



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 6GJ1 / pdb_00006gj1
EMDB ID : EMD-0009
Title : The baseplate complex from the type VI secretion system
Authors : Rapisarda, C.; Fronzes, R.
Deposited on : 2018-05-15
Resolution : 4.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

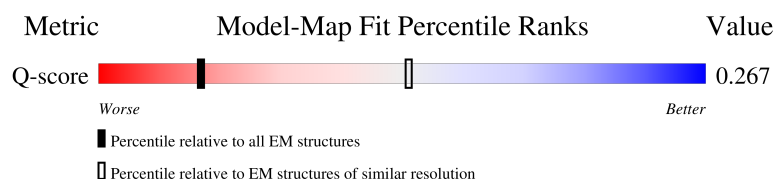
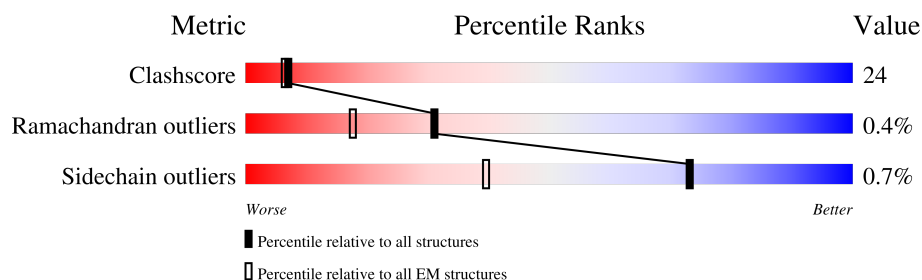
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	
2	C	366	
3	D	143	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13013 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 Putative type VI secretion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	584	Total	C	N	O	S	0	0
			4655	2961	825	844	25		
1	B	583	Total	C	N	O	S	0	0
			4651	2959	824	843	25		

- Molecule 2 is a protein called TssG.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	350	Total	C	N	O	S	0	0
			2737	1739	503	484	11		

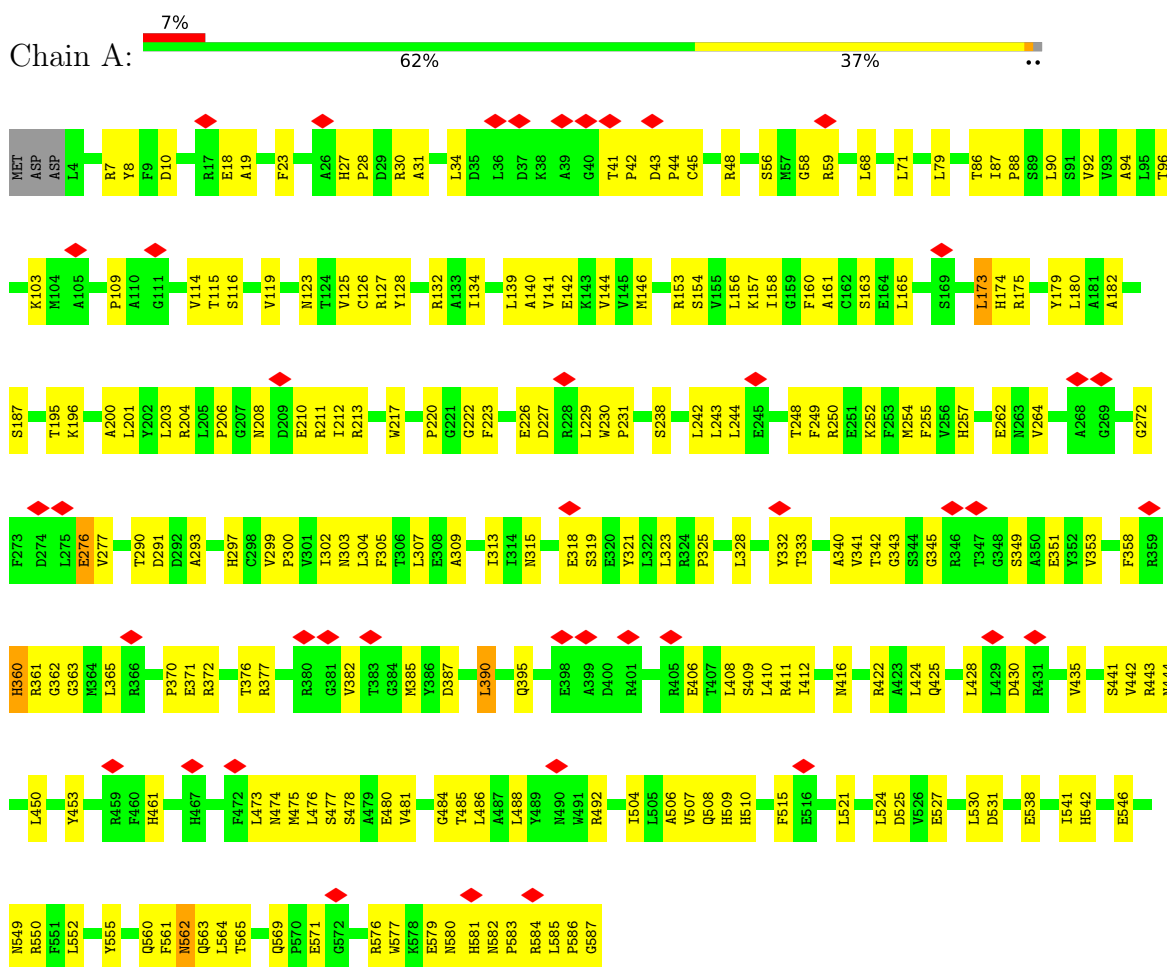
- Molecule 3 is a protein called TssE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	121	Total	C	N	O	S	0	0
			970	612	173	181	4		

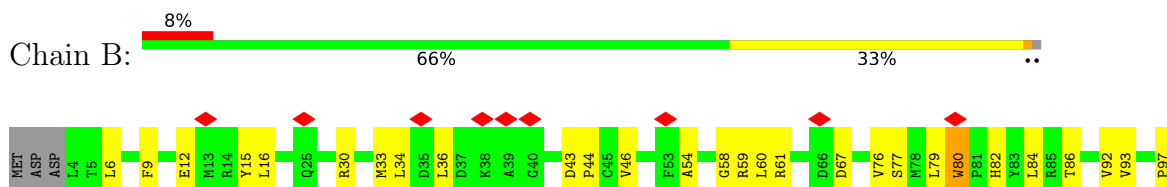
3 Residue-property plots

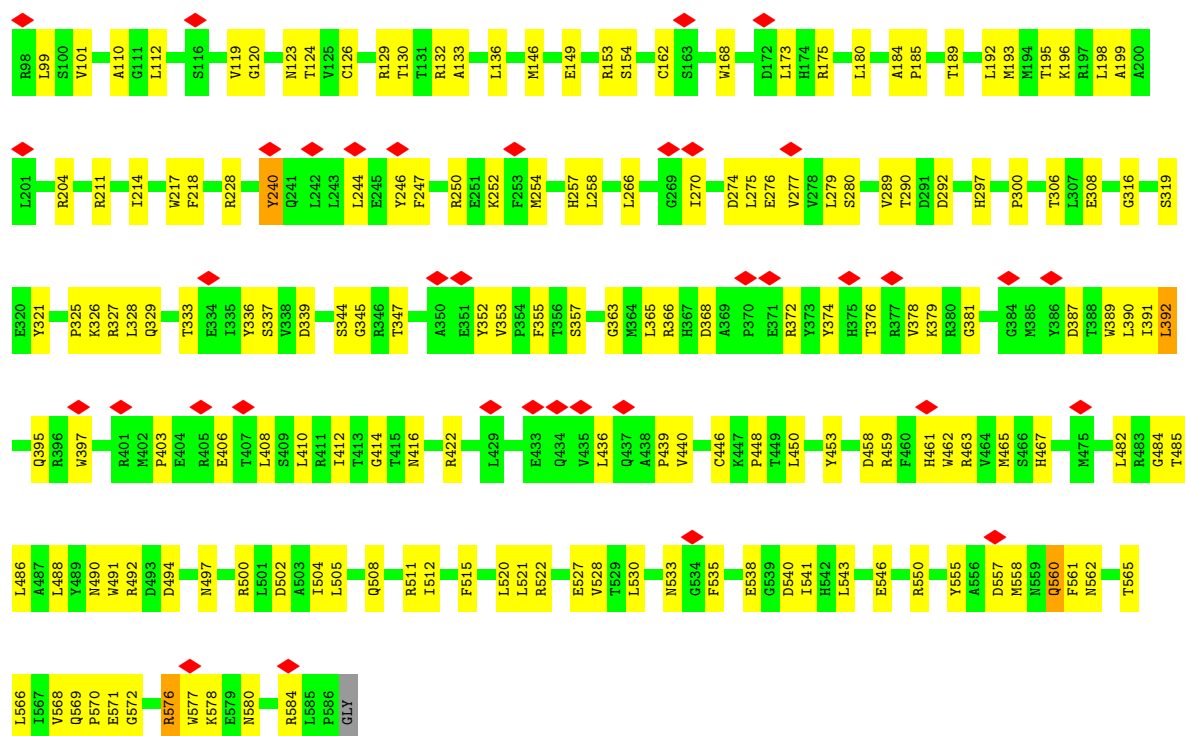
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Putative type VI secretion protein

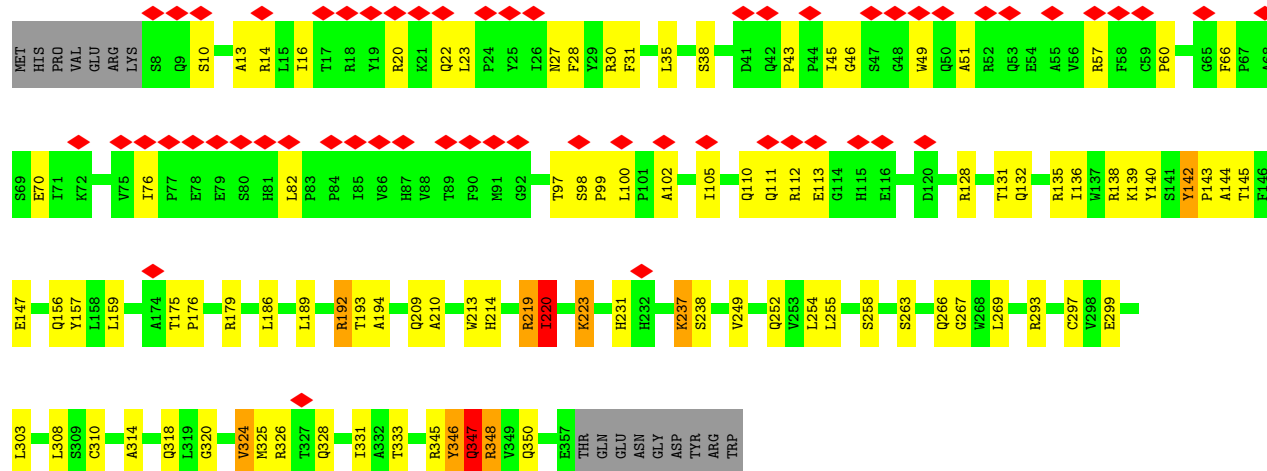


• Molecule 1: Putative type VI secretion protein

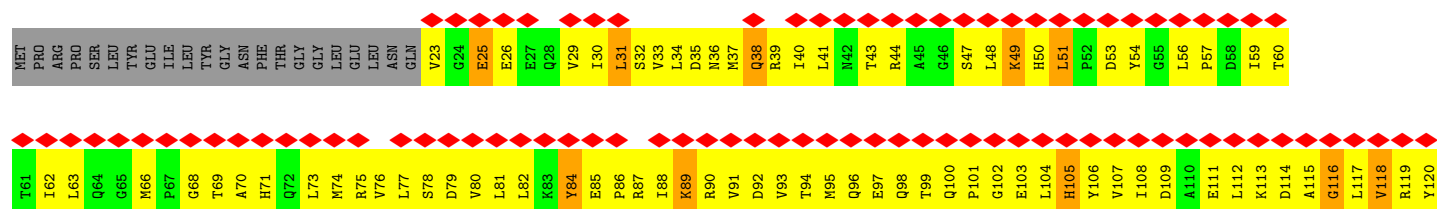
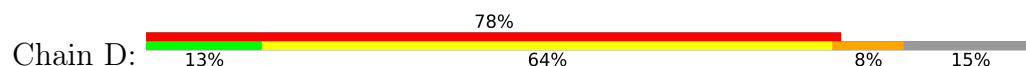




