:LEU:HD21	4:D:1192:LEU:HD21	2.00	0.44
2:B:682:ALA:HB2	2:B:697:ALA:HB3	1.99	0.44
3:C:502:VAL:HG23	3:C:514:PHE:HB3	1.99	0.44
3:C:603:ARG:HG2	3:C:606:ILE:HG22	2.00	0.44
6:F:553:VAL:HG22	6:F:560:ALA:HA	2.00	0.44
6:F:951:TRP:HA	6:F:954:ALA:HB3	2.00	0.44
1:A:163:TRP:CH2	2:B:1004:GLN:HB3	2.53	0.43
3:C:783:LEU:HD13	3:C:783:LEU:HA	1.90	0.43
4:D:1575:ASN:OD1	4:D:1575:ASN:N	2.50	0.43
5:E:581:VAL:HG22	5:E:591:LEU:HG	1.99	0.43
5:E:823:LEU:HD13	5:E:833:LEU:HD23	2.00	0.43
6:F:764:ARG:NH1	6:F:769:GLN:OE1	2.49	0.43
6:F:789:SER:O	6:F:792:TYR:HB3	2.17	0.43
2:B:420:SER:HB3	2:B:436:ARG:NH2	2.33	0.43
4:D:1056:SER:O	4:D:1058:VAL:N	2.51	0.43
5:E:15:LEU:H	5:E:444:SER:HA	1.82	0.43
3:C:824:TYR:HA	3:C:827:LYS:HG2	1.99	0.43
4:D:901:LEU:HD12	4:D:901:LEU:HA	1.90	0.43
2:B:28:TRP:HB2	2:B:73:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:THR:OG1	2:B:84:ASP:OD1	2.28	0.43
3:C:179:ALA:HB3	3:C:201:SER:HB2	2.01	0.43
4:D:974:ASP:O	4:D:995:HIS:NE2	2.51	0.43
5:E:904:LEU:HD12	5:E:907:LEU:HD23	2.00	0.43
6:F:863:SER:OG	6:F:864:SER:N	2.51	0.43
6:F:944:ALA:HA	6:F:947:GLN:HB3	2.00	0.43
2:B:141:ASN:N	2:B:141:ASN:OD1	2.49	0.43
2:B:154:LYS:HE3	2:B:154:LYS:HB3	1.88	0.43
3:C:383:CYS:HB3	3:C:421:VAL:HG23	2.01	0.43
6:F:902:TYR:HA	6:F:906:CYS:HB2	2.00	0.43
2:B:416:ASP:OD1	2:B:417:MET:N	2.49	0.43
5:E:29:LEU:HD13	5:E:432:THR:HG22	2.00	0.43
5:E:427:ASP:N	5:E:440:CYS:O	2.51	0.43
2:B:101:GLU:OE1	2:B:101:GLU:N	2.50	0.43
2:B:638:ARG:NH1	2:B:640:ASP:OD1	2.52	0.43
5:E:16:LYS:HA	5:E:16:LYS:HD3	1.77	0.43
5:E:26:ARG:HA	5:E:26:ARG:HD3	1.86	0.43
5:E:313:MET:HG2	5:E:327:SER:HA	2.00	0.43
5:E:844:ASN:HD22	5:E:847:ASP:HB2	1.84	0.43
6:F:23:LEU:HD13	6:F:325:SER:HB3	1.99	0.43
6:F:721:LEU:HD23	6:F:724:ILE:HD11	2.01	0.43
2:B:431:TYR:OH	2:B:433:TRP:HB2	2.18	0.43
2:B:576:TRP:CE3	2:B:577:ASN:HB2	2.54	0.43
5:E:188:VAL:HA	5:E:230:ASP:HA	1.99	0.43
5:E:258:LEU:HD22	5:E:315:MET:HG2	2.01	0.43
2:B:633:ASP:N	2:B:633:ASP:OD1	2.51	0.43
2:B:1019:ALA:O	2:B:1022:LEU:HB2	2.19	0.43
3:C:783:LEU:HD12	3:C:787:GLU:HB3	2.01	0.43
6:F:958:ARG:HD2	6:F:971:ILE:HD11	1.99	0.43
2:B:289:ARG:HA	2:B:289:ARG:HD3	1.85	0.42
2:B:491:CYS:SG	2:B:492:VAL:N	2.92	0.42
2:B:533:CYS:SG	2:B:534:ASN:N	2.91	0.42
3:C:36:SER:HB2	3:C:62:ILE:HB	2.01	0.42
3:C:824:TYR:HD1	3:C:827:LYS:HD3	1.84	0.42
4:D:1322:PRO:O	4:D:1325:SER:OG	2.37	0.42
5:E:43:ASN:HD22	5:E:45:GLU:H	1.66	0.42
2:B:244:ARG:NH1	2:B:247:PRO:O	2.43	0.42
3:C:540:VAL:HG21	3:C:555:MET:HE1	2.02	0.42
3:C:884:LEU:HB3	3:C:900:TYR:CE2	2.55	0.42
3:C:1028:LEU:HD23	3:C:1028:LEU:HA	1.85	0.42
5:E:264:ARG:HH12	5:E:282:GLU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ASN:HB2	2:B:73:TRP:CD2	2.54	0.42
5:E:138:VAL:N	5:E:152:ALA:O	2.52	0.42
6:F:461:VAL:HG22	6:F:466:VAL:HG22	2.01	0.42
3:C:733:LEU:O	3:C:737:GLN:HG3	2.20	0.42
3:C:753:LEU:O	3:C:756:SER:OG	2.31	0.42
3:C:1013:ILE:HD11	6:F:700:LEU:HD23	2.01	0.42
2:B:422:VAL:HG23	2:B:435:PHE:HE2	1.85	0.42
2:B:1182:LYS:HE2	2:B:1182:LYS:HB2	1.88	0.42
2:B:1189:ILE:HG23	2:B:1190:LYS:HE3	2.01	0.42
3:C:240:LEU:HA	3:C:240:LEU:HD23	1.76	0.42
3:C:575:PHE:HD2	3:C:603:ARG:HD3	1.84	0.42
4:D:1523:GLU:O	4:D:1527:LEU:HG	2.19	0.42
3:C:917:PRO:HG2	3:C:922:LYS:HE3	2.02	0.42
5:E:381:HIS:CE1	5:E:415:GLU:HB2	2.55	0.42
5:E:1016:MET:HA	5:E:1019:ALA:HB3	2.02	0.42
5:E:1123:LEU:HD22	5:E:1130:LYS:HB2	2.02	0.42
6:F:535:ASN:OD1	6:F:539:THR:N	2.42	0.42
6:F:761:LEU:HD21	6:F:788:ILE:HD11	2.02	0.42
2:B:333:LYS:HD3	2:B:333:LYS:HA	1.84	0.42
3:C:439:GLN:HE21	3:C:455:LYS:HE2	1.84	0.42
3:C:1245:GLU:OE1	5:E:1205:SER:OG	2.34	0.42
4:D:1178:LEU:HB2	4:D:1516:CYS:SG	2.59	0.42
5:E:112:VAL:HA	5:E:115:ILE:HG22	2.02	0.42
6:F:348:LEU:HD11	6:F:386:ASP:HB3	2.00	0.42
6:F:352:ALA:HB2	6:F:390:ILE:HG13	2.01	0.42
6:F:621:THR:HG21	6:F:652:GLN:H	1.85	0.42
1:A:154:LEU:HG	4:D:1313:HIS:CD2	2.55	0.42
2:B:378:CYS:SG	2:B:379:VAL:N	2.92	0.42
2:B:493:SER:HB2	2:B:531:VAL:HG11	2.01	0.42
3:C:21:VAL:HG23	3:C:286:GLY:HA2	2.02	0.42
6:F:529:LEU:HD13	6:F:543:TYR:HD2	1.85	0.42
6:F:533:PHE:O	6:F:575:TRP:NE1	2.40	0.41
2:B:4:TYR:CZ	2:B:322:ASN:HB2	2.55	0.41
4:D:919:GLU:O	4:D:923:GLU:HG2	2.20	0.41
5:E:455:LYS:HB3	5:E:493:VAL:HG12	2.02	0.41
6:F:925:ILE:HA	6:F:928:TYR:HB3	2.01	0.41
