Full wwPDB EM Validation Report (i)

Jul 17, 2024 – 12:17 pm BST

PDB ID	:	7ZU0
EMDB ID	:	EMD-14964
Title	:	HOPS tethering complex from yeast
Authors	:	Shvarev, D.; Schoppe, J.; Koenig, C.; Perz, A.; Fuellbrunn, N.; Kiontke, S.; Langemeyer, L.; Januliene, D.; Schnelle, K.; Kuemmel, D.; Froehlich, F.; Moeller, A.; Ungermann, C.
Deposited on	:	2022-05-11
Resolution	:	4.40 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 (i) 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 (i)) were used in the production of this report:

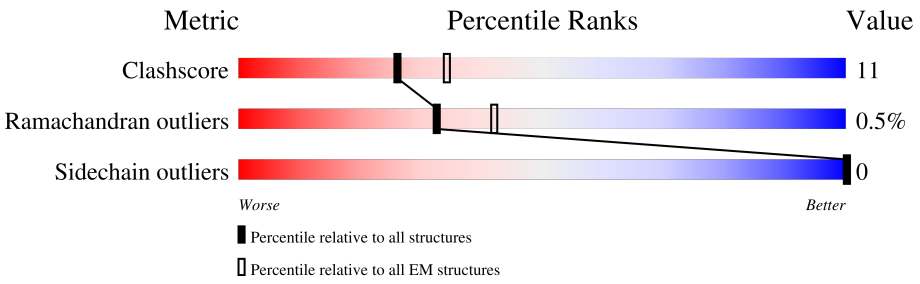
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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 <=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	1029	29% 68% 25% 7%
2	B	798	32% 66% 25% 8%
3	C	918	7% 72% 19% • 8%
4	D	691	35% 64% 22% 14%
5	E	1049	9% 29% • 67%
6	F	1016	• 8% • 89%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25763 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 E3 ubiquitin-protein ligase PEP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	954	6914	4395	1185	1315	19	0	0

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5981	3862	980	1110	29	0	0

- Molecule 3 is a protein called Vacuolar membrane protein PEP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	842	5549	3476	989	1063	21	0	0

- Molecule 4 is a protein called Vacuolar protein sorting-associated protein 33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	597	4749	3036	789	904	20	0	0

- Molecule 5 is a protein called Vacuolar morphogenesis protein 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	343	1704	1018	343	343	0	0

- Molecule 6 is a protein called Vacuolar protein sorting-associated protein 41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	112	866	549	144	170	3	0	0

There are 24 discrepancies between the modelled and reference sequences:

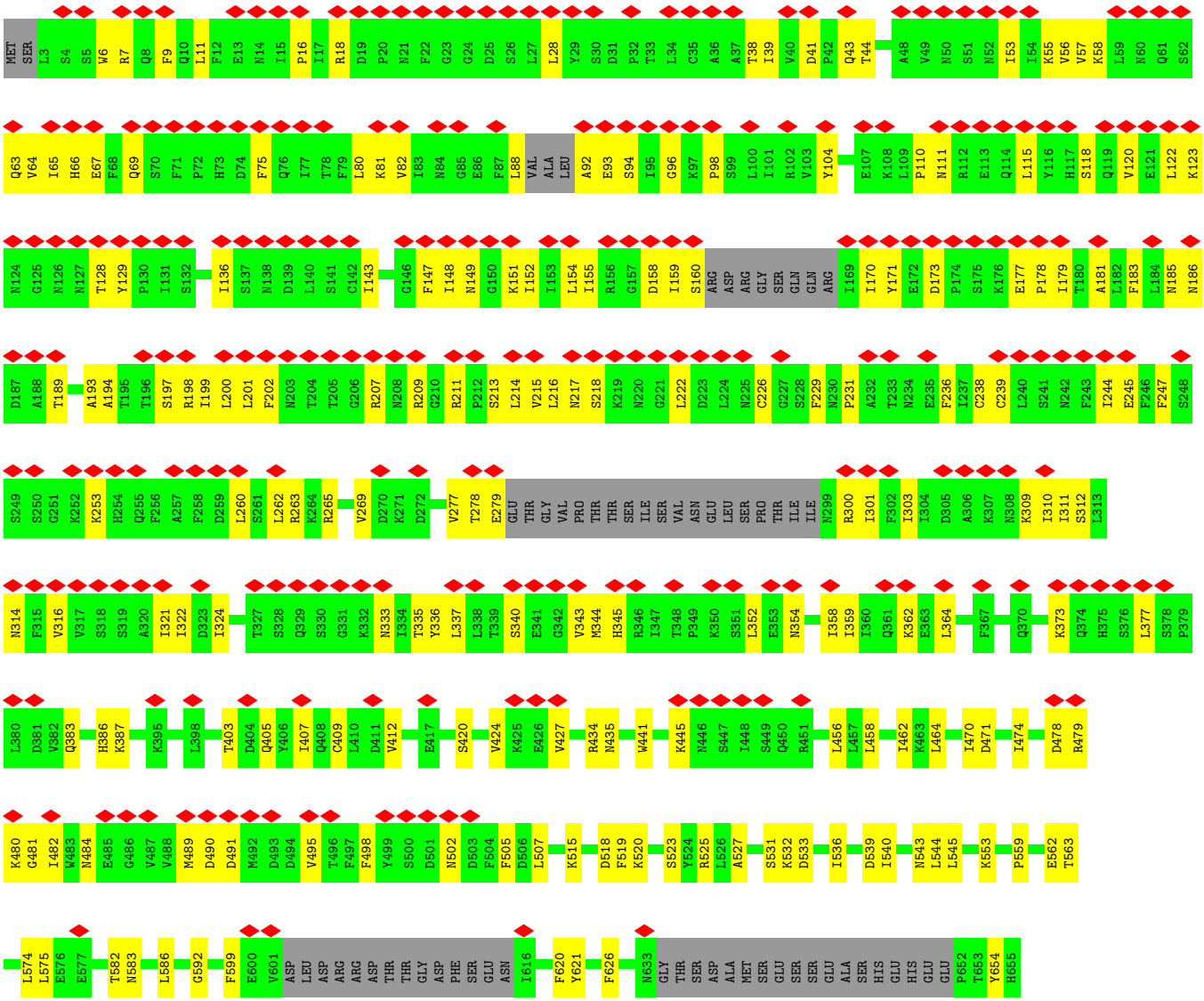
Chain	Residue	Modelled	Actual	Comment	Reference
F	993	ASP	-	expression tag	UNP P38959
F	994	TYR	-	expression tag	UNP P38959
F	995	LYS	-	expression tag	UNP P38959
F	996	ASP	-	expression tag	UNP P38959
F	997	ASP	-	expression tag	UNP P38959
F	998	ASP	-	expression tag	UNP P38959
F	999	ASP	-	expression tag	UNP P38959
F	1000	LYS	-	expression tag	UNP P38959
F	1001	ASP	-	expression tag	UNP P38959
F	1002	TYR	-	expression tag	UNP P38959
F	1003	LYS	-	expression tag	UNP P38959
F	1004	ASP	-	expression tag	UNP P38959
F	1005	ASP	-	expression tag	UNP P38959
F	1006	ASP	-	expression tag	UNP P38959
F	1007	ASP	-	expression tag	UNP P38959
F	1008	LYS	-	expression tag	UNP P38959
F	1009	ASP	-	expression tag	UNP P38959
F	1010	TYR	-	expression tag	UNP P38959
F	1011	LYS	-	expression tag	UNP P38959
F	1012	ASP	-	expression tag	UNP P38959
F	1013	ASP	-	expression tag	UNP P38959
F	1014	ASP	-	expression tag	UNP P38959
F	1015	ASP	-	expression tag	UNP P38959
F	1016	LYS	-	expression tag	UNP P38959

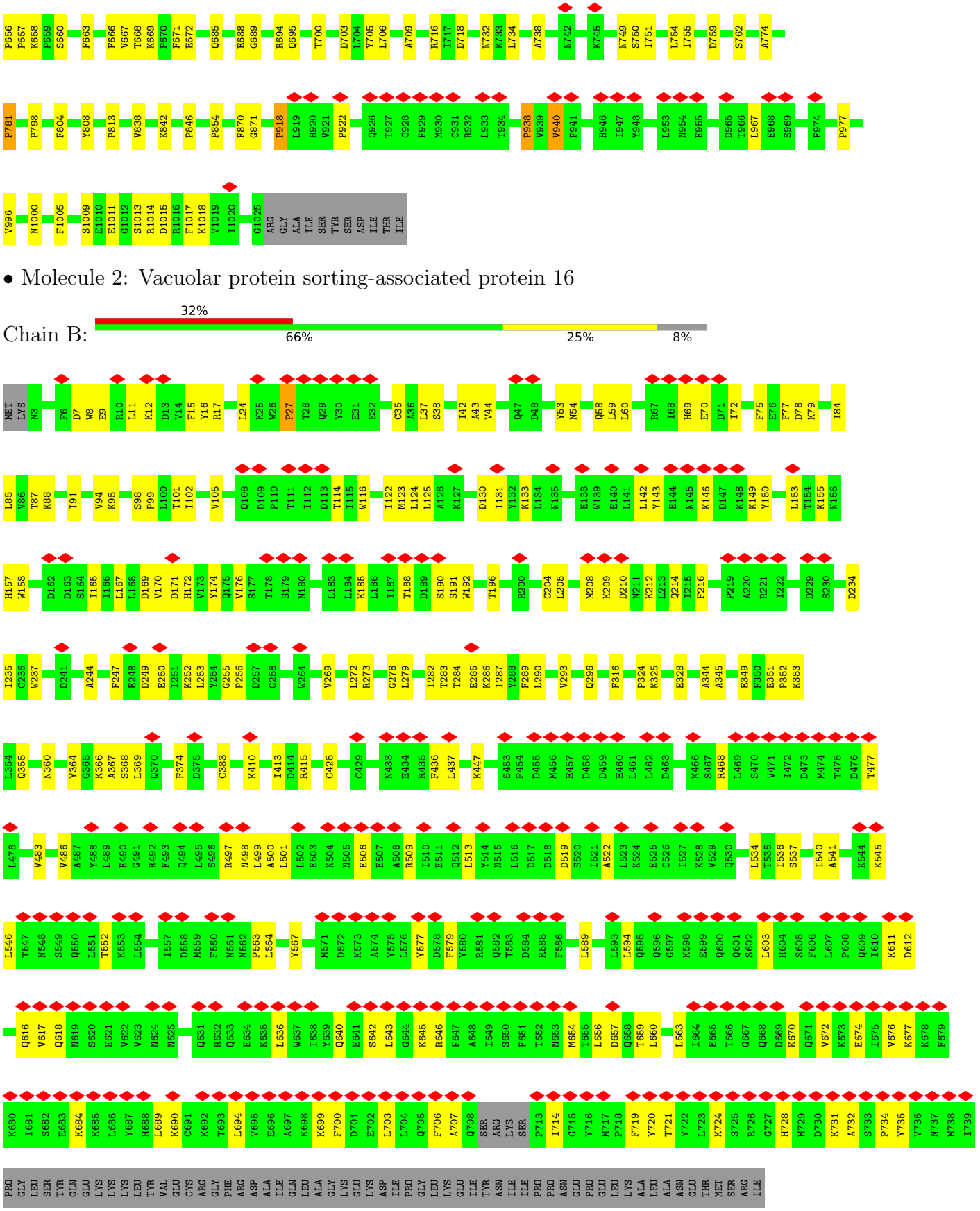
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: E3 ubiquitin-protein ligase PEP5

Chain A:



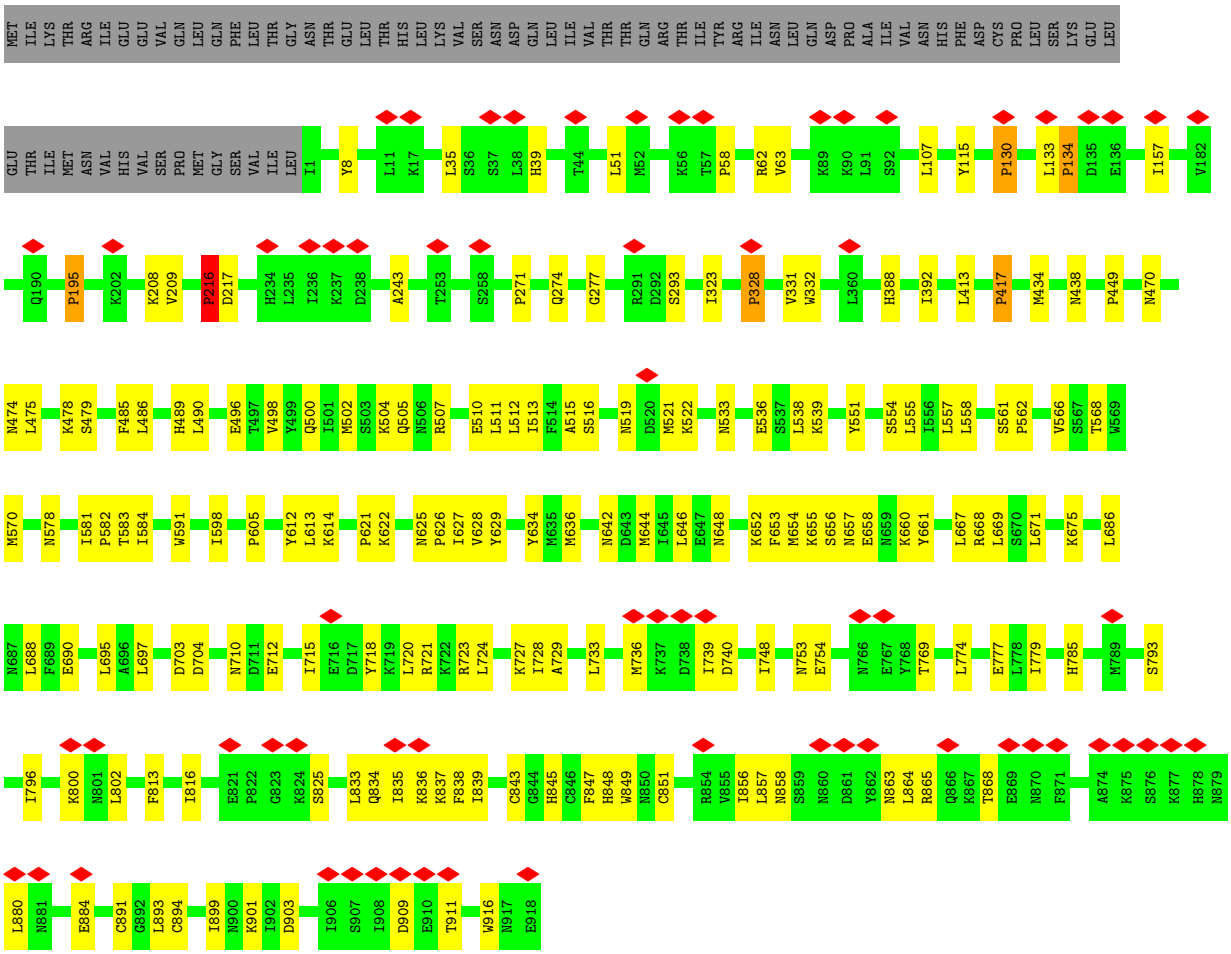


• Molecule 2: Vacuolar protein sorting-associated protein 16

Chain B:

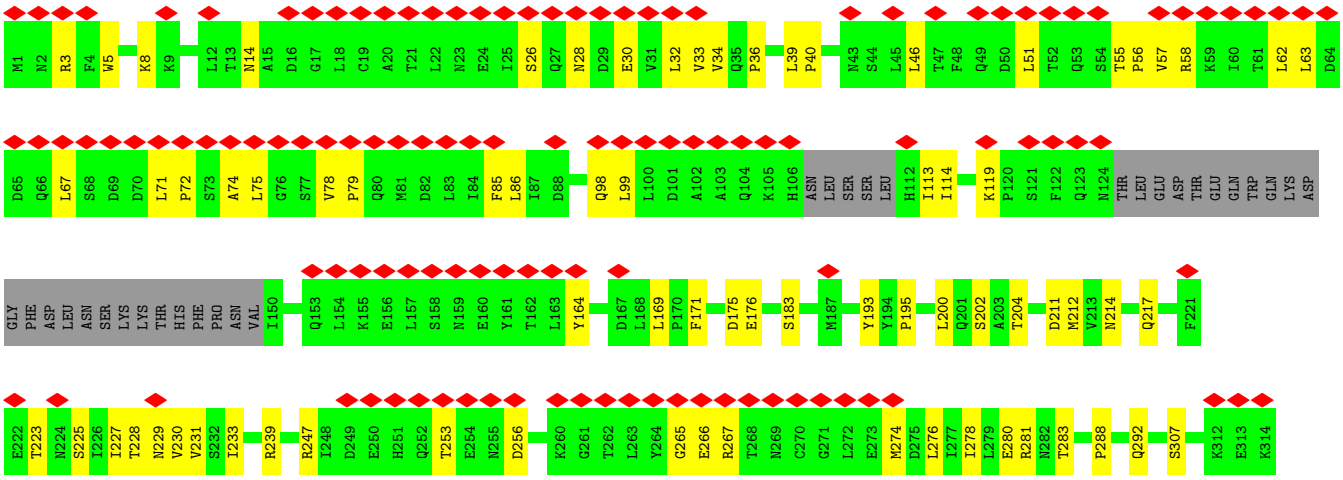
- Molecule 3: Vacuolar membrane protein PEP3

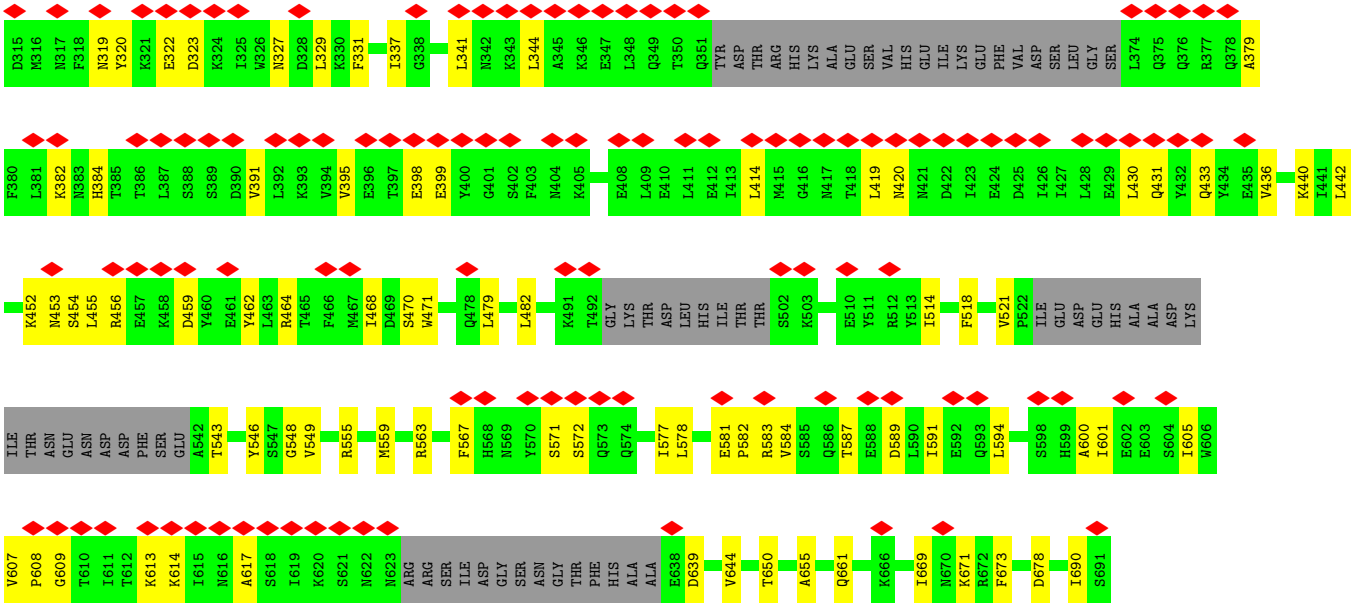
Chain C:



- Molecule 4: Vacuolar protein sorting-associated protein 33

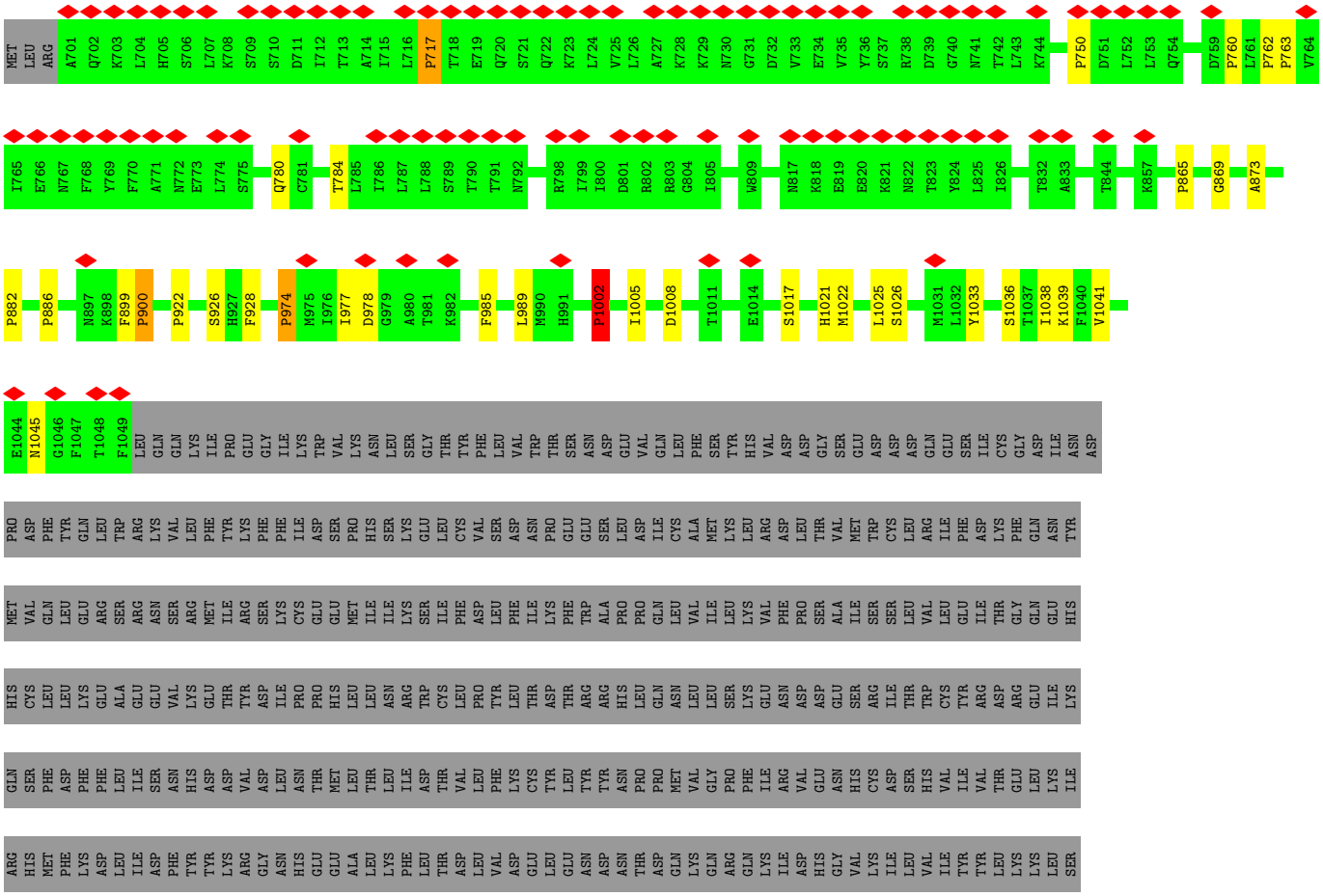
Chain D:





- Molecule 5: Vacuolar morphogenesis protein 6

Chain E:



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

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

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

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

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

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

- Molecule 6: Vacuolar protein sorting-associated protein 41

Chain F: 8% 89%

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

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

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

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

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

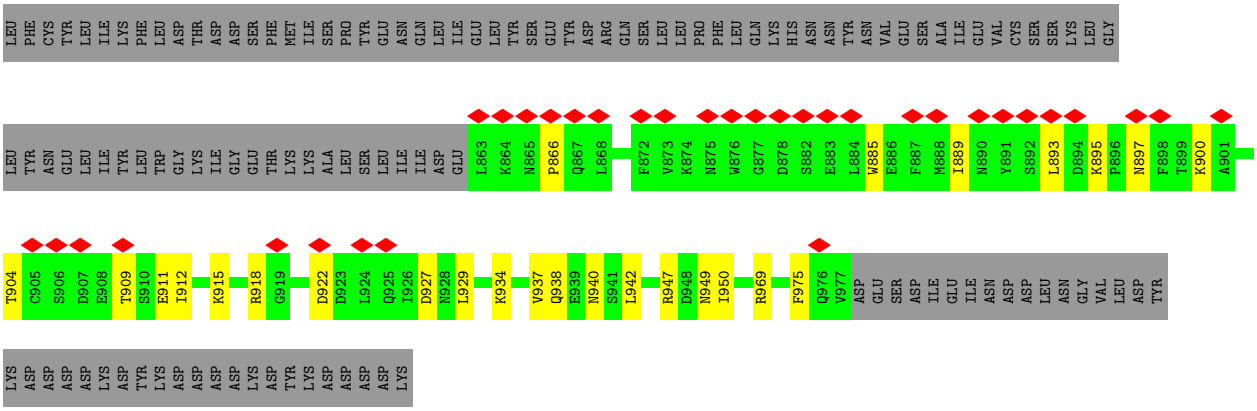
ASP LYS THR THR PRO GLU TYR TYR LEU ILE SER SER ASN ASP ALA ILE ARG VAL GLN GLU LEU SER LEU LYS ASP HIS PHE ASP TRP PHE MET GLU ARG LYS GLN TYR TYR LYS ALA TRP LYS ILE GLY LYS TYR VAL ILE GLY SER GLU GLU ARG PHE SER ILE GLY LEU LYS PHE LEU

