



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 08:51 AM JST

PDB ID : 7WUI
EMDB ID : EMD-32836
Title : Tethered peptide activation mechanism of adhesion GPCRs ADGRG2 and ADGRG4
Authors : Guo, S.C.; He, Q.T.; Xiao, P.; Sun, J.P.; Yu, X.
Deposited on : 2022-02-08
Resolution : 3.10 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

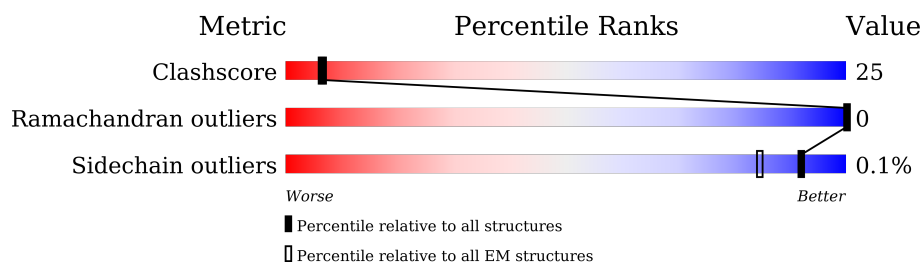
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	361	
2	B	358	
3	G	58	
4	N	128	
5	R	1149	
6	S	250	
7	L	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	4PH	L	601	-	X	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9666 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 mini-Gs.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1905	1205	339	353	8		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total	C	N	O	S	0	0
			2601	1604	467	509	21		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLN	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit

gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	55	Total	C	N	O	S	0	0
			424	266	75	80	3		

- Molecule 4 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

- Molecule 5 is a protein called Adhesion G-protein coupled receptor G2,mCherry.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	245	Total	C	N	O	S	0	0
			1985	1354	306	311	14		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	22	MET	-	expression tag	UNP Q8CJ12
R	23	LYS	-	expression tag	UNP Q8CJ12
R	24	THR	-	expression tag	UNP Q8CJ12
R	25	ILE	-	expression tag	UNP Q8CJ12
R	26	ILE	-	expression tag	UNP Q8CJ12
R	27	ALA	-	expression tag	UNP Q8CJ12
R	28	LEU	-	expression tag	UNP Q8CJ12
R	29	SER	-	expression tag	UNP Q8CJ12
R	30	TYR	-	expression tag	UNP Q8CJ12
R	31	ILE	-	expression tag	UNP Q8CJ12
R	32	PHE	-	expression tag	UNP Q8CJ12
R	33	CYS	-	expression tag	UNP Q8CJ12
R	34	LEU	-	expression tag	UNP Q8CJ12
R	35	VAL	-	expression tag	UNP Q8CJ12
R	36	PHE	-	expression tag	UNP Q8CJ12
R	37	ALA	-	expression tag	UNP Q8CJ12
R	597	ALA	HIS	engineered mutation	UNP Q8CJ12
R	599	ALA	THR	engineered mutation	UNP Q8CJ12
R	892	PHE	-	linker	UNP Q8CJ12
R	893	TRP	-	linker	UNP Q8CJ12
R	894	PHE	-	linker	UNP Q8CJ12
R	895	PRO	-	linker	UNP Q8CJ12
R	896	GLU	-	linker	UNP Q8CJ12

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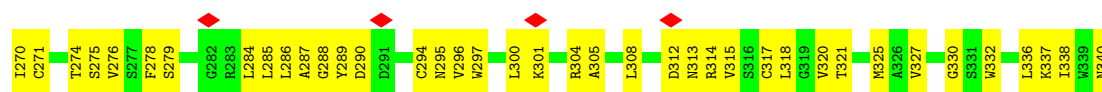
Chain	Residue	Modelled	Actual	Comment	Reference
R	897	LYS	-	linker	UNP Q8CJ12
R	898	GLY	-	linker	UNP Q8CJ12
R	899	ALA	-	linker	UNP Q8CJ12
R	900	ILE	-	linker	UNP Q8CJ12
R	901	LEU	-	linker	UNP Q8CJ12
R	902	THR	-	linker	UNP Q8CJ12
R	903	ASP	-	linker	UNP Q8CJ12
R	904	THR	-	linker	UNP Q8CJ12
R	905	SER	-	linker	UNP Q8CJ12
R	906	VAL	-	linker	UNP Q8CJ12
R	907	LYS	-	linker	UNP Q8CJ12
R	908	ARG	-	linker	UNP Q8CJ12
R	909	ASN	-	linker	UNP Q8CJ12
R	910	ASP	-	linker	UNP Q8CJ12
R	911	LEU	-	linker	UNP Q8CJ12
R	912	SER	-	linker	UNP Q8CJ12
R	913	ILE	-	linker	UNP Q8CJ12
R	914	ILE	-	linker	UNP Q8CJ12
R	915	SER	-	linker	UNP Q8CJ12
R	916	GLY	-	linker	UNP Q8CJ12
R	917	HIS	-	linker	UNP Q8CJ12
R	918	HIS	-	linker	UNP Q8CJ12
R	919	HIS	-	linker	UNP Q8CJ12
R	920	HIS	-	linker	UNP Q8CJ12
R	921	HIS	-	linker	UNP Q8CJ12
R	922	HIS	-	linker	UNP Q8CJ12
R	923	HIS	-	linker	UNP Q8CJ12
R	924	HIS	-	linker	UNP Q8CJ12
R	925	GLY	-	linker	UNP Q8CJ12
R	926	SER	-	linker	UNP Q8CJ12
R	927	ALA	-	linker	UNP Q8CJ12
R	928	GLU	-	linker	UNP Q8CJ12
R	929	ASN	-	linker	UNP Q8CJ12
R	930	LEU	-	linker	UNP Q8CJ12
R	931	TYR	-	linker	UNP Q8CJ12
R	932	PHE	-	linker	UNP Q8CJ12
R	933	GLN	-	linker	UNP Q8CJ12
R	934	GLY	-	linker	UNP Q8CJ12

- Molecule 6 is a protein called scFv16.

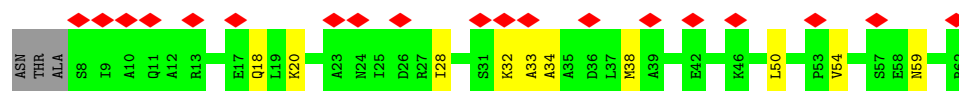
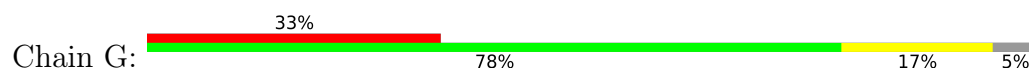
Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	220	Total	C	N	O	S	0	0
			1703	1082	283	328	10		

- Molecule 7 is a protein called IP15.

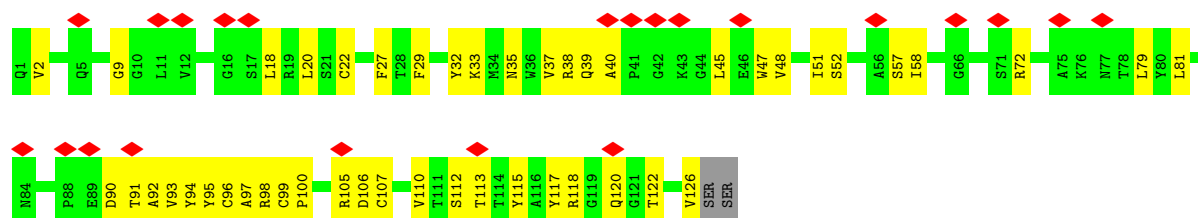
Mol	Chain	Residues	Atoms				AltConf	Trace
7	L	11	Total	C	N	O	0	0
			87	58	14	15		



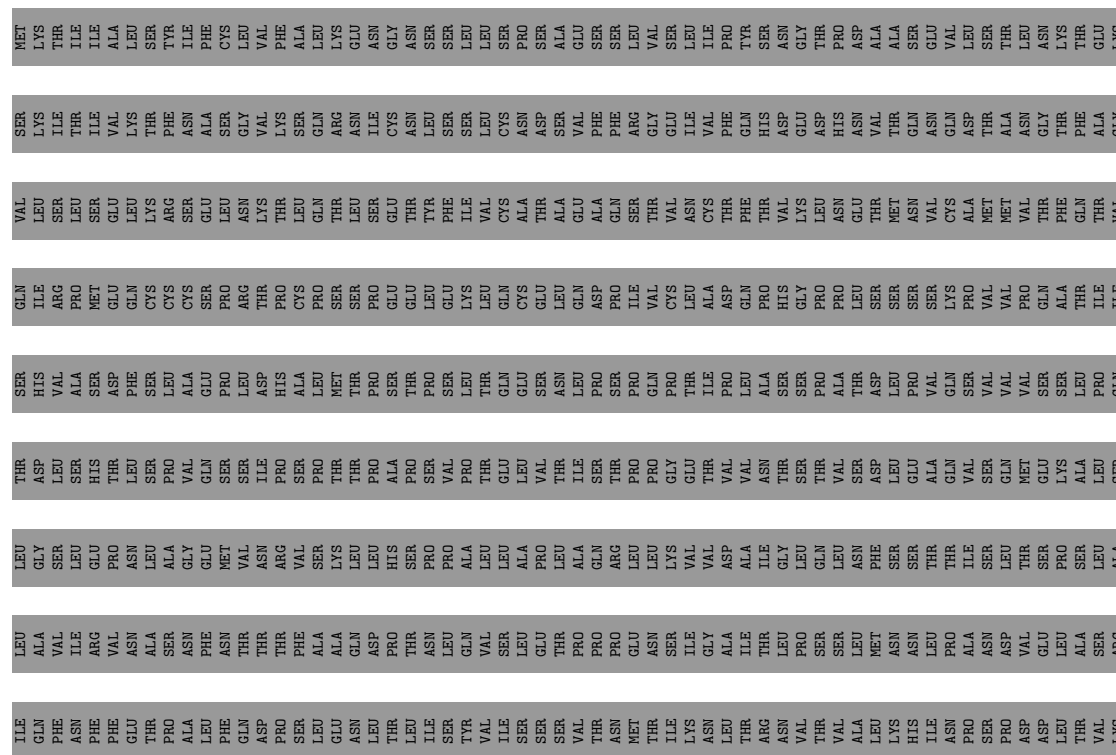
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

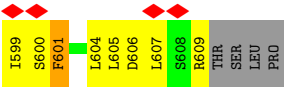


- Molecule 4: Nanobody-35



- Molecule 5: Adhesion G-protein coupled receptor G2,mCherry





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1095986	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	256.0, 256.0, 256.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	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: 4PH

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	0.32	0/1942	0.65	0/2613
2	B	0.34	0/2648	0.73	0/3589
3	G	0.30	0/430	0.58	0/580
4	N	0.33	0/981	0.67	0/1329
5	R	0.32	0/2038	0.62	0/2767
6	S	0.32	0/1742	0.66	0/2353
7	L	0.57	0/73	0.91	0/95
All	All	0.33	0/9854	0.67	0/13326

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	1905	0	1878	77	0
2	B	2601	0	2505	123	0
3	G	424	0	436	11	0
4	N	961	0	932	60	0
5	R	1985	0	2051	163	0
6	S	1703	0	1640	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	87	0	95	47	0
All	All	9666	0	9537	477	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 25.