1:A:163:TRP:CD2	1:A:183:LEU:HD13	2.56	0.41
2:B:405:THR:O	2:B:406:ARG:NH1	2.42	0.41
2:B:844:LEU:HD11	2:B:868:GLY:HA3	2.02	0.41
2:B:1223:GLU:HA	2:B:1226:VAL:HG12	2.02	0.41
3:C:104:ALA:HB3	3:C:117:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:839:LYS:HA	3:C:839:LYS:HD3	1.87	0.41
3:C:1046:ARG:HD3	3:C:1064:CYS:HB2	2.02	0.41
4:D:1046:ILE:HD11	4:D:1107:LEU:HB2	2.02	0.41
5:E:194:VAL:HG23	5:E:227:LEU:HD11	2.02	0.41
5:E:276:GLU:OE1	5:E:278:TYR:OH	2.39	0.41
2:B:575:VAL:HG22	2:B:592:GLU:HB3	2.01	0.41
2:B:1066:GLU:OE1	2:B:1149:ARG:NH2	2.35	0.41
3:C:471:ARG:HH22	3:C:512:ILE:HD11	1.85	0.41
4:D:1160:ASP:HA	4:D:1163:ARG:HB2	2.02	0.41
4:D:1318:LEU:HD12	4:D:1321:LEU:HD12	2.02	0.41
6:F:489:THR:HG23	6:F:505:THR:HB	2.02	0.41
2:B:1044:LEU:HD13	2:B:1044:LEU:HA	1.83	0.41
3:C:718:ASP:OD1	3:C:718:ASP:N	2.53	0.41
3:C:731:LYS:HE3	3:C:731:LYS:HB3	1.91	0.41
4:D:1078:SER:HA	4:D:1081:THR:HG22	2.02	0.41
4:D:1312:ARG:O	4:D:1316:GLN:HG3	2.20	0.41
6:F:550:LEU:HD23	6:F:594:PHE:HE2	1.85	0.41
3:C:147:THR:OG1	3:C:152:THR:O	2.38	0.41
5:E:509:ASP:HB3	5:E:511:TYR:CE1	2.56	0.41
2:B:911:ILE:HD13	2:B:927:LEU:HG	2.02	0.41
2:B:1216:VAL:HG21	2:B:1237:THR:HG21	2.02	0.41
3:C:439:GLN:NE2	3:C:455:LYS:HE2	2.36	0.41
3:C:576:ASP:O	3:C:580:GLU:HG2	2.20	0.41
2:B:1027:ASP:OD1	2:B:1027:ASP:N	2.54	0.41
3:C:42:LEU:HD22	3:C:51:LEU:HD11	2.03	0.41
5:E:969:LYS:HB3	5:E:969:LYS:HE3	1.70	0.41
2:B:3:VAL:HG21	2:B:280:PHE:CE2	2.55	0.41
2:B:1026:ASP:OD1	2:B:1026:ASP:N	2.53	0.41
4:D:878:LEU:HD11	4:D:886:LYS:HE2	2.02	0.41
2:B:64:HIS:ND1	2:B:84:ASP:HB2	2.36	0.41
2:B:95:HIS:HB2	2:B:100:PHE:CE2	2.55	0.41
2:B:462:ILE:HD12	2:B:468:VAL:HG21	2.03	0.41
3:C:905:ALA:HB2	3:C:932:CYS:HB2	2.03	0.41
3:C:939:TYR:OH	3:C:978:ILE:O	2.31	0.41
4:D:1181:HIS:HA	4:D:1553:ASN:OD1	2.21	0.41
2:B:365:VAL:HG11	2:B:368:LEU:HD13	2.03	0.40
2:B:398:ALA:HB3	3:C:587:ALA:HB1	2.03	0.40
2:B:886:ARG:HD3	2:B:886:ARG:HA	1.92	0.40
2:B:896:LYS:HE3	2:B:896:LYS:HB3	1.84	0.40
3:C:122:TRP:HE1	3:C:165:LEU:HD23	1.86	0.40
3:C:505:ASN:HB3	3:C:508:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:LEU:O	3:C:709:GLU:HG2	2.22	0.40
4:D:1152:GLU:OE2	4:D:1156:ASN:ND2	2.53	0.40
5:E:657:MET:HE3	5:E:670:ILE:HG22	2.03	0.40
2:B:460:ARG:HE	2:B:460:ARG:HB3	1.72	0.40
3:C:107:HIS:CE1	3:C:114:LEU:HD22	2.57	0.40
3:C:203:ASP:N	3:C:203:ASP:OD1	2.54	0.40
4:D:1118:GLU:HA	4:D:1122:THR:OG1	2.21	0.40
5:E:332:LEU:HB2	5:E:345:LEU:HB3	2.03	0.40
5:E:776:GLU:OE1	5:E:776:GLU:N	2.53	0.40
5:E:965:LEU:HD22	5:E:970:ARG:HB2	2.03	0.40
6:F:670:ASN:HB3	6:F:679:SER:HB3	2.03	0.40
1:A:199:LEU:HD23	2:B:915:ARG:HH22	1.85	0.40
3:C:143:CYS:SG	3:C:144:ALA:N	2.94	0.40
3:C:408:ARG:HD2	3:C:410:TRP:CZ2	2.56	0.40
3:C:433:VAL:O	3:C:440:VAL:HA	2.22	0.40
3:C:531:TYR:HB2	3:C:564:HIS:HD2	1.86	0.40
4:D:1217:GLU:OE1	4:D:1222:ASN:ND2	2.44	0.40
4:D:1255:VAL:HG23	4:D:1259:GLN:O	2.22	0.40
2:B:857:ILE:HG22	2:B:862:PRO:HB3	2.03	0.40
3:C:618:LYS:H	3:C:618:LYS:HD2	1.85	0.40
4:D:1597:LYS:HD2	4:D:1597:LYS:HA	1.83	0.40
5:E:869:VAL:HG13	5:E:895:ILE:HG23	2.02	0.40
6:F:204:LEU:HB2	6:F:207:THR:HB	2.04	0.40
2:B:363:LYS:NZ	2:B:400:GLY:O	2.30	0.40
2:B:385:ASP:HB3	2:B:388:GLN:HB3	2.02	0.40
3:C:176:ARG:HA	3:C:176:ARG:HH11	1.86	0.40
3:C:1233:ASN:HB2	3:C:1259:TYR:CZ	2.57	0.40
4:D:1634:ASP:OD1	4:D:1634:ASP:N	2.55	0.40
6:F:367:ILE:HG13	6:F:383:VAL:HG21	2.03	0.40
6:F:853:ILE:O	6:F:857:MET:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	73/368 (20%)	69 (94%)	4 (6%)	0	100	100
2	B	1120/1247 (90%)	1070 (96%)	50 (4%)	0	100	100
3	C	1170/1292 (91%)	1133 (97%)	37 (3%)	0	100	100
4	D	596/1642 (36%)	567 (95%)	27 (4%)	2 (0%)	41	72
5	E	1039/1654 (63%)	1001 (96%)	38 (4%)	0	100	100
6	F	966/1376 (70%)	946 (98%)	20 (2%)	0	100	100
All	All	4964/7579 (66%)	4786 (96%)	176 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1058	VAL
4	D	1057	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	A	64/288 (22%)	64 (100%)	0	100	100
2	B	956/1046 (91%)	927 (97%)	29 (3%)	41	68
3	C	1012/1094 (92%)	987 (98%)	25 (2%)	47	72
4	D	505/1320 (38%)	487 (96%)	18 (4%)	35	63
5	E	892/1373 (65%)	879 (98%)	13 (2%)	65	82
6	F	822/1177 (70%)	809 (98%)	13 (2%)	62	81
All	All	4251/6298 (68%)	4153 (98%)	98 (2%)	53	74