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

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

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

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


LEU PHE CYS TYR LEU ILE LYS PHE LEU ASP THR ASP ASP SER PHE MET ILE SER PRO TYR GLU ASN GLN LEU ILE GLU LEU TYR SER GLU TYR ASP ARG GLN SER LEU LEU PRO PHE LEU GLN LYS HIS ASN ASN TYR ASN VAL GLU SER ALA ILE GLU VAL CYS SER SER LYS LEU GLY
LEU TYR ASN GLU LEU ILE TYR LEU TRP GLY LYS ILE GLY GLU THR LYS LYS ALA LEU SER LEU ILE ILE ASP GLU L863 K864 N865 P866 Q867 L868 F872 V873 K874 N875 W876 G877 D878 S882 E883 L884 W885 E886 F887 M888 I889 N890 Y891 S892 L893 D894 K895 P896 N897 F898 T899 K900 A901
T904 C905 S906 D907 E908 T909 S910 E911 I912 K915 R918 G919 D922 D923 L924 Q925 I926 D927 N928 L929 K934 V937 Q938 E939 N940 S941 L942 R947 D948 N949 I950 R969 F975 Q976 V977 ASP GLU SER ASP ILE GLU ILE ASN ASP ASP LEU ASN GLY VAL LEU ASP TYR
LYS ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP LYS ASP TYR LYS ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	244661	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.893	Depositor
Minimum map value	-0.818	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	620.92804, 620.92804, 620.92804	wwPDB
Map dimensions	672, 672, 672	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9240001, 0.9240001, 0.9240001	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	A	0.26	0/7025	0.50	9/9555 (0.1%)
2	B	0.28	0/6101	0.49	1/8240 (0.0%)
3	C	0.26	0/5601	0.49	9/7644 (0.1%)
4	D	0.26	0/4827	0.47	2/6533 (0.0%)
5	E	0.44	0/1702	0.65	12/2373 (0.5%)
6	F	0.28	0/875	0.52	1/1180 (0.1%)
All	All	0.28	0/26131	0.50	34/35525 (0.1%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1002	PRO	N-CA-CB	6.80	111.46	103.30
3	C	134	PRO	N-CA-CB	6.75	111.40	103.30
3	C	216	PRO	N-CA-CB	6.63	111.26	103.30
3	C	195	PRO	N-CA-CB	6.58	111.20	103.30
5	E	900	PRO	N-CA-CB	6.50	111.10	103.30
1	A	938	PRO	N-CA-CB	6.35	110.92	103.30
3	C	130	PRO	N-CA-CB	6.31	110.88	103.30
5	E	974	PRO	N-CA-CB	6.31	110.88	103.30
1	A	781	PRO	N-CA-CB	6.25	110.80	103.30
1	A	854	PRO	N-CA-CB	6.06	110.57	103.30
1	A	922	PRO	N-CA-CB	6.05	110.56	103.30
3	C	271	PRO	N-CA-CB	5.94	110.43	103.30
6	F	866	PRO	N-CA-CB	5.84	110.31	103.30
3	C	449	PRO	N-CA-CB	5.78	110.24	103.30
4	D	72	PRO	N-CA-CB	5.74	110.18	103.30
5	E	717	PRO	N-CA-CB	5.74	110.18	103.30
3	C	417	PRO	N-CA-CB	5.73	110.17	103.30
1	A	846	PRO	N-CA-CB	5.72	110.17	103.30
3	C	328	PRO	N-CA-CB	5.72	110.17	103.30
5	E	760	PRO	N-CA-CB	5.72	110.16	103.30
5	E	886	PRO	N-CA-CB	5.71	110.16	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	922	PRO	N-CA-CB	5.71	110.15	103.30
5	E	865	PRO	N-CA-CB	5.70	110.14	103.30
5	E	763	PRO	N-CA-CB	5.69	110.13	103.30
5	E	882	PRO	N-CA-CB	5.67	110.11	103.30
4	D	79	PRO	N-CA-CB	5.67	110.10	103.30
5	E	762	PRO	N-CA-CB	5.66	110.09	103.30
5	E	750	PRO	N-CA-CB	5.65	110.08	103.30
3	C	58	PRO	N-CA-CB	5.64	110.07	103.30
1	A	798	PRO	N-CA-CB	5.64	110.07	103.30
1	A	813	PRO	N-CA-CB	5.64	110.07	103.30
1	A	977	PRO	N-CA-CB	5.64	110.07	103.30
2	B	27	PRO	N-CA-CB	5.57	109.98	103.30
1	A	918	PRO	N-CA-CB	5.50	109.90	103.30

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	6914	0	6244	166	0
2	B	5981	0	6031	148	0
3	C	5549	0	4384	129	0
4	D	4749	0	4710	96	0
5	E	1704	0	731	20	0
6	F	866	0	830	23	0
All	All	25763	0	22930	546	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 11.

