



Full wwPDB EM Validation Report ⓘ

Jul 27, 2026 – 05:52 PM EDT

PDB ID : 9PRO / pdb_00009pro
EMDB ID : EMD-71810
Title : Human 19S proteasome bound to TXNL1 PITH domain and PSMD5
Authors : Chen, X.; Negi, H.; Walters, K.J.
Deposited on : 2025-07-24
Resolution : 4.07 Å(reported)
Based on initial models : ., 7WSI, 1WWY

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:

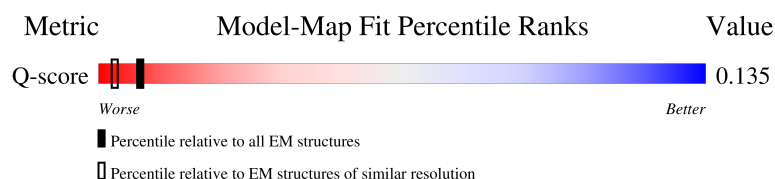
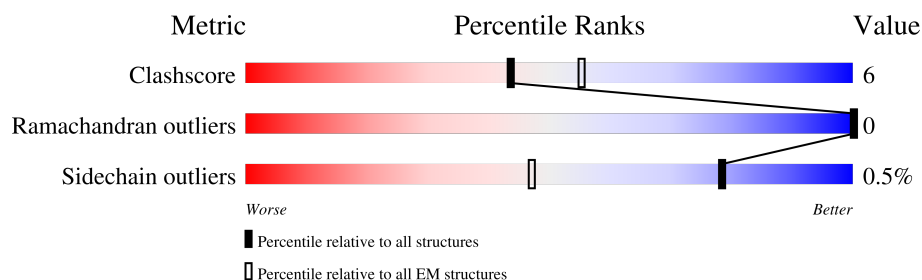
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 4.07 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.



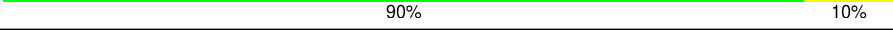
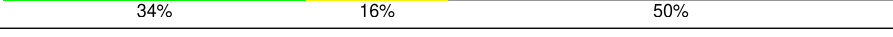
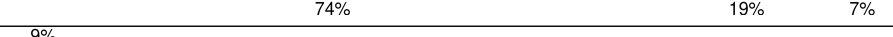
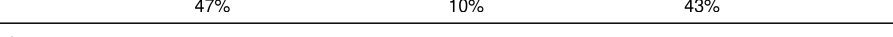
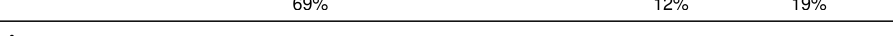
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6427 (3.58 - 4.57)

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	433	 5% 69% 14% 12%
2	B	440	 1% 67% 17% 15%
3	C	406	 69% 22% 9%
4	D	418	 69% 18% 12%

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Mol	Chain	Length	Quality of chain
5	E	389	
6	F	439	
7	U	953	
8	V	534	
9	W	456	
10	X	422	
11	Y	389	
12	Z	324	
13	a	376	
14	b	377	
15	c	310	
16	d	350	
17	e	70	
18	f	908	
19	g	289	
20	z	504	

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 57756 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 RPT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	361	Total	C	N	O	S	0	0
			2833	1782	504	530	17		

- Molecule 2 is a protein called RPT2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	373	Total	C	N	O	S	0	0
			2948	1855	502	576	15		

- Molecule 3 is a protein called RPT6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	0
			2912	1831	523	541	17		

- Molecule 4 is a protein called RPT3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	369	Total	C	N	O	S	0	0
			2935	1857	507	558	13		

- Molecule 5 is a protein called RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	380	Total	C	N	O	S	0	0
			3025	1900	542	567	16		

- Molecule 6 is a protein called RPT5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	374	Total	C	N	O	S	0	0
			2930	1845	506	561	18		

- Molecule 7 is a protein called RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	831	Total	C	N	O	S	0	0
			6472	4108	1099	1221	44		