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	67	THR
2	B	104	VAL
2	B	176	HIS
2	B	211	GLU
2	B	378	CYS
2	B	380	LEU
2	B	383	ARG
2	B	415	TYR
2	B	533	CYS
2	B	583	ASP
2	B	617	PHE
2	B	630	LEU
2	B	659	ASP
2	B	673	ASN
2	B	680	LEU
2	B	739	LEU
2	B	743	VAL
2	B	807	ARG
2	B	828	MET
2	B	881	LEU
2	B	894	LEU
2	B	907	LEU
2	B	921	ASP
2	B	1000	LEU
2	B	1044	LEU
2	B	1047	ASN
2	B	1055	PHE
2	B	1065	ASP
2	B	1225	VAL
3	C	26	TYR
3	C	32	TYR
3	C	147	THR
3	C	317	VAL
3	C	374	ARG
3	C	385	THR
3	C	418	LEU
3	C	481	LEU
3	C	484	LEU
3	C	511	ASN
3	C	525	THR
3	C	550	LEU
3	C	711	TYR
3	C	722	LYS

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Mol	Chain	Res	Type
3	C	730	LEU
3	C	780	CYS
3	C	783	LEU
3	C	787	GLU
3	C	790	LEU
3	C	799	ARG
3	C	831	ARG
3	C	908	TYR
3	C	1069	VAL
3	C	1072	PHE
3	C	1272	ILE
4	D	891	TYR
4	D	972	LEU
4	D	993	ASP
4	D	1031	ARG
4	D	1093	PHE
4	D	1118	GLU
4	D	1175	TYR
4	D	1242	CYS
4	D	1255	VAL
4	D	1309	ASP
4	D	1328	ARG
4	D	1404	LEU
4	D	1522	ILE
4	D	1531	TYR
4	D	1541	ASP
4	D	1575	ASN
4	D	1584	TRP
4	D	1624	THR
5	E	50	THR
5	E	130	ARG
5	E	291	ARG
5	E	325	PHE
5	E	366	MET
5	E	509	ASP
5	E	511	TYR
5	E	522	PHE
5	E	805	HIS
5	E	964	LEU
5	E	1215	GLN
5	E	1224	MET
5	E	1232	MET