All (546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:HH22	1:A:490:ASP:HA	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:HB2	2:B:157:HIS:CE1	2.19	0.78
3:C:834:GLN:HA	3:C:838:PHE:HZ	1.48	0.77
2:B:447:LYS:HG2	2:B:486:VAL:HG21	1.67	0.76
1:A:750:SER:HB2	3:C:627:ILE:HD13	1.65	0.76
3:C:591:TRP:NE1	3:C:605:PRO:O	2.19	0.76
3:C:8:TYR:HA	3:C:331:VAL:HA	1.69	0.75
2:B:37:LEU:HG	2:B:42:ILE:HG12	1.67	0.75
5:E:1022:MET:HA	5:E:1025:LEU:CB	2.18	0.73
1:A:505:PHE:HB2	1:A:507:LEU:HD22	1.70	0.72
3:C:613:LEU:HD12	3:C:628:VAL:HG23	1.71	0.72
2:B:191:SER:HB3	2:B:209:LYS:HZ3	1.55	0.72
3:C:502:MET:O	3:C:505:GLN:NE2	2.22	0.72
1:A:734:LEU:HA	1:A:738:ALA:HB3	1.72	0.71
1:A:269:VAL:O	1:A:333:ASN:ND2	2.23	0.71
4:D:228:THR:HG22	4:D:229:ASN:H	1.56	0.71
4:D:212:MET:HE1	4:D:678:ASP:HB3	1.72	0.70
1:A:732:ASN:ND2	1:A:774:ALA:O	2.21	0.70
2:B:116:TRP:O	2:B:155:LYS:NZ	2.25	0.70
4:D:399:GLU:HG2	4:D:436:VAL:HA	1.74	0.70
1:A:154:LEU:HB3	1:A:170:ILE:HD12	1.75	0.69
1:A:55:LYS:HE2	1:A:67:GLU:HG3	1.74	0.69
2:B:272:LEU:HD23	2:B:279:LEU:HD21	1.74	0.69
2:B:88:LYS:O	2:B:114:THR:OG1	2.11	0.69
6:F:895:LYS:HZ3	6:F:897:ASN:HB2	1.59	0.68
2:B:190:SER:HB2	2:B:192:TRP:CD1	2.29	0.67
2:B:703:LEU:HA	2:B:706:PHE:HB3	1.76	0.67
3:C:612:TYR:HD2	3:C:613:LEU:HD22	1.58	0.67
3:C:486:LEU:O	3:C:490:LEU:N	2.27	0.67
1:A:7:ARG:HB2	1:A:310:ILE:HD11	1.76	0.67
3:C:505:GLN:O	3:C:507:ARG:NH1	2.27	0.67
3:C:521:MET:HG2	3:C:522:LYS:HG3	1.77	0.66
3:C:880:LEU:O	3:C:884:GLU:N	2.26	0.66
2:B:364:TYR:O	6:F:969:ARG:NH1	2.27	0.66
2:B:204:CYS:HB2	2:B:237:TRP:HZ3	1.58	0.66
4:D:320:TYR:O	4:D:327:ASN:ND2	2.26	0.66
1:A:539:ASP:OD1	1:A:543:ASN:ND2	2.24	0.66
1:A:940:VAL:HA	5:E:978:ASP:HA	1.77	0.66
2:B:249:ASP:HA	2:B:269:VAL:HG23	1.78	0.66
1:A:427:VAL:HG11	6:F:909:THR:HG22	1.78	0.66
3:C:243:ALA:O	5:E:1041:VAL:HA	1.94	0.66
3:C:845:HIS:ND1	3:C:891:CYS:SG	2.69	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ILE:O	2:B:167:LEU:HG	1.96	0.66
4:D:414:LEU:HD13	4:D:549:VAL:HG21	1.78	0.66
2:B:190:SER:HB2	2:B:192:TRP:HD1	1.62	0.65
2:B:149:LYS:O	2:B:150:TYR:CD1	2.49	0.64
4:D:578:LEU:HB3	4:D:669:ILE:HD11	1.79	0.64
1:A:703:ASP:OD2	3:C:668:ARG:NH1	2.31	0.64
1:A:667:VAL:HG12	1:A:668:THR:HG23	1.80	0.63
1:A:424:VAL:HG11	3:C:796:ILE:HG21	1.79	0.63
4:D:431:GLN:OE1	4:D:471:TRP:NE1	2.30	0.63
1:A:706:LEU:HD11	1:A:759:ASP:HB2	1.81	0.63
2:B:122:ILE:HD12	2:B:122:ILE:H	1.64	0.63
2:B:38:SER:HB2	2:B:77:PHE:HB2	1.81	0.63
4:D:14:ASN:HD21	4:D:169:LEU:H	1.46	0.63
2:B:612:ASP:OD2	2:B:616:GLN:NE2	2.31	0.63
2:B:328:GLU:HG2	3:C:802:LEU:HD22	1.80	0.63
3:C:837:LYS:HB2	3:C:849:TRP:HB2	1.80	0.63
3:C:323:ILE:HA	3:C:332:TRP:HA	1.81	0.62
2:B:410:LYS:HG2	2:B:437:LEU:HD11	1.81	0.62
3:C:277:GLY:HA2	3:C:293:SER:HA	1.81	0.62
1:A:181:ALA:HB3	1:A:194:ALA:HB3	1.80	0.62
2:B:149:LYS:O	2:B:150:TYR:CG	2.52	0.62
1:A:118:SER:HB2	1:A:159:ILE:HB	1.82	0.62
3:C:793:SER:HB3	6:F:947:ARG:HH22	1.63	0.62
4:D:51:LEU:O	4:D:55:THR:OG1	2.18	0.61
2:B:11:LEU:HD13	2:B:255:GLY:HA3	1.83	0.61
2:B:131:ILE:HB	2:B:143:TYR:HB3	1.81	0.61
1:A:424:VAL:O	6:F:947:ARG:NH2	2.28	0.61
3:C:533:ASN:ND2	3:C:536:GLU:OE1	2.34	0.61
2:B:69:HIS:O	2:B:70:GLU:HG2	2.01	0.61
4:D:46:LEU:HD13	4:D:51:LEU:HB2	1.82	0.61
3:C:697:LEU:HD11	3:C:728:ILE:HA	1.82	0.61
2:B:670:LYS:O	2:B:674:GLU:N	2.29	0.60
4:D:214:ASN:OD1	4:D:247:ARG:NH1	2.34	0.60
2:B:35:CYS:HB3	2:B:44:VAL:HG22	1.82	0.60
1:A:322:ILE:HG13	1:A:340:SER:HB3	1.83	0.60
1:A:217:ASN:ND2	1:A:245:GLU:OE1	2.34	0.60
1:A:303:ILE:HB	1:A:312:SER:HB2	1.82	0.60
2:B:204:CYS:SG	2:B:205:LEU:N	2.74	0.60
3:C:578:ASN:HD21	3:C:625:ASN:H	1.49	0.60
4:D:581:GLU:OE1	4:D:583:ARG:NH2	2.33	0.60
1:A:239:CYS:O	1:A:263:ARG:NH1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ASP:OD1	2:B:170:VAL:N	2.34	0.59
3:C:634:TYR:HD1	3:C:669:LEU:HD11	1.67	0.59
3:C:777:GLU:OE2	3:C:777:GLU:N	2.28	0.59
4:D:229:ASN:HB3	4:D:605:ILE:HG13	1.82	0.59
1:A:244:ILE:HD11	1:A:260:LEU:HD11	1.84	0.59
3:C:658:GLU:O	3:C:660:LYS:NZ	2.29	0.59
6:F:895:LYS:NZ	6:F:897:ASN:HB2	2.18	0.59
4:D:74:ALA:O	4:D:78:VAL:N	2.35	0.59
3:C:690:GLU:OE2	3:C:727:LYS:NZ	2.35	0.59
3:C:834:GLN:HA	3:C:838:PHE:CZ	2.36	0.59
1:A:703:ASP:HB3	1:A:755:ILE:HD13	1.84	0.58
2:B:283:THR:OG1	2:B:286:LYS:O	2.19	0.58
2:B:611:LYS:O	2:B:611:LYS:NZ	2.34	0.58
2:B:468:ARG:HH21	3:C:916:TRP:HE1	1.51	0.58
4:D:26:SER:OG	4:D:28:ASN:OD1	2.21	0.58
1:A:583:ASN:ND2	1:A:672:GLU:O	2.33	0.58
3:C:485:PHE:O	3:C:489:HIS:N	2.33	0.58
1:A:110:PRO:HA	1:A:115:LEU:HD13	1.86	0.58
3:C:703:ASP:OD1	3:C:704:ASP:N	2.36	0.58
3:C:538:LEU:HB3	3:C:568:THR:HG21	1.85	0.58
3:C:578:ASN:OD1	3:C:625:ASN:ND2	2.36	0.58
3:C:652:LYS:NZ	3:C:656:SER:OG	2.36	0.58
3:C:838:PHE:HB2	6:F:975:PHE:HB2	1.86	0.58
1:A:171:TYR:CE2	1:A:173:ASP:HB3	2.38	0.58
3:C:686:LEU:HB3	3:C:688:LEU:HD23	1.84	0.58
3:C:843:CYS:SG	3:C:845:HIS:ND1	2.65	0.58
4:D:521:VAL:HG22	4:D:549:VAL:HG22	1.85	0.58
1:A:527:ALA:O	1:A:531:SER:OG	2.15	0.57
2:B:636:LEU:HD21	2:B:656:LEU:HD12	1.86	0.57
2:B:497:ARG:HG3	2:B:498:ASN:N	2.19	0.57
4:D:609:GLY:O	4:D:613:LYS:N	2.33	0.57
1:A:471:ASP:OD1	1:A:525:ARG:NH1	2.37	0.57
4:D:227:ILE:HA	4:D:274:MET:HB3	1.86	0.57
1:A:967:LEU:H	5:E:977:ILE:HA	1.68	0.57
5:E:1022:MET:O	5:E:1026:SER:N	2.38	0.57
2:B:349:GLU:O	2:B:355:GLN:NE2	2.33	0.57
2:B:703:LEU:O	2:B:707:ALA:N	2.36	0.57
1:A:7:ARG:HH11	1:A:364:LEU:HD21	1.70	0.57
1:A:265:ARG:HD3	1:A:321:ILE:HD13	1.87	0.57
3:C:413:LEU:O	3:C:417:PRO:N	2.37	0.57
3:C:581:ILE:HD13	3:C:627:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:THR:OG1	2:B:285:GLU:OE1	2.22	0.57
1:A:515:LYS:HG3	1:A:544:LEU:HD11	1.87	0.57
2:B:37:LEU:O	2:B:273:ARG:NH2	2.38	0.57
2:B:660:LEU:HD22	2:B:689:LEU:HD23	1.87	0.57
3:C:718:TYR:HA	3:C:721:ARG:HG2	1.86	0.56
4:D:71:LEU:O	4:D:75:LEU:N	2.38	0.56
2:B:497:ARG:O	2:B:500:ALA:N	2.39	0.56
2:B:53:TYR:HE1	2:B:59:LEU:HD13	1.70	0.56
1:A:194:ALA:HB1	1:A:222:LEU:HD13	1.87	0.56
1:A:262:LEU:HD23	1:A:279:GLU:HB3	1.87	0.56
4:D:67:LEU:O	4:D:98:GLN:NE2	2.39	0.56
4:D:543:THR:HB	4:D:548:GLY:HA2	1.88	0.56
4:D:281:ARG:HD2	4:D:288:PRO:HG2	1.87	0.55
2:B:617:VAL:HG23	2:B:618:GLN:H	1.71	0.55
4:D:14:ASN:HD22	4:D:171:PHE:HD2	1.54	0.55
2:B:643:LEU:HD21	2:B:663:LEU:HD11	1.89	0.55
3:C:513:ILE:O	3:C:516:SER:OG	2.20	0.55
3:C:712:GLU:HA	3:C:715:ILE:HB	1.87	0.55
4:D:8:LYS:NZ	4:D:176:GLU:OE2	2.40	0.55
1:A:56:VAL:HG13	1:A:65:ILE:HB	1.89	0.55
2:B:8:TRP:HE3	2:B:15:PHE:HD2	1.54	0.55
4:D:464:ARG:O	4:D:468:ILE:HG12	2.06	0.55
1:A:88:LEU:N	1:A:104:TYR:O	2.40	0.55
1:A:479:ARG:NH1	1:A:491:ASP:O	2.40	0.55
1:A:519:PHE:O	1:A:523:SER:OG	2.25	0.55
2:B:174:TYR:HE1	2:B:185:LYS:HD3	1.72	0.55
4:D:14:ASN:ND2	4:D:169:LEU:O	2.40	0.55
1:A:479:ARG:NH2	1:A:490:ASP:HA	2.17	0.54
6:F:911:GLU:O	6:F:915:LYS:NZ	2.40	0.54
2:B:79:LYS:O	2:B:415:ARG:NH2	2.40	0.54
1:A:695:GLN:NE2	1:A:749:ASN:OD1	2.37	0.54
1:A:871:GLY:N	5:E:926:SER:O	2.40	0.54
1:A:38:THR:OG1	1:A:80:LEU:O	2.25	0.54
3:C:856:ILE:HG21	3:C:868:THR:HG21	1.89	0.54
4:D:3:ARG:HH11	4:D:267:ARG:HH12	1.54	0.54
4:D:571:SER:OG	4:D:572:SER:N	2.37	0.54
1:A:479:ARG:NH2	1:A:491:ASP:H	2.06	0.54
2:B:700:PHE:CE2	2:B:703:LEU:HB2	2.42	0.54
1:A:759:ASP:O	1:A:762:SER:OG	2.22	0.54
2:B:192:TRP:CD1	2:B:205:LEU:HD13	2.43	0.54
3:C:825:SER:H	3:C:833:LEU:HD22	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:SER:O	1:A:1013:SER:N	2.29	0.54
6:F:934:LYS:O	6:F:937:VAL:HG12	2.06	0.54
2:B:483:VAL:HG12	2:B:499:LEU:HD13	1.90	0.54
4:D:119:LYS:HD3	4:D:169:LEU:HD11	1.90	0.54
3:C:498:VAL:O	3:C:502:MET:N	2.37	0.54
3:C:710:ASN:HA	3:C:721:ARG:HH22	1.72	0.54
4:D:419:LEU:HD23	4:D:420:ASN:N	2.23	0.54
2:B:721:THR:HG21	4:D:433:GLN:HE21	1.73	0.53
3:C:736:MET:HB3	3:C:739:ILE:HD13	1.90	0.53
2:B:94:VAL:HG22	2:B:102:ILE:HG22	1.90	0.53
2:B:247:PHE:O	2:B:250:GLU:HB3	2.09	0.53
6:F:922:ASP:OD1	6:F:922:ASP:N	2.41	0.53
1:A:482:ILE:HG22	1:A:484:ASN:H	1.72	0.53
3:C:858:ASN:O	3:C:901:LYS:NZ	2.30	0.53
1:A:9:PHE:HE1	1:A:362:LYS:HG2	1.72	0.53
2:B:244:ALA:HB2	2:B:253:LEU:HD23	1.89	0.53
2:B:501:LEU:HA	2:B:509:ARG:HD2	1.90	0.53
2:B:700:PHE:HE2	2:B:703:LEU:HB2	1.73	0.53
2:B:351:GLU:HG2	2:B:353:LYS:H	1.73	0.53
1:A:98:PRO:HG3	1:A:128:THR:HA	1.90	0.53
1:A:705:TYR:O	1:A:709:ALA:N	2.38	0.53
2:B:413:ILE:HD12	2:B:425:CYS:HB3	1.90	0.53
1:A:311:ILE:HG21	1:A:314:ASN:HD21	1.74	0.53
2:B:98:SER:HB3	2:B:99:PRO:HD3	1.90	0.53
2:B:690:LYS:HD3	2:B:706:PHE:CZ	2.44	0.52
4:D:559:MET:O	4:D:563:ARG:NH1	2.42	0.52
4:D:39:LEU:HD22	4:D:62:LEU:HD11	1.91	0.52
1:A:75:PHE:HE2	1:A:92:ALA:HB1	1.75	0.52
2:B:75:PHE:HB3	2:B:85:LEU:HD23	1.91	0.52
3:C:512:LEU:HA	3:C:515:ALA:HB3	1.92	0.52
3:C:658:GLU:H	3:C:660:LYS:HZ1	1.56	0.52
4:D:518:PHE:HB3	4:D:555:ARG:HG3	1.92	0.52
1:A:688:GLU:CD	1:A:689:GLY:H	2.14	0.52
2:B:146:LYS:HG2	2:B:149:LYS:HG2	1.91	0.52
1:A:93:GLU:OE2	1:A:93:GLU:N	2.43	0.52
4:D:175:ASP:OD1	4:D:176:GLU:N	2.42	0.52
1:A:28:LEU:HD22	1:A:57:VAL:HG11	1.92	0.52
1:A:238:CYS:HB3	1:A:245:GLU:HB2	1.92	0.52
1:A:269:VAL:HG22	1:A:335:THR:HG21	1.92	0.52
1:A:583:ASN:HD22	1:A:672:GLU:HB3	1.74	0.52
2:B:17:ARG:HD2	2:B:293:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:331:PHE:CD1	4:D:655:ALA:HB2	2.45	0.51
1:A:185:ASN:ND2	1:A:189:THR:OG1	2.41	0.51
2:B:205:LEU:HD12	2:B:216:PHE:HE2	1.75	0.51
3:C:558:LEU:HD12	3:C:562:PRO:HA	1.92	0.51
4:D:614:LYS:HA	4:D:617:ALA:HB3	1.93	0.51
1:A:43:GLN:HB3	1:A:58:LYS:HE2	1.91	0.51
3:C:621:PRO:O	3:C:622:LYS:HG2	2.11	0.51
3:C:785:HIS:NE2	6:F:940:ASN:O	2.37	0.51
1:A:94:SER:OG	1:A:96:GLY:O	2.29	0.51
2:B:158:TRP:HB2	2:B:167:LEU:HD23	1.91	0.51
2:B:192:TRP:CG	2:B:205:LEU:HD13	2.46	0.51
3:C:39:HIS:HA	3:C:51:LEU:HA	1.93	0.51
3:C:729:ALA:HB2	3:C:748:ILE:HD11	1.93	0.51
3:C:274:GLN:N	3:C:277:GLY:O	2.44	0.51
3:C:845:HIS:HE1	3:C:894:CYS:SG	2.34	0.51
1:A:53:ILE:HG13	1:A:69:GLN:HA	1.93	0.51
3:C:779:ILE:HD13	6:F:918:ARG:HH21	1.76	0.51
3:C:909:ASP:OD2	3:C:911:THR:OG1	2.28	0.51
4:D:56:PRO:HA	4:D:58:ARG:HH21	1.75	0.51
4:D:329:LEU:HB3	4:D:337:ILE:HD12	1.93	0.51
4:D:639:ASP:HB2	4:D:671:LYS:HD3	1.93	0.51
1:A:403:THR:O	1:A:407:ILE:HG12	2.11	0.51
3:C:836:LYS:HG3	3:C:837:LYS:H	1.76	0.51
1:A:277:VAL:HG23	1:A:301:ILE:HG13	1.93	0.50
1:A:996:VAL:O	1:A:1000:ASN:N	2.42	0.50
2:B:694:LEU:HB3	2:B:700:PHE:CD1	2.46	0.50
3:C:847:PHE:HZ	3:C:893:LEU:HG	1.76	0.50
2:B:567:TYR:HB2	4:D:200:LEU:HD22	1.93	0.50
1:A:28:LEU:HD21	1:A:64:VAL:HG22	1.94	0.50
2:B:324:PRO:HG2	2:B:325:LYS:HE2	1.92	0.50
2:B:72:ILE:HD13	2:B:87:THR:HG22	1.93	0.50
2:B:130:ASP:OD1	2:B:131:ILE:N	2.45	0.50
2:B:214:GLN:HG2	2:B:216:PHE:CE1	2.47	0.50
2:B:296:GLN:HG2	2:B:344:ALA:HB3	1.93	0.50
4:D:567:PHE:HA	4:D:571:SER:HB2	1.94	0.50
2:B:54:ASN:HD21	2:B:58:GLN:HB2	1.76	0.50
2:B:196:THR:HG21	2:B:235:ILE:O	2.11	0.50
1:A:918:PRO:O	5:E:1002:PRO:N	2.45	0.50
2:B:506:GLU:OE1	2:B:509:ARG:NH2	2.44	0.50
1:A:478:ASP:HB3	1:A:481:GLY:H	1.77	0.50
3:C:536:GLU:HA	3:C:539:LYS:HG3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:581:ILE:HA	3:C:584:ILE:HG22	1.93	0.50
4:D:591:ILE:HG21	4:D:600:ALA:HB3	1.93	0.50
1:A:518:ASP:OD1	1:A:518:ASP:N	2.45	0.49
3:C:644:MET:O	3:C:648:ASN:N	2.45	0.49
1:A:441:TRP:O	1:A:445:LYS:HG2	2.12	0.49
6:F:900:LYS:HZ3	6:F:927:ASP:H	1.60	0.49
1:A:201:LEU:HD22	1:A:214:LEU:HD12	1.94	0.49
2:B:37:LEU:HD21	2:B:282:ILE:HD11	1.93	0.49
3:C:498:VAL:O	3:C:502:MET:HG2	2.11	0.49
2:B:91:ILE:HG23	2:B:105:VAL:HB	1.94	0.49
2:B:594:LEU:HD12	2:B:603:LEU:HD11	1.92	0.49
1:A:660:SER:HA	1:A:663:PHE:CD2	2.48	0.49
5:E:1033:TYR:HA	5:E:1036:SER:CB	2.43	0.49
1:A:177:GLU:OE2	1:A:197:SER:OG	2.25	0.49
1:A:479:ARG:HB2	1:A:480:LYS:HZ2	1.78	0.49
2:B:124:LEU:HD23	2:B:125:LEU:O	2.12	0.49
4:D:85:PHE:HB2	4:D:113:ILE:HG22	1.93	0.49
4:D:223:THR:HG1	4:D:225:SER:HG	1.60	0.49
4:D:482:LEU:HD23	4:D:690:ILE:HD13	1.95	0.49
1:A:11:LEU:HD13	1:A:312:SER:HA	1.94	0.49
1:A:158:ASP:OD1	1:A:160:SER:OG	2.27	0.49
2:B:165:ILE:HB	2:B:176:VAL:HB	1.93	0.49
2:B:366:LYS:HZ1	3:C:843:CYS:HB2	1.77	0.49
1:A:186:ASN:ND2	1:A:231:PRO:O	2.40	0.48
3:C:434:MET:O	3:C:438:ASN:N	2.39	0.48
6:F:947:ARG:HA	6:F:950:ILE:HD12	1.94	0.48
1:A:63:GLN:NE2	1:A:65:ILE:HD13	2.28	0.48
1:A:403:THR:HG21	1:A:435:ASN:HB3	1.95	0.48
1:A:685:GLN:HG2	1:A:694:ARG:HH11	1.79	0.48
1:A:703:ASP:N	1:A:703:ASP:OD1	2.45	0.48