- Molecule 8 is a protein called RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V	463	Total	C	N	O	S	0	0
			3731	2370	665	683	13		

- Molecule 9 is a protein called RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	W	437	Total	C	N	O	S	0	0
			3564	2258	609	674	23		

- Molecule 10 is a protein called RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	105	Total	C	N	O	S	0	0
			844	542	140	160	2		

- Molecule 11 is a protein called RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 12 is a protein called RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	287	Total	C	N	O	S	0	0
			2290	1462	394	429	5		

- Molecule 13 is a protein called RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 14 is a protein called RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	189	Total	C	N	O	S	0	0
			1449	905	259	277	8		

- Molecule 15 is a protein called RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 16 is a protein called RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	265	Total	C	N	O	S	0	0
			2166	1402	355	400	9		

- Molecule 17 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 18 is a protein called RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	736	Total	C	N	O	S	0	0
			5695	3586	973	1096	40		

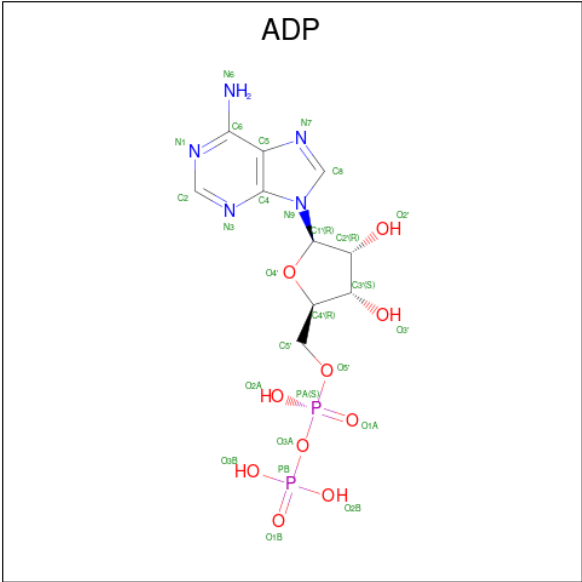
- Molecule 19 is a protein called TXNL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	173	Total	C	N	O	S	0	0
			1383	869	227	278	9		

- Molecule 20 is a protein called PSMD5.

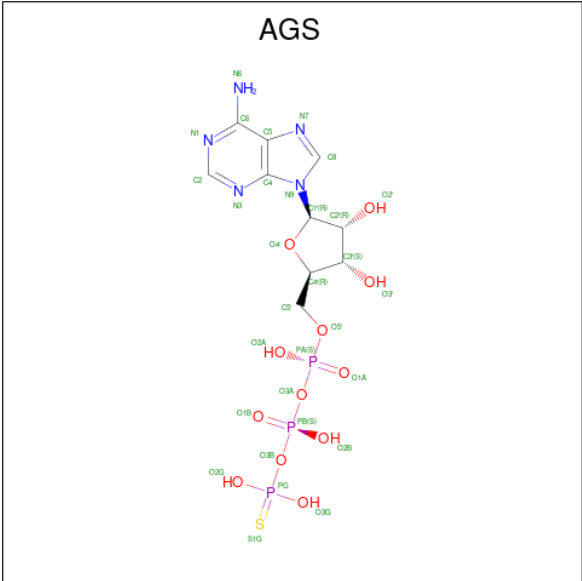
Mol	Chain	Residues	Atoms					AltConf	Trace
20	z	472	Total	C	N	O	S	0	0
			3704	2354	628	706	16		

- Molecule 21 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
21	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 22 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
22	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

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Mol	Chain	Residues	Atoms						AltConf
22	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
22	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
23	C	1	Total	Mg	0
			1	1	
23	D	1	Total	Mg	0
			1	1	
23	E	1	Total	Mg	0
			1	1	