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Mol	Chain	Res	Type
6	F	1	MET
6	F	401	VAL
6	F	627	TYR
6	F	628	THR
6	F	643	ASN
6	F	659	LEU
6	F	678	TRP
6	F	695	LYS
6	F	707	ARG
6	F	766	ASP
6	F	806	LEU
6	F	823	THR
6	F	863	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	417	GLN
4	D	1221	ASN
4	D	1223	ASN
4	D	1622	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

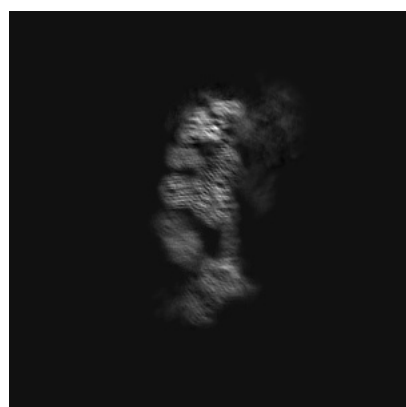
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28867. These allow visual inspection of the internal detail of the map and identification of artifacts.

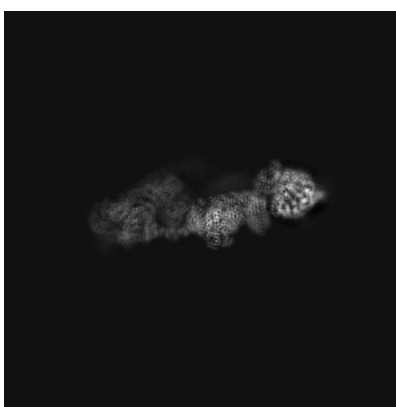
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

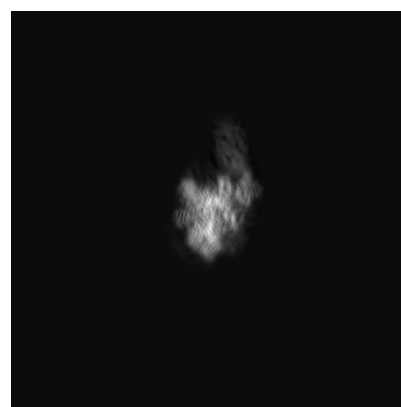
6.1.1 Primary map



X



Y



Z

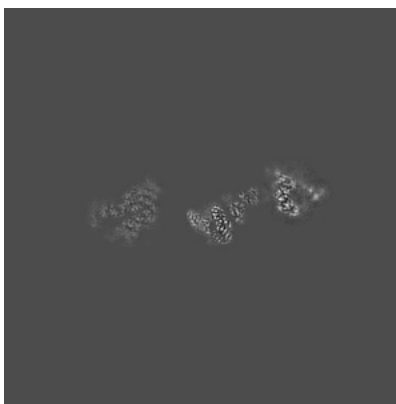
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

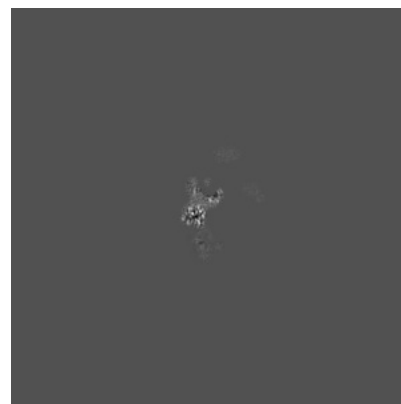
6.2.1 Primary map



X Index: 310



Y Index: 310



Z Index: 310

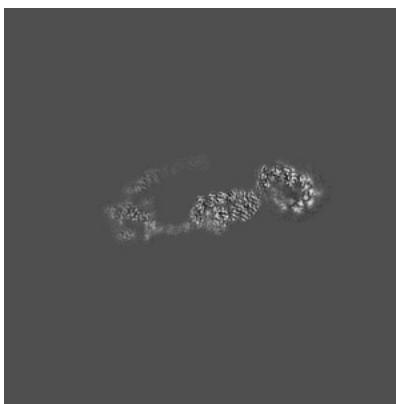
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 306



