Full wwPDB EM Validation Report (i)

Nov 29, 2022 – 07:17 PM JST

PDB ID	:	7WUQ
EMDB ID	:	EMD-32838
Title	:	Tethered peptide activation mechanism of adhesion GPCRs ADGRG2 and ADGRG4
Authors	:	He, Q.T.; Guo, S.C.; Xiao, P.; Sun, J.P.; Yu, X.; Gou, L.; Kong, L.L.; Zhang, L.
Deposited on	:	2022-02-09
Resolution	:	2.90 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:

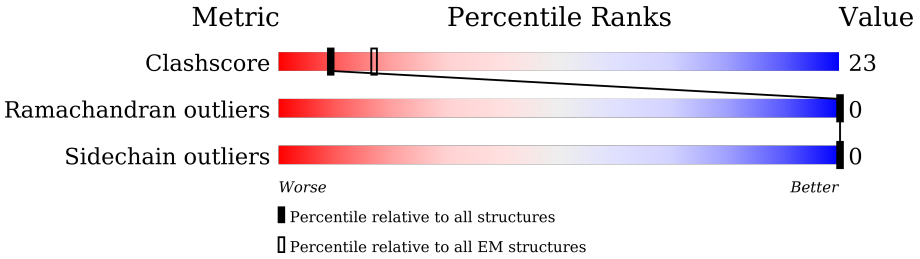
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 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	394	7%, 38%, 16%, 45%
2	B	358	9%, 64%, 29%, 7%
3	G	71	25%, 68%, 10%, 23%
4	N	128	11%, 71%, 28%, .
5	R	683	., 26%, 14%, 59%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7973 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	215	1795	1135	325	330	5	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P63092
A	226	ALA	GLY	engineered mutation	UNP P63092
A	268	ALA	GLU	engineered mutation	UNP P63092
A	271	LYS	ASN	engineered mutation	UNP P63092
A	274	ASP	LYS	engineered mutation	UNP P63092
A	280	LYS	ARG	engineered mutation	UNP P63092
A	284	ASP	THR	engineered mutation	UNP P63092
A	285	THR	ILE	engineered mutation	UNP P63092

- 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
			Total	C	N	O	S		
2	B	334	2564	1583	462	498	21	0	0

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
			Total	C	N	O	S		
3	G	55	421	265	75	78	3	0	0

- Molecule 4 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	127	967	602	169	190	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	R	278	2226	1505	352	355	14	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	581	MET	-	expression tag	UNP Q8CJ12
R	582	LYS	-	expression tag	UNP Q8CJ12
R	583	THR	-	expression tag	UNP Q8CJ12
R	584	ILE	-	expression tag	UNP Q8CJ12
R	585	ILE	-	expression tag	UNP Q8CJ12
R	586	ALA	-	expression tag	UNP Q8CJ12
R	587	LEU	-	expression tag	UNP Q8CJ12

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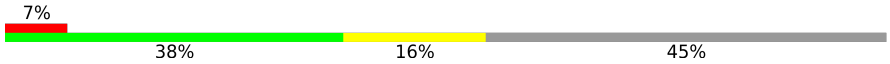
Chain	Residue	Modelled	Actual	Comment	Reference
R	588	SER	-	expression tag	UNP Q8CJ12
R	589	TYR	-	expression tag	UNP Q8CJ12
R	590	ILE	-	expression tag	UNP Q8CJ12
R	591	PHE	-	expression tag	UNP Q8CJ12
R	592	CYS	-	expression tag	UNP Q8CJ12
R	593	LEU	-	expression tag	UNP Q8CJ12
R	594	VAL	-	expression tag	UNP Q8CJ12
R	595	PHE	-	expression tag	UNP Q8CJ12
R	596	ALA	-	expression tag	UNP Q8CJ12
R	1010	HIS	-	linker	UNP Q8CJ12
R	1011	HIS	-	linker	UNP Q8CJ12
R	1012	HIS	-	linker	UNP Q8CJ12
R	1013	HIS	-	linker	UNP Q8CJ12
R	1014	HIS	-	linker	UNP Q8CJ12
R	1015	HIS	-	linker	UNP Q8CJ12
R	1016	HIS	-	linker	UNP Q8CJ12
R	1017	HIS	-	linker	UNP Q8CJ12
R	1018	GLY	-	linker	UNP Q8CJ12
R	1019	SER	-	linker	UNP Q8CJ12
R	1020	ALA	-	linker	UNP Q8CJ12
R	1021	GLU	-	linker	UNP Q8CJ12
R	1022	ASN	-	linker	UNP Q8CJ12
R	1023	LEU	-	linker	UNP Q8CJ12
R	1024	TYR	-	linker	UNP Q8CJ12
R	1025	PHE	-	linker	UNP Q8CJ12
R	1026	GLN	-	linker	UNP Q8CJ12
R	1027	GLY	-	linker	UNP Q8CJ12

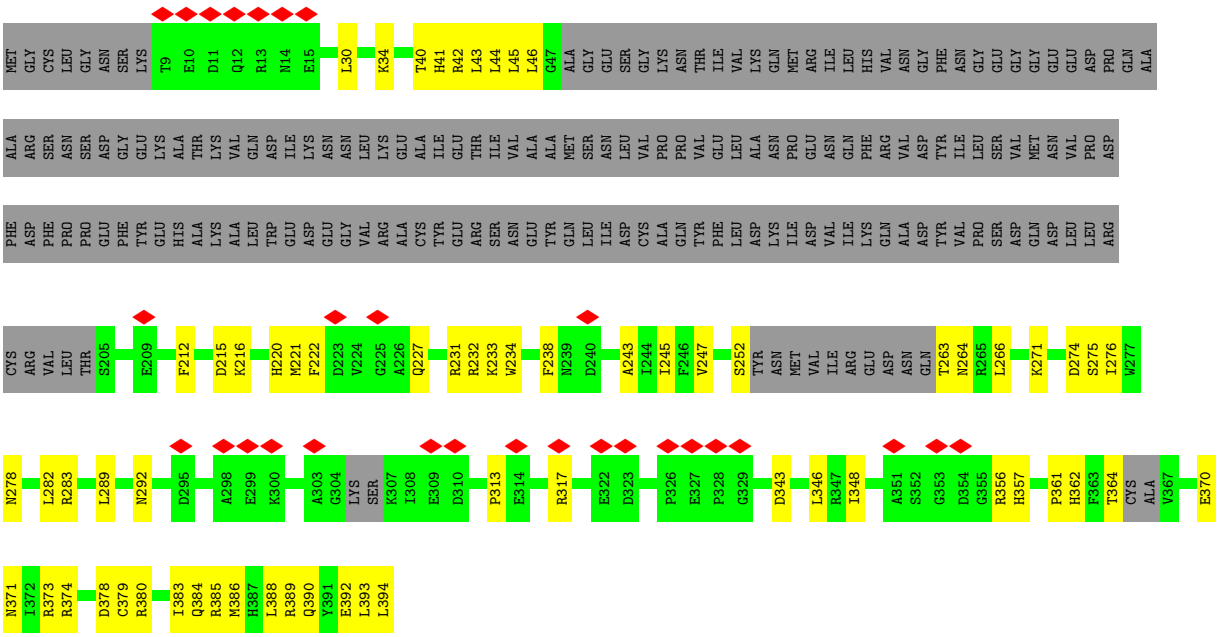
3 Residue-property plots (i)

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: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

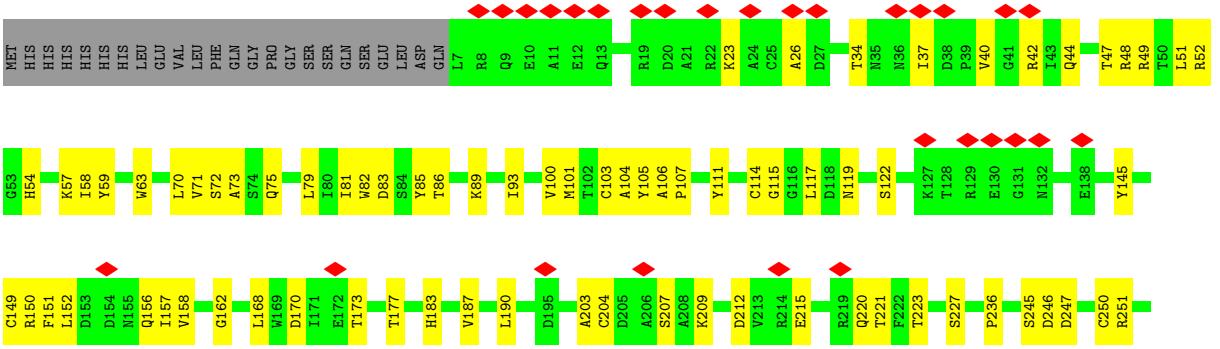
Chain A:





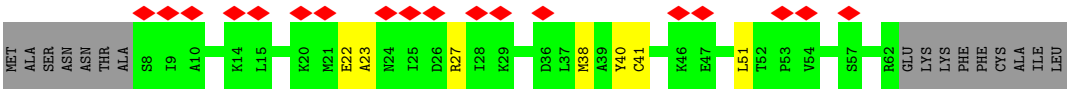
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



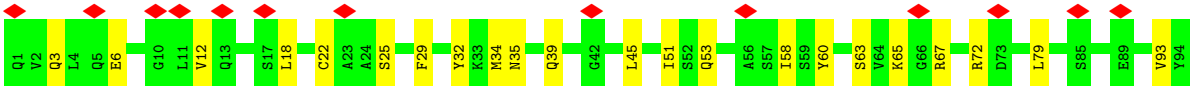
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

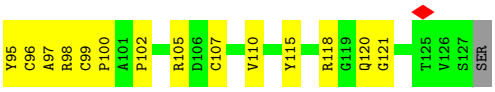
Chain G:



• Molecule 4: Nanobody-35

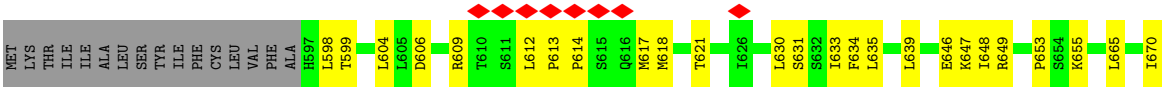
Chain N:

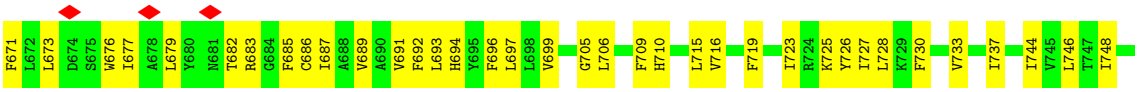


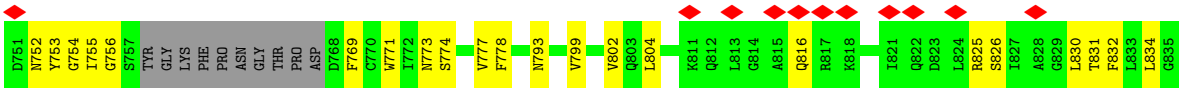


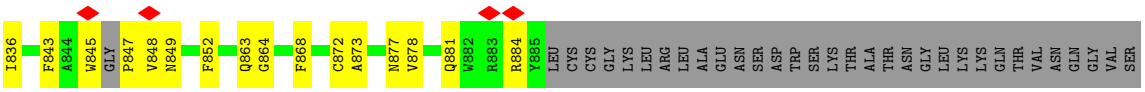
• Molecule 5: Adhesion G-protein coupled receptor G2,mCherry

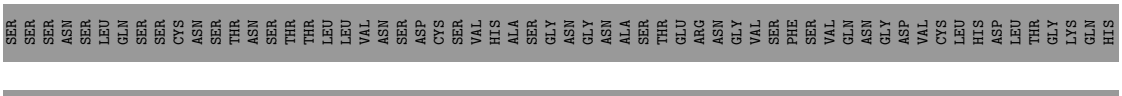
Chain R:

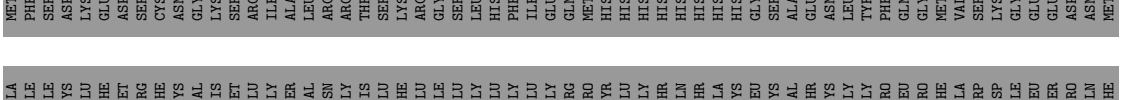


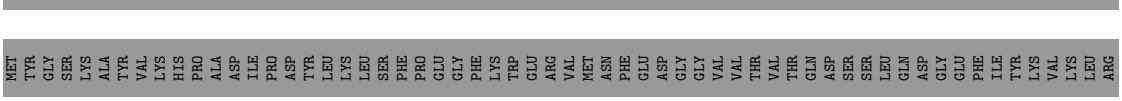












GLY THR ASN PHE PRO SER ASP GLY PRO VAL MET GLN LYS LYS THR MET GLY TRP GLU ALA SER SER GLU ARG MET TYR PRO GLU ASP GLY ALA LEU LYS GLY GLU ILE LYS GLN ARG LEU LYS LEU LYS ASP GLY GLY HIS TYR ASP ALA GLU VAL LYS THR THR TYR LYS ALA LYS LYS

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3743997	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 ($e^-/Å^2$)	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	0.226	Depositor
Minimum map value	-0.155	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.026	Depositor
Map size (Å)	192.0, 192.0, 192.0	wwPDB
Map dimensions	192, 192, 192	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)

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	0.34	0/1828	0.65	0/2456
2	B	0.35	0/2611	0.73	0/3539
3	G	0.28	0/427	0.58	0/576
4	N	0.35	0/987	0.67	0/1337
5	R	0.31	0/2284	0.61	0/3101
All	All	0.34	0/8137	0.66	0/11009

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	1795	0	1766	59	0
2	B	2564	0	2474	100	0
3	G	421	0	434	12	0
4	N	967	0	937	48	0
5	R	2226	0	2302	168	0
All	All	7973	0	7913	358	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 23.