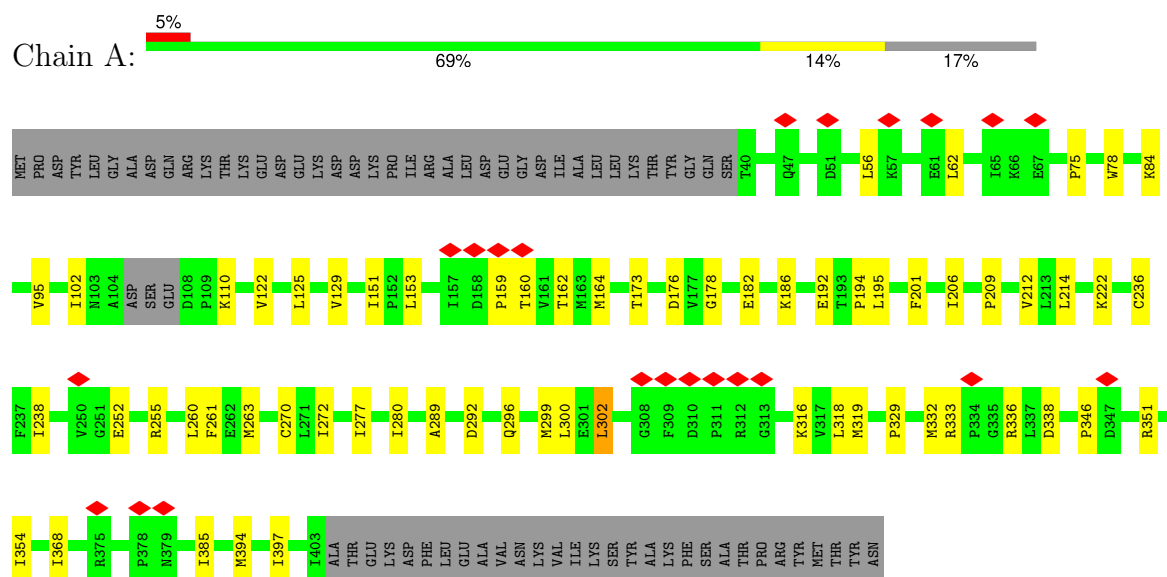
- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	c	1	Total	Zn	0
			1	1	