Y Index: 328



Z Index: 330

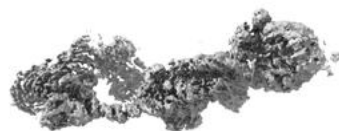
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

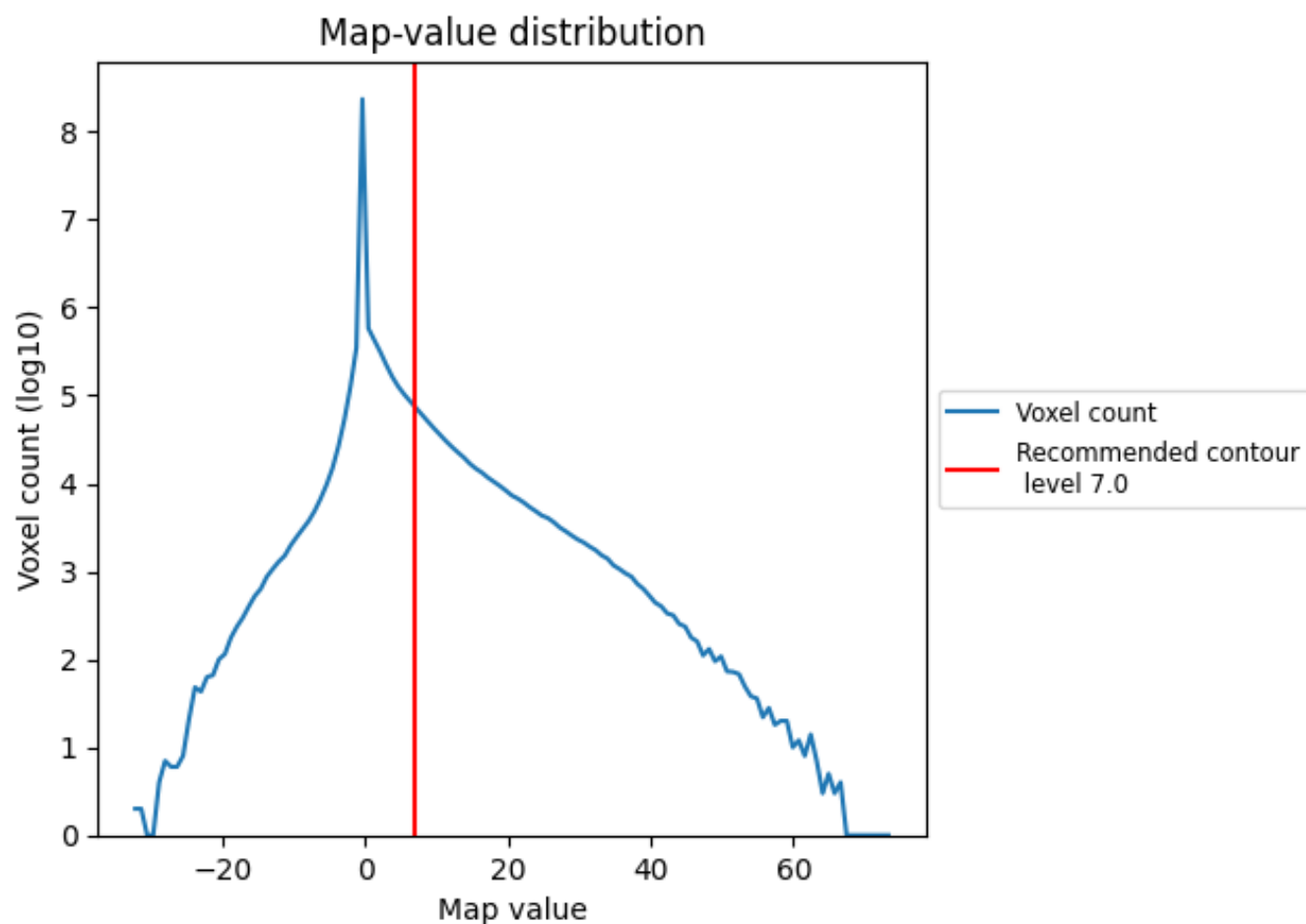
6.5 Mask visualisation

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

7 Map analysis [i](#)

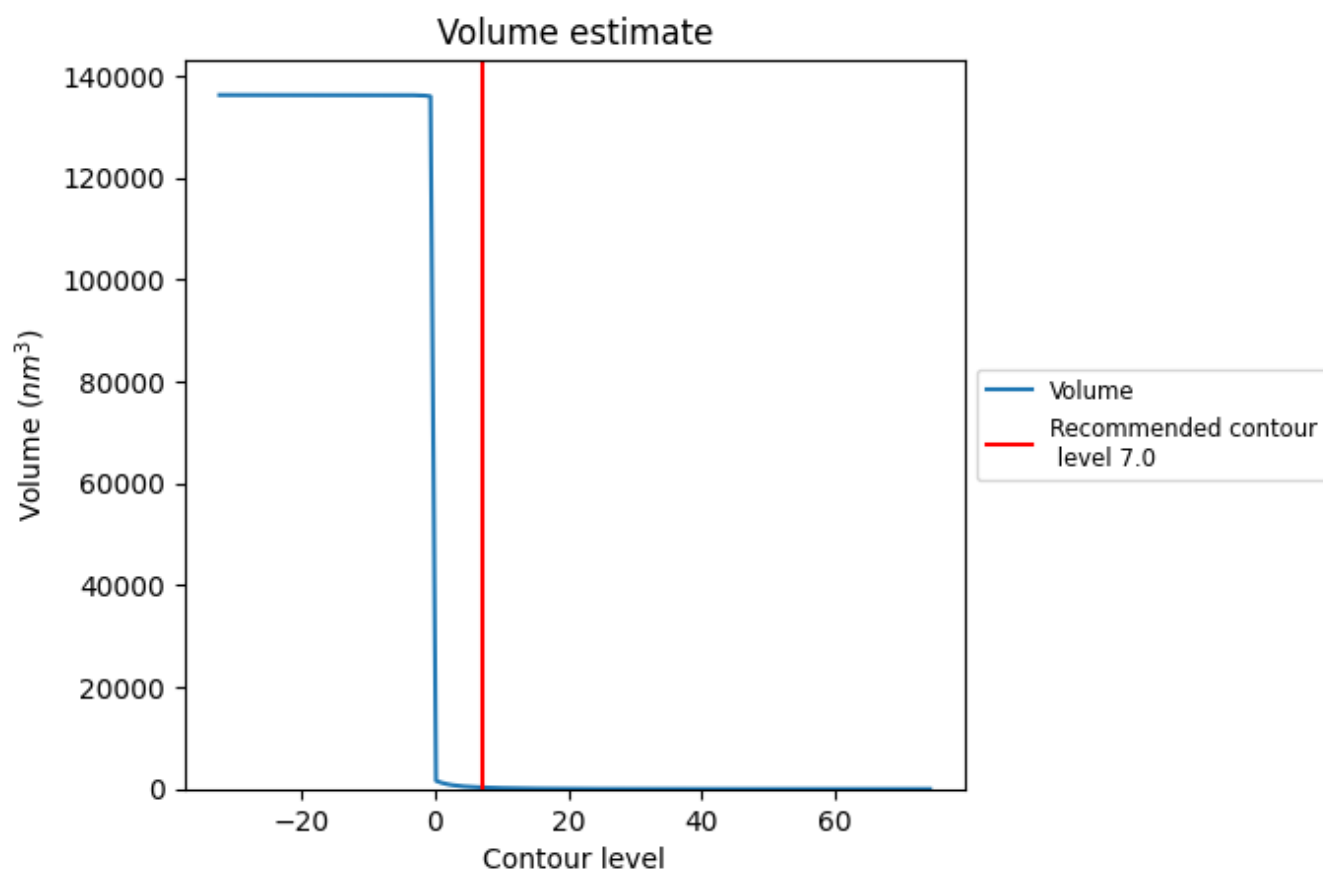