• Molecule 2: TssG



• Molecule 3: TssE



G121	T122	T123	F124	I125	P126	E127	G128	R129	V130	L131	L132	R133	H134	L135	K136	Q137	Q138	R139	Y140	V141	Q142	T143
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32504	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 ($e^-/\text{\AA}^2$)	1.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	16.808	Depositor
Minimum map value	-9.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size ($\text{\AA}$)	220.0, 220.0, 220.0	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

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	0.46	0/4769	0.78	0/6476
1	B	0.44	0/4765	0.82	3/6471 (0.0%)
2	C	0.46	0/2808	0.92	9/3822 (0.2%)
3	D	1.37	0/985	1.61	13/1332 (1.0%)
All	All	0.57	0/13327	0.91	25/18101 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	10
2	C	0	10
All	All	0	28

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	126	PRO	N-CA-C	-9.11	97.05	110.80
3	D	68	GLY	N-CA-C	-9.04	99.39	114.76
3	D	84	TYR	CA-CB-CG	-7.52	100.36	113.90
1	B	557	ASP	CA-C-N	7.17	135.23	121.54
1	B	557	ASP	C-N-CA	7.17	135.23	121.54
2	C	345	ARG	CA-C-N	6.99	134.89	121.54
2	C	345	ARG	C-N-CA	6.99	134.89	121.54
2	C	324	VAL	N-CA-C	-6.60	106.81	113.47
2	C	220	ILE	N-CA-C	6.42	122.76	108.88
3	D	129	ARG	N-CA-C	-6.12	100.59	110.32
2	C	219	ARG	CA-C-N	6.08	133.37	122.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	219	ARG	C-N-CA	6.08	133.37	122.13
3	D	129	ARG	CA-C-N	-5.67	113.96	122.01
3	D	129	ARG	C-N-CA	-5.67	113.96	122.01
1	B	246	TYR	N-CA-C	-5.62	106.56	113.41
2	C	348	ARG	N-CA-C	5.45	115.31	108.45
3	D	68	GLY	CA-C-N	5.42	128.09	120.28
3	D	68	GLY	C-N-CA	5.42	128.09	120.28
3	D	53	ASP	CA-CB-CG	-5.25	107.35	112.60
3	D	116	GLY	CA-C-N	5.23	128.26	120.31
3	D	116	GLY	C-N-CA	5.23	128.26	120.31
3	D	79	ASP	CA-CB-CG	-5.09	107.50	112.60
3	D	120	TYR	N-CA-C	-5.07	105.65	111.07
2	C	192	ARG	CA-C-N	5.02	130.73	121.70
2	C	192	ARG	C-N-CA	5.02	130.73	121.70

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	LEU	Peptide
1	A	276	GLU	Peptide
1	A	360	HIS	Peptide
1	A	390	LEU	Peptide
1	A	435	VAL	Peptide
1	A	453	TYR	Peptide
1	A	530	LEU	Peptide
1	A	562	ASN	Peptide
1	B	240	TYR	Peptide
1	B	247	PHE	Peptide
1	B	257	HIS	Peptide
1	B	363	GLY	Peptide
1	B	467	HIS	Peptide
1	B	515	PHE	Peptide
1	B	560	GLN	Peptide
1	B	576	ARG	Peptide
1	B	578	LYS	Peptide
1	B	80	TRP	Peptide
2	C	142	TYR	Peptide
2	C	219	ARG	Peptide
2	C	220	ILE	Peptide
2	C	231	HIS	Peptide
2	C	237	LYS	Peptide

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Mol	Chain	Res	Type	Group
2	C	249	VAL	Peptide
2	C	308	LEU	Peptide
2	C	310	CYS	Peptide
2	C	346	TYR	Peptide
2	C	347	GLN	Peptide

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	4655	0	4621	185	0
1	B	4651	0	4624	123	0
2	C	2737	0	2732	74	0
3	D	970	0	990	304	0
All	All	13013	0	12967	624	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 24.