All (477) 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:R:697:LEU:HD13	7:L:604:LEU:CD2	1.50	1.40
2:B:278:PHE:CZ	2:B:285:LEU:HD12	1.59	1.37
5:R:775:ASN:HA	7:L:609:ARG:NH1	1.39	1.35
5:R:697:LEU:CD1	7:L:604:LEU:HD23	1.59	1.31
1:A:26:ILE:HG13	2:B:89:LYS:O	1.34	1.25
6:S:97:VAL:HG21	6:S:108:PHE:CD2	1.71	1.24
5:R:693:LEU:HD23	5:R:771:TRP:CZ3	1.73	1.22
2:B:284:LEU:HD11	2:B:296:VAL:CG1	1.70	1.21
6:S:38:ARG:NH1	6:S:48:VAL:HG22	1.61	1.14
5:R:774:SER:HB3	5:R:777:VAL:CG1	1.78	1.13
1:A:283:ARG:HB2	1:A:356:ARG:NH1	1.63	1.12
6:S:35:HIS:HB2	6:S:97:VAL:HG13	1.28	1.12
5:R:845:TRP:CD1	7:L:607:LEU:HB3	1.86	1.10
5:R:693:LEU:HD23	5:R:771:TRP:CE3	1.86	1.09
2:B:284:LEU:HD11	2:B:296:VAL:HG11	1.36	1.07
2:B:314:ARG:HD3	2:B:332:TRP:CZ3	1.89	1.07
6:S:38:ARG:HH11	6:S:48:VAL:HG22	0.95	1.06
2:B:314:ARG:HD3	2:B:332:TRP:CE3	1.90	1.06
5:R:774:SER:HB3	5:R:777:VAL:HG12	1.32	1.06
5:R:845:TRP:HD1	7:L:607:LEU:CB	1.70	1.04
5:R:838:TRP:HH2	7:L:601:4PH:HE1	1.24	1.02
6:S:45:LEU:HD11	6:S:239:PHE:CD1	1.94	1.02
2:B:284:LEU:CD1	2:B:296:VAL:CG1	2.39	1.00
2:B:48:ARG:HE	2:B:340:ASN:HB2	1.24	1.00
5:R:772:ILE:HG21	5:R:777:VAL:HG13	1.43	0.99
5:R:771:TRP:HE1	5:R:778:PHE:HE1	1.10	0.99
2:B:269:ILE:HG21	2:B:289:TYR:CE2	1.97	0.98
5:R:674:ASP:OD2	5:R:689:VAL:HG12	1.63	0.98
1:A:352:SER:HB2	4:N:105:ARG:HH22	1.31	0.96
6:S:93:MET:SD	6:S:95:TYR:OH	2.24	0.94
5:R:693:LEU:CD2	5:R:771:TRP:CZ3	2.50	0.94
1:A:352:SER:HB3	4:N:105:ARG:HH12	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:775:ASN:HA	7:L:609:ARG:HH11	0.94	0.92
5:R:694:HIS:HD1	5:R:753:TYR:HH	1.09	0.91
5:R:775:ASN:CA	7:L:609:ARG:NH1	2.31	0.91
2:B:269:ILE:HG21	2:B:289:TYR:HE2	1.34	0.91
6:S:38:ARG:HH11	6:S:48:VAL:CG2	1.82	0.91
5:R:774:SER:CB	5:R:777:VAL:HG12	2.01	0.91
6:S:21:SER:HA	6:S:79:LEU:O	1.71	0.90
5:R:838:TRP:CH2	7:L:601:4PH:HE1	2.07	0.89
5:R:623:ILE:HD13	5:R:858:ILE:HA	1.54	0.89
6:S:93:MET:HE1	6:S:95:TYR:OH	1.73	0.88
2:B:314:ARG:NH1	2:B:332:TRP:CE2	2.40	0.88
6:S:4:LEU:HD23	6:S:96:CYS:SG	2.14	0.87
5:R:687:ILE:CD1	5:R:753:TYR:O	2.23	0.87
5:R:771:TRP:CZ2	7:L:604:LEU:HG	2.10	0.87
2:B:314:ARG:NH1	2:B:332:TRP:CZ2	2.43	0.87
6:S:97:VAL:HG23	6:S:108:PHE:HA	1.56	0.87
5:R:787:CYS:SG	5:R:842:PHE:HZ	1.96	0.87
6:S:93:MET:CE	6:S:95:TYR:OH	2.23	0.86
5:R:687:ILE:HD13	5:R:753:TYR:O	1.76	0.86
5:R:845:TRP:CD1	7:L:607:LEU:CB	2.51	0.86
5:R:686:CYS:SG	5:R:754:GLY:HA2	2.17	0.84
2:B:284:LEU:HD11	2:B:296:VAL:HG13	1.57	0.84
5:R:699:VAL:HA	5:R:702:THR:HG22	1.58	0.84
6:S:177:PHE:HE2	6:S:230:MET:SD	2.00	0.83
5:R:787:CYS:HG	5:R:842:PHE:HZ	0.85	0.83
6:S:177:PHE:CE2	6:S:230:MET:SD	2.72	0.83
5:R:774:SER:HB3	5:R:777:VAL:HG11	1.59	0.83
5:R:693:LEU:HD23	5:R:771:TRP:HZ3	1.40	0.82
1:A:279:ASN:HA	4:N:106:ASP:OD2	1.79	0.82
5:R:697:LEU:HD13	7:L:604:LEU:HD23	0.82	0.82
6:S:45:LEU:HD11	6:S:239:PHE:CE1	2.13	0.82
7:L:599:ILE:HD12	7:L:600:SER:O	1.79	0.82
1:A:352:SER:CB	4:N:105:ARG:HH12	1.93	0.82
6:S:97:VAL:CG2	6:S:108:PHE:HA	2.10	0.82
1:A:352:SER:HB2	4:N:105:ARG:NH2	1.95	0.82
5:R:787:CYS:SG	5:R:842:PHE:CZ	2.73	0.81
5:R:671:PHE:HD1	5:R:693:LEU:HD11	1.44	0.81
5:R:690:ALA:HB3	5:R:753:TYR:HB3	1.63	0.81
5:R:668:ASN:O	5:R:672:LEU:HD13	1.80	0.80
5:R:674:ASP:HA	5:R:689:VAL:HG11	1.63	0.80
5:R:702:THR:HG21	5:R:734:GLY:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:778:PHE:CE2	7:L:609:ARG:HD3	2.17	0.80
6:S:45:LEU:CD1	6:S:239:PHE:CD1	2.65	0.79
5:R:769:PHE:CG	7:L:599:ILE:HG12	2.16	0.79
2:B:318:LEU:HD12	2:B:318:LEU:O	1.83	0.79
5:R:671:PHE:HA	5:R:693:LEU:HD13	1.62	0.79
1:A:283:ARG:HB2	1:A:356:ARG:HH12	1.41	0.79
2:B:314:ARG:CD	2:B:332:TRP:CE3	2.64	0.78
1:A:59:GLN:NE2	1:A:371:ASN:HD22	1.81	0.78
5:R:781:THR:O	5:R:785:TYR:HB3	1.84	0.78
6:S:97:VAL:HG21	6:S:108:PHE:CG	2.19	0.78
1:A:228:ARG:CZ	1:A:230:GLU:OE2	2.31	0.77
5:R:772:ILE:CG2	5:R:777:VAL:HG13	2.13	0.77
2:B:270:ILE:HD12	2:B:270:ILE:O	1.85	0.77
5:R:674:ASP:OD2	5:R:689:VAL:CG1	2.33	0.77
2:B:278:PHE:CZ	2:B:285:LEU:CD1	2.55	0.77
5:R:702:THR:CG2	5:R:734:GLY:O	2.34	0.76
2:B:287:ALA:O	2:B:289:TYR:HD1	1.69	0.76
6:S:180:ARG:HG2	6:S:183:GLN:HE21	1.49	0.76
1:A:373:ARG:HA	1:A:373:ARG:NE	2.00	0.76
6:S:230:MET:SD	6:S:239:PHE:CE1	2.78	0.76
1:A:352:SER:HB3	4:N:105:ARG:NH1	2.02	0.74
6:S:230:MET:SD	6:S:239:PHE:CZ	2.81	0.74
2:B:286:LEU:HD21	2:B:327:VAL:HG21	1.67	0.74
6:S:45:LEU:HD12	6:S:45:LEU:O	1.87	0.74
4:N:99:CYS:HG	4:N:107:CYS:HG	0.83	0.74
6:S:45:LEU:CD1	6:S:239:PHE:CG	2.71	0.74
2:B:288:GLY:H	2:B:318:LEU:HD21	1.51	0.73
2:B:278:PHE:HZ	2:B:285:LEU:HD12	1.42	0.73
5:R:778:PHE:CZ	7:L:604:LEU:O	2.42	0.72
5:R:694:HIS:CE1	5:R:781:THR:HG21	2.25	0.72
5:R:683:ARG:HG3	5:R:683:ARG:HH11	1.55	0.72
5:R:682:THR:OG1	5:R:685:PHE:HB2	1.90	0.71
5:R:621:THR:CG2	5:R:625:TYR:HE2	2.04	0.71
5:R:775:ASN:CA	7:L:609:ARG:HH11	1.89	0.71
6:S:35:HIS:HB2	6:S:97:VAL:CG1	2.16	0.71
5:R:769:PHE:CD2	7:L:599:ILE:HG12	2.26	0.71
5:R:621:THR:CG2	5:R:625:TYR:CE2	2.74	0.70
5:R:621:THR:HG22	5:R:625:TYR:CE2	2.26	0.70
5:R:690:ALA:HB1	5:R:753:TYR:HD2	1.56	0.70
5:R:771:TRP:NE1	5:R:778:PHE:HE1	1.86	0.70
5:R:693:LEU:CD2	5:R:771:TRP:CE3	2.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:45:LEU:HD12	6:S:239:PHE:CG	2.27	0.69
2:B:276:VAL:HA	2:B:286:LEU:O	1.92	0.69
4:N:9:GLY:H	4:N:18:LEU:HD21	1.56	0.69
5:R:694:HIS:HE1	5:R:781:THR:HG21	1.56	0.69
5:R:697:LEU:CD1	7:L:604:LEU:CD2	2.40	0.69
6:S:174:LEU:HA	6:S:230:MET:O	1.91	0.69
2:B:48:ARG:NE	2:B:340:ASN:HB2	2.04	0.69
5:R:772:ILE:HG22	5:R:774:SER:H	1.56	0.69