This section contains the results of statistical analysis of the map.

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.

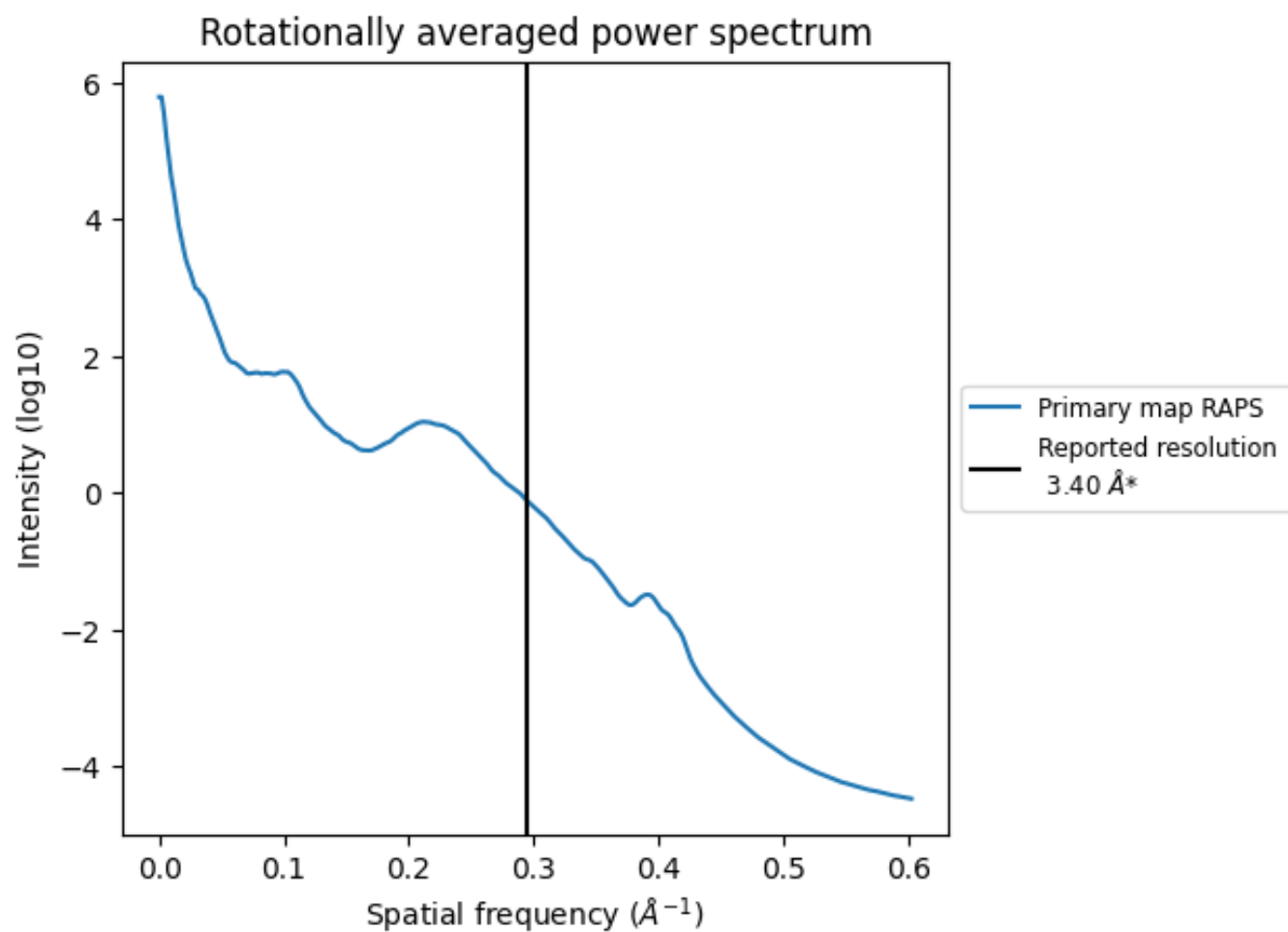
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 303 nm³; this corresponds to an approximate mass of 273 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