All (624) 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:41:THR:CB	3:D:86:PRO:HB2	0.96	1.44
1:A:41:THR:CB	3:D:86:PRO:CB	1.93	1.44
3:D:43:THR:HG21	3:D:54:TYR:CE2	1.51	1.43
1:A:41:THR:HB	3:D:86:PRO:CB	1.50	1.40
3:D:38:GLN:HE22	3:D:137:GLN:NE2	1.21	1.39
3:D:40:ILE:HG22	3:D:54:TYR:CZ	1.61	1.36
1:A:41:THR:CG2	3:D:86:PRO:HB2	1.55	1.34
3:D:38:GLN:NE2	3:D:137:GLN:NE2	1.80	1.30
3:D:40:ILE:HG22	3:D:54:TYR:OH	1.24	1.27
1:A:41:THR:CG2	3:D:86:PRO:CB	2.13	1.23
1:A:41:THR:HG21	3:D:86:PRO:CB	1.73	1.17
3:D:40:ILE:CG2	3:D:54:TYR:OH	1.93	1.17
3:D:90:ARG:HB2	3:D:125:ILE:HG22	1.15	1.14
3:D:43:THR:CG2	3:D:54:TYR:CE2	2.31	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:63:LEU:HD13	3:D:141:VAL:HB	1.21	1.13
2:C:105:ILE:CD1	3:D:35:ASP:OD2	1.96	1.13
1:A:41:THR:HG21	3:D:86:PRO:HB3	1.18	1.12
3:D:38:GLN:HE22	3:D:137:GLN:CD	1.57	1.10
3:D:59:ILE:HG22	3:D:62:ILE:HG23	1.36	1.06
3:D:125:ILE:HG23	3:D:126:PRO:HD3	1.32	1.06
3:D:30:ILE:HB	3:D:133:ARG:CG	1.86	1.05
3:D:37:MET:CE	3:D:112:LEU:HD23	1.87	1.05
3:D:30:ILE:HB	3:D:133:ARG:HG2	1.36	1.05
1:A:43:ASP:HB2	3:D:118:VAL:CG2	1.90	1.02
3:D:48:LEU:HD22	3:D:51:LEU:H	1.19	1.02
3:D:37:MET:HE2	3:D:112:LEU:CD2	1.90	1.02
3:D:43:THR:HG21	3:D:54:TYR:CD2	1.95	1.01
3:D:40:ILE:HG22	3:D:54:TYR:CE1	1.98	0.99
3:D:90:ARG:H	3:D:115:ALA:HB3	1.28	0.98
1:A:43:ASP:HB2	3:D:118:VAL:HG21	1.47	0.97
2:C:105:ILE:HD13	3:D:35:ASP:OD2	1.66	0.96
3:D:30:ILE:HB	3:D:133:ARG:CD	1.97	0.95
3:D:30:ILE:HD11	3:D:134:HIS:O	1.67	0.95
3:D:63:LEU:HD21	3:D:106:TYR:HB3	1.49	0.94
3:D:59:ILE:CG2	3:D:62:ILE:HG23	1.98	0.93
1:A:43:ASP:O	3:D:85:GLU:CD	2.11	0.93
3:D:37:MET:HE2	3:D:112:LEU:HD23	1.46	0.93
3:D:56:LEU:HD13	3:D:77:LEU:HD22	1.51	0.93
3:D:63:LEU:CD2	3:D:106:TYR:HB3	1.99	0.92
3:D:63:LEU:HD13	3:D:141:VAL:CB	1.98	0.92
3:D:43:THR:CG2	3:D:54:TYR:HE2	1.72	0.92
1:A:41:THR:HB	3:D:86:PRO:CG	2.02	0.90
1:A:42:PRO:O	3:D:87:ARG:N	2.07	0.88
2:C:97:THR:HG22	3:D:50:HIS:CD2	2.09	0.88
3:D:115:ALA:HA	3:D:123:THR:HG21	1.56	0.87
1:A:41:THR:OG1	3:D:86:PRO:HB2	1.73	0.87
1:B:44:PRO:HG2	3:D:119:ARG:HE	1.40	0.87
3:D:135:LEU:CD2	3:D:137:GLN:HG3	2.06	0.86
3:D:103:GLU:HG2	3:D:104:LEU:H	1.38	0.86
1:A:41:THR:CG2	3:D:86:PRO:HB3	1.93	0.86
3:D:34:LEU:HA	3:D:135:LEU:CD1	2.06	0.86
3:D:135:LEU:HD23	3:D:136:LYS:N	1.91	0.85
1:A:109:PRO:HG3	1:A:134:ILE:H	1.40	0.85
3:D:93:VAL:HG22	3:D:112:LEU:HD13	1.58	0.85
3:D:94:THR:HG22	3:D:111:GLU:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:100:GLN:HB3	3:D:101:PRO:HD3	1.57	0.84
3:D:56:LEU:HD23	3:D:80:VAL:HG11	1.58	0.84
1:A:44:PRO:O	3:D:85:GLU:OE2	1.96	0.82
3:D:77:LEU:HD12	3:D:93:VAL:HG11	1.61	0.82
3:D:135:LEU:HD21	3:D:137:GLN:HG3	1.62	0.82
3:D:40:ILE:CG2	3:D:54:TYR:CZ	2.56	0.81
1:B:44:PRO:HG2	3:D:119:ARG:NE	1.94	0.81
1:A:41:THR:HB	3:D:86:PRO:HB2	0.81	0.80
3:D:30:ILE:HB	3:D:133:ARG:HD3	1.62	0.80
3:D:59:ILE:O	3:D:62:ILE:HG12	1.80	0.80
3:D:115:ALA:HA	3:D:123:THR:CG2	2.12	0.80
3:D:59:ILE:HG23	3:D:62:ILE:H	1.47	0.79
3:D:73:LEU:HD11	3:D:77:LEU:HD11	1.64	0.79
3:D:30:ILE:CB	3:D:133:ARG:HG2	2.11	0.79
3:D:73:LEU:HB3	3:D:95:MET:HE3	1.64	0.78
3:D:37:MET:HE1	3:D:112:LEU:HD23	1.64	0.78
3:D:56:LEU:HD21	3:D:80:VAL:CG2	2.13	0.78
3:D:56:LEU:HD13	3:D:77:LEU:CD2	2.13	0.78
3:D:88:ILE:HG21	3:D:91:VAL:HG22	1.65	0.77
1:A:43:ASP:O	3:D:85:GLU:OE2	2.02	0.77
3:D:90:ARG:N	3:D:115:ALA:HB3	1.99	0.77
3:D:56:LEU:HD21	3:D:80:VAL:HG21	1.66	0.77
3:D:70:ALA:O	3:D:74:MET:HG3	1.85	0.76
3:D:90:ARG:HB2	3:D:125:ILE:CG2	2.08	0.76
3:D:115:ALA:HB1	3:D:126:PRO:HD2	1.64	0.76
3:D:117:LEU:O	3:D:117:LEU:HD13	1.86	0.76
3:D:57:PRO:HD2	3:D:76:VAL:HG21	1.66	0.76
2:C:105:ILE:HD12	3:D:35:ASP:OD2	1.86	0.75
3:D:95:MET:HG3	3:D:108:ILE:CG2	2.16	0.75
3:D:77:LEU:O	3:D:81:LEU:HD23	1.84	0.75
3:D:99:THR:HA	3:D:106:TYR:CE2	2.21	0.75
1:A:43:ASP:HB2	3:D:118:VAL:HG23	1.70	0.74
1:A:48:ARG:HD3	3:D:84:TYR:HD1	1.52	0.74
3:D:94:THR:CG2	3:D:111:GLU:HB3	2.17	0.74
3:D:37:MET:SD	3:D:135:LEU:HD13	2.27	0.74
3:D:43:THR:HG21	3:D:54:TYR:HE2	0.97	0.74
3:D:30:ILE:CB	3:D:133:ARG:CG	2.66	0.73
3:D:116:GLY:O	3:D:121:GLY:HA2	1.88	0.73
3:D:56:LEU:CD1	3:D:77:LEU:HD22	2.18	0.73
3:D:123:THR:HA	3:D:131:LEU:O	1.88	0.73
3:D:90:ARG:CB	3:D:125:ILE:HG22	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:TYR:O	2:C:192:ARG:NH1	2.22	0.72
3:D:98:GLN:HB3	3:D:101:PRO:HD2	1.70	0.72
3:D:130:VAL:O	3:D:131:LEU:HD23	1.89	0.72
3:D:48:LEU:HD22	3:D:51:LEU:N	2.02	0.72
3:D:66:MET:HB3	3:D:106:TYR:OH	1.89	0.72
3:D:80:VAL:HG23	3:D:81:LEU:HD22	1.72	0.71
3:D:49:LYS:HD2	3:D:49:LYS:C	2.14	0.71
3:D:30:ILE:CD1	3:D:134:HIS:O	2.38	0.71
3:D:115:ALA:HA	3:D:123:THR:CB	2.20	0.71
3:D:30:ILE:CB	3:D:133:ARG:HD3	2.21	0.70
3:D:73:LEU:HD13	3:D:77:LEU:HG	1.74	0.70
3:D:98:GLN:HB3	3:D:101:PRO:CD	2.21	0.70
1:A:45:CYS:N	3:D:85:GLU:OE1	2.25	0.70
3:D:56:LEU:HD23	3:D:80:VAL:CG1	2.22	0.70
3:D:49:LYS:HD2	3:D:49:LYS:O	1.91	0.69
3:D:115:ALA:CA	3:D:123:THR:HG21	2.22	0.69
1:A:254:MET:HE2	1:A:552:LEU:HD12	1.75	0.69
1:A:315:ASN:HB3	2:C:22:GLN:HE22	1.58	0.69
3:D:70:ALA:HA	3:D:95:MET:SD	2.33	0.69
3:D:70:ALA:HB2	3:D:97:GLU:OE1	1.92	0.68
1:B:199:ALA:HB1	1:B:277:VAL:HB	1.74	0.68
2:C:138:ARG:HD3	2:C:139:LYS:HG3	1.76	0.68
3:D:73:LEU:O	3:D:76:VAL:HG12	1.93	0.68
3:D:34:LEU:HA	3:D:135:LEU:HD12	1.73	0.68
1:A:44:PRO:C	3:D:85:GLU:OE1	2.37	0.68
2:C:100:LEU:HB2	2:C:111:GLN:HE21	1.58	0.67
1:A:48:ARG:HD3	3:D:84:TYR:CD1	2.28	0.67
1:A:119:VAL:HG23	1:A:422:ARG:HD2	1.77	0.67
3:D:125:ILE:HG23	3:D:126:PRO:CD	2.17	0.67
3:D:133:ARG:HA	3:D:133:ARG:NE	2.09	0.67
3:D:77:LEU:O	3:D:80:VAL:HG22	1.94	0.67
3:D:88:ILE:CG2	3:D:91:VAL:HG22	2.24	0.67
3:D:101:PRO:HB2	3:D:106:TYR:CA	2.25	0.67
3:D:111:GLU:CD	3:D:136:LYS:HE2	2.20	0.66
1:B:132:ARG:HB2	1:B:250:ARG:HD3	1.76	0.66
1:A:41:THR:OG1	3:D:86:PRO:CB	2.38	0.66
1:B:527:GLU:HB2	1:B:566:LEU:HB2	1.77	0.66
1:B:422:ARG:NH2	1:B:448:PRO:O	2.28	0.66
3:D:56:LEU:HD21	3:D:77:LEU:HA	1.78	0.66
3:D:71:HIS:HA	3:D:74:MET:HE2	1.76	0.66
3:D:73:LEU:O	3:D:77:LEU:HG	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:H	1:B:372:ARG:HB3	1.59	0.65
1:A:584:ARG:HG2	1:A:585:LEU:HG	1.77	0.65
2:C:299:GLU:HA	2:C:331:ILE:HA	1.77	0.65
1:B:92:VAL:HG21	1:B:446:CYS:H	1.61	0.65
1:A:19:ALA:HA	1:A:23:PHE:HB3	1.79	0.65
1:A:141:VAL:HA	1:A:158:ILE:HG22	1.78	0.65
3:D:101:PRO:HB2	3:D:106:TYR:N	2.12	0.65
3:D:111:GLU:CG	3:D:136:LYS:HE2	2.26	0.65
1:B:555:TYR:HB3	1:B:560:GLN:HB2	1.79	0.64
1:A:43:ASP:CB	3:D:118:VAL:HG21	2.24	0.64
2:C:46:GLY:HA3	2:C:135:ARG:HH21	1.61	0.64
1:A:351:GLU:HB3	1:A:372:ARG:HD2	1.78	0.64
3:D:93:VAL:HG22	3:D:112:LEU:CD1	2.28	0.64
1:A:525:ASP:HA	1:A:563:GLN:HB2	1.79	0.64
1:B:173:LEU:HB2	1:B:214:ILE:HG21	1.80	0.64
3:D:43:THR:O	3:D:47:SER:OG	2.14	0.64
3:D:63:LEU:HD23	3:D:63:LEU:O	1.98	0.64
1:A:127:ARG:HA	1:A:303:ASN:HA	1.80	0.64
3:D:95:MET:HG3	3:D:108:ILE:HG23	1.78	0.64
3:D:101:PRO:HB2	3:D:106:TYR:HA	1.80	0.64
1:B:569:GLN:HG3	1:B:571:GLU:H	1.61	0.63
3:D:123:THR:HG22	3:D:131:LEU:O	1.98	0.63
1:A:361:ARG:HD3	1:A:371:GLU:HG2	1.80	0.63
1:B:374:TYR:O	1:B:395:GLN:NE2	2.29	0.63
3:D:122:THR:OG1	3:D:129:ARG:HB2	1.98	0.63
1:A:179:TYR:HB3	1:A:222:GLY:H	1.64	0.63
1:A:201:LEU:HA	1:A:262:GLU:HG2	1.81	0.63
3:D:43:THR:CG2	3:D:54:TYR:CD2	2.75	0.63
3:D:69:THR:HG23	3:D:95:MET:SD	2.39	0.63
1:A:139:LEU:HD21	1:A:165:LEU:HD21	1.81	0.62
3:D:63:LEU:HD23	3:D:106:TYR:HB3	1.80	0.62
1:B:522:ARG:HH12	1:B:562:ASN:HB3	1.64	0.62
1:A:341:VAL:HG22	1:A:410:LEU:HG	1.80	0.62
3:D:38:GLN:NE2	3:D:137:GLN:CD	2.34	0.62
1:B:458:ASP:HB3	1:B:461:HIS:HB2	1.82	0.62
3:D:73:LEU:CD1	3:D:77:LEU:HD11	2.29	0.62
1:A:227:ASP:O	1:A:492:ARG:NH2	2.33	0.62
1:B:146:MET:H	1:B:289:VAL:HG21	1.65	0.62
1:B:486:LEU:O	1:B:490:ASN:ND2	2.33	0.62
3:D:57:PRO:HD2	3:D:76:VAL:CG2	2.29	0.62
3:D:101:PRO:HG2	3:D:107:VAL:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:33:VAL:HB	3:D:37:MET:HE3	1.81	0.61
3:D:95:MET:HG2	3:D:96:GLN:N	2.14	0.61
2:C:97:THR:CG2	3:D:50:HIS:CD2	2.83	0.61
3:D:62:ILE:HG13	3:D:63:LEU:N	2.15	0.61
3:D:88:ILE:HG12	3:D:114:ASP:OD2	2.00	0.61
2:C:98:SER:HB3	3:D:39:ARG:HH12	1.66	0.61
3:D:63:LEU:HD21	3:D:105:HIS:O	2.00	0.61
1:B:129:ARG:HH21	1:B:306:THR:HB	1.66	0.61
3:D:115:ALA:HB1	3:D:123:THR:OG1	2.00	0.61
3:D:38:GLN:NE2	3:D:137:GLN:HE22	1.96	0.61
1:B:463:ARG:HE	2:C:159:LEU:HD22	1.66	0.61
2:C:136:ILE:HA	2:C:140:TYR:HB2	1.83	0.61
3:D:73:LEU:HD13	3:D:73:LEU:C	2.25	0.61
3:D:73:LEU:HD13	3:D:73:LEU:O	2.01	0.61
1:A:132:ARG:NH1	1:A:248:THR:O	2.34	0.61
3:D:54:TYR:HA	3:D:84:TYR:CZ	2.35	0.61
1:A:313:ILE:HD13	1:A:406:GLU:H	1.66	0.60
1:A:315:ASN:OD1	2:C:30:ARG:NH2	2.29	0.60
3:D:75:ARG:NH1	3:D:75:ARG:HB3	2.15	0.60
1:B:562:ASN:O	1:B:580:ASN:ND2	2.35	0.60
3:D:63:LEU:HD23	3:D:63:LEU:C	2.26	0.60
3:D:115:ALA:HA	3:D:123:THR:HB	1.84	0.60
2:C:326:ARG:HH21	2:C:328:GLN:HE21	1.50	0.60
3:D:135:LEU:HD21	3:D:137:GLN:CG	2.32	0.60
3:D:116:GLY:N	3:D:123:THR:HG21	2.17	0.60
1:B:97:PRO:HD2	1:B:440:VAL:HG13	1.83	0.60
3:D:95:MET:CG	3:D:108:ILE:HG23	2.31	0.60
3:D:104:LEU:HD12	3:D:104:LEU:N	2.16	0.60
3:D:51:LEU:N	3:D:51:LEU:HD22	2.16	0.59
2:C:145:THR:HG22	2:C:156:GLN:HB3	1.83	0.59
2:C:176:PRO:O	2:C:179:ARG:NH1	2.34	0.59
1:B:365:LEU:HB3	1:B:368:ASP:HB2	1.85	0.59
2:C:66:PHE:HB3	2:C:70:GLU:HB2	1.85	0.59
3:D:91:VAL:HG13	3:D:112:LEU:HD11	1.83	0.59
1:A:44:PRO:C	3:D:85:GLU:OE2	2.44	0.59
1:B:43:ASP:HB2	1:B:46:VAL:HG22	1.85	0.59
2:C:314:ALA:H	2:C:318:GLN:HE22	1.51	0.59
1:A:27:HIS:O	1:A:31:ALA:N	2.36	0.58
1:A:94:ALA:HB3	1:A:443:ARG:HB2	1.84	0.58
1:A:507:VAL:HB	1:A:527:GLU:HB2	1.85	0.58
1:B:336:TYR:HA	1:B:416:ASN:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:HD21	1:B:576:ARG:HD2	1.86	0.58
1:A:44:PRO:C	3:D:85:GLU:CD	2.71	0.58
1:B:276:GLU:HA	1:B:279:LEU:HB3	1.83	0.58
2:C:193:THR:OG1	2:C:194:ALA:N	2.34	0.58
3:D:117:LEU:HD13	3:D:117:LEU:C	2.28	0.58
1:B:204:ARG:HD3	1:B:266:LEU:HD11	1.84	0.58
3:D:132:LEU:N	3:D:132:LEU:HD12	2.19	0.58
1:A:425:GLN:HA	1:A:444:ASN:HD22	1.68	0.58
1:B:80:TRP:HA	1:B:82:HIS:HD2	1.69	0.58
2:C:20:ARG:HG3	2:C:23:LEU:HD12	1.85	0.58
1:A:18:GLU:OE2	1:B:59:ARG:NH2	2.37	0.57
2:C:297:CYS:HA	2:C:333:THR:HA	1.86	0.57
1:A:96:THR:HB	1:A:441:SER:HB2	1.85	0.57
1:A:328:LEU:HA	1:A:332:TYR:HB2	1.86	0.57
1:B:465:MET:HB2	1:B:488:LEU:HD21	1.86	0.57
3:D:48:LEU:HD21	3:D:50:HIS:HB2	1.87	0.57
1:A:139:LEU:HB3	1:A:160:PHE:HB3	1.86	0.57
3:D:23:VAL:HG23	3:D:23:VAL:O	2.04	0.57
1:A:318:GLU:OE1	2:C:30:ARG:NH2	2.37	0.57
2:C:16:ILE:HG21	2:C:76:ILE:HD12	1.86	0.57
3:D:101:PRO:HB2	3:D:106:TYR:H	1.68	0.57
1:B:325:PRO:HA	1:B:328:LEU:HB3	1.85	0.57
1:B:565:THR:OG1	2:C:350:GLN:NE2	2.37	0.57
1:B:149:GLU:H	1:B:153:ARG:H	1.53	0.57
3:D:98:GLN:C	3:D:101:PRO:HD2	2.30	0.57
3:D:121:GLY:O	3:D:128:GLY:HA3	2.04	0.57
1:A:361:ARG:HD2	1:A:370:PRO:HA	1.87	0.56
1:A:318:GLU:HB2	2:C:30:ARG:HH12	1.70	0.56
1:A:564:LEU:HB3	1:A:577:TRP:HB2	1.86	0.56
1:B:192:LEU:O	1:B:196:LYS:N	2.32	0.56
1:B:327:ARG:HE	1:B:337:SER:HA	1.69	0.56
2:C:266:GLN:HA	2:C:269:LEU:HG	1.86	0.56
1:A:510:HIS:HA	1:A:524:LEU:HA	1.87	0.56
3:D:122:THR:HG23	3:D:122:THR:O	2.05	0.56
3:D:30:ILE:CG2	3:D:133:ARG:HD3	2.35	0.56
3:D:40:ILE:CG2	3:D:54:TYR:CE1	2.82	0.56
3:D:89:LYS:C	3:D:89:LYS:HD3	2.31	0.56
1:A:307:LEU:HB2	1:A:412:ILE:HG23	1.88	0.56
1:A:319:SER:OG	2:C:27:ASN:ND2	2.39	0.55
1:A:560:GLN:OE1	1:A:562:ASN:ND2	2.40	0.55
3:D:118:VAL:HG12	3:D:119:ARG:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLY:O	1:B:61:ARG:NH2	2.37	0.55
3:D:130:VAL:O	3:D:130:VAL:HG23	2.05	0.55
1:B:33:MET:HG3	1:B:36:LEU:HD12	1.88	0.55
1:B:535:PHE:HB2	1:B:538:GLU:HG2	1.88	0.55
3:D:89:LYS:HD2	3:D:125:ILE:HG21	1.88	0.55
1:B:390:LEU:HB3	1:B:392:LEU:HD23	1.87	0.55
1:B:217:TRP:CD1	1:B:258:LEU:HB2	2.42	0.55
3:D:116:GLY:H	3:D:123:THR:CG2	2.19	0.55
3:D:141:VAL:HG22	3:D:142:GLN:N	2.20	0.55
3:D:69:THR:HG23	3:D:95:MET:HE1	1.89	0.55
1:A:210:GLU:O	1:A:213:ARG:NH1	2.39	0.55
1:B:12:GLU:HG3	1:B:58:GLY:HA3	1.88	0.55
1:A:174:HIS:HA	1:A:217:TRP:HB3	1.89	0.55
1:A:226:GLU:HA	1:A:230:TRP:CD1	2.42	0.55
3:D:25:GLU:HA	3:D:25:GLU:OE1	2.07	0.54
3:D:103:GLU:HG2	3:D:104:LEU:N	2.16	0.54
2:C:60:PRO:HG2	2:C:76:ILE:HG12	1.88	0.54
3:D:38:GLN:CD	3:D:137:GLN:NE2	2.60	0.54
3:D:96:GLN:HB3	3:D:109:ASP:HB2	1.89	0.54
1:B:120:GLY:HA3	1:B:123:ASN:HB3	1.89	0.54
3:D:135:LEU:HD23	3:D:135:LEU:C	2.33	0.54
1:A:41:THR:HB	3:D:86:PRO:HG2	1.86	0.54
3:D:56:LEU:CD2	3:D:77:LEU:HA	2.36	0.54
1:A:581:HIS:HA	1:A:586:PRO:HA	1.90	0.54
2:C:99:PRO:O	3:D:39:ARG:NH1	2.40	0.54
3:D:50:HIS:C	3:D:51:LEU:HD22	2.33	0.54
1:A:504:ILE:HG13	1:A:531:ASP:HB2	1.90	0.54
1:B:500:ARG:NH1	1:B:533:ASN:OD1	2.39	0.54
3:D:40:ILE:HG23	3:D:54:TYR:OH	1.99	0.54
1:A:546:GLU:OE2	1:A:550:ARG:NE	2.41	0.53
3:D:30:ILE:HG23	3:D:31:LEU:HD13	1.90	0.53
3:D:34:LEU:CA	3:D:135:LEU:HD12	2.34	0.53
1:B:319:SER:HA	1:B:391:ILE:HG23	1.90	0.53
2:C:189:LEU:HB3	2:C:192:ARG:HD2	1.89	0.53
1:B:184:ALA:HA	1:B:189:THR:HB	1.89	0.53
1:A:7:ARG:HA	1:A:10:ASP:HB2	1.91	0.53
3:D:98:GLN:O	3:D:101:PRO:HD2	2.09	0.53
1:A:142:GLU:HB2	1:A:157:LYS:HG3	1.90	0.53
1:B:30:ARG:HB2	1:B:34:LEU:HB2	1.91	0.53
1:A:309:ALA:HB2	1:A:325:PRO:HB3	1.89	0.53
3:D:34:LEU:HA	3:D:135:LEU:HD11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:56:LEU:CD2	3:D:80:VAL:HG21	2.38	0.53
3:D:70:ALA:HA	3:D:95:MET:CE	2.38	0.53
1:B:168:TRP:HB2	1:B:211:ARG:HG3	1.91	0.53
1:A:290:THR:OG1	1:A:291:ASP:N	2.41	0.53
1:A:333:THR:N	1:A:416:ASN:OD1	2.40	0.53
1:A:538:GLU:HB2	1:A:541:ILE:HB	1.89	0.53
1:B:84:LEU:HD13	1:B:491:TRP:HH2	1.74	0.52
3:D:73:LEU:HB3	3:D:95:MET:CE	2.38	0.52
3:D:80:VAL:HG23	3:D:81:LEU:N	2.23	0.52
2:C:192:ARG:HB3	2:C:193:THR:HB	1.92	0.52
1:A:43:ASP:OD2	3:D:29:VAL:HB	2.10	0.52
1:A:153:ARG:HB3	1:A:277:VAL:HG23	1.90	0.52
1:A:382:VAL:HG11	1:A:385:MET:HB2	1.92	0.52
1:A:182:ALA:HB3	1:A:187:SER:HB3	1.91	0.52
1:B:252:LYS:HG3	1:B:254:MET:H	1.74	0.52
3:D:38:GLN:OE1	3:D:137:GLN:OE1	2.27	0.52