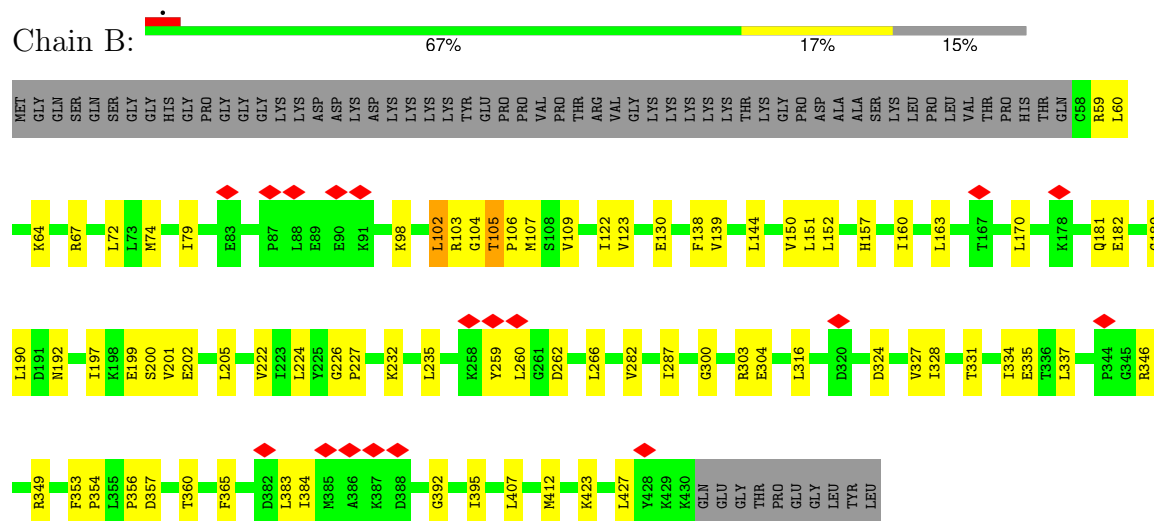
3 Residue-property plots

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: RPT1



• Molecule 2: RPT2



• Molecule 3: RPT6

Response	Percentage
Yes	69%
No	22%
Don't know	9%



69% 18% 12%

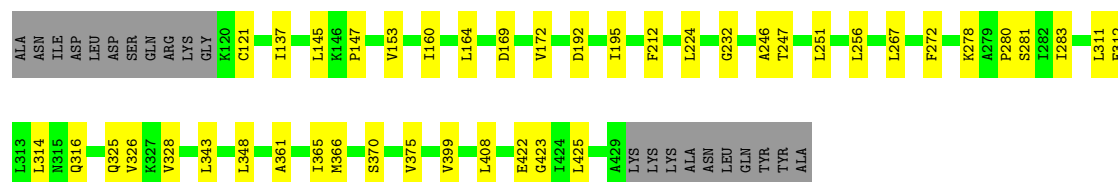


Response	Percentage
Yes, it is a crisis	76%
No, it is not a crisis	22%



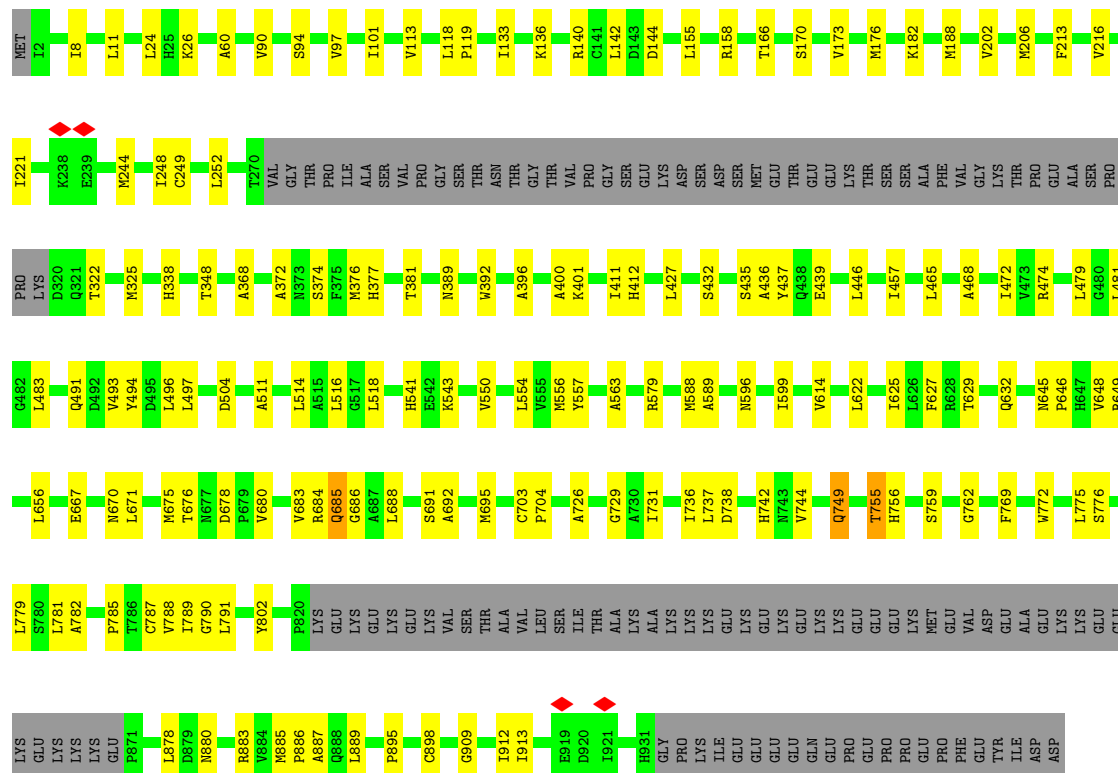
Response	Percentage
U.S. should take action to reduce greenhouse gas emissions	73%
U.S. should not take action to reduce greenhouse gas emissions	12%
U.S. should not take action to reduce greenhouse gas emissions (Unsure)	15%