2:B:286:LEU:CD2	2:B:327:VAL:HG11	2.23	0.69
5:R:771:TRP:CH2	7:L:604:LEU:HG	2.28	0.68
5:R:778:PHE:CE1	7:L:604:LEU:O	2.46	0.68
1:A:24:LYS:O	1:A:28:LYS:HG3	1.94	0.68
2:B:284:LEU:CD1	2:B:296:VAL:HG11	2.15	0.68
5:R:671:PHE:CD1	5:R:693:LEU:HD11	2.29	0.67
4:N:35:ASN:OD1	4:N:99:CYS:SG	2.52	0.67
2:B:49:ARG:HB2	2:B:338:ILE:HD12	1.75	0.67
2:B:287:ALA:O	2:B:289:TYR:CD1	2.46	0.67
5:R:772:ILE:CG2	5:R:777:VAL:CG1	2.73	0.67
5:R:845:TRP:HD1	7:L:607:LEU:HB2	1.58	0.67
4:N:39:GLN:O	4:N:92:ALA:HB1	1.95	0.67
6:S:97:VAL:HG11	6:S:108:PHE:CE2	2.30	0.67
5:R:623:ILE:HD13	5:R:858:ILE:CA	2.24	0.67
2:B:48:ARG:HG3	2:B:340:ASN:OD1	1.95	0.66
2:B:226:GLU:O	4:N:98:ARG:NH2	2.27	0.66
2:B:314:ARG:HD3	2:B:332:TRP:CD2	2.31	0.66
6:S:95:TYR:HE1	6:S:114:GLY:HA3	1.61	0.66
5:R:778:PHE:CD2	7:L:609:ARG:NE	2.64	0.66
2:B:210:LEU:HB3	2:B:220:GLN:HB2	1.78	0.65
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.78	0.65
1:A:228:ARG:NH2	1:A:230:GLU:OE2	2.29	0.65
5:R:841:ALA:HB1	7:L:607:LEU:HD23	1.78	0.65
5:R:774:SER:O	5:R:777:VAL:HG12	1.98	0.64
1:A:59:GLN:HE22	1:A:371:ASN:HB2	1.63	0.64
2:B:314:ARG:HD3	2:B:332:TRP:CH2	2.32	0.64
1:A:278:ASN:C	4:N:106:ASP:HB3	2.18	0.64
2:B:286:LEU:HD23	2:B:327:VAL:HG11	1.79	0.64
2:B:278:PHE:CE2	2:B:285:LEU:HD12	2.30	0.64
5:R:769:PHE:CB	7:L:599:ILE:HG12	2.28	0.64
5:R:674:ASP:HB2	5:R:689:VAL:CG1	2.28	0.64
2:B:60:ALA:HA	2:B:317:CYS:HB3	1.79	0.63
5:R:674:ASP:HB2	5:R:689:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:93:VAL:HG23	4:N:122:THR:C	2.19	0.63
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.80	0.62
5:R:696:PHE:HA	5:R:699:VAL:HG22	1.80	0.62
6:S:39:GLN:HB3	6:S:45:LEU:HB3	1.80	0.62
6:S:12:VAL:HG12	6:S:118:THR:O	1.99	0.62
1:A:373:ARG:HA	1:A:373:ARG:HE	1.65	0.62
1:A:283:ARG:O	1:A:356:ARG:HG2	2.00	0.61
1:A:283:ARG:CB	1:A:356:ARG:NH1	2.53	0.61
2:B:83:ASP:HB3	2:B:88:ASN:HB2	1.83	0.61
5:R:683:ARG:HH11	5:R:683:ARG:CG	2.14	0.61
4:N:33:LYS:HG3	4:N:52:SER:HA	1.81	0.61
5:R:690:ALA:CB	5:R:753:TYR:HB3	2.31	0.61
5:R:771:TRP:CE2	7:L:604:LEU:HA	2.35	0.61
5:R:690:ALA:CB	5:R:753:TYR:HD2	2.14	0.60
5:R:697:LEU:HD13	7:L:604:LEU:HD21	1.73	0.60
5:R:702:THR:HB	5:R:785:TYR:OH	2.01	0.60
5:R:725:LYS:HG2	5:R:728:LEU:HB2	1.84	0.60
5:R:674:ASP:CB	5:R:689:VAL:CG1	2.80	0.60
2:B:256:ARG:HH21	3:G:33:ALA:HA	1.67	0.60
6:S:39:GLN:CD	6:S:95:TYR:HE2	2.05	0.60
2:B:315:VAL:HG13	2:B:315:VAL:O	2.01	0.60
5:R:778:PHE:HB3	7:L:609:ARG:NH1	2.16	0.60
5:R:786:PHE:CZ	5:R:838:TRP:HB3	2.37	0.60
6:S:45:LEU:CD1	6:S:239:PHE:CE1	2.85	0.60
1:A:26:ILE:HG21	2:B:89:LYS:HB3	1.85	0.59
2:B:34:THR:HG23	3:G:38:MET:HE2	1.84	0.59
2:B:314:ARG:CD	2:B:332:TRP:CZ3	2.76	0.59
5:R:621:THR:HG22	5:R:625:TYR:CD2	2.36	0.59
5:R:694:HIS:CE1	5:R:781:THR:CG2	2.85	0.59
2:B:325:MET:O	2:B:340:ASN:ND2	2.36	0.59
6:S:38:ARG:HB3	6:S:94:TYR:CD1	2.37	0.59
2:B:231:ALA:HB1	2:B:276:VAL:HG22	1.85	0.59
1:A:266:LEU:HD21	1:A:341:ILE:HD12	1.85	0.59
5:R:694:HIS:CD2	5:R:698:LEU:HD13	2.37	0.59
1:A:275:SER:HA	4:N:106:ASP:HB2	1.84	0.59
1:A:352:SER:CB	4:N:105:ARG:NH1	2.62	0.58
1:A:207:ILE:HD11	1:A:222:PHE:HB3	1.83	0.58
2:B:152:LEU:HD11	2:B:213:VAL:HG21	1.84	0.58
2:B:242:ALA:CB	2:B:285:LEU:HD11	2.32	0.58
4:N:112:SER:O	4:N:118:ARG:NH1	2.30	0.58
4:N:93:VAL:HG13	4:N:93:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:699:VAL:HA	5:R:702:THR:CG2	2.33	0.57
4:N:115:TYR:HD2	4:N:118:ARG:HG3	1.69	0.57
2:B:207:SER:HA	2:B:222:PHE:O	2.04	0.57
4:N:97:ALA:HA	4:N:118:ARG:HG2	1.87	0.57
5:R:624:THR:HG23	7:L:601:4PH:HD2	1.85	0.57
6:S:32:PHE:CE1	6:S:98:ARG:NH1	2.72	0.57
1:A:16:ASP:OD2	6:S:169:ASN:ND2	2.36	0.57
2:B:75:GLN:NE2	2:B:100:VAL:O	2.38	0.57
4:N:98:ARG:HB3	4:N:117:TYR:HB3	1.87	0.57
5:R:674:ASP:CA	5:R:689:VAL:HG11	2.35	0.57
5:R:769:PHE:CD2	7:L:599:ILE:CG1	2.88	0.56
6:S:39:GLN:HA	6:S:45:LEU:HA	1.86	0.56
2:B:296:VAL:O	2:B:305:ALA:N	2.39	0.56
5:R:771:TRP:NE1	7:L:604:LEU:HA	2.19	0.56
5:R:771:TRP:NE1	5:R:778:PHE:CE1	2.69	0.56
4:N:91:THR:HG23	4:N:126:VAL:H	1.69	0.56
1:A:13:SER:OG	1:A:14:ALA:N	2.38	0.56
2:B:8:ARG:HD3	4:N:120:GLN:HG3	1.87	0.56
5:R:786:PHE:CE2	7:L:605:LEU:HD13	2.40	0.56
6:S:97:VAL:CG2	6:S:108:PHE:CD2	2.67	0.56
2:B:288:GLY:N	2:B:318:LEU:HD21	2.19	0.56
6:S:142:GLN:HG3	6:S:242:GLY:H	1.71	0.56
4:N:20:LEU:HB3	4:N:81:LEU:HB3	1.88	0.56
2:B:34:THR:HG23	3:G:38:MET:CE	2.37	0.55
1:A:22:ARG:O	1:A:25:MET:HB3	2.07	0.55
1:A:346:LEU:HD21	1:A:361:PRO:HG3	1.88	0.55
5:R:772:ILE:HD12	5:R:782:VAL:CG2	2.37	0.55
5:R:671:PHE:HA	5:R:693:LEU:CD1	2.32	0.55
1:A:214:VAL:HG22	1:A:373:ARG:HH21	1.71	0.55
6:S:63:THR:HG23	6:S:64:VAL:HG13	1.89	0.55
4:N:22:CYS:HB3	4:N:79:LEU:HB3	1.90	0.54
2:B:279:SER:HA	2:B:320:VAL:HG11	1.89	0.54
2:B:118:ASP:N	2:B:118:ASP:OD1	2.40	0.54
5:R:854:TYR:O	5:R:858:ILE:HG22	2.08	0.54
1:A:342:ARG:NH2	1:A:361:PRO:O	2.40	0.54
2:B:250:CYS:HB3	2:B:264:TYR:HB2	1.90	0.54
1:A:344:GLU:OE1	1:A:347:ARG:NH1	2.40	0.54
2:B:284:LEU:CD1	2:B:296:VAL:HG13	2.26	0.54
2:B:50:THR:O	2:B:50:THR:HG23	2.08	0.54
6:S:177:PHE:O	6:S:227:TYR:HA	2.07	0.54
1:A:20:VAL:HG12	1:A:24:LYS:NZ	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:CG2	2:B:289:TYR:CE2	2.85	0.53
2:B:314:ARG:CG	2:B:332:TRP:CE3	2.91	0.53
4:N:35:ASN:HB2	4:N:97:ALA:O	2.08	0.53
4:N:112:SER:HB2	4:N:115:TYR:HB2	1.90	0.53
4:N:2:VAL:HG11	4:N:98:ARG:HE	1.73	0.53
5:R:699:VAL:CA	5:R:702:THR:HG22	2.36	0.53
2:B:321:THR:OG1	2:B:325:MET:N	2.42	0.53
5:R:775:ASN:HA	7:L:609:ARG:HH12	1.60	0.53
1:A:38:ARG:NH2	2:B:55:LEU:O	2.42	0.53
2:B:67:SER:HB3	2:B:321:THR:HB	1.90	0.53