3:D:73:LEU:HD22	3:D:76:VAL:CG1	2.39	0.52
1:B:146:MET:HG3	1:B:154:SER:HB2	1.92	0.52
1:B:329:GLN:O	1:B:333:THR:N	2.43	0.52
3:D:75:ARG:HB3	3:D:75:ARG:HH11	1.74	0.52
3:D:76:VAL:HG13	3:D:77:LEU:N	2.24	0.52
3:D:66:MET:HG3	3:D:66:MET:O	2.09	0.52
1:B:112:LEU:H	1:B:130:THR:HG22	1.74	0.52
2:C:10:SER:O	2:C:14:ARG:N	2.40	0.52
1:B:450:LEU:O	1:B:492:ARG:NH2	2.30	0.51
3:D:104:LEU:H	3:D:104:LEU:HD12	1.74	0.51
1:A:473:LEU:HD11	2:C:192:ARG:HE	1.74	0.51
1:A:579:GLU:HB3	1:A:587:GLY:HA3	1.93	0.51
3:D:135:LEU:HD22	3:D:137:GLN:HG3	1.90	0.51
1:A:204:ARG:HD2	1:A:264:VAL:HG11	1.93	0.51
1:A:480:GLU:O	1:A:484:GLY:N	2.33	0.51
1:B:505:LEU:H	1:B:528:VAL:HG11	1.76	0.51
3:D:71:HIS:HA	3:D:74:MET:CE	2.40	0.51
1:A:569:GLN:HG3	1:A:571:GLU:HB2	1.93	0.51
2:C:142:TYR:O	2:C:144:ALA:N	2.44	0.51
1:B:308:GLU:O	1:B:326:LYS:NZ	2.38	0.50
2:C:128:ARG:O	2:C:131:THR:OG1	2.28	0.50
1:A:132:ARG:HD2	1:A:249:PHE:HA	1.92	0.50
1:B:93:VAL:HA	1:B:300:PRO:HA	1.93	0.50
1:A:250:ARG:HG2	1:A:252:LYS:HB2	1.94	0.50
3:D:48:LEU:HD23	3:D:50:HIS:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:TYR:HH	1:B:397:TRP:CD1	2.28	0.50
1:A:173:LEU:HB3	1:A:217:TRP:HE3	1.77	0.50
1:A:340:ALA:O	1:A:411:ARG:N	2.43	0.50
1:A:387:ASP:N	1:A:387:ASP:OD1	2.44	0.50
1:B:562:ASN:OD1	1:B:562:ASN:N	2.45	0.50
3:D:100:GLN:HB3	3:D:101:PRO:CD	2.37	0.50
1:B:357:SER:HB2	1:B:374:TYR:H	1.75	0.50
1:B:568:VAL:HB	1:B:572:GLY:HA3	1.93	0.50
1:A:165:LEU:HD12	1:A:211:ARG:HB2	1.93	0.49
1:A:180:LEU:HA	1:A:297:HIS:HE1	1.77	0.49
1:A:42:PRO:C	3:D:87:ARG:CA	2.63	0.49
1:B:67:ASP:O	1:B:459:ARG:NH1	2.42	0.49
1:A:507:VAL:O	1:A:527:GLU:N	2.46	0.49
3:D:38:GLN:NE2	3:D:137:GLN:HE21	1.97	0.49
1:B:196:LYS:HE2	1:B:275:LEU:HB2	1.92	0.49
1:B:512:ILE:H	1:B:522:ARG:HA	1.77	0.49
1:B:352:TYR:HA	1:B:372:ARG:HD3	1.94	0.49
1:A:360:HIS:HB3	1:A:365:LEU:H	1.77	0.49
3:D:30:ILE:CG1	3:D:133:ARG:CG	2.90	0.49
1:A:579:GLU:HB2	1:A:581:HIS:CE1	2.48	0.49
1:B:290:THR:HG22	1:B:292:ASP:H	1.77	0.49
3:D:78:SER:O	3:D:82:LEU:HG	2.12	0.49
2:C:237:LYS:HD3	2:C:238:SER:HA	1.94	0.49
3:D:116:GLY:O	3:D:126:PRO:HG2	2.13	0.49
2:C:105:ILE:HG12	2:C:111:GLN:HG3	1.94	0.48
3:D:76:VAL:HG13	3:D:77:LEU:HD23	1.95	0.48
1:B:576:ARG:HB2	1:B:577:TRP:CD1	2.48	0.48
3:D:139:ARG:CZ	3:D:140:TYR:H	2.26	0.48
3:D:89:LYS:HD2	3:D:125:ILE:CG2	2.43	0.48
1:B:540:ASP:HA	1:B:543:LEU:HD23	1.96	0.48
1:A:486:LEU:HB3	1:A:488:LEU:H	1.78	0.48
1:A:583:PRO:O	2:C:214:HIS:N	2.46	0.48
3:D:59:ILE:HG22	3:D:62:ILE:CG2	2.25	0.48
3:D:90:ARG:HD3	3:D:124:PHE:HB3	1.95	0.48
3:D:111:GLU:HG3	3:D:136:LYS:CE	2.43	0.48
1:A:128:TYR:N	1:A:302:ILE:O	2.42	0.48
3:D:139:ARG:HA	3:D:139:ARG:NE	2.29	0.48
1:A:8:TYR:HB3	1:A:59:ARG:HD2	1.96	0.48
1:A:569:GLN:O	1:A:571:GLU:N	2.47	0.48
1:B:228:ARG:NH1	1:B:494:ASP:OD2	2.42	0.48
3:D:122:THR:O	3:D:123:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:135:LEU:HD23	3:D:136:LYS:C	2.39	0.48
1:A:42:PRO:C	3:D:87:ARG:HA	2.39	0.48
1:A:103:LYS:HG2	1:A:163:SER:HA	1.96	0.48
1:A:560:GLN:HE22	1:A:562:ASN:HA	1.78	0.48
1:B:381:GLY:N	1:B:387:ASP:O	2.47	0.48
3:D:90:ARG:HB3	3:D:115:ALA:HB2	1.96	0.48
3:D:92:ASP:HB2	3:D:113:LYS:HB2	1.96	0.48
3:D:122:THR:HA	3:D:128:GLY:HA3	1.96	0.48
3:D:40:ILE:HA	3:D:43:THR:HG22	1.95	0.48
1:A:474:ASN:HA	1:A:480:GLU:HB3	1.95	0.48
2:C:314:ALA:H	2:C:318:GLN:NE2	2.11	0.48
3:D:122:THR:O	3:D:131:LEU:HB2	2.14	0.47
1:B:374:TYR:HH	1:B:376:THR:HG1	1.58	0.47
3:D:50:HIS:CB	3:D:51:LEU:HD22	2.44	0.47
2:C:347:GLN:HB3	2:C:348:ARG:HB3	1.97	0.47
1:A:28:PRO:HA	1:A:31:ALA:HB3	1.96	0.47
2:C:57:ARG:HG2	2:C:82:LEU:HD23	1.96	0.47
3:D:101:PRO:CB	3:D:106:TYR:H	2.27	0.47
1:A:88:PRO:HG2	1:A:302:ILE:HD12	1.96	0.47
1:A:538:GLU:O	1:A:542:HIS:ND1	2.41	0.47
2:C:145:THR:HB	2:C:157:TYR:HE1	1.79	0.47
3:D:30:ILE:HG21	3:D:133:ARG:HD3	1.97	0.47
3:D:103:GLU:HG2	3:D:104:LEU:HD12	1.97	0.47
1:A:86:THR:OG1	1:A:87:ILE:N	2.48	0.47
1:A:180:LEU:HD22	1:A:293:ALA:HB1	1.96	0.47
2:C:132:GLN:HA	2:C:135:ARG:HB2	1.96	0.47
3:D:94:THR:O	3:D:94:THR:HG23	2.15	0.47
1:A:146:MET:HB3	1:A:154:SER:HB2	1.96	0.47
1:A:231:PRO:HG2	1:A:492:ARG:HH22	1.79	0.47
1:A:360:HIS:CD2	1:A:363:GLY:HA3	2.50	0.47
1:A:509:HIS:N	1:A:525:ASP:O	2.47	0.47
1:A:584:ARG:HA	2:C:213:TRP:CD1	2.49	0.47
1:B:274:ASP:HB3	1:B:276:GLU:HG3	1.97	0.47
1:B:504:ILE:HA	1:B:528:VAL:HG11	1.94	0.47
3:D:56:LEU:CD2	3:D:80:VAL:HG11	2.38	0.47
3:D:70:ALA:HA	3:D:95:MET:HE3	1.96	0.47
2:C:49:TRP:HZ3	2:C:128:ARG:HD2	1.79	0.47
2:C:16:ILE:HG13	2:C:23:LEU:HD11	1.97	0.47
1:A:30:ARG:O	1:A:34:LEU:N	2.42	0.47
3:D:56:LEU:HD21	3:D:80:VAL:HG22	1.93	0.47
1:A:96:THR:O	1:A:441:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:PRO:HD2	1:A:328:LEU:HD13	1.97	0.46
3:D:48:LEU:CD2	3:D:50:HIS:HB2	2.45	0.46
3:D:63:LEU:CD1	3:D:141:VAL:HB	2.16	0.46
2:C:43:PRO:HG2	2:C:45:ILE:HG12	1.97	0.46
3:D:88:ILE:HG23	3:D:114:ASP:OD2	2.14	0.46
3:D:101:PRO:HB3	3:D:105:HIS:HB3	1.97	0.46
3:D:139:ARG:HA	3:D:139:ARG:HE	1.80	0.46
1:A:128:TYR:HB2	1:A:304:LEU:HB2	1.97	0.46
1:B:316:GLY:H	1:B:403:PRO:HB3	1.80	0.46
2:C:252:GLN:HE22	2:C:293:ARG:HB2	1.80	0.46
3:D:73:LEU:CB	3:D:95:MET:HE3	2.42	0.46
3:D:63:LEU:HD13	3:D:141:VAL:CA	2.44	0.46
3:D:69:THR:HG23	3:D:95:MET:CE	2.46	0.46
1:A:114:VAL:HG21	1:A:127:ARG:HB2	1.97	0.46
1:A:243:LEU:HD23	1:A:244:LEU:HG	1.97	0.46
1:A:390:LEU:HD12	1:A:390:LEU:HA	1.75	0.46
1:A:195:THR:HG23	1:A:196:LYS:HG3	1.98	0.46
1:A:376:THR:O	1:A:377:ARG:NE	2.48	0.46
1:B:484:GLY:HA2	1:B:485:THR:HA	1.68	0.46
1:B:490:ASN:HB3	1:B:497:ASN:HD21	1.79	0.46
1:B:410:LEU:HD22	1:B:412:ILE:HD11	1.98	0.46
3:D:115:ALA:C	3:D:123:THR:HG21	2.40	0.46
1:A:90:LEU:HD12	1:A:300:PRO:HB2	1.97	0.46
1:A:560:GLN:NE2	1:A:561:PHE:O	2.49	0.46
1:A:43:ASP:CB	3:D:118:VAL:CG2	2.79	0.45
2:C:143:PRO:HB3	2:C:147:GLU:HB2	1.98	0.45
3:D:73:LEU:CB	3:D:95:MET:CE	2.95	0.45
1:A:132:ARG:NH1	1:A:299:VAL:HG11	2.31	0.45
1:B:530:LEU:HD23	1:B:570:PRO:HD2	1.98	0.45
3:D:73:LEU:HD13	3:D:77:LEU:CG	2.45	0.45
1:A:179:TYR:CG	1:A:223:PHE:HB2	2.51	0.45
3:D:36:ASN:C	3:D:36:ASN:HD22	2.24	0.45
1:A:116:SER:O	1:A:428:LEU:N	2.50	0.45
1:A:161:ALA:HB2	1:A:208:ASN:HB3	1.98	0.45
1:A:538:GLU:H	1:A:542:HIS:CE1	2.35	0.45
3:D:88:ILE:CG2	3:D:91:VAL:CG2	2.94	0.45
1:A:220:PRO:HG2	1:A:257:HIS:HB3	1.99	0.45
1:A:323:LEU:HB3	1:A:390:LEU:HD23	1.97	0.45
1:B:76:VAL:HG12	1:B:82:HIS:HB3	1.99	0.45
1:B:175:ARG:HA	1:B:218:PHE:HB3	1.99	0.45
1:A:358:PHE:HZ	1:A:362:GLY:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:210:ALA:HB1	2:C:255:LEU:HD11	1.98	0.45
3:D:48:LEU:CD2	3:D:50:HIS:H	2.30	0.45
3:D:73:LEU:CD1	3:D:77:LEU:CD1	2.95	0.45
1:B:195:THR:HA	1:B:198:LEU:HG	1.98	0.45
1:B:458:ASP:O	1:B:462:TRP:N	2.49	0.45
3:D:60:THR:HG22	3:D:141:VAL:HG23	1.99	0.45
1:A:321:TYR:HE2	1:A:390:LEU:HD23	1.81	0.45
3:D:30:ILE:CG1	3:D:133:ARG:HG3	2.47	0.45
3:D:54:TYR:HD1	3:D:84:TYR:CE1	2.34	0.45
1:A:509:HIS:HB2	1:A:525:ASP:HB2	1.99	0.44
1:A:342:THR:O	1:A:409:SER:N	2.50	0.44
1:A:345:GLY:N	1:A:349:SER:O	2.38	0.44
2:C:303:LEU:HG	2:C:320:GLY:HA3	1.98	0.44
3:D:111:GLU:HB2	3:D:136:LYS:HE2	1.98	0.44
1:A:461:HIS:CE1	1:B:366:ARG:HE	2.35	0.44
3:D:36:ASN:C	3:D:36:ASN:ND2	2.73	0.44
1:A:115:THR:HG21	1:A:442:VAL:HG21	1.99	0.44
1:A:238:SER:HA	2:C:186:LEU:HD21	1.99	0.44
1:A:565:THR:HG22	1:A:576:ARG:HG2	2.00	0.44
1:B:15:TYR:HB2	2:C:51:ALA:HA	2.00	0.44
1:B:511:ARG:HA	1:B:522:ARG:HA	2.00	0.44
1:B:378:VAL:HG12	1:B:390:LEU:HG	2.00	0.44
1:B:511:ARG:HG3	1:B:521:LEU:O	2.17	0.44
2:C:131:THR:OG1	2:C:132:GLN:N	2.51	0.44
1:B:79:LEU:HD23	1:B:79:LEU:HA	1.87	0.44
1:B:119:VAL:HG23	1:B:124:THR:HA	2.00	0.44
2:C:98:SER:HB3	3:D:39:ARG:NH1	2.31	0.44
1:A:206:PRO:HA	1:A:272:GLY:HA3	1.99	0.44
1:A:180:LEU:HD13	1:A:293:ALA:HA	2.00	0.43
1:A:343:GLY:HA3	1:A:408:LEU:N	2.33	0.43
3:D:23:VAL:HB	3:D:26:GLU:HB2	2.00	0.43
3:D:60:THR:HG22	3:D:141:VAL:CG2	2.48	0.43
1:B:77:SER:HA	1:B:82:HIS:CD2	2.53	0.43
3:D:48:LEU:CD2	3:D:50:HIS:N	2.81	0.43
1:A:515:PHE:HB2	1:A:521:LEU:HD13	1.99	0.43
1:B:482:LEU:HD11	1:B:502:ASP:HA	2.00	0.43
1:B:508:GLN:HG2	2:C:346:TYR:HE1	1.84	0.43
1:A:68:LEU:HD23	1:A:71:LEU:HD12	1.99	0.43
1:B:339:ASP:H	1:B:414:GLY:HA2	1.83	0.43
2:C:28:PHE:HA	2:C:31:PHE:HB3	1.99	0.43
1:A:56:SER:HB2	1:A:59:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:C	3:D:85:GLU:OE2	2.61	0.43
1:B:347:THR:OG1	1:B:406:GLU:N	2.52	0.43
1:B:154:SER:N	1:B:279:LEU:HD11	2.33	0.43
3:D:37:MET:CE	3:D:112:LEU:CD2	2.61	0.43
3:D:38:GLN:CD	3:D:137:GLN:CD	2.87	0.43
1:B:86:THR:HG22	1:B:453:TYR:HE1	1.84	0.43
1:B:16:LEU:HD11	1:B:54:ALA:HB3	2.01	0.43
1:B:436:LEU:HD23	1:B:439:PRO:HA	2.01	0.43
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.92	0.43
1:B:101:VAL:HG11	1:B:162:CYS:HB3	2.01	0.43
3:D:102:GLY:O	3:D:103:GLU:HB3	2.19	0.43
3:D:118:VAL:CG1	3:D:119:ARG:N	2.81	0.43
1:A:115:THR:HG22	1:A:430:ASP:HA	2.01	0.42
1:B:336:TYR:HD1	1:B:416:ASN:HB3	1.84	0.42
3:D:76:VAL:CG1	3:D:77:LEU:N	2.82	0.42
1:A:119:VAL:N	1:A:123:ASN:O	2.51	0.42
1:A:360:HIS:HA	1:A:363:GLY:H	1.84	0.42
1:B:136:LEU:HD13	1:B:297:HIS:CG	2.54	0.42
1:B:276:GLU:O	1:B:280:SER:N	2.51	0.42
2:C:10:SER:HA	2:C:13:ALA:HB3	2.00	0.42
2:C:135:ARG:HB3	2:C:140:TYR:CZ	2.54	0.42
3:D:133:ARG:HA	3:D:133:ARG:HE	1.81	0.42
1:B:240:TYR:HB3	1:B:244:LEU:HD23	2.01	0.42
1:B:521:LEU:HB3	1:B:561:PHE:CD2	2.55	0.42
2:C:209:GLN:O	2:C:258:SER:N	2.53	0.42
3:D:63:LEU:HD11	3:D:105:HIS:O	2.19	0.42
3:D:69:THR:HG23	3:D:70:ALA:N	2.34	0.42
3:D:73:LEU:HA	3:D:76:VAL:HG12	2.00	0.42
1:B:266:LEU:HB3	1:B:270:ILE:HB	2.00	0.42
1:B:538:GLU:HA	1:B:541:ILE:HB	2.01	0.42
3:D:56:LEU:CD2	3:D:80:VAL:CG1	2.95	0.42
1:A:229:LEU:HD22	1:A:549:ASN:HD22	1.84	0.42
1:A:542:HIS:O	1:A:546:GLU:HB2	2.20	0.42
1:A:580:ASN:HB3	1:A:582:ASN:HD21	1.83	0.42
1:B:482:LEU:HD12	1:B:504:ILE:HB	2.01	0.42
2:C:175:THR:HA	2:C:176:PRO:HD3	1.87	0.42
3:D:30:ILE:HD12	3:D:133:ARG:CD	2.49	0.42
1:A:92:VAL:HG22	1:A:300:PRO:HD3	2.02	0.42
1:A:144:VAL:HG12	1:A:157:LYS:H	1.84	0.42
2:C:102:ALA:HB2	3:D:32:SER:O	2.15	0.42
2:C:223:LYS:HE3	2:C:223:LYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:111:GLU:CG	3:D:136:LYS:CE	2.95	0.42
1:A:200:ALA:O	1:A:203:LEU:HB2	2.20	0.42
1:A:242:LEU:HD23	1:A:242:LEU:HA	1.90	0.42
1:B:189:THR:O	1:B:193:MET:HB2	2.20	0.42
1:A:212:ILE:HG13	1:A:213:ARG:H	1.85	0.42
2:C:263:SER:O	2:C:267:GLY:N	2.52	0.42
3:D:103:GLU:HG2	3:D:104:LEU:CD1	2.50	0.42
1:B:344:SER:HB2	1:B:355:PHE:CZ	2.55	0.41
1:B:379:LYS:N	1:B:389:TRP:O	2.53	0.41
1:B:505:LEU:N	1:B:528:VAL:HG11	2.34	0.41
2:C:35:LEU:O	2:C:38:SER:OG	2.28	0.41
3:D:89:LYS:HG3	3:D:126:PRO:HG3	2.01	0.41
1:B:196:LYS:HG2	1:B:275:LEU:HD22	2.01	0.41
1:B:321:TYR:HB3	1:B:391:ILE:HD13	2.02	0.41
2:C:331:ILE:H	2:C:331:ILE:HG13	1.76	0.41
3:D:30:ILE:HG13	3:D:133:ARG:HG3	2.02	0.41
3:D:50:HIS:HB2	3:D:51:LEU:HD22	2.02	0.41
3:D:54:TYR:HD1	3:D:84:TYR:CD1	2.37	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.88	0.41
1:A:140:ALA:HB2	1:A:160:PHE:HB2	2.01	0.41
1:A:371:GLU:HB3	1:A:395:GLN:HG3	2.02	0.41
1:A:508:GLN:HB3	1:B:584:ARG:HH21	1.86	0.41
1:B:110:ALA:HB2	1:B:133:ALA:H	1.85	0.41
1:A:475:MET:HE2	1:A:475:MET:HB3	1.87	0.41
1:A:481:VAL:O	1:A:485:THR:OG1	2.26	0.41
2:C:110:GLN:H	2:C:112:ARG:HB2	1.85	0.41
2:C:326:ARG:HG3	2:C:328:GLN:H	1.85	0.41
1:A:116:SER:HB2	1:A:125:VAL:HB	2.02	0.41
1:B:450:LEU:H	1:B:492:ARG:HH12	1.69	0.41
3:D:37:MET:HE2	3:D:112:LEU:HD22	1.93	0.41
3:D:89:LYS:HB3	3:D:126:PRO:CD	2.50	0.41
1:A:144:VAL:HB	1:A:156:LEU:HA	2.02	0.41
1:A:276:GLU:H	1:A:277:VAL:HG22	1.86	0.41
1:A:422:ARG:HB3	1:A:424:LEU:HD21	2.02	0.41
3:D:80:VAL:CG2	3:D:81:LEU:N	2.83	0.41
1:A:126:CYS:HB3	1:A:305:PHE:CE1	2.56	0.41
3:D:73:LEU:HD21	3:D:77:LEU:HD21	2.02	0.41
1:A:45:CYS:HB2	3:D:36:ASN:OD1	2.21	0.41
1:A:360:HIS:CG	1:A:363:GLY:HA3	2.56	0.41
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.90	0.41
2:C:324:VAL:HB	2:C:325:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:51:LEU:N	3:D:51:LEU:CD2	2.83	0.41
3:D:98:GLN:CB	3:D:101:PRO:HD2	2.44	0.41
3:D:106:TYR:O	3:D:106:TYR:CD1	2.74	0.41
1:A:353:VAL:H	1:A:372:ARG:HB3	1.86	0.41
1:B:126:CYS:SG	1:B:416:ASN:ND2	2.94	0.41
1:B:196:LYS:HE3	1:B:279:LEU:HB2	2.03	0.41
2:C:223:LYS:H	2:C:223:LYS:HD2	1.86	0.41
3:D:123:THR:HA	3:D:131:LEU:H	1.86	0.41
1:A:30:ARG:HA	1:A:30:ARG:HD3	1.84	0.40
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.80	0.40
1:A:161:ALA:HB1	1:A:211:ARG:NE	2.36	0.40
1:A:476:LEU:HB3	1:A:477:SER:H	1.64	0.40
3:D:142:GLN:HG2	3:D:143:THR:O	2.21	0.40
1:A:255:PHE:HD1	1:A:255:PHE:HA	1.73	0.40
1:B:511:ARG:HH22	1:B:520:LEU:HB3	1.87	0.40
3:D:38:GLN:OE1	3:D:38:GLN:N	2.54	0.40
3:D:89:LYS:HB3	3:D:90:ARG:H	1.69	0.40
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.85	0.40
1:A:174:HIS:CD2	1:A:175:ARG:HG3	2.56	0.40
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.91	0.40
1:A:478:SER:OG	1:A:506:ALA:N	2.42	0.40
1:B:6:LEU:HA	1:B:9:PHE:HB3	2.04	0.40
1:B:345:GLY:HA2	1:B:408:LEU:HG	2.03	0.40
2:C:254:LEU:HD13	2:C:293:ARG:HD3	2.03	0.40
3:D:77:LEU:HD12	3:D:93:VAL:CG1	2.41	0.40
3:D:106:TYR:O	3:D:106:TYR:HD1	2.04	0.40
3:D:115:ALA:CA	3:D:123:THR:CB	2.95	0.40
3:D:135:LEU:CD2	3:D:135:LEU:C	2.94	0.40
1:B:546:GLU:HB3	1:B:550:ARG:CZ	2.51	0.40
2:C:112:ARG:HG3	2:C:113:GLU:H	1.86	0.40
3:D:60:THR:HA	3:D:141:VAL:HG23	2.03	0.40
3:D:117:LEU:C	3:D:117:LEU:CD1	2.94	0.40
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.88	0.40
1:B:327:ARG:HH21	1:B:337:SER:HA	1.85	0.40
3:D:41:LEU:HD23	3:D:56:LEU:HD12	2.03	0.40
3:D:48:LEU:HD23	3:D:48:LEU:C	2.47	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	582/587 (99%)	474 (81%)	108 (19%)	0	100	100
1	B	581/587 (99%)	471 (81%)	109 (19%)	1 (0%)	43	78
2	C	348/366 (95%)	271 (78%)	75 (22%)	2 (1%)	21	59
3	D	119/143 (83%)	110 (92%)	6 (5%)	3 (2%)	4	26
All	All	1630/1683 (97%)	1326 (81%)	298 (18%)	6 (0%)	31	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	44	ARG
3	D	105	HIS
3	D	118	VAL
2	C	220	ILE
2	C	347	GLN
1	B	558	MET