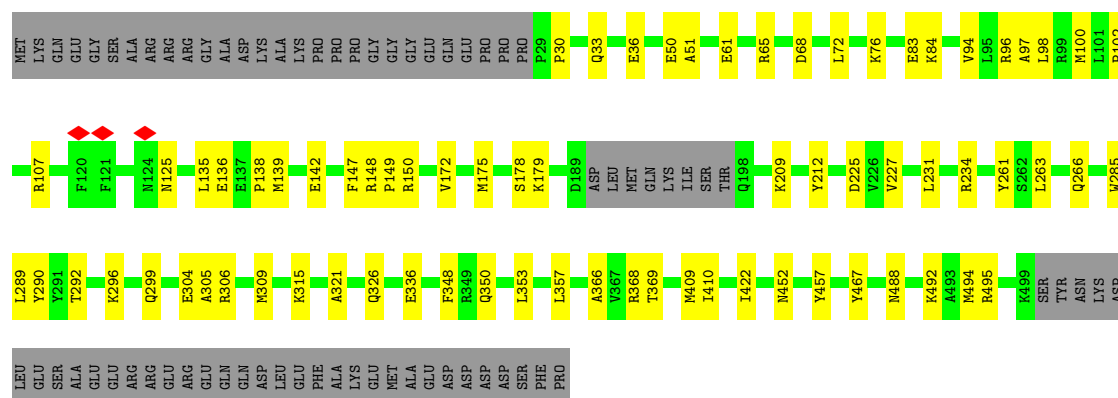
• Molecule 7: RPN2

Chain U: 71% 16% 13%



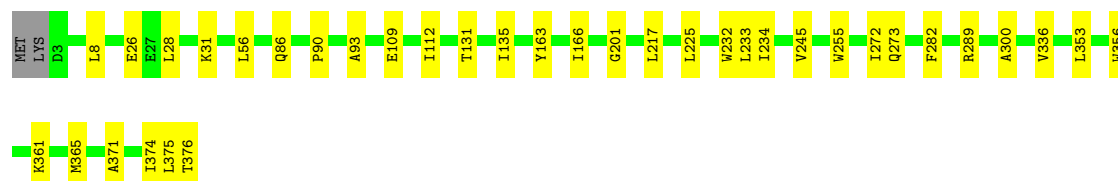
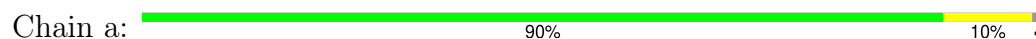
• Molecule 8: RPN3

Chain V: 73% 14% 13%

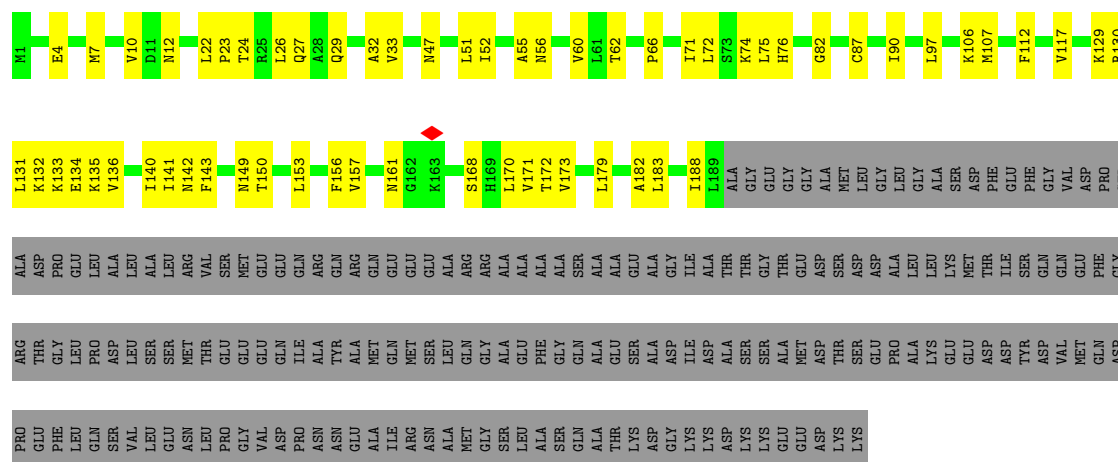
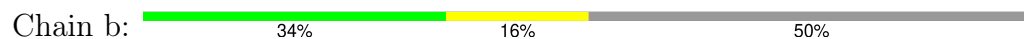