All (358) 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:845:TRP:C	5:R:847:PRO:HD2	1.32	1.47
4:N:95:TYR:CE1	4:N:121:GLY:HA3	1.55	1.41
5:R:845:TRP:CA	5:R:849:ASN:HB2	1.57	1.34
5:R:679:LEU:CD1	5:R:689:VAL:HG11	1.56	1.31
5:R:648:ILE:HD12	5:R:877:ASN:ND2	1.46	1.31
1:A:41:HIS:CE1	1:A:383:ILE:HD13	1.71	1.24
5:R:648:ILE:CD1	5:R:877:ASN:HD22	1.49	1.24
4:N:35:ASN:HB2	4:N:97:ALA:O	1.38	1.21
5:R:598:LEU:HD21	5:R:617:MET:CG	1.74	1.17
5:R:598:LEU:HD21	5:R:617:MET:HG3	1.19	1.14
5:R:630:LEU:HD12	5:R:633:ILE:HD11	1.32	1.11
5:R:634:PHE:CE1	5:R:868:PHE:CE2	2.40	1.10
5:R:845:TRP:O	5:R:847:PRO:HD2	1.52	1.10
5:R:679:LEU:HD11	5:R:689:VAL:HG11	1.34	1.07
5:R:679:LEU:HD12	5:R:689:VAL:HG11	1.32	1.07
1:A:41:HIS:CE1	1:A:383:ILE:CD1	2.37	1.06
5:R:845:TRP:C	5:R:847:PRO:CD	2.25	1.05
5:R:679:LEU:CD1	5:R:689:VAL:CG1	2.33	1.05
2:B:81:ILE:CG2	2:B:105:TYR:HE2	1.68	1.05
5:R:670:ILE:CD1	5:R:692:PHE:HB3	1.87	1.04
5:R:845:TRP:HA	5:R:849:ASN:HB2	1.32	1.03
5:R:670:ILE:CD1	5:R:692:PHE:CB	2.37	1.02
4:N:95:TYR:CE1	4:N:121:GLY:CA	2.44	1.01
5:R:845:TRP:C	5:R:849:ASN:HB2	1.81	1.00
5:R:670:ILE:HD11	5:R:692:PHE:CB	1.92	0.99
5:R:670:ILE:HD12	5:R:692:PHE:HB3	1.45	0.98
2:B:81:ILE:HG23	2:B:105:TYR:HE2	1.26	0.97
5:R:648:ILE:HD12	5:R:877:ASN:HD22	0.83	0.97
5:R:670:ILE:HD11	5:R:692:PHE:HB2	1.42	0.97
5:R:744:ILE:O	5:R:748:ILE:HG12	1.65	0.97
4:N:95:TYR:HE1	4:N:121:GLY:HA3	1.26	0.95
2:B:318:LEU:HD12	2:B:318:LEU:O	1.68	0.94
1:A:43:LEU:HD23	1:A:243:ALA:HB3	1.48	0.93
1:A:42:ARG:HG2	1:A:222:PHE:HE2	1.34	0.93
2:B:37:ILE:HD13	3:G:38:MET:CE	1.99	0.92
2:B:156:GLN:HE21	2:B:168:LEU:HD11	1.31	0.92
5:R:845:TRP:HA	5:R:849:ASN:CB	1.99	0.92
2:B:81:ILE:HG23	2:B:105:TYR:CE2	2.04	0.92
2:B:81:ILE:CG2	2:B:105:TYR:CE2	2.55	0.90
4:N:95:TYR:CD1	4:N:121:GLY:HA3	2.05	0.90
4:N:93:VAL:HG11	4:N:95:TYR:OH	1.72	0.89
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:HIS:HE1	1:A:383:ILE:HD13	1.36	0.88
5:R:634:PHE:HE1	5:R:868:PHE:CE2	1.90	0.88
5:R:845:TRP:CA	5:R:849:ASN:CB	2.49	0.88
5:R:634:PHE:CD1	5:R:868:PHE:CD2	2.63	0.87
5:R:845:TRP:N	5:R:849:ASN:HB2	1.88	0.86
2:B:157:ILE:O	2:B:157:ILE:HG23	1.77	0.85
5:R:673:LEU:O	5:R:677:ILE:HG12	1.76	0.85
4:N:95:TYR:HE1	4:N:120:GLN:O	1.59	0.84
5:R:634:PHE:CD1	5:R:868:PHE:CE2	2.67	0.82
2:B:37:ILE:CD1	3:G:38:MET:CE	2.58	0.81
5:R:755:ILE:HD11	5:R:769:PHE:O	1.81	0.81
5:R:670:ILE:HD13	5:R:692:PHE:C	2.01	0.81
4:N:95:TYR:CD1	4:N:121:GLY:CA	2.64	0.80
5:R:843:PHE:O	5:R:848:VAL:HG23	1.82	0.79
5:R:744:ILE:O	5:R:748:ILE:CG1	2.31	0.79
2:B:288:GLY:N	2:B:318:LEU:HD21	1.98	0.79
5:R:845:TRP:N	5:R:849:ASN:HD22	1.82	0.78
5:R:673:LEU:O	5:R:677:ILE:CG1	2.32	0.78
5:R:648:ILE:HG22	5:R:648:ILE:O	1.83	0.77
5:R:679:LEU:HD11	5:R:689:VAL:CG1	2.06	0.77
5:R:634:PHE:HE1	5:R:868:PHE:CZ	2.03	0.76
4:N:93:VAL:HG12	4:N:95:TYR:CZ	2.22	0.75
4:N:93:VAL:CG1	4:N:95:TYR:CZ	2.71	0.74
2:B:183:HIS:CE1	2:B:209:LYS:HG2	2.22	0.73
4:N:97:ALA:HB1	4:N:110:VAL:HB	1.71	0.73
5:R:744:ILE:O	5:R:748:ILE:CD1	2.36	0.73
1:A:43:LEU:HD21	1:A:379:CYS:SG	2.28	0.72
1:A:43:LEU:CD2	1:A:243:ALA:HB3	2.18	0.72
5:R:682:THR:HG23	5:R:682:THR:O	1.87	0.71
5:R:845:TRP:O	5:R:849:ASN:N	2.20	0.71
5:R:598:LEU:HD21	5:R:617:MET:HG2	1.68	0.71
1:A:41:HIS:CE1	1:A:383:ILE:HD11	2.25	0.71
4:N:35:ASN:CB	4:N:97:ALA:O	2.29	0.71
5:R:694:HIS:HD1	5:R:753:TYR:HH	1.39	0.71
2:B:37:ILE:CD1	3:G:38:MET:HE3	2.21	0.71
5:R:754:GLY:O	5:R:773:ASN:ND2	2.24	0.70
4:N:95:TYR:CE1	4:N:120:GLN:O	2.44	0.68
5:R:845:TRP:H	5:R:849:ASN:HD22	1.40	0.68
2:B:71:VAL:HG12	2:B:105:TYR:HB2	1.75	0.68
5:R:634:PHE:CE1	5:R:868:PHE:CZ	2.80	0.68
5:R:755:ILE:CD1	5:R:769:PHE:O	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:693:LEU:HD21	5:R:769:PHE:CZ	2.30	0.67
5:R:774:SER:OG	5:R:777:VAL:HB	1.95	0.67
5:R:679:LEU:HD13	5:R:686:CYS:HA	1.76	0.66
5:R:673:LEU:O	5:R:677:ILE:CG2	2.43	0.66
5:R:670:ILE:CD1	5:R:692:PHE:C	2.64	0.66
5:R:845:TRP:O	5:R:849:ASN:HB2	1.94	0.66
5:R:845:TRP:C	5:R:849:ASN:CB	2.63	0.65
1:A:392:GLU:OE1	5:R:825:ARG:NH2	2.27	0.65
4:N:95:TYR:HE1	4:N:121:GLY:CA	2.00	0.65
5:R:793:ASN:ND2	5:R:834:LEU:O	2.30	0.65
5:R:634:PHE:HD1	5:R:868:PHE:CD2	2.15	0.64
5:R:845:TRP:HA	5:R:849:ASN:ND2	2.13	0.64
5:R:848:VAL:HB	5:R:852:PHE:CE2	2.33	0.64
4:N:97:ALA:CB	4:N:110:VAL:HB	2.28	0.63
5:R:752:ASN:O	5:R:773:ASN:HB2	1.99	0.63
2:B:75:GLN:NE2	2:B:100:VAL:O	2.31	0.63
5:R:635:LEU:HD13	5:R:864:GLY:CA	2.28	0.63
5:R:848:VAL:HB	5:R:852:PHE:CD2	2.33	0.63
1:A:362:HIS:NE2	1:A:378:ASP:OD2	2.33	0.62
5:R:679:LEU:HD12	5:R:689:VAL:CG1	2.14	0.62
5:R:673:LEU:O	5:R:677:ILE:HG23	2.00	0.62
2:B:318:LEU:HD12	2:B:318:LEU:C	2.20	0.61
2:B:158:VAL:HG13	2:B:190:LEU:HD21	1.82	0.61
2:B:283:ARG:N	3:G:41:CYS:SG	2.74	0.61
5:R:845:TRP:H	5:R:849:ASN:ND2	1.97	0.61
2:B:156:GLN:NE2	2:B:168:LEU:HD11	2.08	0.61
5:R:748:ILE:HD13	5:R:748:ILE:N	2.15	0.61
2:B:72:SER:HG	2:B:82:TRP:HE1	1.47	0.61
5:R:845:TRP:N	5:R:849:ASN:CB	2.63	0.61
2:B:37:ILE:CD1	3:G:38:MET:HE2	2.29	0.61
4:N:35:ASN:ND2	4:N:107:CYS:SG	2.73	0.60
1:A:42:ARG:HG2	1:A:222:PHE:CE2	2.26	0.60
2:B:156:GLN:HE21	2:B:168:LEU:CD1	2.09	0.60
4:N:35:ASN:ND2	4:N:99:CYS:SG	2.72	0.60
1:A:41:HIS:ND1	1:A:383:ILE:HD11	2.16	0.59
2:B:157:ILE:O	2:B:157:ILE:CG2	2.49	0.59
4:N:35:ASN:HD21	4:N:107:CYS:HG	1.50	0.59
5:R:598:LEU:CD2	5:R:617:MET:HG3	2.13	0.59
4:N:39:GLN:HB2	4:N:45:LEU:HD13	1.85	0.59
5:R:633:ILE:HG13	5:R:634:PHE:N	2.16	0.59
4:N:99:CYS:HG	4:N:107:CYS:CB	2.10	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:673:LEU:O	5:R:677:ILE:CD1	2.51	0.58