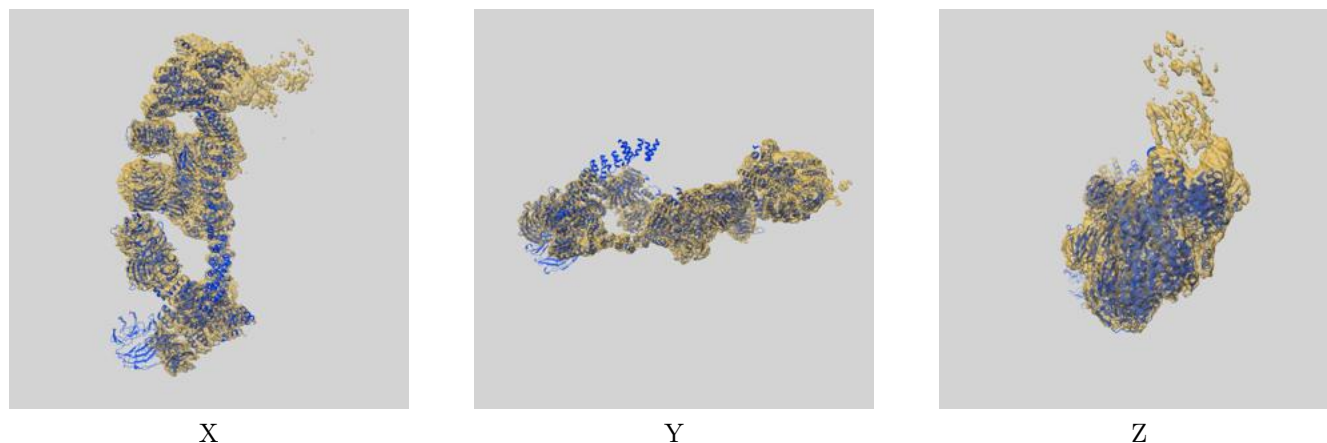
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

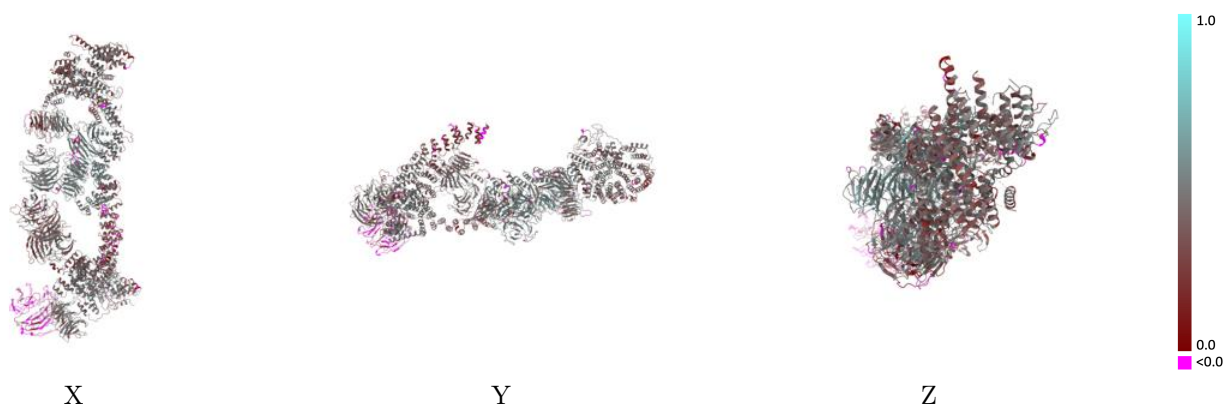
This section contains information regarding the fit between EMDB map EMD-28867 and PDB model 8F5P. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