5:R:701:PHE:O	5:R:789:ILE:HG21	2.09	0.53
5:R:772:ILE:CD1	5:R:782:VAL:HG23	2.38	0.53
5:R:631:SER:O	5:R:635:LEU:HB2	2.08	0.53
5:R:793:ASN:ND2	5:R:834:LEU:O	2.42	0.53
2:B:124:TYR:HB3	2:B:133:VAL:HG12	1.91	0.53
5:R:691:VAL:HA	5:R:753:TYR:CE2	2.44	0.53
4:N:29:PHE:O	4:N:72:ARG:NH2	2.42	0.53
5:R:778:PHE:CB	7:L:609:ARG:NH1	2.72	0.53
6:S:27:PHE:CZ	6:S:98:ARG:HD3	2.44	0.53
1:A:231:ARG:NH1	1:A:272:ASP:OD2	2.42	0.52
1:A:393:LEU:HD23	5:R:826:SER:HB2	1.91	0.52
4:N:20:LEU:HD21	4:N:94:TYR:HB2	1.89	0.52
4:N:52:SER:O	4:N:72:ARG:NH1	2.42	0.52
4:N:95:TYR:HB3	4:N:118:ARG:HD2	1.91	0.52
6:S:12:VAL:HG21	6:S:86:LEU:HD12	1.89	0.52
2:B:47:THR:HG21	2:B:337:LYS:HD2	1.92	0.52
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.91	0.52
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.90	0.52
6:S:20:LEU:N	6:S:20:LEU:HD12	2.24	0.52
2:B:149:CYS:O	2:B:150:ARG:NH1	2.42	0.52
5:R:628:CYS:HG	5:R:861:THR:HG1	1.58	0.52
5:R:844:ALA:HB2	5:R:852:PHE:HB2	1.91	0.52
2:B:284:LEU:CD1	2:B:296:VAL:HG12	2.38	0.52
5:R:778:PHE:CE2	7:L:609:ARG:CD	2.92	0.51
2:B:22:ARG:NH2	2:B:221:THR:O	2.43	0.51
2:B:49:ARG:HB2	2:B:338:ILE:HB	1.91	0.51
5:R:841:ALA:HB1	7:L:607:LEU:CD2	2.40	0.51
4:N:40:ALA:HA	4:N:92:ALA:HB2	1.91	0.51
4:N:51:ILE:HG22	4:N:58:ILE:HG12	1.92	0.51
6:S:93:MET:HE2	6:S:114:GLY:HA3	1.91	0.51
5:R:774:SER:CB	5:R:777:VAL:CG1	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:CYS:SG	3:G:18:GLN:NE2	2.84	0.51
2:B:286:LEU:N	2:B:286:LEU:HD12	2.25	0.51
4:N:97:ALA:CB	4:N:110:VAL:HB	2.40	0.51
1:A:214:VAL:CG2	1:A:373:ARG:HH21	2.24	0.51
2:B:312:ASP:OD2	5:R:650:ARG:NE	2.41	0.51
6:S:45:LEU:CD1	6:S:239:PHE:CD2	2.94	0.51
1:A:21:GLU:OE1	6:S:52:SER:OG	2.25	0.50
2:B:314:ARG:CG	2:B:332:TRP:CD2	2.94	0.50
5:R:844:ALA:HB2	5:R:852:PHE:CB	2.40	0.50
1:A:280:ARG:HA	1:A:283:ARG:HE	1.77	0.50
5:R:855:LEU:O	5:R:858:ILE:HG22	2.12	0.50
5:R:738:PRO:HA	5:R:741:VAL:HG12	1.94	0.50
6:S:11:LEU:HD12	6:S:11:LEU:O	2.12	0.50
2:B:248:ALA:HB1	2:B:269:ILE:O	2.11	0.50
2:B:275:SER:CB	2:B:318:LEU:HG	2.42	0.50
1:A:315:PHE:O	1:A:336:ARG:NH2	2.45	0.50
2:B:275:SER:HB2	2:B:318:LEU:HG	1.94	0.50
5:R:649:ARG:HB2	5:R:655:LYS:HG3	1.94	0.50
1:A:25:MET:SD	6:S:54:GLY:HA3	2.52	0.49
2:B:93:ILE:HG21	2:B:133:VAL:HB	1.92	0.49
6:S:178:LEU:HB2	6:S:188:LEU:HD11	1.94	0.49
1:A:27:GLU:HG2	2:B:89:LYS:HD2	1.92	0.49
2:B:340:ASN:HD22	3:G:50:LEU:HD21	1.76	0.49
5:R:693:LEU:CD2	5:R:771:TRP:HZ3	2.08	0.49
6:S:95:TYR:CE1	6:S:114:GLY:HA3	2.46	0.49
5:R:690:ALA:CB	5:R:753:TYR:CD2	2.95	0.49
6:S:97:VAL:HG11	6:S:108:PHE:HE2	1.76	0.49
2:B:14:LEU:HD21	3:G:20:LYS:HA	1.94	0.49
1:A:383:ILE:HA	1:A:386:MET:HG2	1.94	0.49
4:N:98:ARG:O	4:N:115:TYR:OH	2.23	0.49
5:R:683:ARG:CG	5:R:683:ARG:NH1	2.73	0.49
5:R:804:LEU:HD22	5:R:827:ILE:HD11	1.94	0.49
1:A:59:GLN:HE22	1:A:371:ASN:CB	2.26	0.49
1:A:393:LEU:HA	5:R:826:SER:HB2	1.95	0.49
2:B:96:ARG:NH1	2:B:138:GLU:OE2	2.46	0.49
4:N:32:TYR:CE1	4:N:98:ARG:NH1	2.79	0.49
5:R:769:PHE:HB2	7:L:599:ILE:HG12	1.94	0.49
5:R:776:VAL:HG13	5:R:777:VAL:N	2.27	0.49
1:A:368:ASP:N	1:A:368:ASP:OD1	2.44	0.49
6:S:52:SER:OG	6:S:53:SER:N	2.46	0.49
1:A:208:PHE:HB2	1:A:223:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:HG21	2:B:300:LEU:HB3	1.95	0.48
6:S:38:ARG:HD3	6:S:94:TYR:CE1	2.48	0.48
1:A:21:GLU:HG3	6:S:57:THR:HG23	1.95	0.48
5:R:702:THR:HG21	5:R:738:PRO:HG2	1.95	0.48
1:A:232:ARG:CD	4:N:100:PRO:CB	2.91	0.48
5:R:691:VAL:HG22	5:R:753:TYR:CZ	2.48	0.48
6:S:38:ARG:HB3	6:S:94:TYR:CE1	2.48	0.48
6:S:179:GLN:O	6:S:225:GLY:CA	2.62	0.48
1:A:294:GLN:HG3	1:A:363:PHE:HB3	1.95	0.48
2:B:314:ARG:HG2	2:B:332:TRP:CE3	2.47	0.48
4:N:27:PHE:CE1	4:N:98:ARG:HD3	2.49	0.48
4:N:79:LEU:HD23	4:N:96:CYS:SG	2.52	0.48
1:A:229:ASP:OD2	4:N:113:THR:N	2.40	0.48
5:R:668:ASN:O	5:R:672:LEU:CD1	2.56	0.48
5:R:691:VAL:HG13	5:R:742:VAL:HG11	1.95	0.48
1:A:57:VAL:HG13	1:A:210:THR:HG21	1.96	0.48
6:S:187:LEU:HD21	6:S:190:TYR:HB3	1.96	0.48
6:S:6:GLU:HB3	6:S:22:CYS:HA	1.96	0.48
2:B:108:SER:OG	2:B:154:ASP:OD1	2.31	0.48
5:R:697:LEU:HD22	5:R:771:TRP:CH2	2.48	0.48
1:A:279:ASN:CA	4:N:106:ASP:OD2	2.59	0.47
5:R:741:VAL:HA	5:R:744:ILE:HG12	1.95	0.47
6:S:11:LEU:HD12	6:S:11:LEU:C	2.35	0.47
6:S:93:MET:CE	6:S:95:TYR:CE1	2.97	0.47
6:S:93:MET:CE	6:S:95:TYR:CZ	2.97	0.47
6:S:235:TYR:O	6:S:237:LEU:N	2.47	0.47
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.95	0.47
2:B:313:ASN:ND2	2:B:332:TRP:O	2.47	0.47
2:B:318:LEU:HD12	2:B:318:LEU:C	2.35	0.47
6:S:95:TYR:CD1	6:S:114:GLY:HA2	2.50	0.47
1:A:232:ARG:HD2	4:N:100:PRO:CB	2.44	0.47
6:S:229:CYS:O	6:S:239:PHE:HA	2.14	0.47
1:A:362:HIS:NE2	1:A:378:ASP:OD2	2.45	0.47
2:B:8:ARG:NH1	4:N:120:GLN:OE1	2.48	0.47
2:B:274:THR:OG1	2:B:314:ARG:NH2	2.48	0.47
5:R:620:LEU:HG	7:L:600:SER:HB3	1.96	0.47
5:R:621:THR:HG21	5:R:625:TYR:HE2	1.77	0.47
6:S:230:MET:CG	6:S:239:PHE:CE1	2.97	0.47
6:S:177:PHE:HB2	6:S:228:TYR:HB2	1.96	0.47
2:B:278:PHE:CE1	2:B:285:LEU:HD12	2.36	0.47
2:B:313:ASN:ND2	2:B:332:TRP:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:674:ASP:CB	5:R:689:VAL:HG11	2.44	0.47
5:R:845:TRP:CD1	7:L:607:LEU:C	2.88	0.47
5:R:866:PHE:HA	5:R:869:ILE:HG12	1.97	0.47
1:A:232:ARG:CD	4:N:100:PRO:HB3	2.44	0.46
4:N:38:ARG:HD3	4:N:48:VAL:HG22	1.97	0.46
4:N:37:VAL:HG22	4:N:47:TRP:HA	1.97	0.46
1:A:232:ARG:HD2	4:N:100:PRO:HB2	1.98	0.46
2:B:30:LEU:HD13	3:G:34:ALA:HB1	1.96	0.46
2:B:295:ASN:OD1	2:B:304:ARG:NH2	2.49	0.46
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.97	0.46