3:C:653:PHE:O	3:C:657:ASN:N	2.42	0.48
3:C:507:ARG:O	3:C:511:LEU:HG	2.13	0.48
3:C:557:LEU:O	3:C:561:SER:OG	2.22	0.48
4:D:546:TYR:HH	4:D:650:THR:HG1	1.59	0.48
1:A:209:ARG:HB3	1:A:211:ARG:HG2	1.94	0.48
2:B:153:LEU:HD21	2:B:170:VAL:HG22	1.95	0.48
3:C:654:MET:HG3	3:C:661:TYR:CZ	2.49	0.48
2:B:172:HIS:ND1	2:B:188:THR:O	2.33	0.48
2:B:534:LEU:O	2:B:537:SER:OG	2.25	0.48
3:C:614:LYS:HD2	3:C:653:PHE:HZ	1.79	0.48
1:A:1005:PHE:O	3:C:500:GLN:NE2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLY:HA3	2:B:289:PHE:CE1	2.49	0.48
1:A:199:ILE:HD11	1:A:236:PHE:CE2	2.49	0.48
2:B:78:ASP:OD1	2:B:78:ASP:N	2.44	0.47
4:D:34:VAL:HG22	4:D:86:LEU:HD23	1.95	0.47
1:A:200:LEU:HD22	1:A:213:SER:HB3	1.95	0.47
2:B:519:ASP:OD1	2:B:519:ASP:N	2.46	0.47
2:B:642:SER:O	2:B:645:LYS:HG2	2.14	0.47
2:B:436:PHE:HA	2:B:477:THR:HG21	1.96	0.47
1:A:39:ILE:HD12	1:A:336:TYR:HE2	1.79	0.47
1:A:321:ILE:HD11	1:A:324:ILE:HG13	1.95	0.47
1:A:383:GLN:HB2	1:A:412:VAL:HG21	1.94	0.47
1:A:337:LEU:O	1:A:344:MET:HG3	2.15	0.47
1:A:754:LEU:HD21	3:C:634:TYR:CD1	2.50	0.47
1:A:159:ILE:HG13	1:A:159:ILE:O	2.14	0.47
1:A:143:ILE:HB	1:A:155:ILE:HG13	1.97	0.47
1:A:300:ARG:HG2	1:A:316:VAL:HG22	1.95	0.47
2:B:703:LEU:HD22	2:B:735:TYR:CE1	2.50	0.47
3:C:769:THR:HA	6:F:929:LEU:HD12	1.95	0.47
4:D:280:GLU:HG3	4:D:283:THR:HG23	1.96	0.47
6:F:885:TRP:HZ3	6:F:912:ILE:HD13	1.79	0.47
2:B:158:TRP:HB2	2:B:167:LEU:CD2	2.45	0.47
4:D:14:ASN:ND2	4:D:169:LEU:H	2.12	0.47
4:D:63:LEU:HD11	4:D:99:LEU:HD12	1.97	0.47
3:C:470:ASN:O	3:C:474:ASN:N	2.40	0.47
3:C:474:ASN:O	3:C:478:LYS:N	2.34	0.47
1:A:41:ASP:OD1	1:A:44:THR:HG22	2.14	0.46
1:A:193:ALA:HB3	1:A:202:PHE:HE2	1.80	0.46
2:B:720:TYR:O	2:B:724:LYS:N	2.33	0.46
3:C:243:ALA:HB3	5:E:1045:ASN:N	2.30	0.46
4:D:253:THR:H	4:D:256:ASP:HB2	1.81	0.46
1:A:479:ARG:HD3	1:A:479:ARG:N	2.30	0.46
3:C:35:LEU:HA	3:C:63:VAL:H	1.80	0.46
4:D:452:LYS:HE3	4:D:456:ARG:HH12	1.80	0.46
1:A:657:PRO:O	1:A:658:LYS:HG3	2.16	0.46
3:C:642:ASN:HB3	3:C:675:LYS:HE3	1.98	0.46
4:D:3:ARG:NH1	4:D:267:ARG:HH12	2.14	0.46
4:D:233:ILE:HG12	4:D:601:ILE:HG12	1.97	0.46
4:D:379:ALA:HA	4:D:382:LYS:HE3	1.96	0.46
3:C:729:ALA:O	3:C:733:LEU:N	2.49	0.46
1:A:247:PHE:HE1	1:A:253:LYS:HE3	1.80	0.46
1:A:575:LEU:HD13	1:A:669:LYS:HG2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLU:O	2:B:16:TYR:N	2.42	0.46
2:B:367:ALA:HB3	6:F:969:ARG:HD2	1.98	0.46
3:C:720:LEU:O	3:C:723:ARG:HG2	2.16	0.46
3:C:857:LEU:HA	3:C:865:ARG:HG3	1.98	0.46
2:B:24:LEU:HG	2:B:287:ILE:HD11	1.96	0.46
2:B:54:ASN:ND2	2:B:58:GLN:HB2	2.31	0.46
1:A:9:PHE:HB2	1:A:11:LEU:HD12	1.98	0.46
1:A:183:PHE:HB3	1:A:229:PHE:HB2	1.98	0.46
1:A:479:ARG:HB2	1:A:480:LYS:NZ	2.30	0.46
1:A:110:PRO:HB3	1:A:115:LEU:HD22	1.97	0.45
1:A:562:GLU:OE1	1:A:562:GLU:N	2.41	0.45
2:B:577:TYR:CD2	2:B:589:LEU:HD11	2.50	0.45
4:D:323:ASP:OD2	4:D:384:HIS:NE2	2.49	0.45
3:C:740:ASP:OD1	3:C:740:ASP:N	2.49	0.45
4:D:30:GLU:HB2	4:D:57:VAL:HG12	1.98	0.45
1:A:1014:ARG:O	1:A:1018:LYS:N	2.45	0.45
3:C:753:ASN:O	3:C:754:GLU:HG3	2.16	0.45
4:D:661:GLN:HB2	4:D:673:PHE:HD2	1.81	0.45
1:A:122:LEU:HD23	1:A:122:LEU:O	2.16	0.45
2:B:210:ASP:O	2:B:212:LYS:HG2	2.16	0.45
2:B:636:LEU:O	2:B:640:GLN:HG3	2.16	0.45
3:C:566:VAL:O	3:C:570:MET:N	2.48	0.45
1:A:456:LEU:HD13	6:F:949:ASN:HB2	1.97	0.45
2:B:7:ASP:OD1	2:B:7:ASP:N	2.47	0.45
1:A:152:ILE:HG13	1:A:179:ILE:HG13	1.99	0.45
1:A:420:SER:OG	3:C:800:LYS:HD2	2.17	0.45
1:A:533:ASP:O	1:A:536:ILE:HG12	2.16	0.45
6:F:938:GLN:O	6:F:942:LEU:N	2.31	0.45
1:A:148:ILE:O	1:A:178:PRO:HB3	2.17	0.45
1:A:470:ILE:O	1:A:474:ILE:HG12	2.16	0.45
2:B:54:ASN:HB3	2:B:60:LEU:HD11	1.99	0.45
4:D:419:LEU:HD23	4:D:420:ASN:H	1.82	0.45
5:E:1022:MET:CA	5:E:1025:LEU:CB	2.93	0.45
1:A:574:LEU:HB3	1:A:582:THR:HG21	1.99	0.45
2:B:208:MET:O	2:B:208:MET:HG2	2.16	0.45
2:B:247:PHE:CE1	2:B:252:LYS:HD3	2.51	0.45
2:B:410:LYS:HB3	2:B:410:LYS:HE2	1.79	0.45
3:C:578:ASN:O	3:C:581:ILE:HG12	2.16	0.45
4:D:183:SER:OG	4:D:211:ASP:OD2	2.28	0.45
1:A:718:ASP:N	1:A:718:ASP:OD1	2.50	0.44
2:B:133:LYS:HD2	2:B:142:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:ILE:HG13	2:B:541:ALA:N	2.33	0.44
3:C:625:ASN:O	3:C:628:VAL:HG12	2.17	0.44
4:D:607:VAL:HA	4:D:608:PRO:HD3	1.70	0.44
3:C:555:LEU:HD13	3:C:583:THR:HG23	1.99	0.44
5:E:869:GLY:O	5:E:873:ALA:N	2.42	0.44
1:A:38:THR:HG21	1:A:82:VAL:H	1.82	0.44
1:A:66:HIS:CE1	1:A:111:ASN:HA	2.52	0.44
1:A:147:PHE:HB2	1:A:151:LYS:HB2	1.99	0.44
1:A:337:LEU:HB2	1:A:345:HIS:HB2	2.00	0.44
1:A:478:ASP:OD1	1:A:479:ARG:N	2.50	0.44
1:A:559:PRO:HG2	1:A:562:GLU:OE1	2.17	0.44
1:A:671:PHE:HE2	1:A:716:ARG:HH12	1.64	0.44
2:B:171:ASP:O	2:B:190:SER:N	2.50	0.44
3:C:671:LEU:HD11	3:C:695:LEU:HD11	1.98	0.44
4:D:577:ILE:HG22	4:D:578:LEU:HG	1.98	0.44
5:E:1005:ILE:N	5:E:1008:ASP:O	2.42	0.44
1:A:621:TYR:HB3	1:A:671:PHE:CE2	2.52	0.44
2:B:536:ILE:HD13	2:B:564:LEU:HG	1.99	0.44
1:A:669:LYS:HG3	1:A:672:GLU:OE1	2.18	0.44
2:B:210:ASP:OD1	2:B:210:ASP:N	2.48	0.44
3:C:634:TYR:CD1	3:C:669:LEU:HD11	2.50	0.44
4:D:341:LEU:HD23	4:D:344:LEU:HD12	1.98	0.44
4:D:398:GLU:OE1	4:D:399:GLU:HG3	2.18	0.44
6:F:900:LYS:O	6:F:904:THR:HG22	2.18	0.44
1:A:16:PRO:HB2	1:A:343:VAL:HG21	2.00	0.44
2:B:191:SER:HB3	2:B:209:LYS:NZ	2.29	0.44
2:B:577:TYR:HD2	2:B:589:LEU:HD11	1.83	0.44
2:B:684:LYS:HE3	2:B:714:ILE:HA	1.98	0.44
4:D:193:TYR:OH	4:D:280:GLU:OE1	2.35	0.44
3:C:35:LEU:HA	3:C:62:ARG:HA	2.00	0.44
3:C:720:LEU:O	3:C:724:LEU:HG	2.18	0.44
1:A:38:THR:HG21	1:A:82:VAL:N	2.32	0.44
3:C:496:GLU:O	3:C:500:GLN:N	2.37	0.44
3:C:863:ASN:OD1	3:C:864:LEU:N	2.50	0.44
1:A:81:LYS:HG2	1:A:136:ILE:HD12	2.00	0.43
1:A:804:PHE:O	1:A:808:TYR:N	2.50	0.43
3:C:614:LYS:CD	3:C:653:PHE:HZ	2.30	0.43
3:C:779:ILE:HD13	6:F:918:ARG:NH2	2.32	0.43
5:E:1017:SER:O	5:E:1021:HIS:N	2.46	0.43
1:A:553:LYS:HZ3	1:A:599:PHE:HA	1.83	0.43
1:A:751:ILE:O	1:A:755:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:TYR:CE1	2:B:185:LYS:HB2	2.53	0.43
3:C:848:HIS:CE1	3:C:851:CYS:HG	2.35	0.43
4:D:430:LEU:O	4:D:436:VAL:HG12	2.17	0.43
5:E:985:PHE:O	5:E:989:LEU:N	2.44	0.43
1:A:495:VAL:HA	1:A:498:PHE:HD2	1.82	0.43
2:B:366:LYS:HG3	2:B:374:PHE:HZ	1.82	0.43
2:B:545:LYS:HG3	2:B:546:LEU:HD22	2.00	0.43
3:C:581:ILE:O	3:C:584:ILE:HG22	2.17	0.43
3:C:857:LEU:O	3:C:865:ARG:NE	2.41	0.43
3:C:209:VAL:N	3:C:216:PRO:O	2.32	0.43
3:C:475:LEU:O	3:C:479:SER:N	2.48	0.43
3:C:566:VAL:O	3:C:570:MET:HG2	2.18	0.43
3:C:652:LYS:HA	3:C:655:LYS:HB2	2.00	0.43
4:D:281:ARG:O	4:D:281:ARG:HD3	2.19	0.43
1:A:502:ASN:OD1	1:A:532:LYS:NZ	2.38	0.43
1:A:559:PRO:O	1:A:563:THR:OG1	2.28	0.43
6:F:889:ILE:O	6:F:893:LEU:HD23	2.18	0.43
1:A:479:ARG:NH2	1:A:489:MET:O	2.52	0.43
1:A:838:VAL:O	1:A:842:LYS:N	2.51	0.43
1:A:358:ILE:HG13	1:A:359:ILE:N	2.34	0.43
2:B:205:LEU:HD12	2:B:216:PHE:CE2	2.54	0.43
2:B:563:PRO:HD2	4:D:202:SER:HB2	2.00	0.43
1:A:434:ARG:HA	1:A:464:LEU:HD11	2.00	0.43
2:B:35:CYS:HA	2:B:43:ALA:O	2.18	0.43
2:B:296:GLN:HB3	2:B:345:ALA:HB2	2.00	0.43
2:B:552:THR:HG23	2:B:579:PHE:CE2	2.54	0.43
3:C:504:LYS:HB3	3:C:507:ARG:HH12	1.84	0.43
4:D:265:GLY:O	4:D:266:GLU:HG2	2.19	0.43
4:D:453:ASN:O	4:D:454:SER:OG	2.30	0.43
3:C:626:PRO:HA	3:C:629:TYR:HD2	1.84	0.43
4:D:591:ILE:HG13	4:D:601:ILE:HD12	2.00	0.43
1:A:120:VAL:HG23	1:A:159:ILE:HD13	2.02	0.42
1:A:129:TYR:CE2	1:A:149:ASN:HB3	2.53	0.42
1:A:373:LYS:HB2	1:A:373:LYS:HE2	1.81	0.42
2:B:352:PRO:HB3	3:C:903:ASP:HB3	2.01	0.42
2:B:366:LYS:NZ	3:C:894:CYS:SG	2.85	0.42
2:B:720:TYR:HE1	2:B:732:ALA:HB1	1.84	0.42
2:B:234:ASP:HB2	2:B:272:LEU:HD13	2.02	0.42
2:B:383:CYS:SG	3:C:899:ILE:HG22	2.59	0.42
3:C:208:LYS:HA	3:C:217:ASP:HA	2.00	0.42
5:E:1022:MET:O	5:E:1025:LEU:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:731:LYS:O	2:B:734:PRO:HD2	2.20	0.42
4:D:40:PRO:HB2	4:D:307:SER:HB2	2.00	0.42
4:D:230:VAL:HG13	4:D:276:LEU:HB3	2.00	0.42
1:A:592:GLY:HA2	1:A:654:TYR:CZ	2.55	0.42
2:B:513:LEU:HB3	2:B:522:ALA:HB2	2.01	0.42
1:A:18:ARG:HB2	1:A:343:VAL:HG12	2.00	0.42
1:A:386:HIS:ND1	1:A:405:GLN:OE1	2.49	0.42
2:B:645:LYS:HG3	2:B:646:ARG:HG3	2.01	0.42
1:A:700:THR:HG22	3:C:668:ARG:HH21	1.85	0.42
2:B:699:LYS:HD2	2:B:728:HIS:NE2	2.35	0.42
4:D:278:ILE:HG12	4:D:644:VAL:HB	2.02	0.42
1:A:870:PHE:N	5:E:928:PHE:O	2.52	0.42
2:B:37:LEU:HD11	2:B:282:ILE:HD11	2.02	0.42
2:B:728:HIS:HD2	2:B:731:LYS:HE2	1.84	0.42
3:C:667:LEU:HD23	3:C:671:LEU:HD23	2.01	0.42
3:C:739:ILE:HD12	3:C:739:ILE:H	1.85	0.42
2:B:316:PHE:CZ	2:B:360:ASN:HB3	2.55	0.42
4:D:239:ARG:HE	4:D:239:ARG:HB3	1.67	0.42
3:C:733:LEU:HD23	3:C:733:LEU:HA	1.91	0.42
3:C:774:LEU:HB2	3:C:777:GLU:OE1	2.20	0.42
2:B:672:VAL:O	2:B:676:VAL:HG23	2.19	0.41
2:B:690:LYS:O	2:B:694:LEU:N	2.41	0.41
3:C:612:TYR:CD2	3:C:613:LEU:HD22	2.47	0.41
5:E:1021:HIS:O	5:E:1025:LEU:N	2.52	0.41
1:A:352:LEU:HD22	1:A:377:LEU:HD21	2.03	0.41
1:A:540:ILE:HA	1:A:544:LEU:HB2	2.01	0.41
3:C:551:TYR:O	3:C:554:SER:OG	2.24	0.41
4:D:584:VAL:O	4:D:587:THR:HG22	2.19	0.41
1:A:336:TYR:O	1:A:337:LEU:HD23	2.20	0.41
1:A:354:ASN:O	1:A:358:ILE:HG23	2.21	0.41
1:A:387:LYS:HB2	1:A:409:CYS:SG	2.60	0.41
1:A:586:LEU:HD13	1:A:666:PHE:HZ	1.85	0.41
3:C:507:ARG:HG3	3:C:510:GLU:OE2	2.20	0.41
3:C:581:ILE:HG13	3:C:582:PRO:HD3	2.03	0.41
1:A:6:TRP:HE1	1:A:309:LYS:HB3	1.84	0.41
2:B:95:LYS:HB3	2:B:101:THR:HG23	2.01	0.41
2:B:123:MET:SD	2:B:124:LEU:N	2.93	0.41
3:C:502:MET:HA	3:C:507:ARG:NH2	2.36	0.41
4:D:319:ASN:HD22	4:D:322:GLU:HG3	1.84	0.41
4:D:391:VAL:O	4:D:395:VAL:HG23	2.20	0.41
4:D:5:TRP:HE1	4:D:223:THR:HG1	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:442:LEU:HD12	4:D:442:LEU:HA	1.89	0.41
5:E:1038:ILE:O	5:E:1039:LYS:C	2.59	0.41
1:A:123:LYS:HA	1:A:123:LYS:HD3	1.82	0.41
1:A:198:ARG:HD3	1:A:218:SER:HB2	2.03	0.41
2:B:253:LEU:HD11	2:B:290:LEU:HD12	2.03	0.41
2:B:369:LEU:HD23	2:B:369:LEU:HA	1.91	0.41
3:C:636:MET:HB3	3:C:646:LEU:HD11	2.03	0.41
4:D:32:LEU:HD12	4:D:32:LEU:HA	1.89	0.41
4:D:440:LYS:H	4:D:440:LYS:HG2	1.75	0.41
1:A:262:LEU:O	1:A:278:THR:HA	2.21	0.41
1:A:520:LYS:HB3	1:A:545:LEU:HD21	2.02	0.41
2:B:279:LEU:O	2:B:279:LEU:HD23	2.20	0.41
2:B:657:ASP:HB2	4:D:470:SER:HA	2.03	0.41
2:B:684:LYS:HE2	2:B:684:LYS:HB3	1.83	0.41
4:D:292:GLN:HG2	4:D:546:TYR:CE1	2.56	0.41
1:A:199:ILE:HG23	1:A:216:LEU:O	2.20	0.41
3:C:515:ALA:O	3:C:519:ASN:N	2.54	0.41
4:D:195:PRO:HB3	4:D:204:THR:HG21	2.03	0.41
1:A:620:PHE:HB3	1:A:626:PHE:HB2	2.03	0.41
1:A:1011:GLU:O	1:A:1015:ASP:N	2.41	0.41
2:B:84:ILE:CG2	2:B:91:ILE:HD11	2.51	0.41
2:B:536:ILE:HD12	2:B:536:ILE:HA	1.93	0.41
2:B:703:LEU:HD11	2:B:719:PHE:HD1	1.86	0.41
3:C:388:HIS:O	3:C:392:ILE:N	2.54	0.41
3:C:813:PHE:O	3:C:816:ILE:HG22	2.21	0.41
3:C:839:ILE:HD11	3:C:849:TRP:HE3	1.86	0.41
4:D:114:ILE:HD13	4:D:164:TYR:HB2	2.03	0.41
1:A:226:CYS:SG	1:A:263:ARG:HD2	2.61	0.41
1:A:656:PRO:HA	1:A:657:PRO:HD3	1.95	0.41
2:B:12:LYS:NZ	2:B:256:PRO:O	2.42	0.41
2:B:677:LYS:HE2	2:B:677:LYS:HB2	1.82	0.41
4:D:36:PRO:HD3	4:D:63:LEU:HB2	2.03	0.41
4:D:589:ASP:OD1	4:D:589:ASP:N	2.54	0.41
1:A:207:ARG:N	1:A:207:ARG:HD2	2.36	0.40
4:D:231:VAL:HG21	4:D:582:PRO:HB2	2.03	0.40
4:D:459:ASP:HA	4:D:462:TYR:HB3	2.02	0.40
4:D:514:ILE:HD11	4:D:594:LEU:HD11	2.03	0.40
3:C:581:ILE:HG13	3:C:582:PRO:CD	2.51	0.40
4:D:33:VAL:HG12	4:D:63:LEU:CD2	2.51	0.40
4:D:217:GLN:OE1	4:D:247:ARG:HB3	2.21	0.40
4:D:455:LEU:HD23	4:D:455:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:1022:MET:C	5:E:1025:LEU:H	2.24	0.40
1:A:75:PHE:CD1	1:A:94:SER:HB3	2.56	0.40
1:A:1013:SER:O	1:A:1017:PHE:N	2.42	0.40
2:B:656:LEU:HA	2:B:659:THR:HG22	2.04	0.40
1:A:458:LEU:O	1:A:462:ILE:HG12	2.20	0.40
2:B:368:SER:OG	6:F:969:ARG:NE	2.54	0.40
2:B:640:GLN:NE2	2:B:654:MET:O	2.53	0.40
5:E:780:GLN:O	5:E:784:THR:N	2.42	0.40
1:A:213:SER:C	1:A:215:VAL:H	2.25	0.40
3:C:107:LEU:O	3:C:115:TYR:N	2.52	0.40
3:C:835:ILE:HG13	3:C:836:LYS:N	2.37	0.40
4:D:479:LEU:HD13	4:D:482:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	940/1029 (91%)	840 (89%)	97 (10%)	3 (0%)	41	76
2	B	729/798 (91%)	646 (89%)	82 (11%)	1 (0%)	51	85
3	C	820/918 (89%)	751 (92%)	61 (7%)	8 (1%)	15	54
4	D	583/691 (84%)	548 (94%)	35 (6%)	0	100	100
5	E	339/1049 (32%)	320 (94%)	14 (4%)	5 (2%)	10	46
6	F	108/1016 (11%)	96 (89%)	12 (11%)	0	100	100
All	All	3519/5501 (64%)	3201 (91%)	301 (9%)	17 (0%)	32	68