2:B:325:MET:O	2:B:340:ASN:ND2	2.36	0.58
1:A:46:LEU:HD23	1:A:231:ARG:HH11	1.67	0.58
2:B:114:CYS:SG	2:B:122:SER:OG	2.61	0.58
5:R:631:SER:O	5:R:635:LEU:N	2.28	0.58
5:R:845:TRP:O	5:R:849:ASN:CB	2.52	0.58
5:R:845:TRP:O	5:R:847:PRO:CD	2.42	0.58
4:N:3:GLN:NE2	4:N:25:SER:OG	2.36	0.58
4:N:95:TYR:HE1	4:N:120:GLN:C	2.07	0.58
1:A:313:PRO:HG2	4:N:65:LYS:HB3	1.86	0.57
5:R:687:ILE:HG23	5:R:753:TYR:HB2	1.86	0.57
1:A:289:LEU:HB3	1:A:361:PRO:HA	1.85	0.57
5:R:845:TRP:H	5:R:849:ASN:CB	2.17	0.57
5:R:648:ILE:O	5:R:648:ILE:CG2	2.51	0.56
2:B:106:ALA:HB2	2:B:111:TYR:O	2.05	0.56
2:B:288:GLY:HA3	2:B:318:LEU:HD23	1.87	0.56
5:R:609:ARG:HD3	5:R:778:PHE:CE2	2.40	0.56
5:R:693:LEU:HD21	5:R:769:PHE:CE2	2.39	0.56
2:B:107:PRO:HD3	2:B:151:PHE:HB2	1.86	0.56
5:R:635:LEU:HD13	5:R:864:GLY:HA3	1.87	0.56
5:R:753:TYR:C	5:R:773:ASN:ND2	2.59	0.56
1:A:40:THR:HG23	1:A:220:HIS:HB2	1.87	0.56
5:R:606:ASP:OD1	5:R:609:ARG:HD2	2.05	0.56
2:B:283:ARG:HD3	2:B:300:LEU:HD12	1.87	0.56
5:R:881:GLN:OE1	5:R:884:ARG:NH2	2.38	0.56
4:N:93:VAL:HG11	4:N:95:TYR:CZ	2.39	0.55
5:R:845:TRP:CA	5:R:849:ASN:HD22	2.19	0.55
2:B:37:ILE:HD13	3:G:38:MET:HE2	1.84	0.55
5:R:648:ILE:HG21	5:R:878:VAL:HG22	1.89	0.55
1:A:380:ARG:NH2	5:R:716:VAL:O	2.39	0.55
1:A:384:GLN:NE2	5:R:715:LEU:O	2.40	0.55
2:B:170:ASP:HB3	2:B:173:THR:HG22	1.89	0.55
5:R:647:LYS:HD3	5:R:881:GLN:HE22	1.72	0.55
1:A:232:ARG:HG3	1:A:233:LYS:HG2	1.89	0.55
5:R:845:TRP:HA	5:R:849:ASN:CG	2.27	0.55
1:A:274:ASP:OD1	1:A:278:ASN:ND2	2.40	0.55
2:B:106:ALA:CB	2:B:111:TYR:O	2.55	0.55
4:N:63:SER:O	4:N:67:ARG:NH1	2.40	0.55
2:B:47:THR:HG23	2:B:337:LYS:HB3	1.88	0.54
5:R:673:LEU:O	5:R:677:ILE:HD13	2.07	0.54
2:B:59:TYR:CD2	2:B:101:MET:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:PRO:HD3	2:B:151:PHE:CB	2.38	0.54
2:B:149:CYS:O	2:B:150:ARG:NH1	2.39	0.54
5:R:604:LEU:HD13	5:R:697:LEU:HD13	1.88	0.54
1:A:232:ARG:HH21	2:B:204:CYS:HB3	1.72	0.54
1:A:215:ASP:OD2	1:A:373:ARG:NH1	2.40	0.54
1:A:227:GLN:NE2	2:B:119:ASN:OD1	2.41	0.54
1:A:283:ARG:O	1:A:357:HIS:ND1	2.41	0.54
2:B:49:ARG:NH1	2:B:85:TYR:O	2.41	0.53
2:B:156:GLN:NE2	2:B:168:LEU:HD21	2.22	0.53
2:B:145:TYR:O	2:B:162:GLY:N	2.41	0.53
5:R:843:PHE:O	5:R:848:VAL:CG2	2.53	0.53
1:A:386:MET:SD	1:A:390:GLN:NE2	2.82	0.53
5:R:609:ARG:NH2	5:R:778:PHE:CG	2.76	0.53
5:R:843:PHE:CD1	5:R:843:PHE:N	2.73	0.53
2:B:251:ARG:NH1	2:B:263:THR:OG1	2.41	0.53
5:R:598:LEU:CD2	5:R:617:MET:CG	2.68	0.53
5:R:754:GLY:O	5:R:773:ASN:OD1	2.27	0.53
1:A:234:TRP:HB2	2:B:117:LEU:HD21	1.91	0.53
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.90	0.52
5:R:606:ASP:OD2	5:R:609:ARG:HD2	2.09	0.52
2:B:54:HIS:NE2	2:B:72:SER:OG	2.37	0.52
5:R:598:LEU:HA	5:R:621:THR:HG21	1.91	0.52
2:B:58:ILE:O	2:B:316:SER:OG	2.28	0.52
5:R:670:ILE:CD1	5:R:692:PHE:HB2	2.17	0.52
5:R:771:TRP:NE1	5:R:778:PHE:CE1	2.71	0.52
5:R:676:TRP:HA	5:R:676:TRP:CE3	2.45	0.52
2:B:288:GLY:CA	2:B:318:LEU:HD23	2.40	0.52
1:A:30:LEU:O	1:A:34:LYS:HB2	2.10	0.52
5:R:755:ILE:HG22	5:R:756:GLY:N	2.24	0.52
5:R:683:ARG:CZ	5:R:687:ILE:HD11	2.39	0.52
5:R:639:LEU:HD12	5:R:665:LEU:HD13	1.92	0.52
2:B:37:ILE:HD11	3:G:38:MET:CE	2.37	0.51
2:B:250:CYS:HB3	2:B:273:ILE:HD13	1.91	0.51
5:R:752:ASN:O	5:R:773:ASN:ND2	2.41	0.51
5:R:753:TYR:O	5:R:773:ASN:ND2	2.43	0.51
1:A:393:LEU:HD23	5:R:826:SER:HB2	1.93	0.51
4:N:99:CYS:SG	4:N:107:CYS:CB	2.99	0.51
5:R:706:LEU:HD11	5:R:733:VAL:HG13	1.92	0.51
2:B:331:SER:OG	2:B:332:TRP:N	2.44	0.51
5:R:799:VAL:HA	5:R:802:VAL:HG12	1.93	0.51
5:R:683:ARG:NE	5:R:687:ILE:HD11	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD11	5:R:830:LEU:HD13	1.92	0.51
4:N:51:ILE:HG13	4:N:58:ILE:HG12	1.92	0.51
5:R:733:VAL:HG23	5:R:737:ILE:HD12	1.93	0.51
5:R:845:TRP:HA	5:R:849:ASN:HD22	1.76	0.51
2:B:187:VAL:HA	2:B:203:ALA:HA	1.94	0.50
5:R:725:LYS:HB3	5:R:728:LEU:HB3	1.92	0.50
2:B:73:ALA:HB2	2:B:103:CYS:HB3	1.92	0.50
5:R:670:ILE:HD13	5:R:693:LEU:N	2.26	0.50
5:R:696:PHE:HA	5:R:699:VAL:HG22	1.94	0.50
5:R:831:THR:HG23	5:R:836:ILE:HB	1.92	0.50
2:B:100:VAL:HG23	2:B:115:GLY:H	1.77	0.50
5:R:655:LYS:HD3	5:R:727:ILE:HG13	1.93	0.49
2:B:220:GLN:HA	3:G:22:GLU:HG3	1.94	0.49
4:N:115:TYR:HD2	4:N:118:ARG:HB2	1.77	0.49
5:R:754:GLY:O	5:R:773:ASN:CG	2.51	0.49
4:N:93:VAL:HG12	4:N:95:TYR:CE2	2.47	0.49
5:R:671:PHE:CE2	5:R:769:PHE:CZ	3.01	0.49
1:A:263:THR:OG1	1:A:264:ASN:N	2.45	0.48
5:R:744:ILE:O	5:R:748:ILE:HD13	2.10	0.48
1:A:233:LYS:NZ	2:B:246:ASP:OD2	2.37	0.48
2:B:288:GLY:CA	2:B:318:LEU:CD2	2.91	0.48
5:R:687:ILE:O	5:R:691:VAL:HG23	2.12	0.48
1:A:317:ARG:O	1:A:317:ARG:HG2	2.14	0.48
1:A:356:ARG:HB2	1:A:389:ARG:HD2	1.96	0.48
1:A:390:GLN:HB3	5:R:653:PRO:HG2	1.96	0.48
2:B:212:ASP:HB3	2:B:215:GLU:HB2	1.95	0.48
2:B:288:GLY:N	2:B:318:LEU:CD2	2.74	0.48
5:R:647:LYS:CD	5:R:881:GLN:HE22	2.26	0.48
1:A:346:LEU:HD11	1:A:361:PRO:HG3	1.96	0.48
2:B:168:LEU:O	2:B:177:THR:N	2.47	0.48
5:R:832:PHE:HB3	5:R:863:GLN:HG3	1.95	0.48
5:R:705:GLY:O	5:R:709:PHE:N	2.42	0.48
5:R:609:ARG:NH2	5:R:778:PHE:CB	2.77	0.48
2:B:318:LEU:O	2:B:318:LEU:CD1	2.53	0.47
5:R:604:LEU:HD22	5:R:697:LEU:HD22	1.94	0.47
2:B:42:ARG:HH11	2:B:306:GLY:HA2	1.80	0.47
2:B:321:THR:OG1	2:B:325:MET:N	2.46	0.47
2:B:83:ASP:OD2	2:B:86:THR:OG1	2.33	0.47
2:B:275:SER:OG	2:B:317:CYS:HA	2.15	0.47
1:A:44:LEU:HD22	1:A:238:PHE:CG	2.50	0.47
2:B:34:THR:HG21	2:B:300:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ILE:HG21	2:B:105:TYR:CE2	2.43	0.47
5:R:606:ASP:CG	5:R:609:ARG:HD2	2.34	0.47
5:R:723:ILE:HB	5:R:726:TYR:HD1	1.79	0.47