1:A:291:LEU:HB3	1:A:294:GLN:HE21	1.79	0.46
6:S:35:HIS:NE2	6:S:101:TYR:OH	2.41	0.46
6:S:95:TYR:CE1	6:S:114:GLY:CA	2.98	0.46
2:B:256:ARG:NH2	3:G:32:LYS:O	2.49	0.46
5:R:715:LEU:O	5:R:803:GLN:NE2	2.48	0.46
6:S:40:ALA:HB3	6:S:43:LYS:HB3	1.98	0.46
1:A:42:ARG:HG2	1:A:222:PHE:HE2	1.80	0.45
5:R:787:CYS:SG	5:R:842:PHE:CE1	3.10	0.45
2:B:57:LYS:HB2	2:B:332:TRP:CD1	2.52	0.45
5:R:667:LEU:O	5:R:671:PHE:HB2	2.16	0.45
6:S:39:GLN:NE2	6:S:95:TYR:HE2	2.15	0.45
4:N:45:LEU:HD23	4:N:113:THR:HA	1.99	0.45
5:R:691:VAL:HG22	5:R:753:TYR:CE1	2.51	0.45
2:B:256:ARG:O	3:G:28:ILE:N	2.45	0.45
1:A:253:TYR:HA	1:A:266:LEU:HB2	1.99	0.45
7:L:601:4PH:HD1	7:L:601:4PH:O	2.17	0.45
1:A:279:ASN:HA	4:N:106:ASP:CG	2.36	0.45
2:B:70:LEU:HG	2:B:82:TRP:HB2	1.99	0.45
5:R:772:ILE:HD12	5:R:782:VAL:HG21	1.99	0.45
5:R:744:ILE:HA	5:R:747:THR:HG22	1.99	0.45
6:S:93:MET:HE2	6:S:95:TYR:HE1	1.81	0.45
4:N:52:SER:HB3	4:N:57:SER:HB3	1.99	0.44
5:R:693:LEU:HD23	5:R:771:TRP:HE3	1.68	0.44
6:S:27:PHE:CZ	6:S:98:ARG:CD	3.00	0.44
1:A:352:SER:HB2	4:N:105:ARG:CZ	2.45	0.44
5:R:772:ILE:HD12	5:R:782:VAL:HG23	1.98	0.44
5:R:694:HIS:NE2	5:R:781:THR:HG22	2.33	0.44
5:R:855:LEU:HA	5:R:858:ILE:HG22	1.98	0.44
6:S:45:LEU:HD12	6:S:239:PHE:CD2	2.53	0.44
2:B:226:GLU:HB2	4:N:27:PHE:HB3	2.00	0.44
4:N:94:TYR:CD1	4:N:94:TYR:N	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:653:PRO:HA	5:R:656:ILE:HG22	1.99	0.44
6:S:93:MET:HE2	6:S:95:TYR:CE1	2.53	0.44
1:A:23:SER:O	1:A:27:GLU:HG3	2.18	0.44
1:A:266:LEU:HD23	1:A:312:PHE:HE2	1.83	0.44
1:A:281:TRP:HH2	2:B:290:ASP:HB3	1.83	0.44
1:A:27:GLU:CG	2:B:89:LYS:HD2	2.49	0.43
2:B:264:TYR:HB3	2:B:297:TRP:CD2	2.53	0.43
1:A:22:ARG:O	1:A:25:MET:CB	2.66	0.43
1:A:44:LEU:HD23	1:A:244:ILE:HG12	2.00	0.43
2:B:288:GLY:H	2:B:318:LEU:CD2	2.27	0.43
5:R:623:ILE:HA	5:R:626:ILE:CG1	2.48	0.43
6:S:109:ASP:OD1	6:S:109:ASP:N	2.49	0.43
1:A:14:ALA:HA	1:A:17:LYS:HB2	2.00	0.43
5:R:697:LEU:HD22	5:R:771:TRP:CZ2	2.54	0.43
5:R:701:PHE:HB3	5:R:789:ILE:HG13	2.00	0.43
2:B:192:LEU:HD23	2:B:199:PHE:HB3	2.00	0.43
5:R:786:PHE:CE2	7:L:605:LEU:CD1	3.02	0.43
2:B:152:LEU:HD13	2:B:196:THR:HG22	2.01	0.42
4:N:29:PHE:HE2	4:N:72:ARG:HG3	1.82	0.42
5:R:694:HIS:HB2	5:R:753:TYR:HE2	1.84	0.42
4:N:33:LYS:HB3	4:N:99:CYS:SG	2.59	0.42
7:L:607:LEU:HD13	7:L:607:LEU:HA	1.90	0.42
2:B:165:THR:HA	2:B:180:PHE:O	2.19	0.42
5:R:771:TRP:CE3	5:R:771:TRP:HA	2.54	0.42
2:B:330:GLY:HA2	2:B:336:LEU:HA	2.02	0.42
2:B:284:LEU:HD12	2:B:296:VAL:CG1	2.42	0.42
4:N:39:GLN:C	4:N:92:ALA:HB1	2.40	0.42
5:R:787:CYS:O	5:R:791:LEU:N	2.42	0.42
1:A:43:LEU:HD13	1:A:245:ILE:HD11	2.02	0.42
4:N:93:VAL:O	4:N:93:VAL:CG1	2.66	0.42
6:S:91:THR:HB	6:S:119:VAL:HG22	2.02	0.42
2:B:288:GLY:N	2:B:318:LEU:CD2	2.83	0.42
5:R:690:ALA:HB1	5:R:753:TYR:CD2	2.45	0.42
3:G:54:VAL:HG12	3:G:59:ASN:HB2	2.01	0.41
5:R:702:THR:HG21	5:R:738:PRO:CG	2.50	0.41
5:R:781:THR:O	5:R:785:TYR:CB	2.64	0.41
5:R:858:ILE:HG23	5:R:859:PHE:N	2.34	0.41
2:B:66:ASP:N	2:B:66:ASP:OD1	2.50	0.41
2:B:39:PRO:HG3	2:B:301:LYS:HE2	2.03	0.41
6:S:159:CYS:SG	6:S:229:CYS:CB	3.07	0.41
1:A:293:LYS:HD3	1:A:296:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:ALA:O	2:B:243:THR:HA	2.21	0.41
1:A:20:VAL:CG1	1:A:24:LYS:NZ	2.84	0.41
1:A:292:ASN:HA	1:A:364:THR:HB	2.03	0.41
2:B:148:CYS:HB3	2:B:190:LEU:HB2	2.03	0.41
5:R:737:ILE:HA	5:R:740:VAL:HG12	2.03	0.41
5:R:772:ILE:CD1	5:R:782:VAL:CG2	2.97	0.41
6:S:12:VAL:HG13	6:S:119:VAL:HG12	2.02	0.41
6:S:200:PRO:HB2	6:S:202:ARG:HG2	2.03	0.41
7:L:599:ILE:CD1	7:L:600:SER:O	2.62	0.41
2:B:245:SER:OG	2:B:247:ASP:OD1	2.26	0.41
5:R:620:LEU:HG	7:L:600:SER:CB	2.51	0.41
5:R:845:TRP:CD1	7:L:607:LEU:HB2	2.42	0.41
1:A:232:ARG:NE	4:N:100:PRO:HB3	2.36	0.41
1:A:373:ARG:O	1:A:373:ARG:HD3	2.20	0.41
1:A:230:GLU:O	1:A:234:TRP:NE1	2.48	0.41
2:B:210:LEU:HD22	2:B:255:LEU:HG	2.03	0.41
5:R:623:ILE:CD1	5:R:858:ILE:HA	2.38	0.41
5:R:771:TRP:CZ2	7:L:604:LEU:HA	2.55	0.41
6:S:111:TRP:HB2	6:S:184:SER:HB2	2.03	0.41
1:A:245:ILE:HA	1:A:288:ILE:O	2.21	0.40
1:A:292:ASN:OD1	1:A:293:LYS:N	2.49	0.40
5:R:778:PHE:HZ	7:L:606:ASP:H	1.67	0.40
5:R:785:TYR:O	5:R:789:ILE:HG12	2.21	0.40
6:S:142:GLN:NE2	6:S:229:CYS:SG	2.94	0.40
2:B:22:ARG:HB3	2:B:259:GLN:HB3	2.03	0.40
2:B:79:LEU:HD22	2:B:114:CYS:SG	2.61	0.40
2:B:225:HIS:ND1	2:B:229:ILE:HG12	2.35	0.40
2:B:256:ARG:HB3	3:G:28:ILE:HD12	2.03	0.40
6:S:151:PRO:HB2	6:S:152:GLY:H	1.74	0.40
2:B:148:CYS:O	2:B:160:SER:N	2.50	0.40
5:R:674:ASP:OD2	5:R:770:CYS:HB2	2.22	0.40
2:B:286:LEU:CD2	2:B:327:VAL:CG1	2.97	0.40
6:S:86:LEU:HD23	6:S:86:LEU:HA	1.87	0.40
4:N:90:ASP:OD1	4:N:90:ASP:N	2.44	0.40
6:S:173:TYR:HB3	6:S:232:HIS:HB2	2.04	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	224/361 (62%)	222 (99%)	2 (1%)	0	100	100
2	B	336/358 (94%)	314 (94%)	22 (6%)	0	100	100
3	G	53/58 (91%)	52 (98%)	1 (2%)	0	100	100
4	N	124/128 (97%)	118 (95%)	6 (5%)	0	100	100
5	R	237/1149 (21%)	230 (97%)	7 (3%)	0	100	100
6	S	210/250 (84%)	198 (94%)	12 (6%)	0	100	100
7	L	8/15 (53%)	7 (88%)	1 (12%)	0	100	100
All	All	1192/2319 (51%)	1141 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	207/315 (66%)	207 (100%)	0	100	100
2	B	281/299 (94%)	281 (100%)	0	100	100
3	G	45/47 (96%)	45 (100%)	0	100	100
4	N	104/106 (98%)	104 (100%)	0	100	100
5	R	212/1014 (21%)	212 (100%)	0	100	100
6	S	186/202 (92%)	185 (100%)	1 (0%)	86	92
7	L	9/13 (69%)	9 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1044/1996 (52%)	1043 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	S	97	VAL