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	501/504 (99%)	501 (100%)	0	100	100
1	B	501/504 (99%)	498 (99%)	3 (1%)	78	81
2	C	287/310 (93%)	286 (100%)	1 (0%)	86	84
3	D	108/127 (85%)	102 (94%)	6 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1397/1445 (97%)	1387 (99%)	10 (1%)	73	79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	99	LEU
1	B	185	PRO
1	B	392	LEU
2	C	223	LYS
3	D	25	GLU
3	D	31	LEU
3	D	38	GLN
3	D	49	LYS
3	D	51	LEU
3	D	89	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	208	ASN
1	A	297	HIS
1	A	303	ASN
1	A	444	ASN
1	A	461	HIS
1	A	560	GLN
1	A	562	ASN
1	A	581	HIS
1	A	582	ASN
1	B	62	GLN
1	B	82	HIS
1	B	208	ASN
1	B	257	HIS
1	B	367	HIS
1	B	461	HIS
1	B	490	ASN
1	B	509	HIS
1	B	580	ASN
2	C	22	GLN
2	C	27	ASN
2	C	111	GLN

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Mol	Chain	Res	Type
2	C	127	HIS
2	C	171	GLN
2	C	252	GLN
2	C	318	GLN
2	C	328	GLN
2	C	350	GLN
2	C	352	HIS
3	D	38	GLN
3	D	50	HIS
3	D	72	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 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.