1:A:385:ARG:HA	1:A:388:LEU:HD12	1.98	0.46
2:B:57:LYS:HD2	2:B:332:TRP:CE2	2.50	0.46
2:B:207:SER:HA	2:B:223:THR:HA	1.95	0.46
5:R:646:GLU:HA	5:R:649:ARG:HE	1.80	0.46
5:R:670:ILE:CD1	5:R:693:LEU:N	2.79	0.46
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.98	0.46
5:R:634:PHE:HD1	5:R:868:PHE:CG	2.33	0.46
1:A:371:ASN:OD1	1:A:374:ARG:NH1	2.48	0.46
4:N:6:GLU:HA	4:N:22:CYS:HA	1.97	0.46
4:N:98:ARG:HH21	4:N:100:PRO:HA	1.81	0.46
5:R:673:LEU:HA	5:R:677:ILE:HG23	1.98	0.45
5:R:868:PHE:HA	5:R:872:CYS:HB3	1.98	0.45
2:B:63:TRP:O	2:B:105:TYR:HB3	2.15	0.45
1:A:252:SER:HB3	1:A:266:LEU:HB3	1.98	0.45
1:A:384:GLN:HG2	5:R:715:LEU:HA	1.99	0.45
2:B:37:ILE:HD11	3:G:38:MET:HE3	1.95	0.45
2:B:320:VAL:HG12	2:B:321:THR:N	2.32	0.45
5:R:693:LEU:CD2	5:R:769:PHE:CZ	2.98	0.45
4:N:22:CYS:SG	4:N:79:LEU:HB3	2.57	0.45
5:R:635:LEU:HD23	5:R:665:LEU:HB2	1.99	0.45
5:R:683:ARG:CZ	5:R:687:ILE:CD1	2.94	0.45
1:A:364:THR:HG22	1:A:371:ASN:HD21	1.80	0.45
1:A:276:ILE:HG23	1:A:282:LEU:HD13	1.97	0.45
1:A:370:GLU:O	1:A:370:GLU:HG3	2.17	0.45
5:R:653:PRO:HD3	5:R:710:HIS:CE1	2.52	0.45
1:A:271:LYS:HD2	1:A:271:LYS:HA	1.82	0.45
2:B:52:ARG:O	2:B:89:LYS:NZ	2.50	0.44
4:N:35:ASN:ND2	4:N:110:VAL:HG11	2.33	0.44
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.99	0.44
1:A:41:HIS:CD2	5:R:719:PHE:HD1	2.34	0.44
1:A:278:ASN:OD1	4:N:105:ARG:NE	2.47	0.44
2:B:23:LYS:HA	2:B:26:ALA:HB2	2.00	0.44
2:B:327:VAL:O	2:B:339:TRP:N	2.49	0.44
2:B:227:SER:OG	4:N:100:PRO:O	2.32	0.44
5:R:679:LEU:CD1	5:R:689:VAL:HG12	2.37	0.44
5:R:635:LEU:HD13	5:R:864:GLY:C	2.37	0.44
1:A:389:ARG:HG2	1:A:394:LEU:HB2	2.00	0.44
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:99:CYS:SG	4:N:107:CYS:HB2	2.58	0.43
5:R:635:LEU:HB3	5:R:665:LEU:HD12	2.00	0.43
1:A:44:LEU:O	1:A:245:ILE:N	2.52	0.43
1:A:364:THR:CG2	1:A:371:ASN:HD21	2.31	0.43
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.35	0.43
4:N:93:VAL:CG1	4:N:95:TYR:CE2	3.01	0.43
4:N:95:TYR:CE1	4:N:120:GLN:C	2.88	0.43
4:N:32:TYR:O	4:N:72:ARG:NH2	2.45	0.43
2:B:57:LYS:HB2	2:B:332:TRP:CD1	2.53	0.43
2:B:275:SER:O	2:B:318:LEU:HD21	2.18	0.43
4:N:60:TYR:HB2	4:N:65:LYS:HG3	2.00	0.43
1:A:275:SER:OG	4:N:107:CYS:O	2.36	0.43
2:B:245:SER:OG	2:B:247:ASP:OD1	2.36	0.43
4:N:34:MET:HB3	4:N:79:LEU:HD22	2.01	0.43
1:A:212:PHE:HE1	1:A:221:MET:HB2	1.83	0.43
4:N:53:GLN:NE2	4:N:102:PRO:O	2.52	0.43
1:A:343:ASP:HA	1:A:346:LEU:HB2	2.01	0.42
3:G:23:ALA:HA	3:G:27:ARG:HH22	1.84	0.42
5:R:693:LEU:HG	5:R:771:TRP:CZ3	2.54	0.42
1:A:388:LEU:HD22	5:R:804:LEU:HD13	2.01	0.42
5:R:682:THR:O	5:R:682:THR:CG2	2.59	0.42
2:B:48:ARG:HE	2:B:340:ASN:HB2	1.83	0.42
5:R:679:LEU:HD23	5:R:679:LEU:HA	1.71	0.42
5:R:679:LEU:HD21	5:R:685:PHE:CD1	2.54	0.42
5:R:694:HIS:ND1	5:R:753:TYR:OH	2.40	0.42
1:A:274:ASP:HA	1:A:348:ILE:HG21	2.02	0.42
4:N:12:VAL:HG21	4:N:18:LEU:HD12	2.01	0.42
1:A:45:LEU:CD2	1:A:247:VAL:HG23	2.50	0.42
5:R:599:THR:H	5:R:621:THR:HG23	1.84	0.42
5:R:730:PHE:HA	5:R:733:VAL:HG12	2.02	0.42
5:R:868:PHE:O	5:R:873:ALA:N	2.51	0.42
2:B:290:ASP:HA	2:B:314:ARG:HG2	2.02	0.41
5:R:612:LEU:HB2	5:R:617:MET:CE	2.50	0.41
5:R:848:VAL:HB	5:R:852:PHE:HE2	1.83	0.41
5:R:613:PRO:HA	5:R:614:PRO:HD3	1.91	0.41
2:B:42:ARG:HG3	2:B:44:GLN:HG2	2.02	0.41
2:B:152:LEU:HB2	2:B:156:GLN:HB3	2.03	0.41
2:B:286:LEU:HD13	2:B:296:VAL:HB	2.02	0.41
2:B:156:GLN:HE21	2:B:168:LEU:HD21	1.83	0.41
5:R:618:MET:SD	5:R:618:MET:O	2.79	0.41
1:A:393:LEU:HA	5:R:826:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:HA	2:B:48:ARG:HD3	1.87	0.41
2:B:275:SER:CB	2:B:318:LEU:H	2.33	0.41
4:N:6:GLU:HG3	4:N:22:CYS:HB3	2.02	0.41
5:R:618:MET:O	5:R:618:MET:HE3	2.20	0.41
5:R:746:LEU:HD23	5:R:746:LEU:HA	1.91	0.41
2:B:70:LEU:O	2:B:82:TRP:N	2.51	0.41
4:N:29:PHE:HE1	4:N:72:ARG:HB2	1.85	0.41
2:B:40:VAL:HG21	3:G:51:LEU:HD22	2.02	0.41
4:N:96:CYS:O	4:N:96:CYS:SG	2.78	0.41
2:B:57:LYS:HE2	2:B:75:GLN:HG3	2.01	0.41
4:N:35:ASN:HD22	4:N:110:VAL:HG11	1.86	0.41
1:A:216:LYS:HE2	1:A:216:LYS:HB2	1.86	0.41
2:B:103:CYS:O	2:B:103:CYS:SG	2.79	0.41
5:R:673:LEU:CA	5:R:677:ILE:HG23	2.51	0.41
5:R:752:ASN:O	5:R:773:ASN:CB	2.67	0.41
2:B:287:ALA:C	2:B:318:LEU:HD21	2.40	0.41
1:A:247:VAL:HG13	1:A:292:ASN:HB2	2.02	0.40
2:B:209:LYS:HB3	2:B:221:THR:HG23	2.04	0.40
5:R:816:GLN:H	5:R:816:GLN:HG3	1.72	0.40
2:B:104:ALA:HB2	2:B:149:CYS:O	2.21	0.40
2:B:151:PHE:CZ	2:B:157:ILE:HD12	2.57	0.40
2:B:317:CYS:SG	2:B:317:CYS:O	2.79	0.40
5:R:753:TYR:C	5:R:773:ASN:HD21	2.24	0.40
1:A:370:GLU:O	1:A:370:GLU:CG	2.70	0.40
5:R:679:LEU:HD13	5:R:689:VAL:CG1	2.44	0.40
5:R:609:ARG:NH2	5:R:778:PHE:CD2	2.89	0.40
5:R:848:VAL:HB	5:R:852:PHE:HD2	1.83	0.40
2:B:236:PRO:HB2	3:G:40:TYR:CE1	2.57	0.40
5:R:754:GLY:C	5:R:773:ASN:HD21	2.25	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	205/394 (52%)	199 (97%)	6 (3%)	0	100	100
2	B	332/358 (93%)	307 (92%)	25 (8%)	0	100	100
3	G	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
4	N	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
5	R	272/683 (40%)	264 (97%)	8 (3%)	0	100	100
All	All	987/1634 (60%)	938 (95%)	49 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/349 (55%)	193 (100%)	0	100	100
2	B	276/299 (92%)	276 (100%)	0	100	100
3	G	44/58 (76%)	44 (100%)	0	100	100
4	N	105/106 (99%)	105 (100%)	0	100	100
5	R	239/592 (40%)	239 (100%)	0	100	100
All	All	857/1404 (61%)	857 (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 (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
2	B	62	HIS
2	B	75	GLN
2	B	156	GLN
5	R	597	HIS
5	R	616	GLN
5	R	773	ASN
5	R	849	ASN