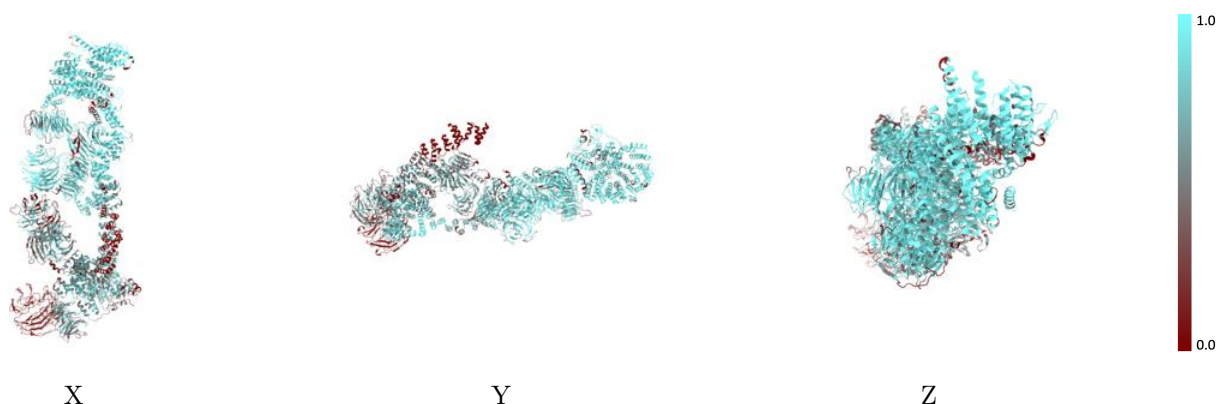
The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



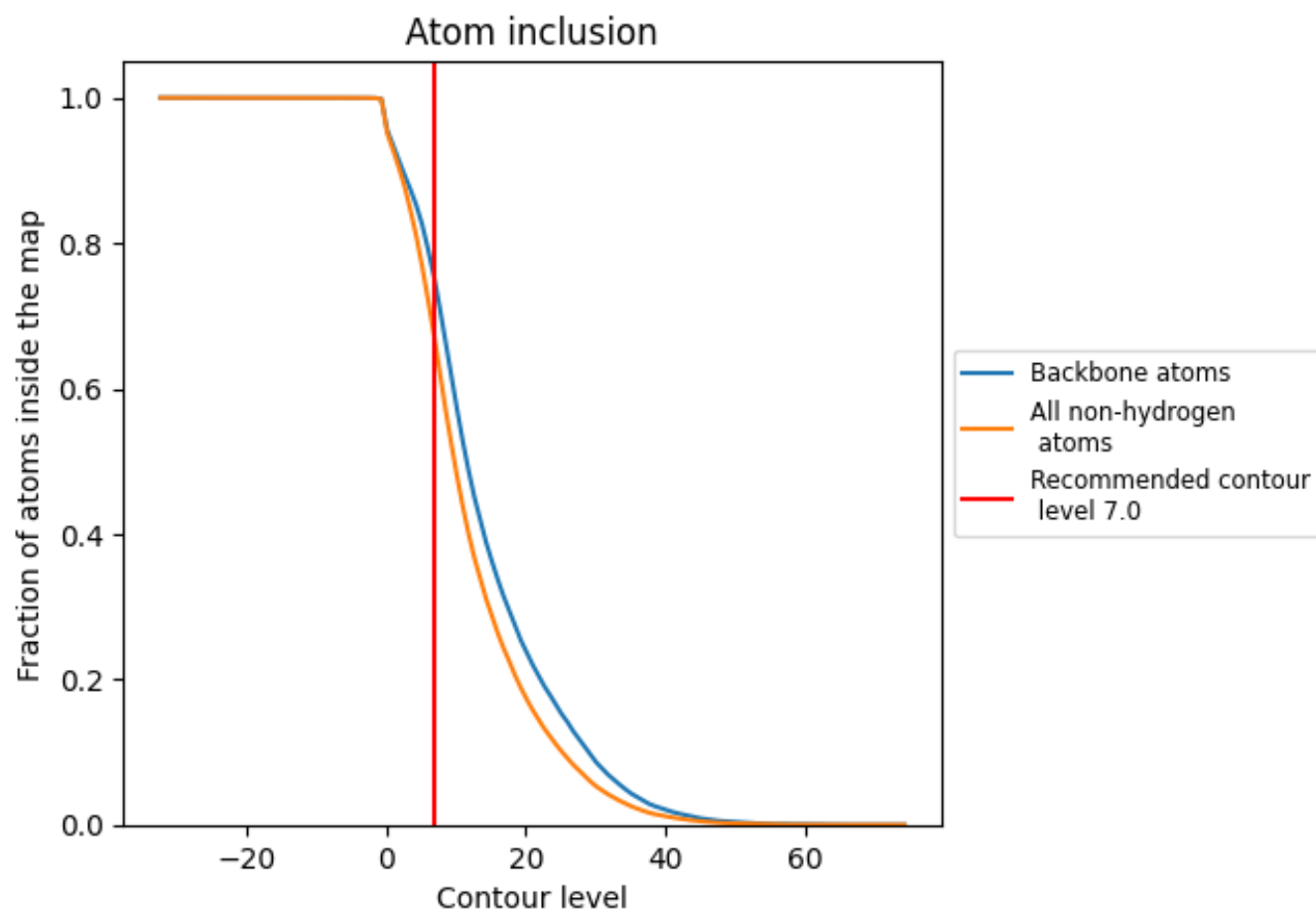
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (7.0).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 67% 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 (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6664	<div></div> 0.3860
A	<div></div> 0.6463	<div></div> 0.3640
B	<div></div> 0.8720	<div></div> 0.4660
C	<div></div> 0.7463	<div></div> 0.4180
D	<div></div> 0.9017	<div></div> 0.3900
E	<div></div> 0.5746	<div></div> 0.3960
F	<div></div> 0.2758	<div></div> 0.2390

1.0

0.0

<0.0