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

Mol	Chain	Res	Type
1	A	59	GLN
3	G	18	GLN
6	S	179	GLN
6	S	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	4PH	L	601	7	11,12,13	5.00	6 (54%)	12,15,17	4.68	11 (91%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	4PH	L	601	7	-	3/5/6/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	601	4PH	CE1-CD1	7.76	1.52	1.38
7	L	601	4PH	CE2-CD2	7.60	1.52	1.38
7	L	601	4PH	CD2-CG	6.99	1.53	1.38
7	L	601	4PH	CD1-CG	6.91	1.53	1.38
7	L	601	4PH	CE1-CZ	5.35	1.53	1.38
7	L	601	4PH	CE2-CZ	5.23	1.53	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	601	4PH	CD1-CE1-CZ	-6.71	112.39	121.38
7	L	601	4PH	CD2-CE2-CZ	-6.51	112.66	121.38
7	L	601	4PH	CE1-CD1-CG	-6.47	112.12	121.03
7	L	601	4PH	CE2-CD2-CG	-6.46	112.14	121.03
7	L	601	4PH	CB-CG-CD2	-5.27	110.44	120.91
7	L	601	4PH	CD1-CG-CD2	-3.98	111.90	118.17
7	L	601	4PH	C33-CZ-CE1	-3.50	110.00	120.94
7	L	601	4PH	C33-CZ-CE2	-3.25	110.79	120.94
7	L	601	4PH	CE1-CZ-CE2	-3.08	111.36	118.11
7	L	601	4PH	CB-CG-CD1	-2.80	115.34	120.91
7	L	601	4PH	CB-CA-C	-2.32	107.12	111.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	601	4PH	C-CA-CB-CG
7	L	601	4PH	N-CA-CB-CG
7	L	601	4PH	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	L	601	4PH	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

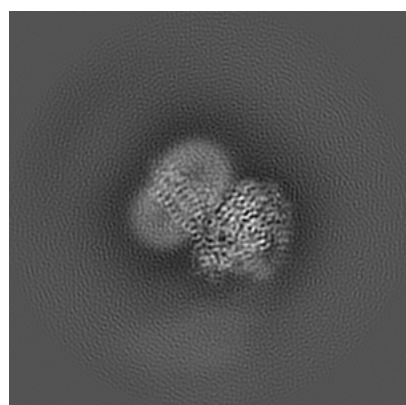
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32836. These allow visual inspection of the internal detail of the map and identification of artifacts.

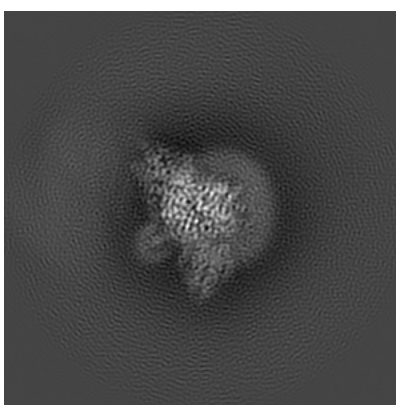
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

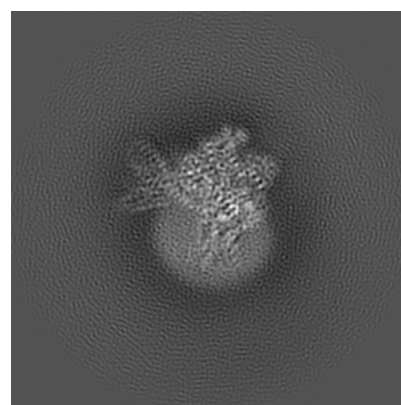
6.1.1 Primary map



X



Y

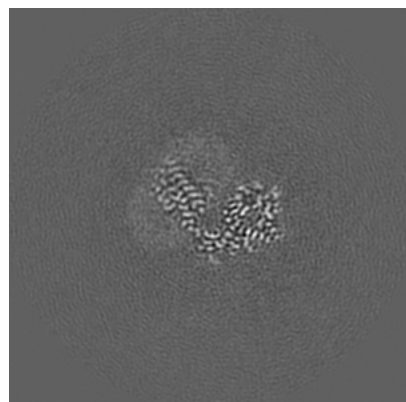


Z

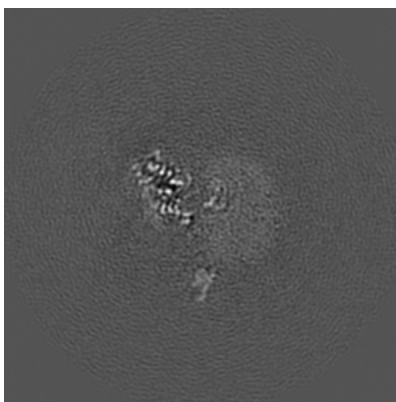
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

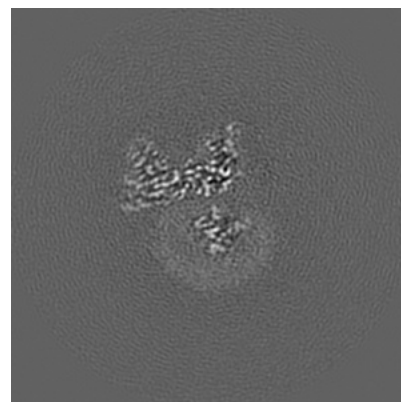
6.2.1 Primary map



X Index: 128



Y Index: 128

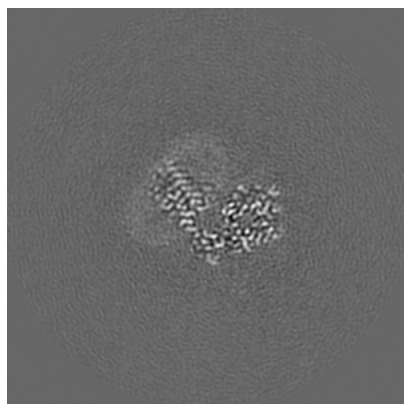


Z Index: 128

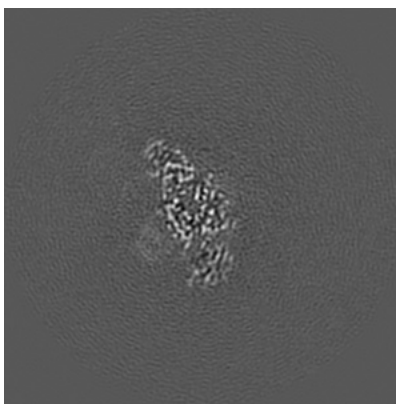
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

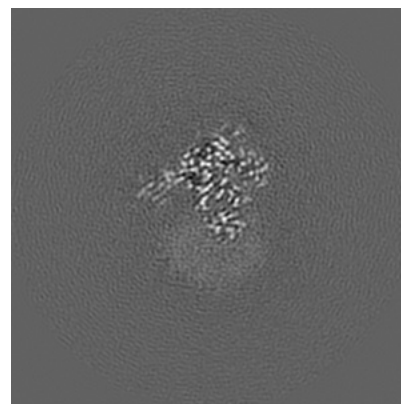
6.3.1 Primary map



X Index: 129



Y Index: 151

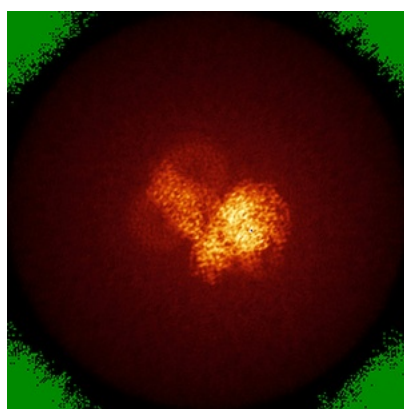


Z Index: 115

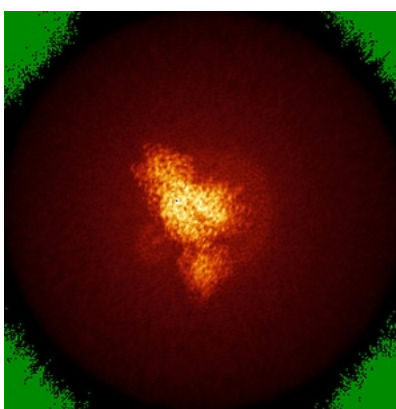
The images above show the largest variance slices of the map in three orthogonal directions.