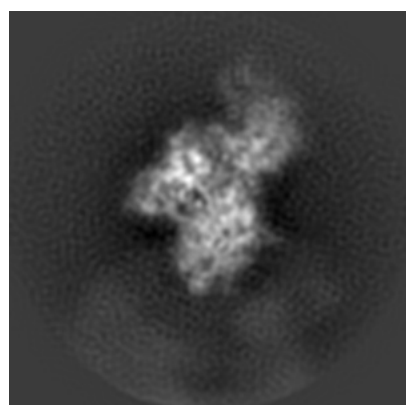
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0009. These allow visual inspection of the internal detail of the map and identification of artifacts.

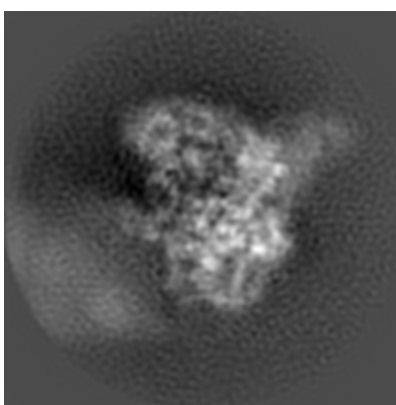
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

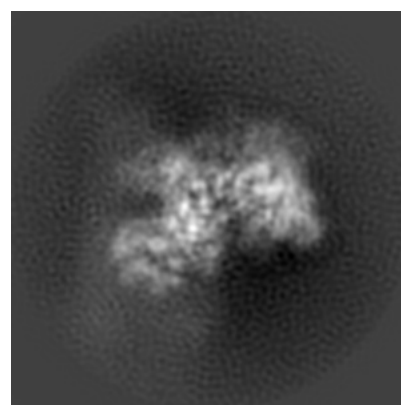
6.1.1 Primary map



X



Y

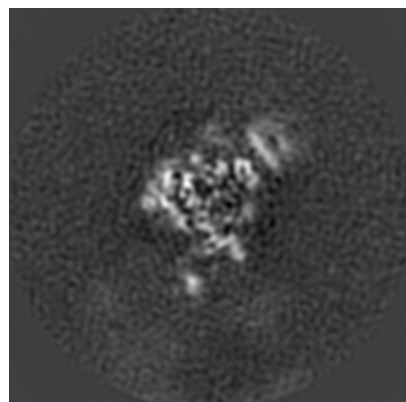


Z

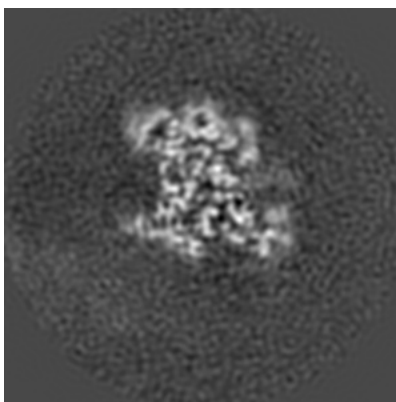
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

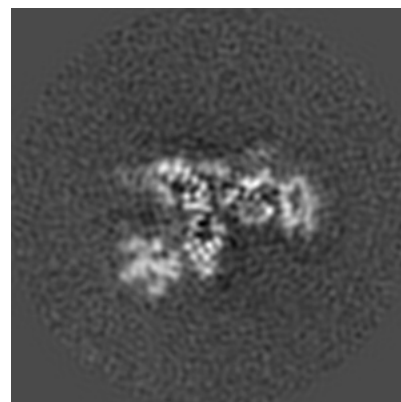
6.2.1 Primary map



X Index: 100



Y Index: 100

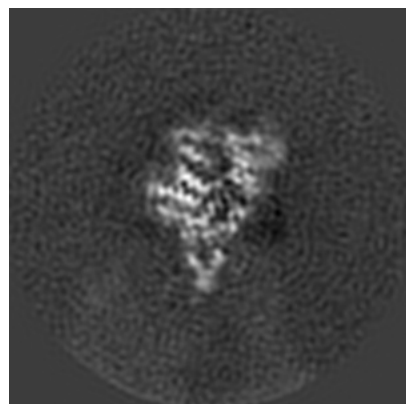


Z Index: 100

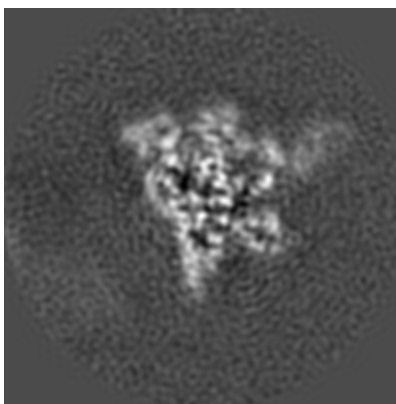
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