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Mol	Chain	Res	Type
5	R	877	ASN

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)

There are no chain breaks in this entry.

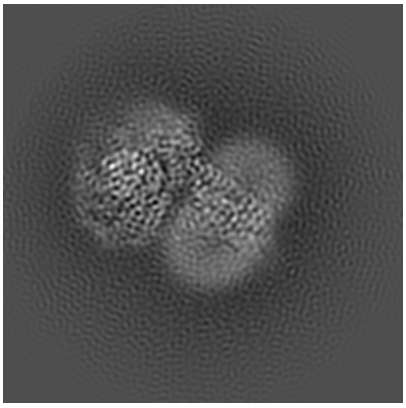
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-32838. These allow visual inspection of the internal detail of the map and identification of artifacts.

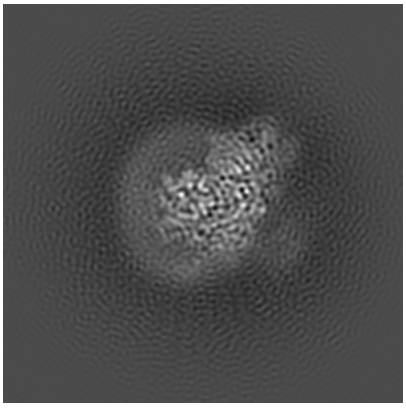
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

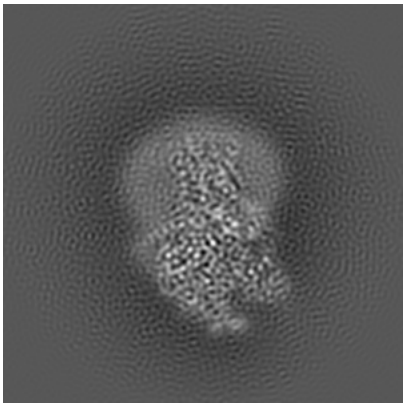
6.1.1 Primary map



X



Y

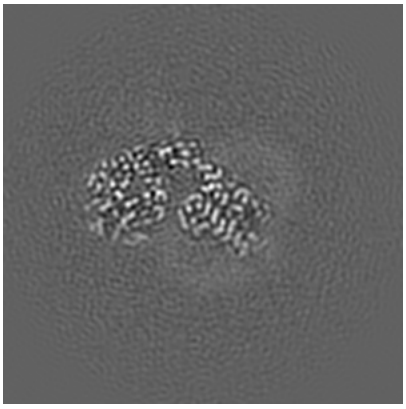


Z

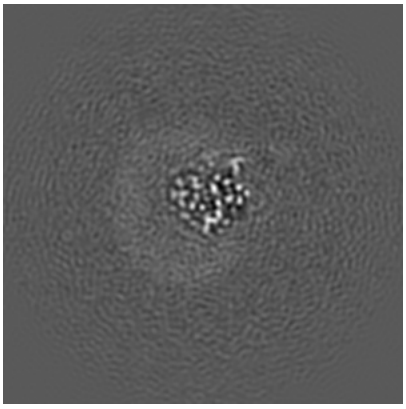
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

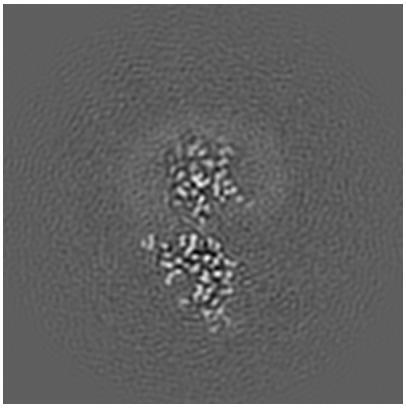
6.2.1 Primary map



X Index: 96



Y Index: 96

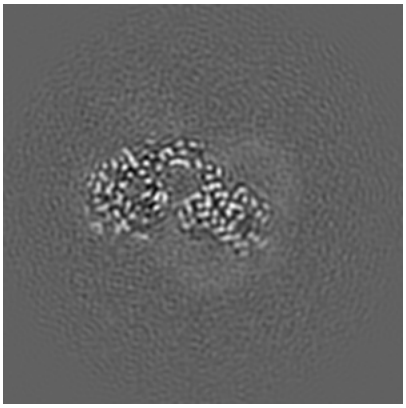


Z Index: 96

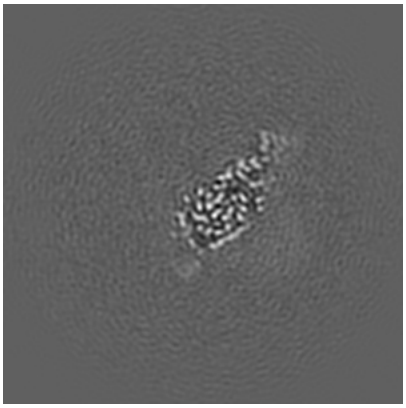
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

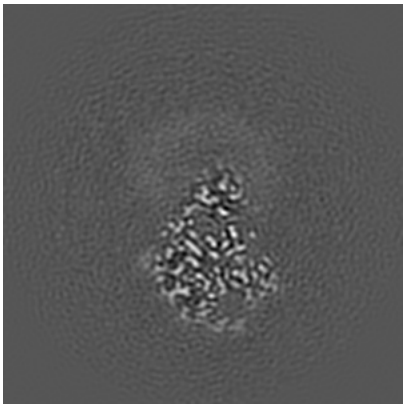
6.3.1 Primary map



X Index: 95



Y Index: 73



Z Index: 109

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.026. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

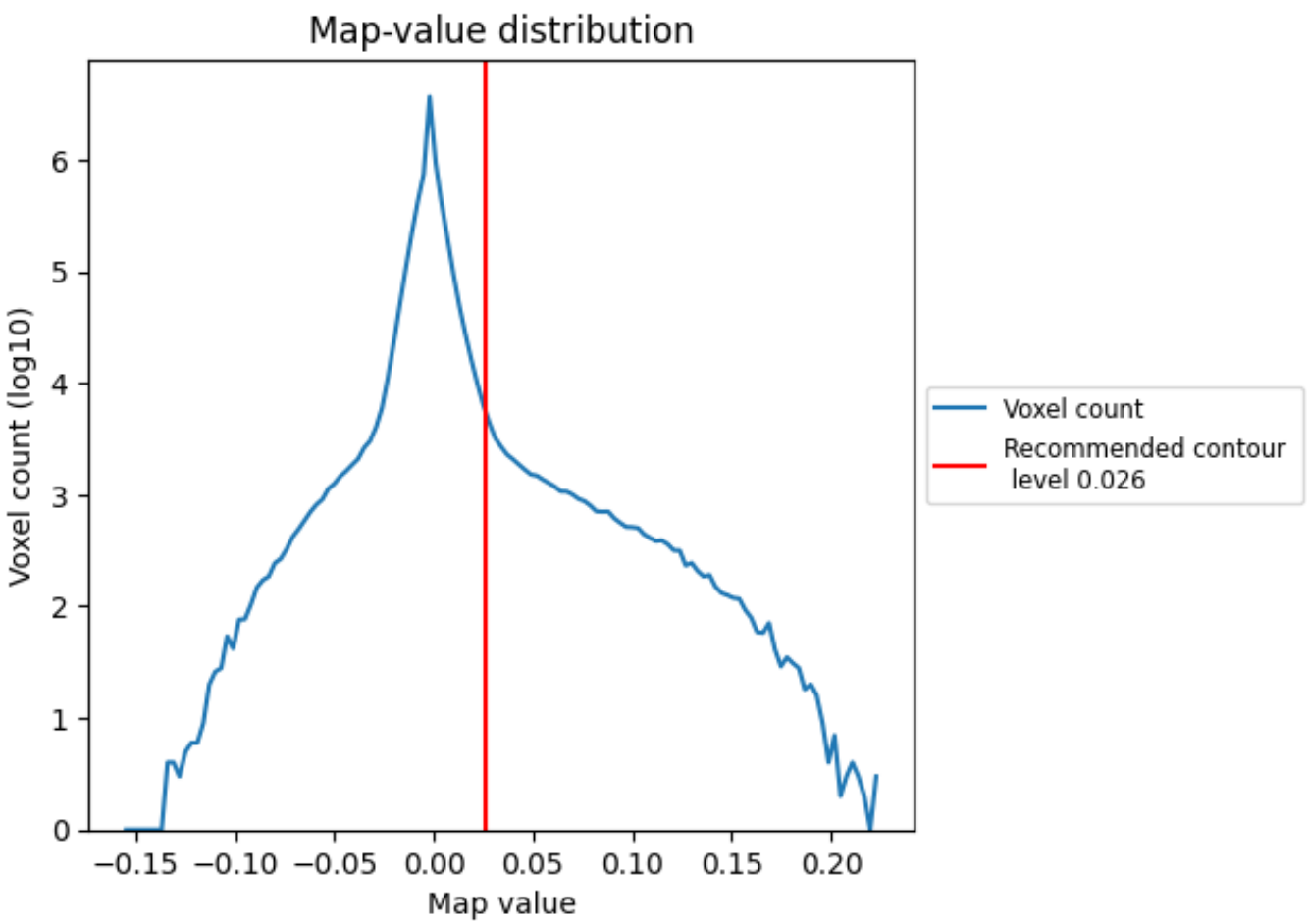
6.5 Mask visualisation (i)