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

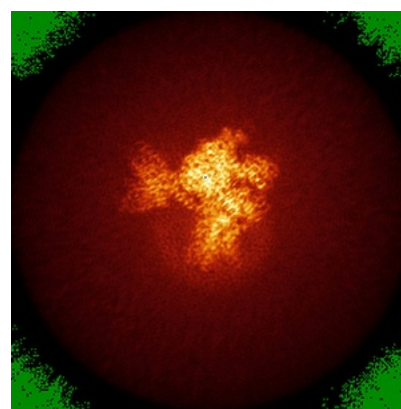
6.4.1 Primary map



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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

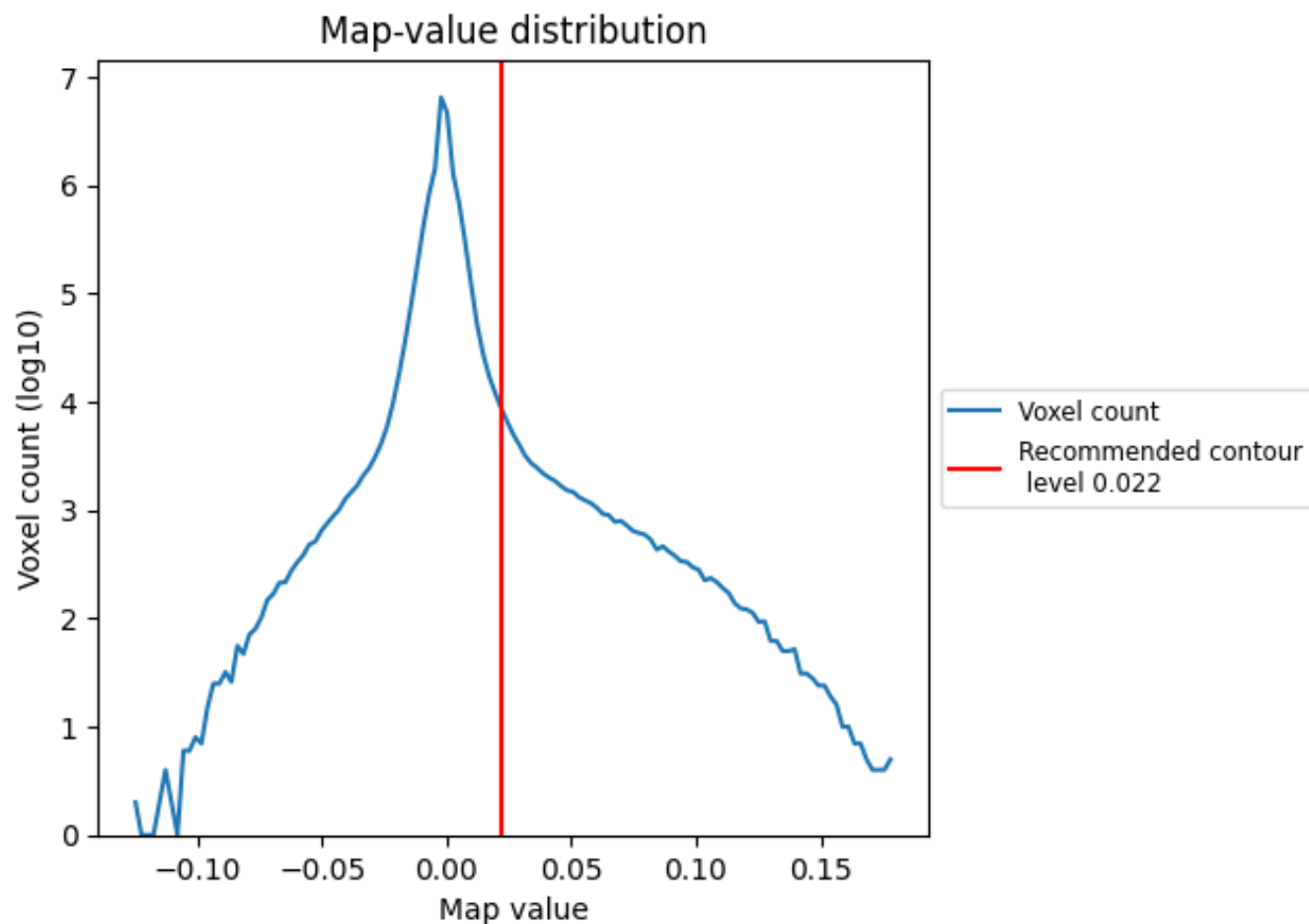
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

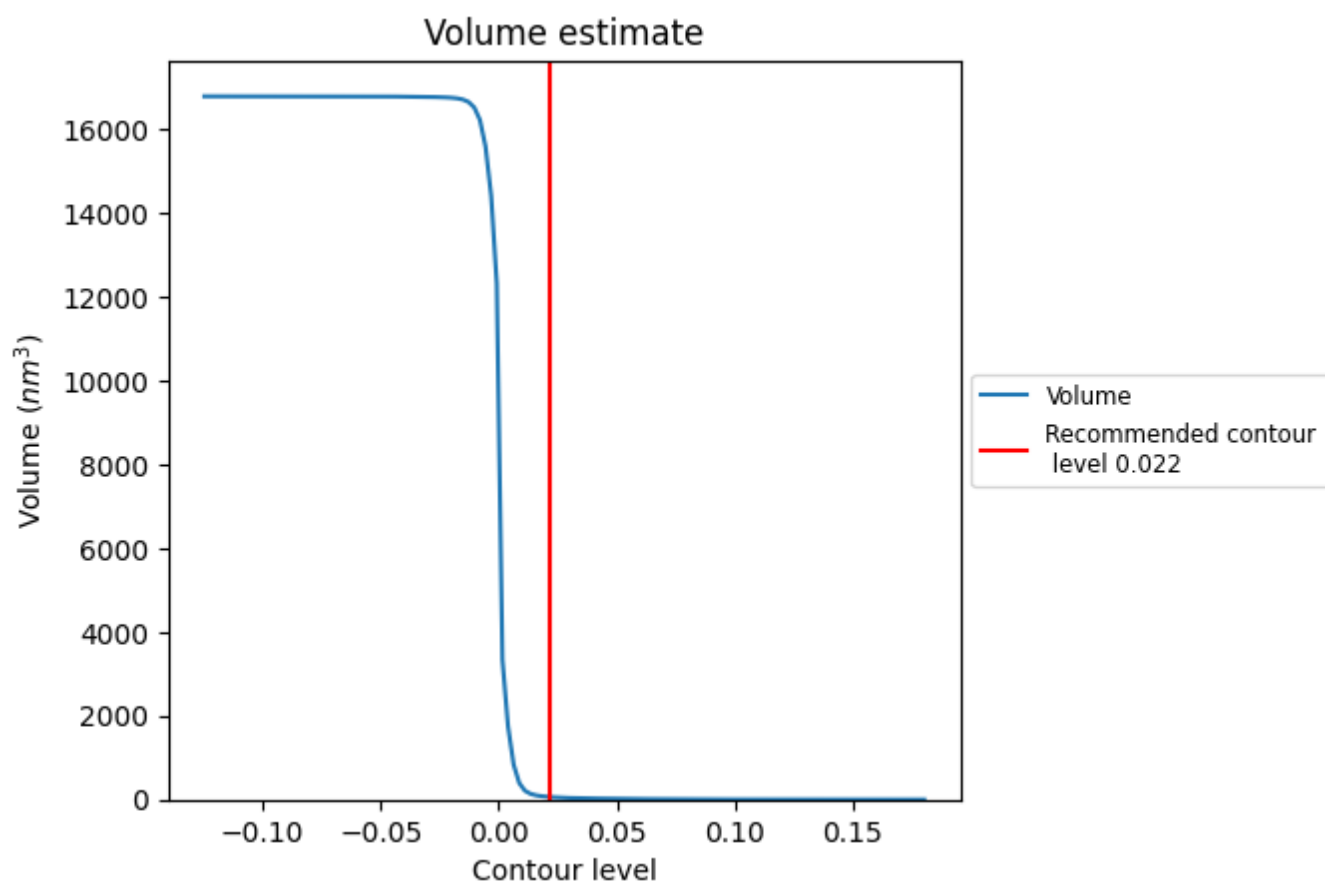
This section contains the results of statistical analysis of the map.

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.