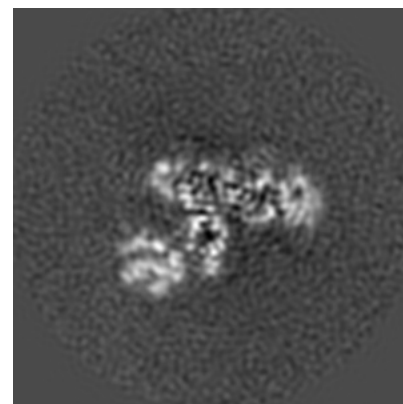
6.3.1 Primary map



X Index: 90



Y Index: 111

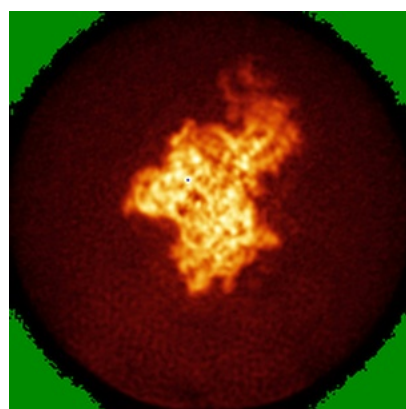


Z Index: 102

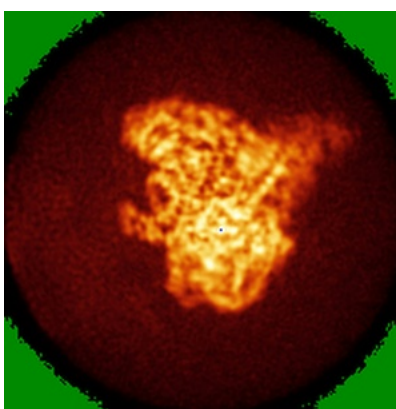
The images above show the largest variance slices of the map in three orthogonal directions.

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

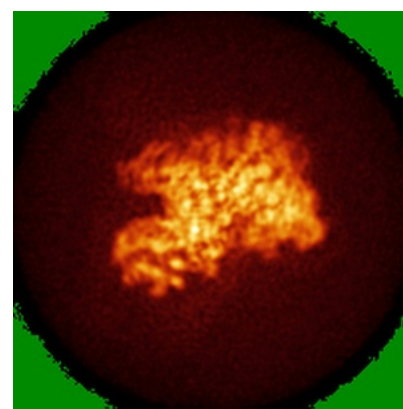
6.4.1 Primary map



X



Y

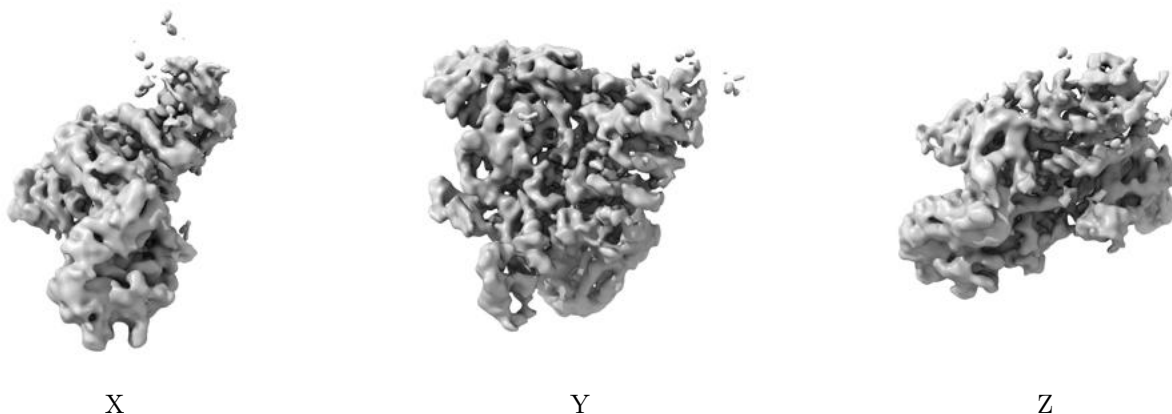


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

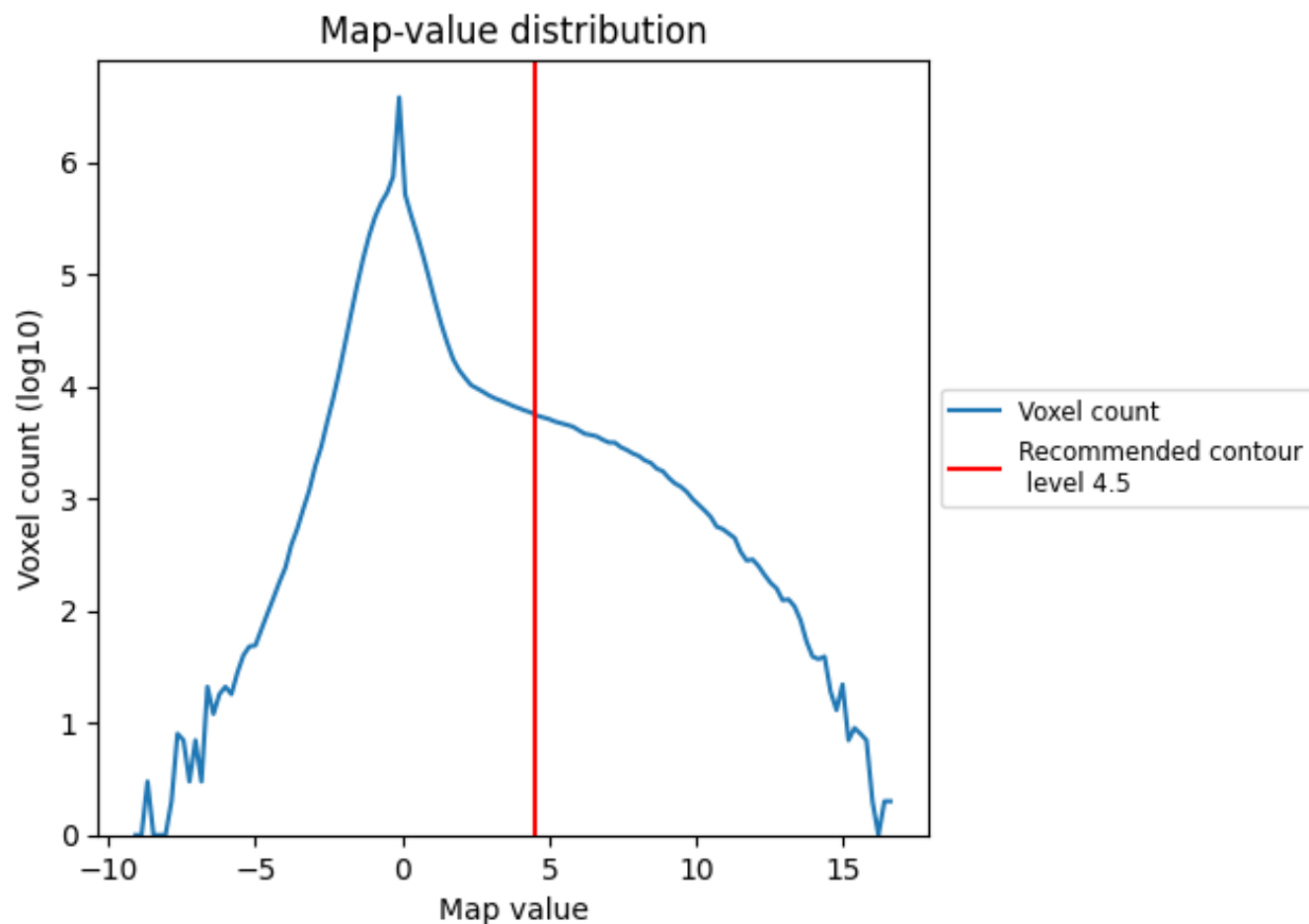
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

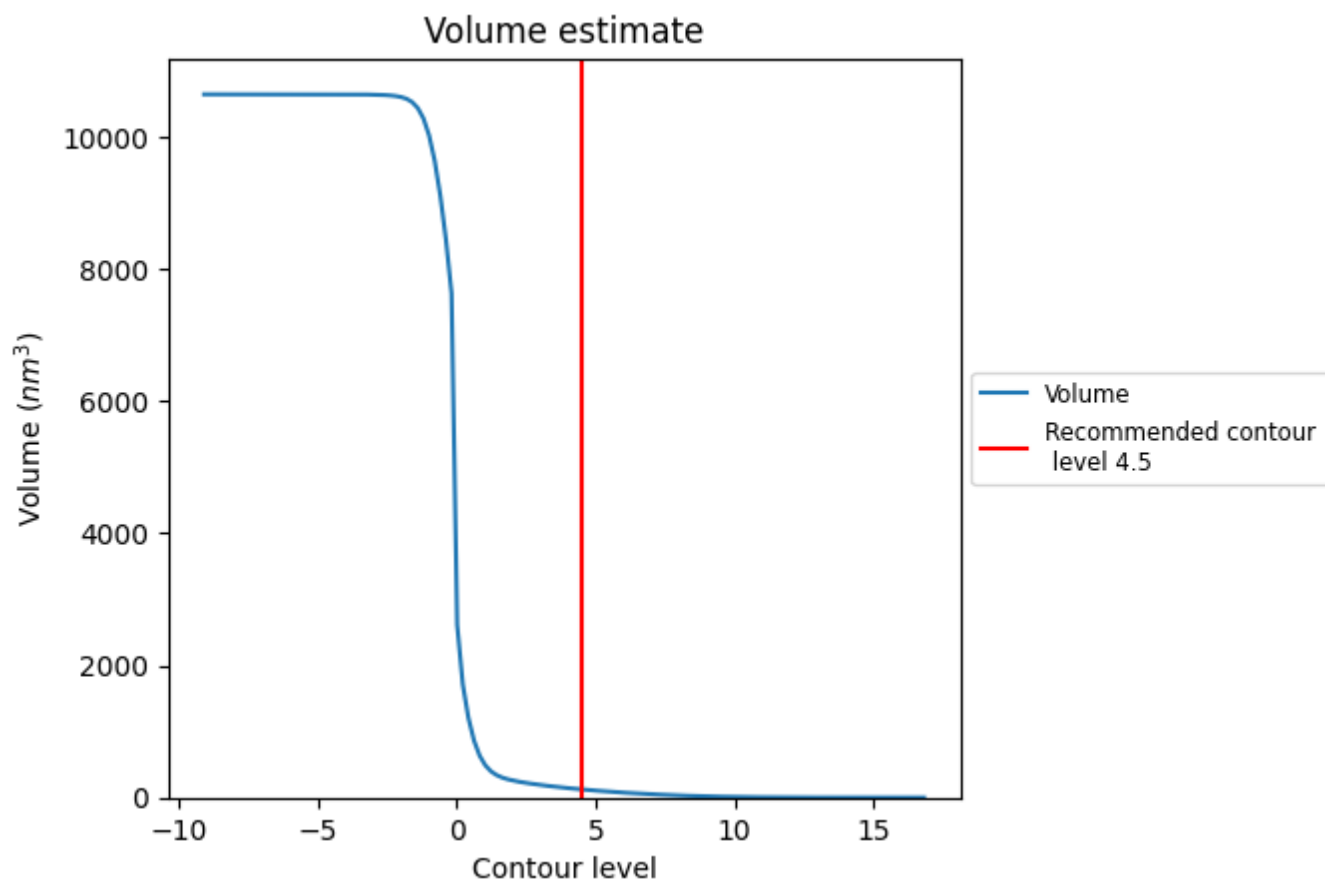
This section contains the results of statistical analysis of the map.

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.