• Molecule 9: RPN5

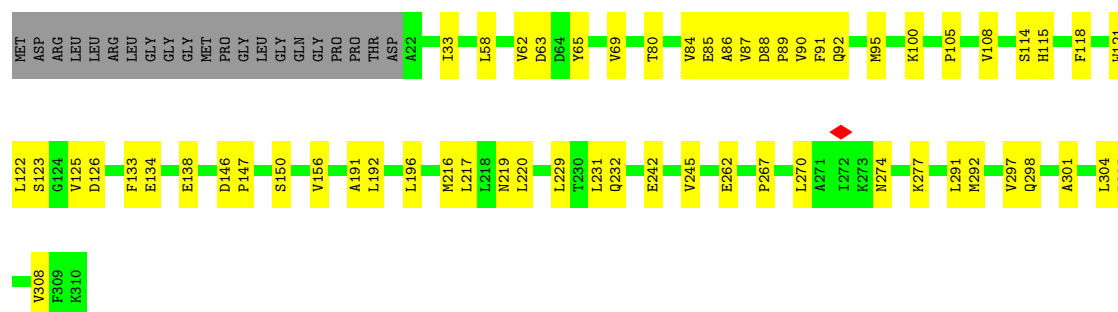
- Molecule 13: RPN9



- Molecule 14: RPN10

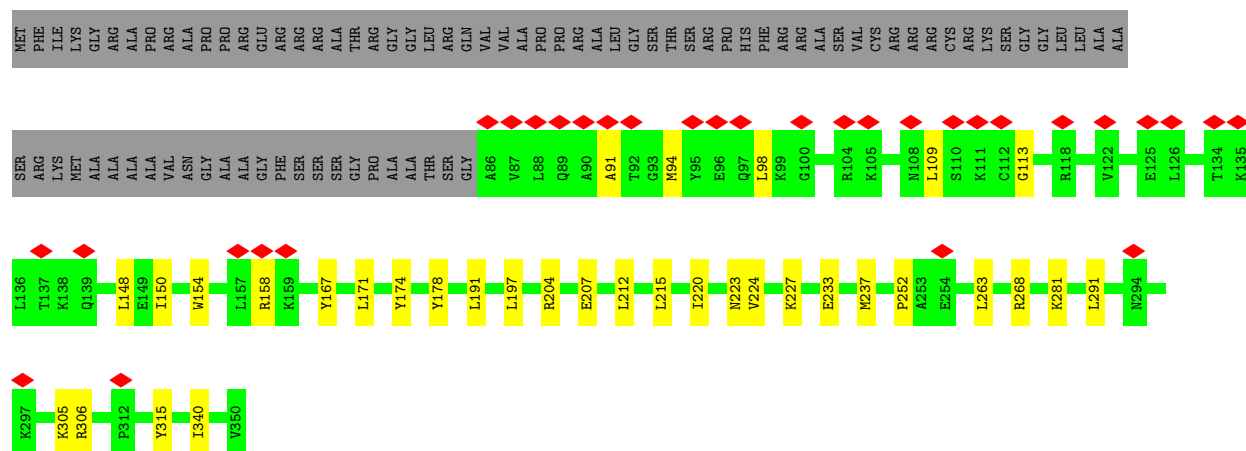


- Molecule 15: RPN11



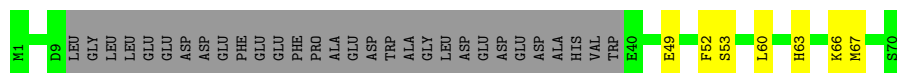
- Molecule 16: RPN12