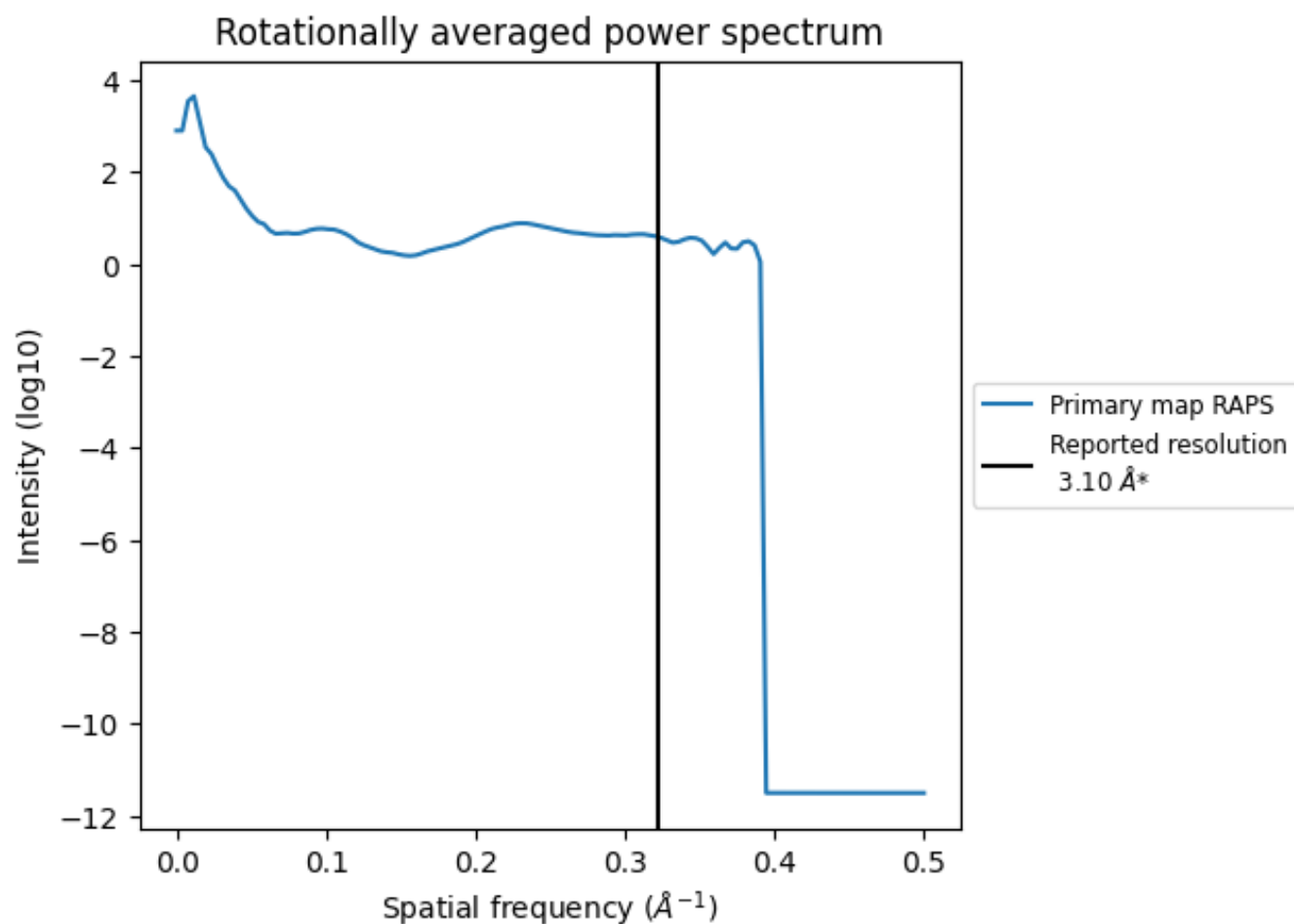
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 60 nm³; this corresponds to an approximate mass of 54 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 0.323 \AA^{-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-32836 and PDB model 7WUI. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



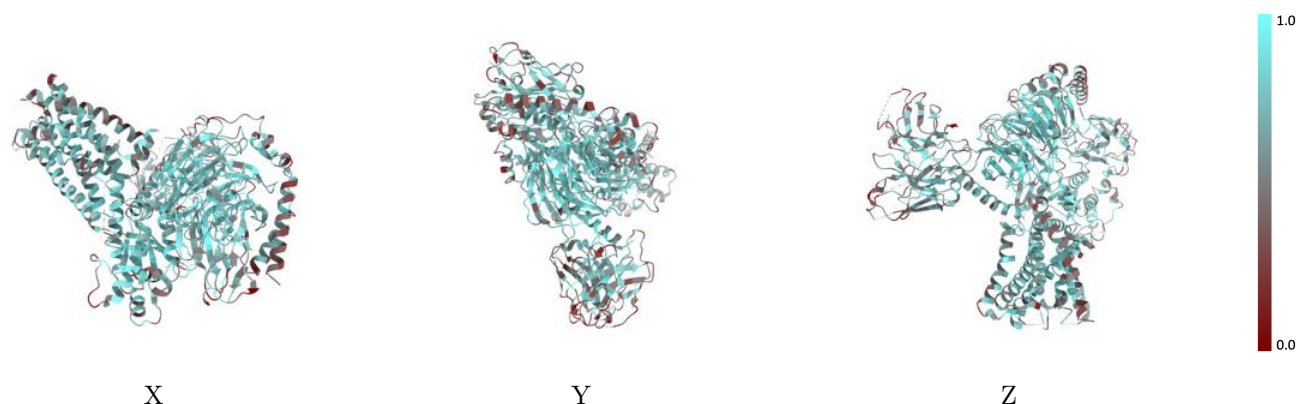
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



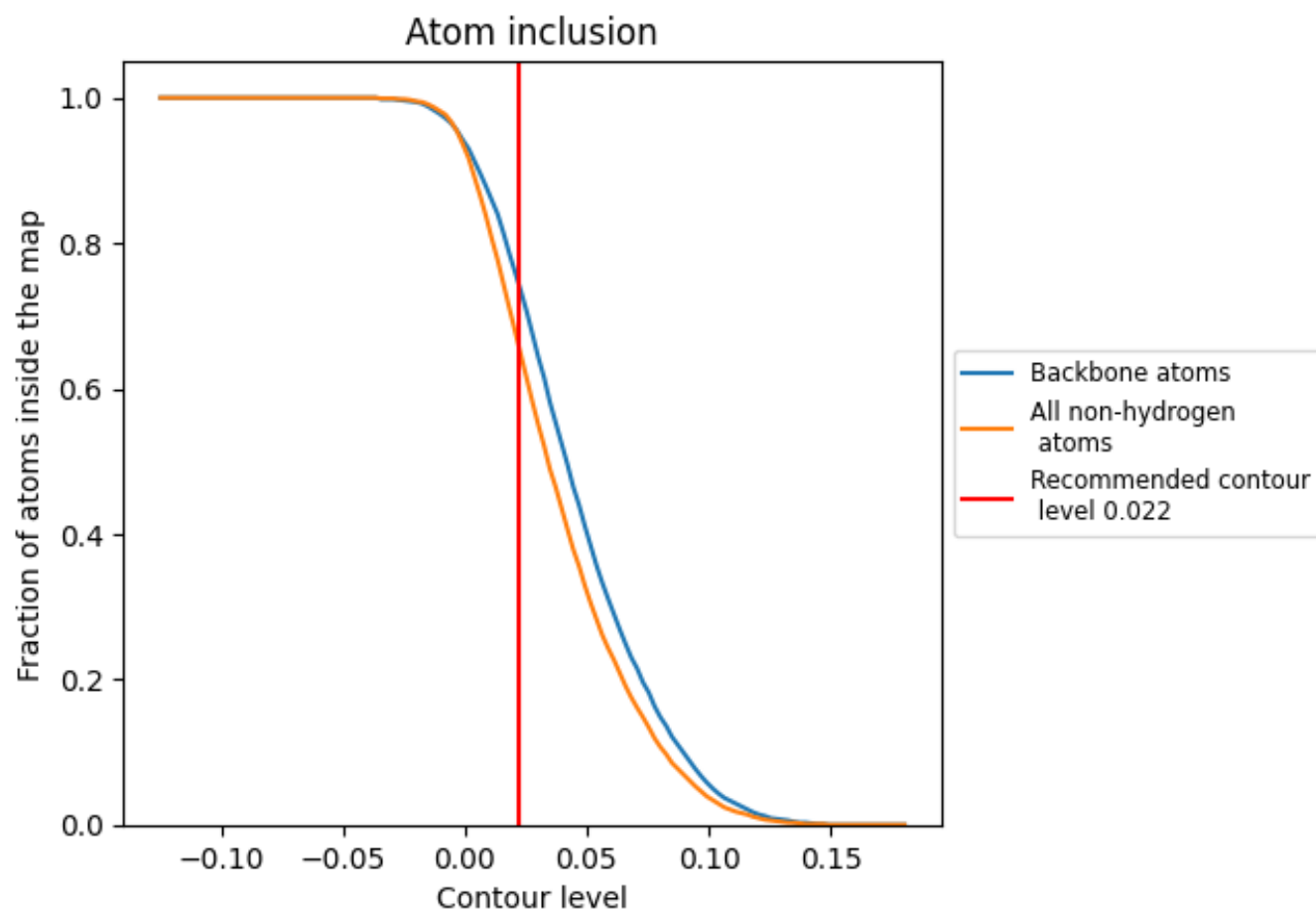
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 66% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.6610</div>	<div><div></div>0.4180</div>
A	<div><div></div>0.7100</div>	<div><div></div>0.4530</div>
B	<div><div></div>0.7190</div>	<div><div></div>0.4330</div>
G	<div><div></div>0.5660</div>	<div><div></div>0.3450</div>
L	<div><div></div>0.5650</div>	<div><div></div>0.4400</div>
N	<div><div></div>0.6440</div>	<div><div></div>0.4080</div>
R	<div><div></div>0.6730</div>	<div><div></div>0.4170</div>
S	<div><div></div>0.5400</div>	<div><div></div>0.3780</div>

1.0

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