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	938	PRO

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Mol	Chain	Res	Type
2	B	27	PRO
3	C	130	PRO
3	C	134	PRO
3	C	195	PRO
3	C	328	PRO
3	C	598	ILE
5	E	717	PRO
5	E	1002	PRO
1	A	781	PRO
5	E	899	PHE
5	E	974	PRO
3	C	216	PRO
1	A	940	VAL
5	E	900	PRO
3	C	157	ILE
3	C	133	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	652/952 (68%)	652 (100%)	0	100	100
2	B	666/730 (91%)	666 (100%)	0	100	100
3	C	396/873 (45%)	396 (100%)	0	100	100
4	D	526/640 (82%)	526 (100%)	0	100	100
6	F	92/938 (10%)	92 (100%)	0	100	100
All	All	2332/4133 (56%)	2332 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	ASN

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Mol	Chain	Res	Type
2	B	494	GLN

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)

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	10
5	E	1
6	F	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	115:TYR	C	121:TRP	N	13.77
1	E	991:HIS	C	998:ASN	N	13.23
1	C	23:GLN	C	27:LEU	N	12.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	140:PHE	C	150:GLU	N	12.97
1	C	11:LEU	C	17:LYS	N	10.46
1	C	294:VAL	C	308:LYS	N	9.65
1	F	878:ASP	C	882:SER	N	9.64
1	C	456:ASN	C	468:LEU	N	9.37
1	C	44:THR	C	49:THR	N	9.20
1	C	172:SER	C	179:ASN	N	8.71
1	C	223:ASP	C	234:HIS	N	8.46
1	C	75:TRP	C	86:TYR	N	6.28
1	A	957:GLU	C	965:ASP	N	6.11

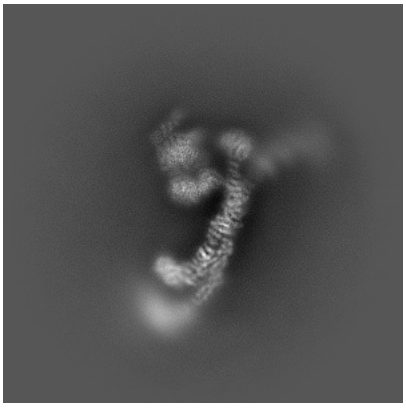
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14964. These allow visual inspection of the internal detail of the map and identification of artifacts.