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

7 Map analysis (i)

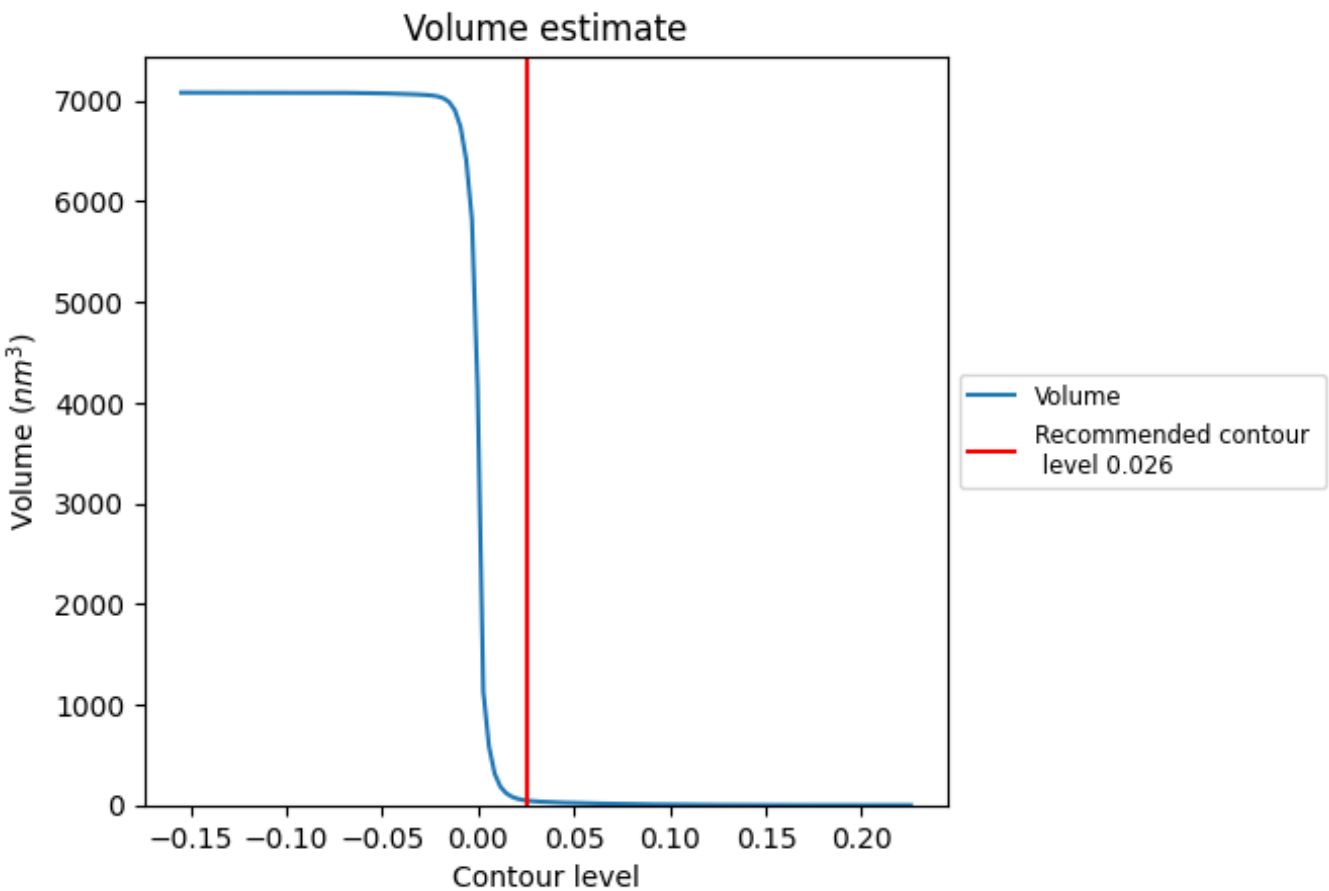
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

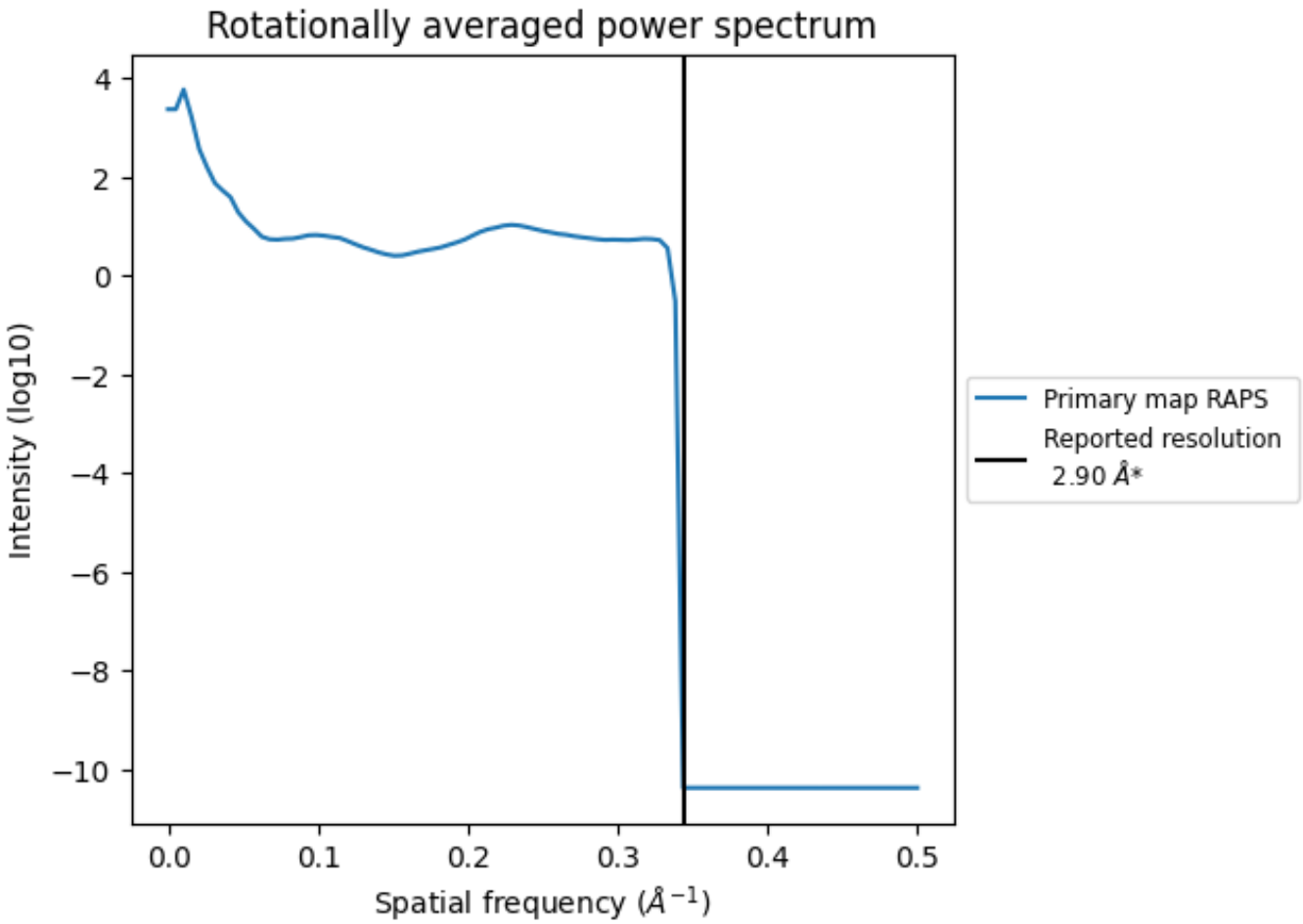
7.2 Volume estimate (i)



The volume at the recommended contour level is 45 nm^3; this corresponds to an approximate mass of 40 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 0.345 Å^{-1}

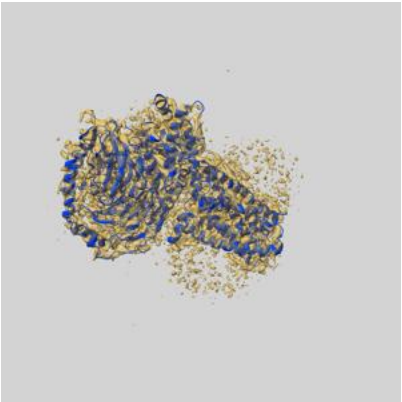
8 Fourier-Shell correlation (i)

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

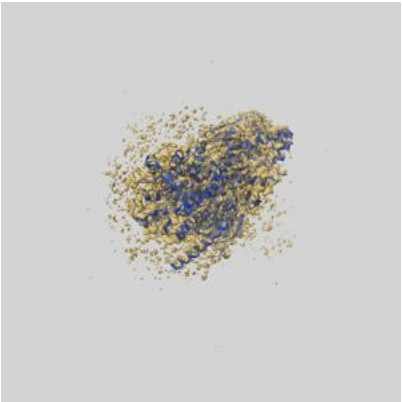
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-32838 and PDB model 7WUQ. Per-residue inclusion information can be found in section 3 on page 6.