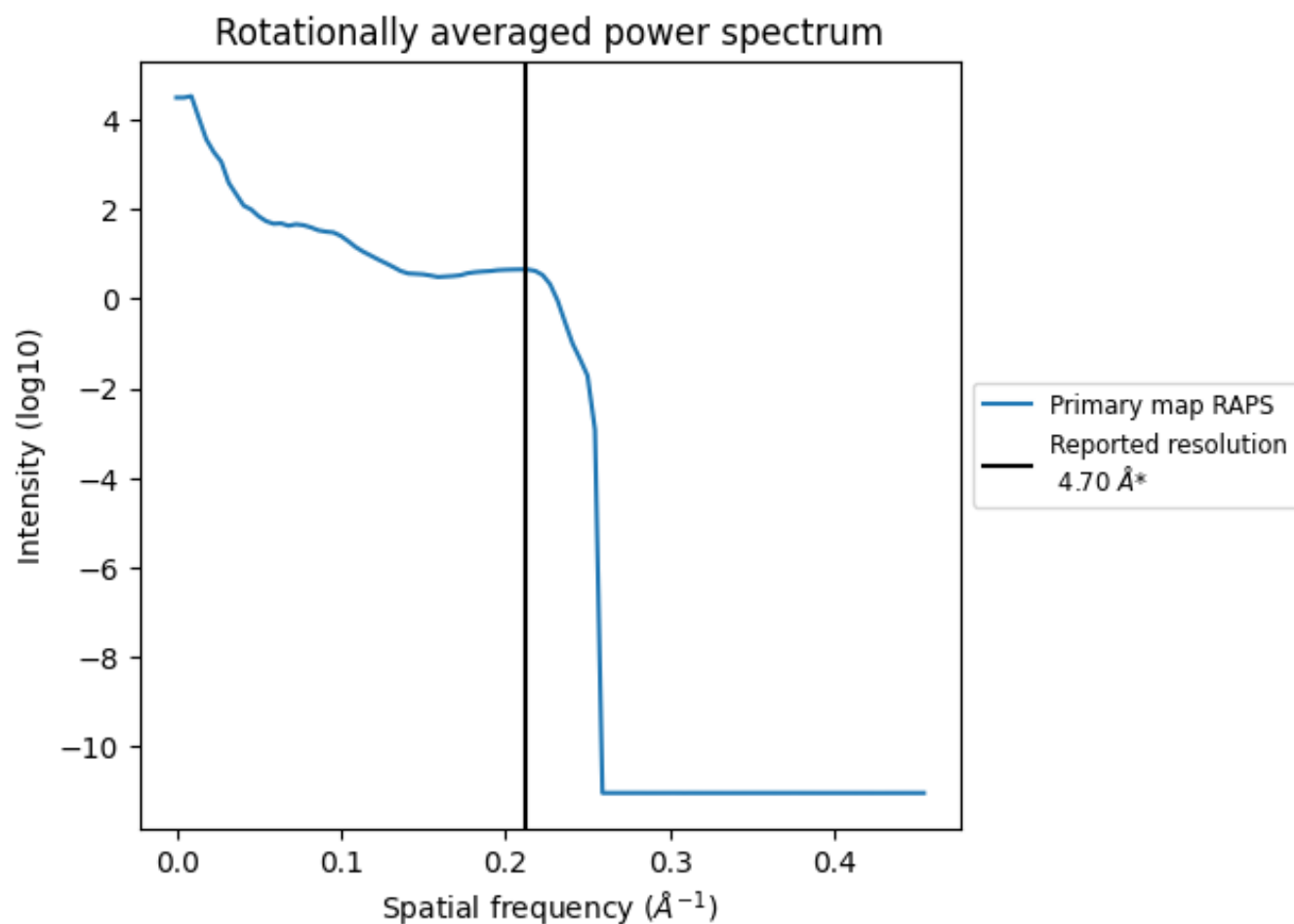
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 123 nm³; this corresponds to an approximate mass of 112 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 0.213 Å⁻¹

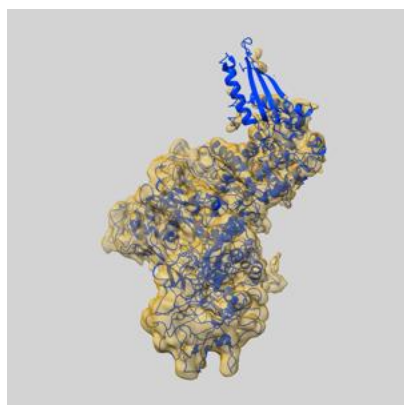
8 Fourier-Shell correlation ⓘ

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

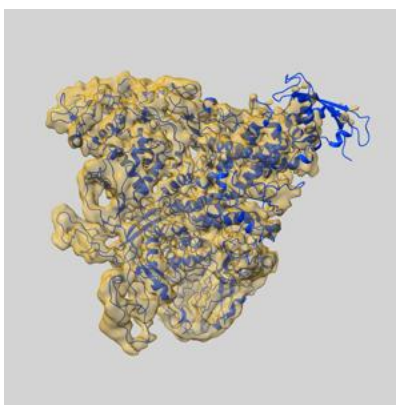
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0009 and PDB model 6GJ1. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

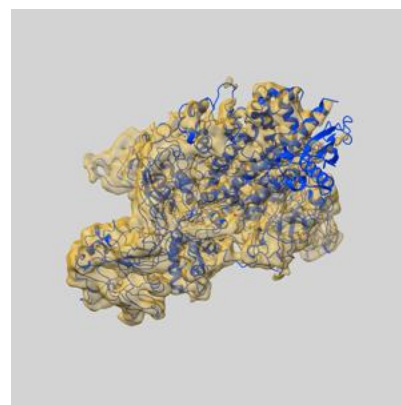
9.1 Map-model overlay [i](#)



X



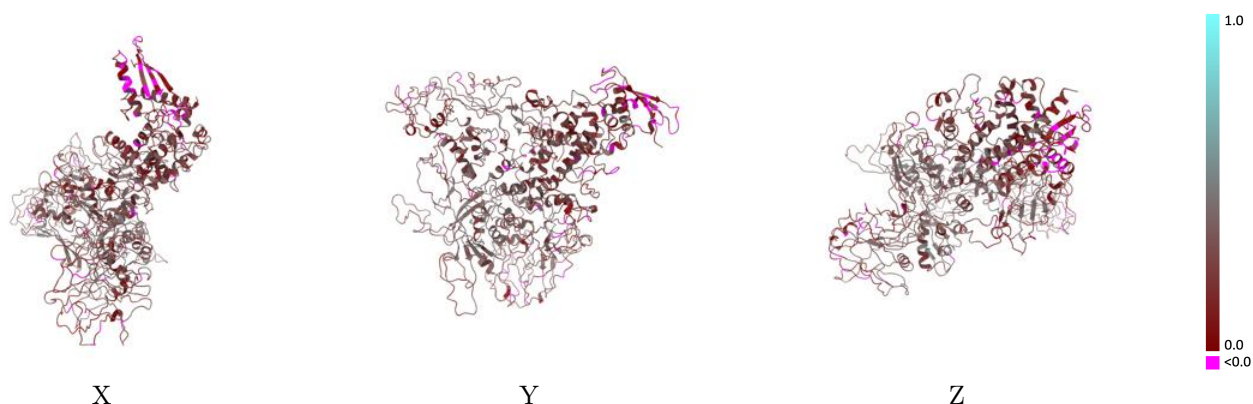
Y



Z

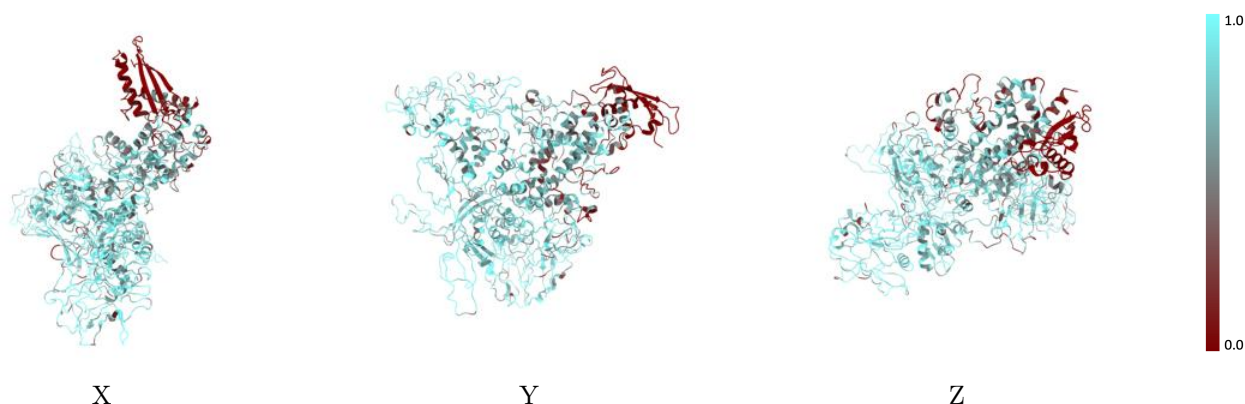
The images above show the 3D surface view of the map at the recommended contour level 4.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



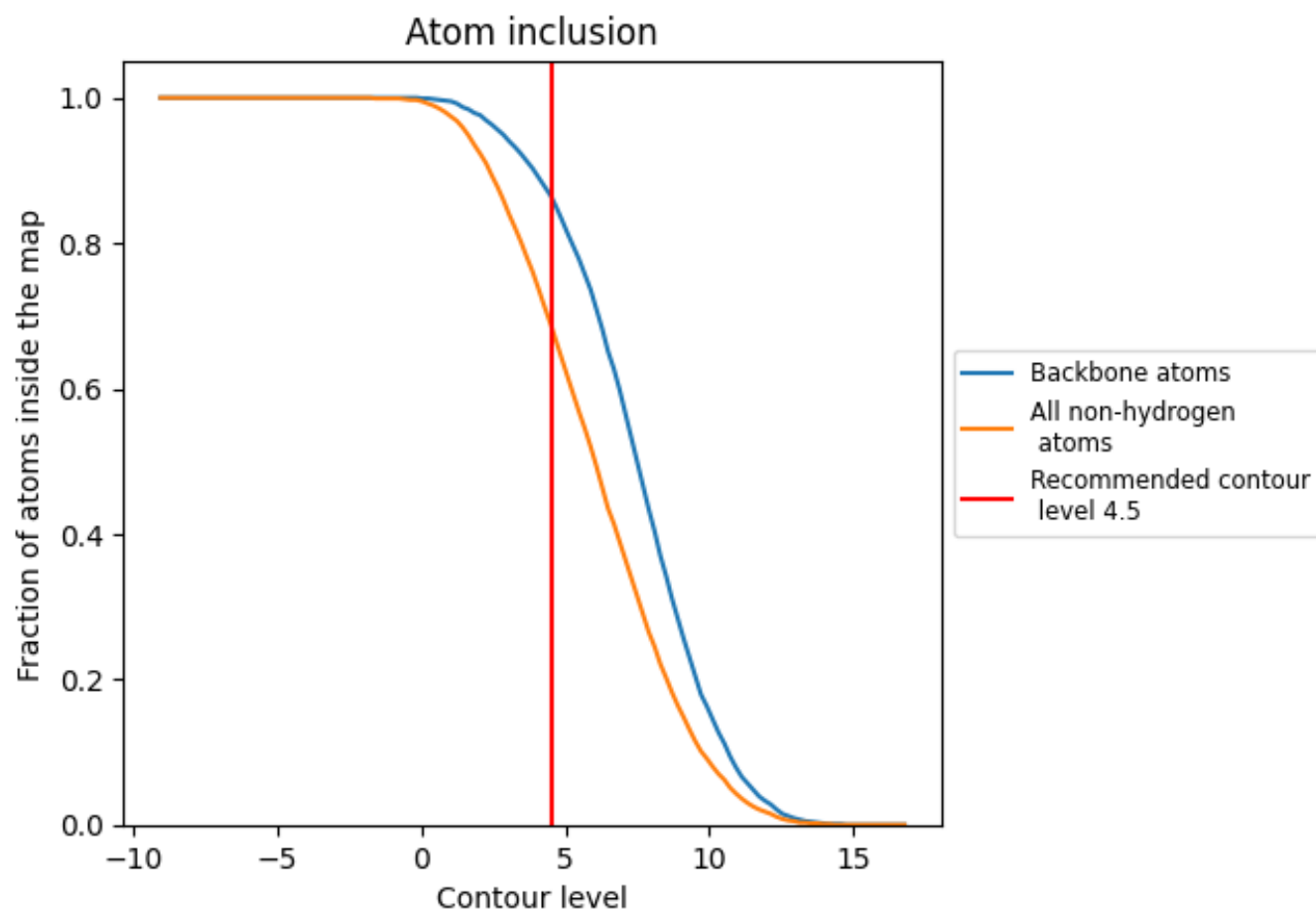
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 69% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6880	0.2670
A	0.7650	0.2740
B	0.7400	0.2690
C	0.6870	0.3040
D	0.0800	0.1160