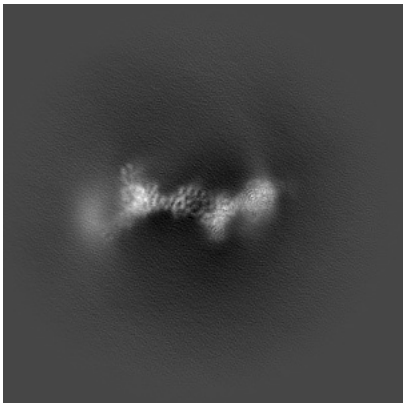
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

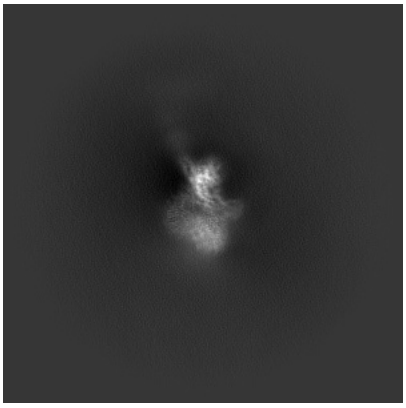
6.1.1 Primary map



X



Y

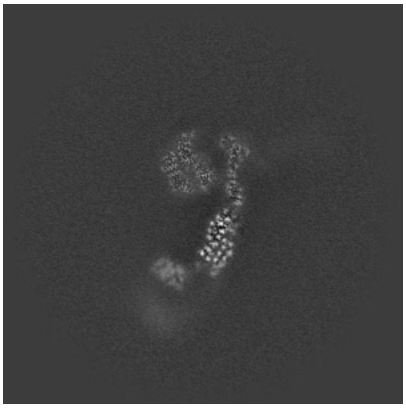


Z

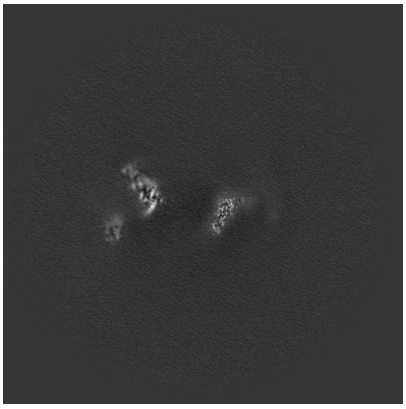
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

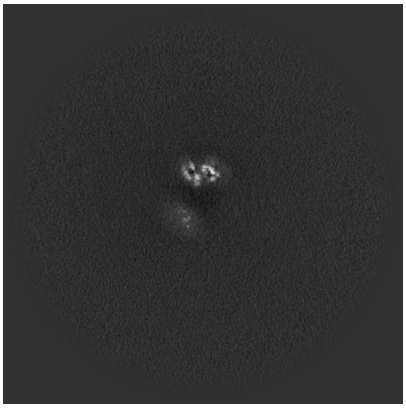
6.2.1 Primary map



X Index: 336



Y Index: 336

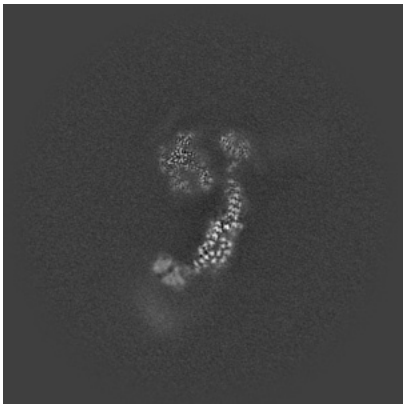


Z Index: 336

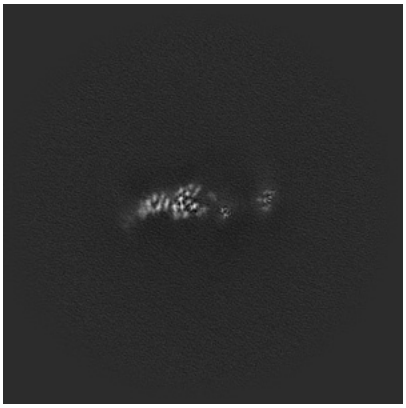
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

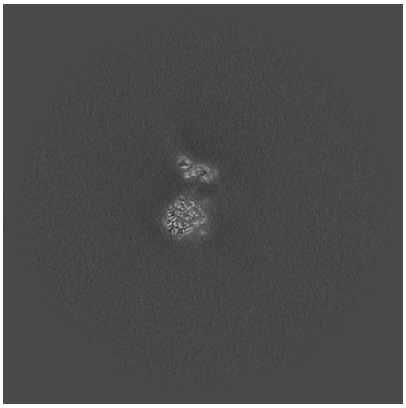
6.3.1 Primary map



X Index: 342



Y Index: 372

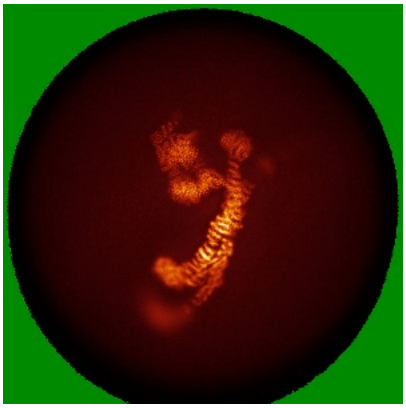


Z Index: 358

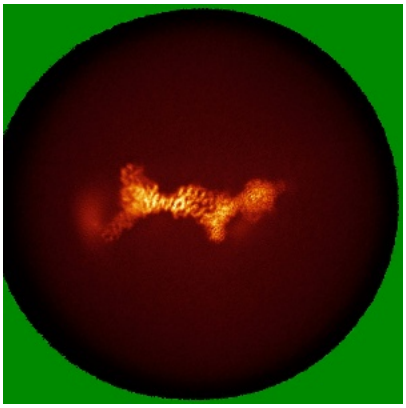
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

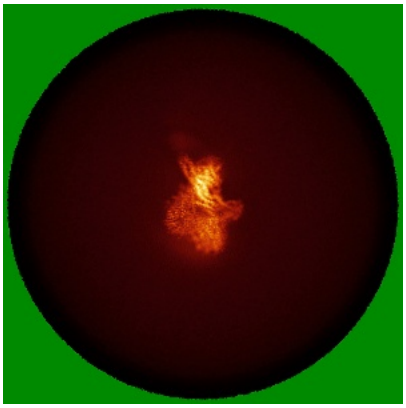
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.35. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

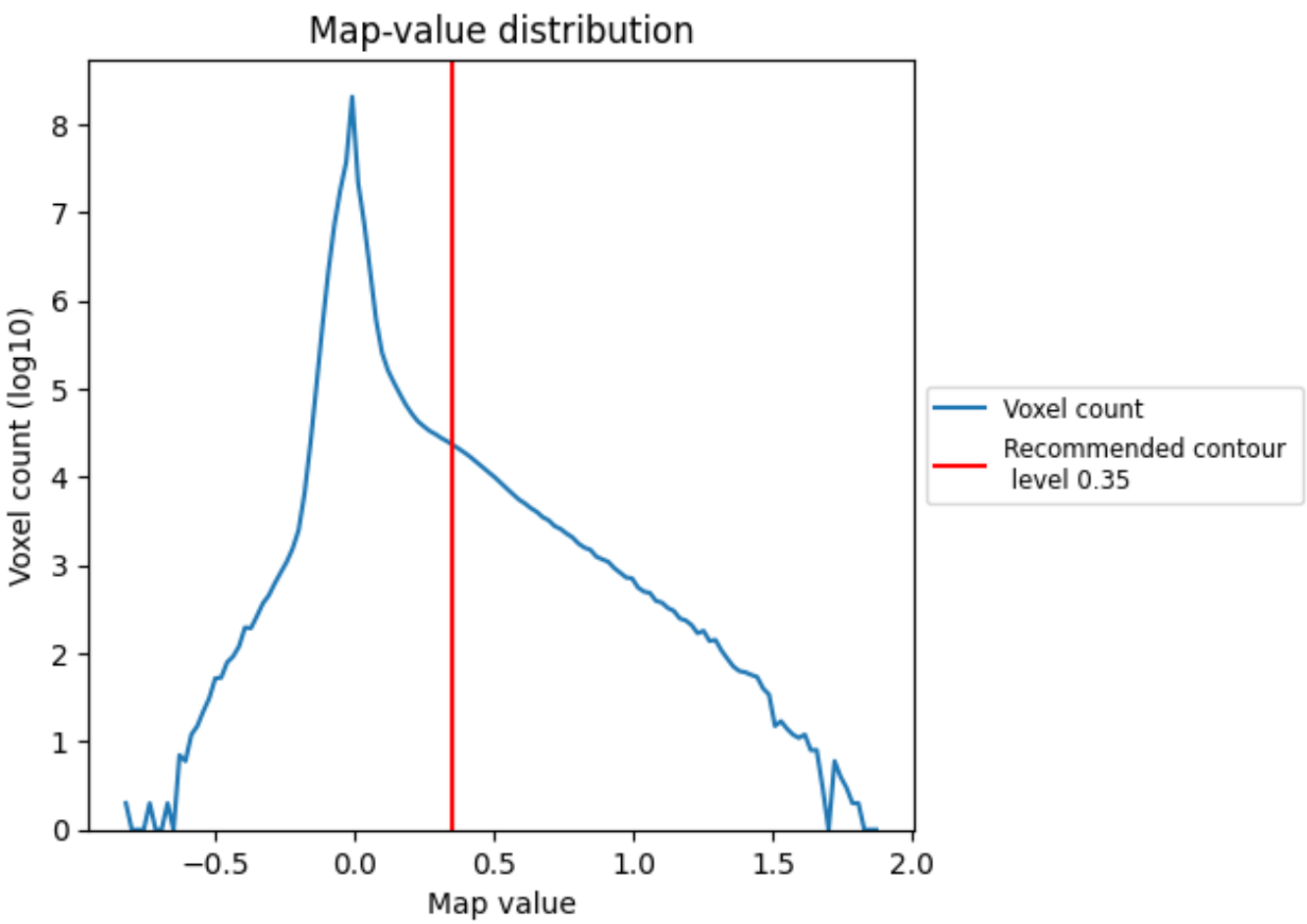
6.6 Mask visualisation (i)

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

7 Map analysis (i)

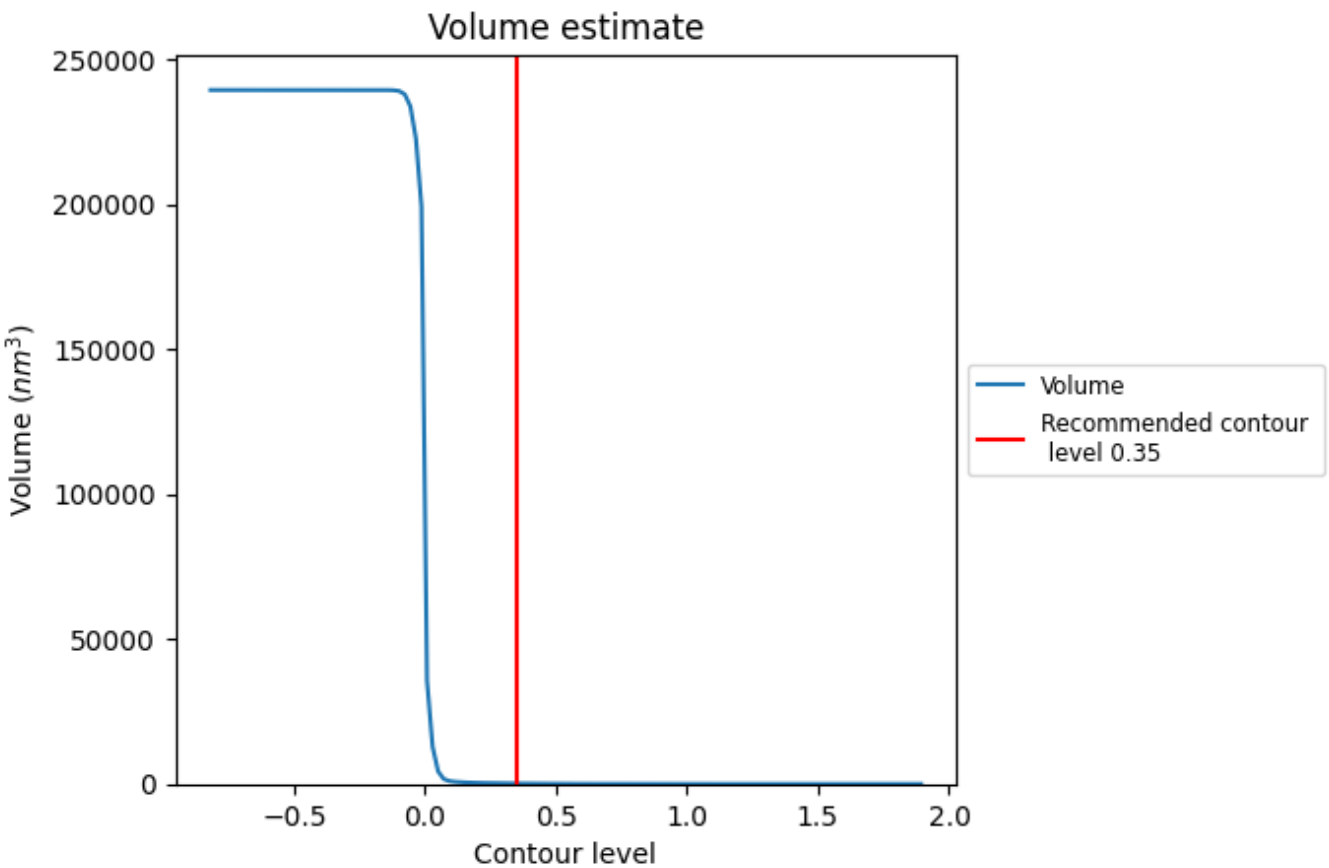
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