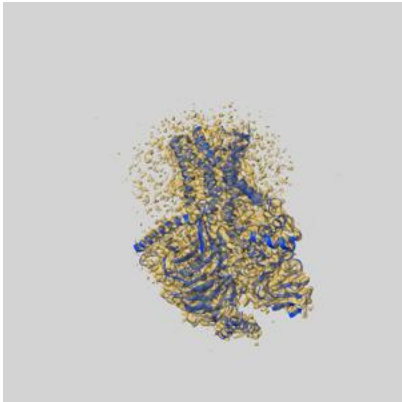
9.1 Map-model overlay (i)



X



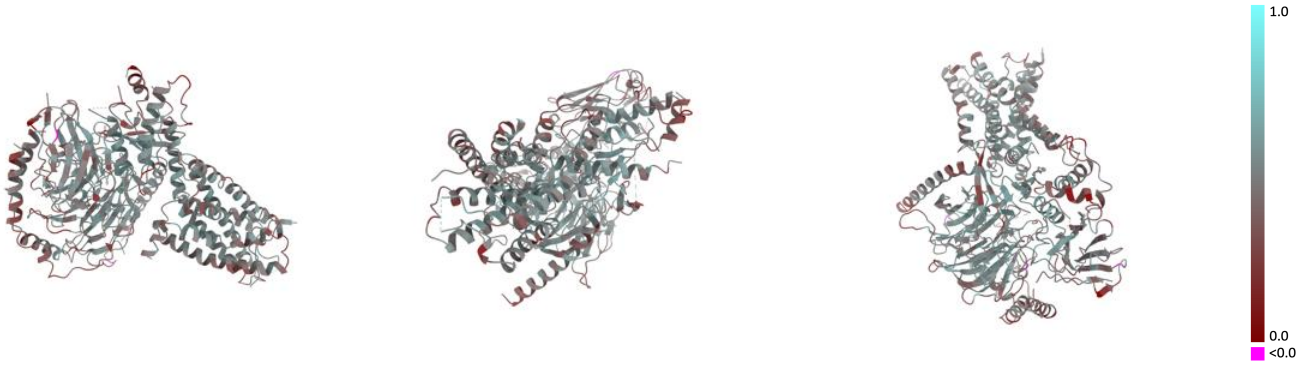
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.026 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.

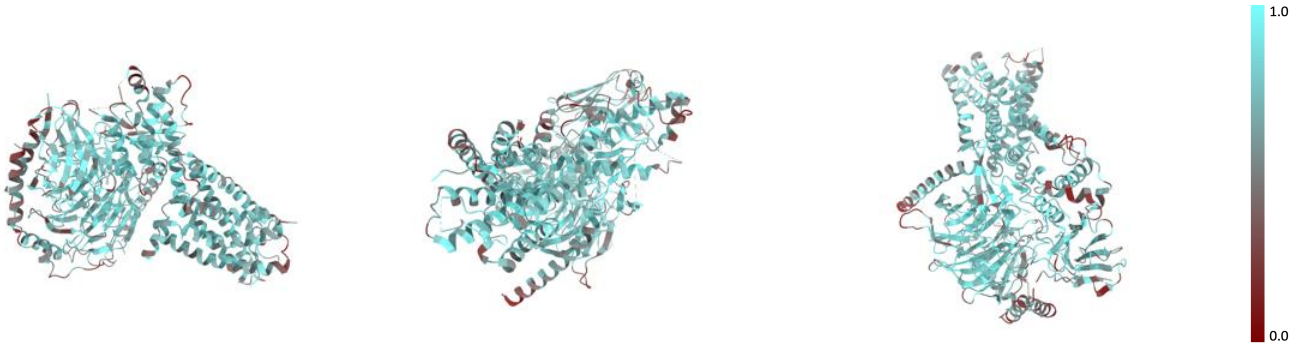
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

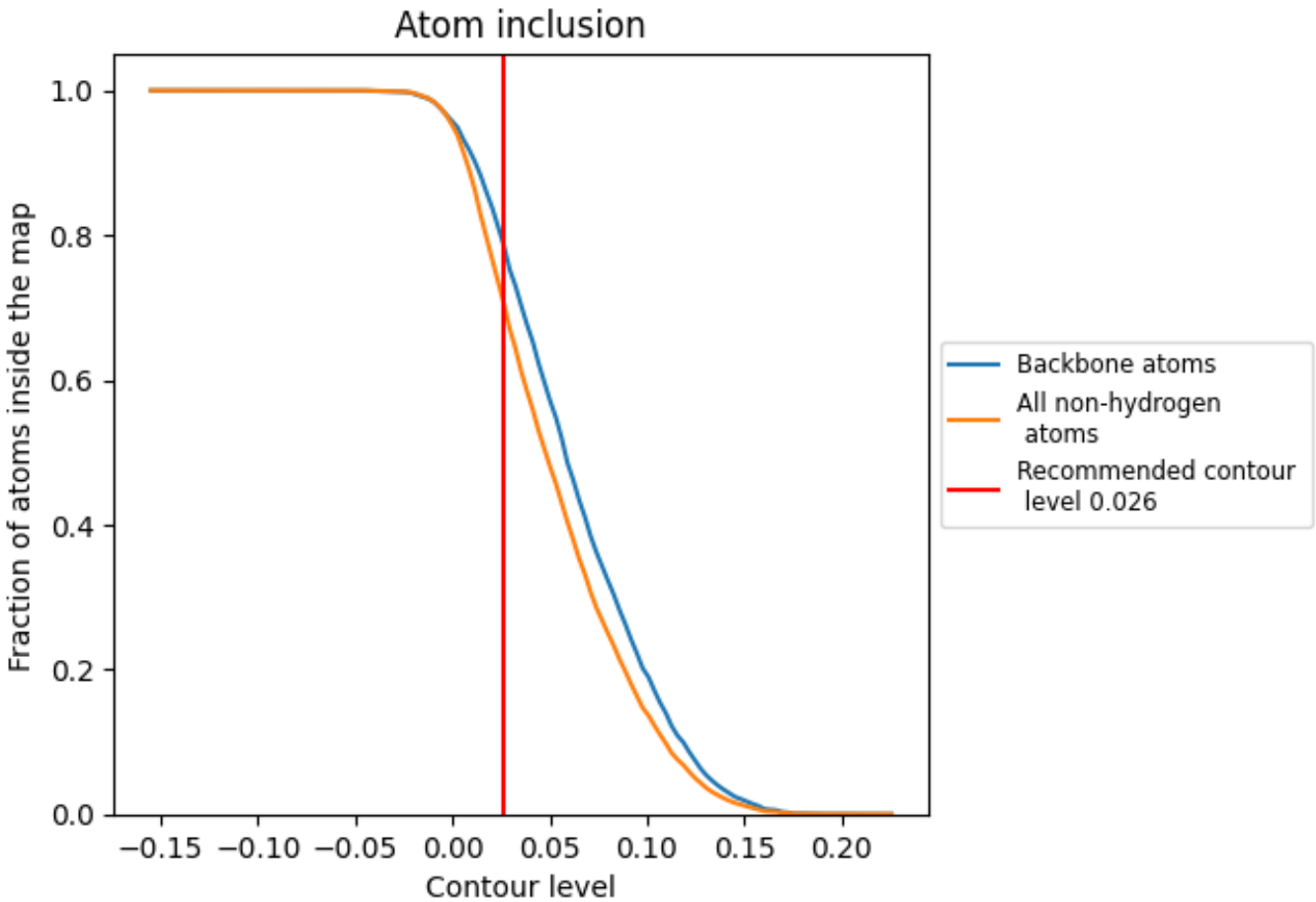
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.026).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 71% 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 (0.026) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7098	0.4650
A	0.7095	0.4660
B	0.7312	0.4690
G	0.5628	0.3790
N	0.7066	0.4620
R	0.7149	0.4780