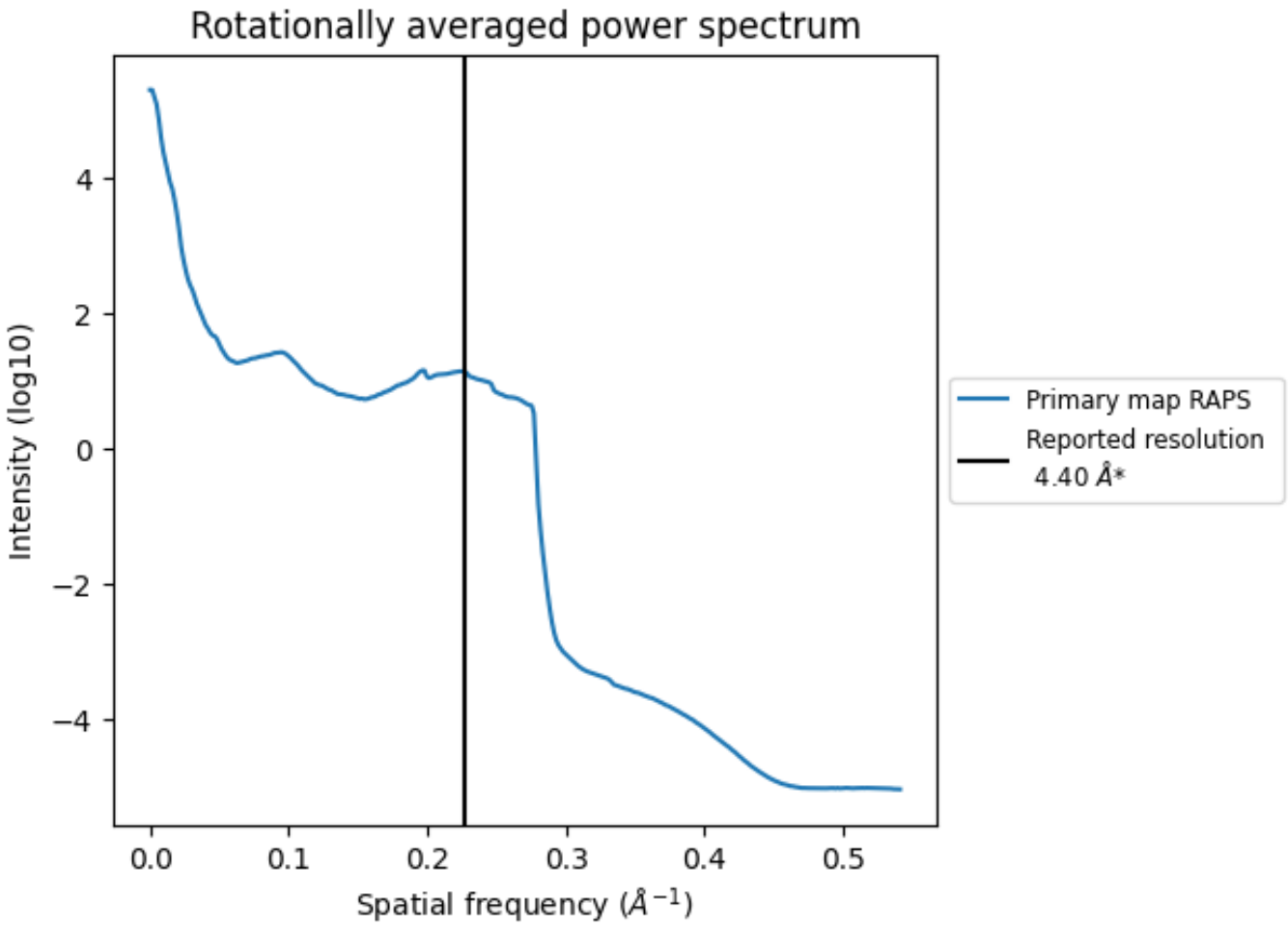
7.2 Volume estimate (i)



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 149 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 (i)



*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

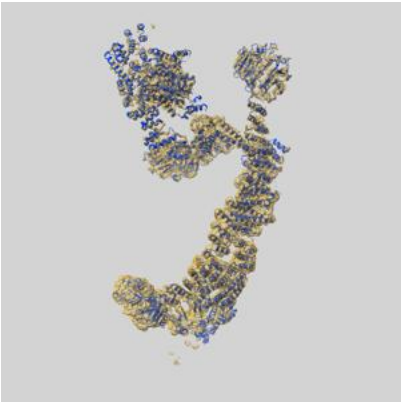
8 Fourier-Shell correlation (i)

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

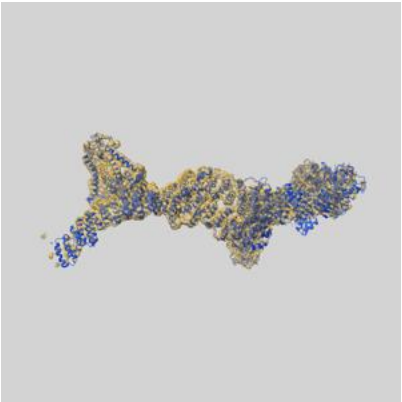
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14964 and PDB model 7ZU0. Per-residue inclusion information can be found in section 3 on page 5.

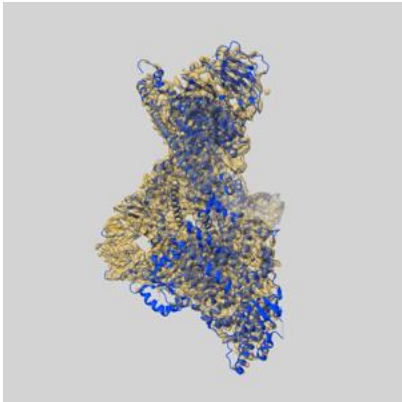
9.1 Map-model overlay (i)



X



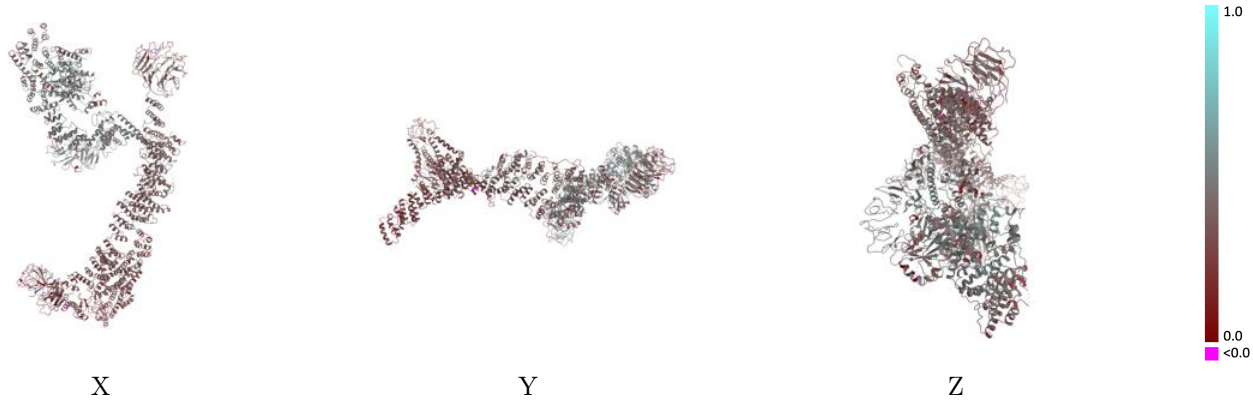
Y



Z

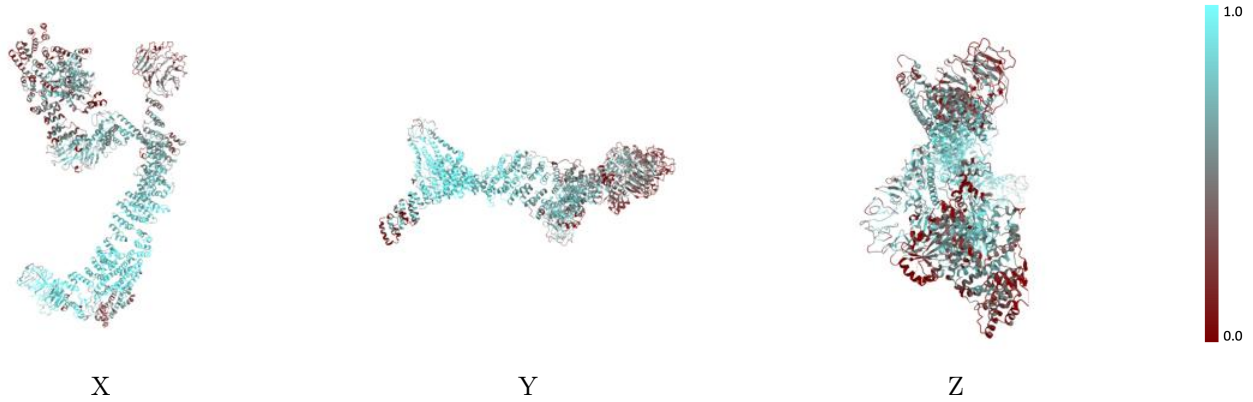
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



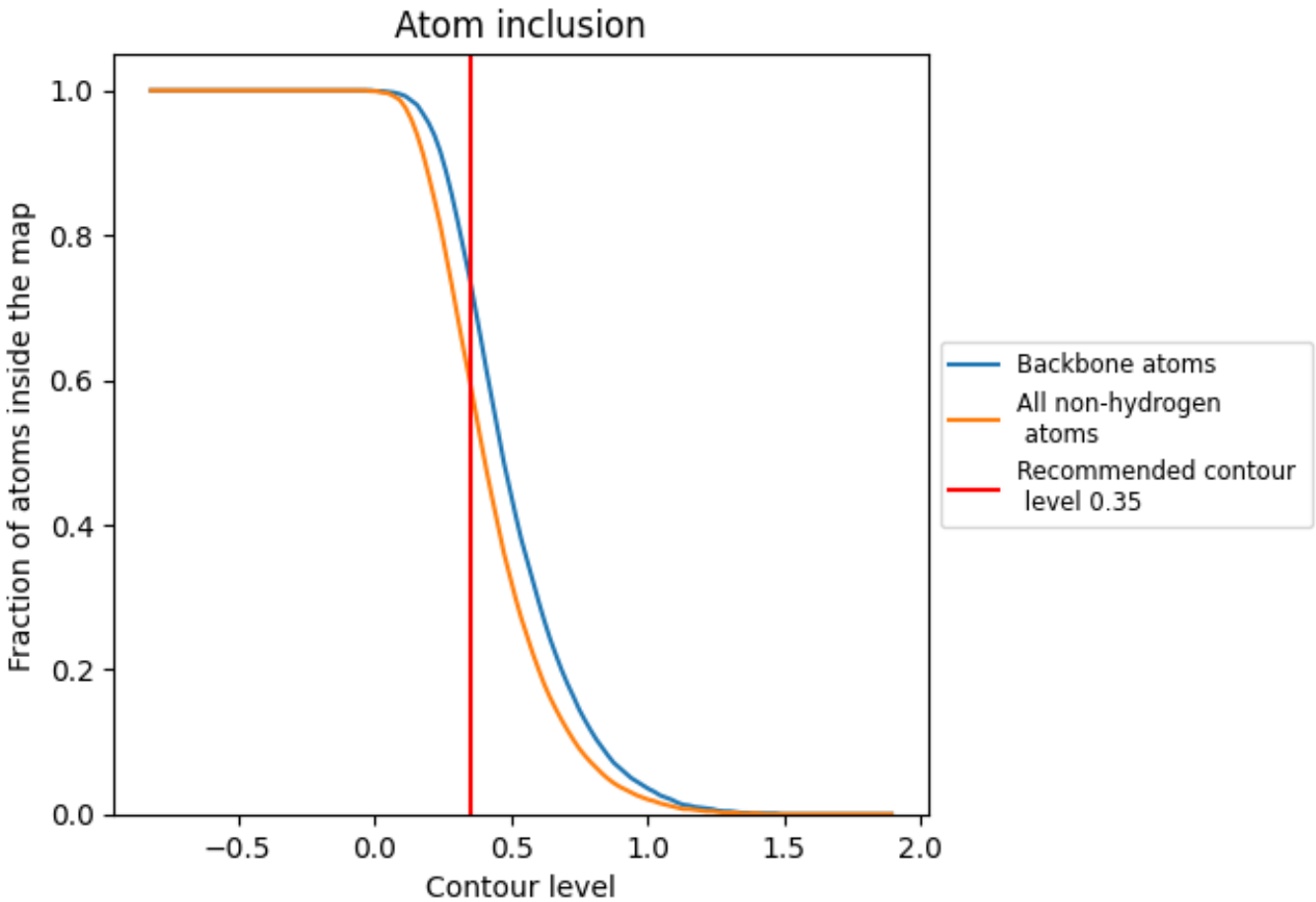
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.35).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5980	0.3930
A	0.5650	0.3590
B	0.5310	0.4490
C	0.8000	0.3510
D	0.4710	0.4620
E	0.6740	0.2820
F	0.5500	0.4010