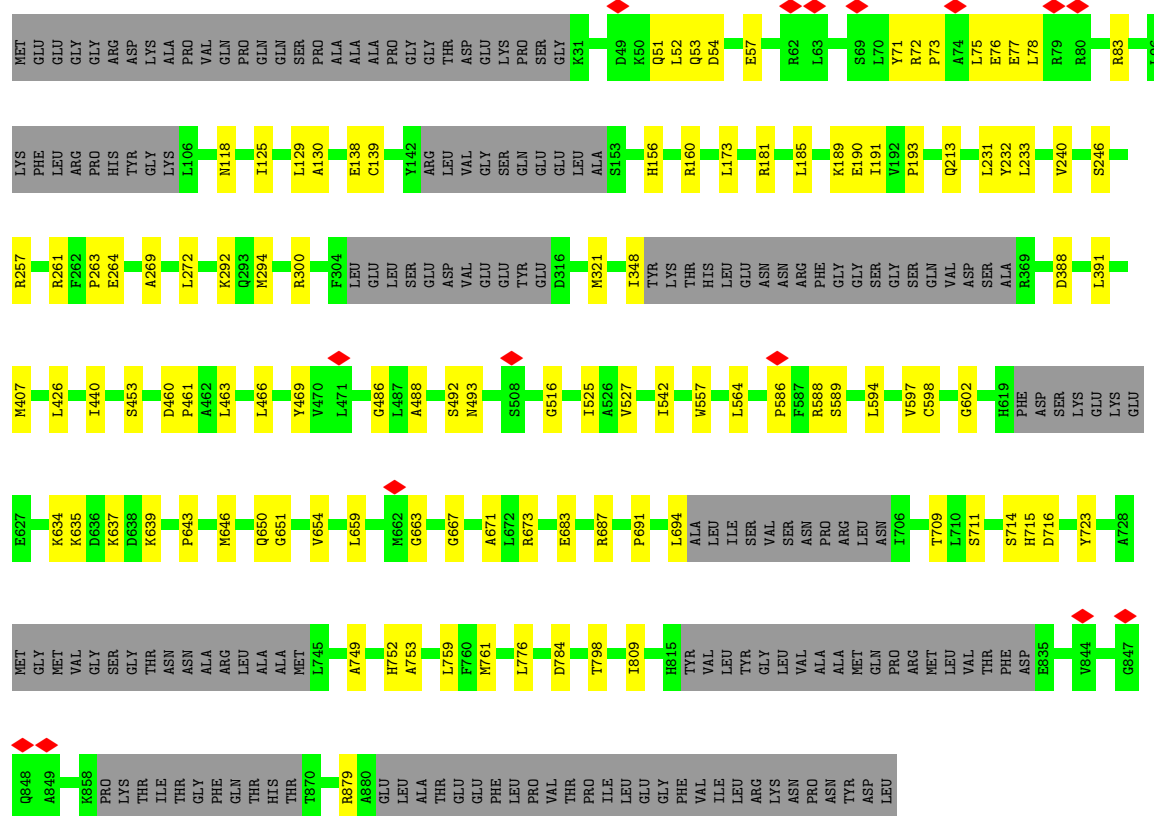
• Molecule 17: DSS1

Chain e: 47% 10% 43%



• Molecule 18: RPN1

Chain f: 69% 12% 19%



• Molecule 19: TXNL1

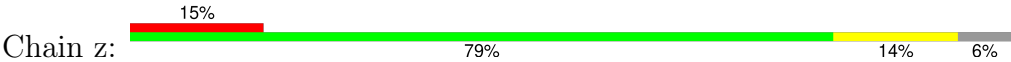


MET	VAL	GLY	VAL	LYS	PRO	VAL	GLY	ASP	PRO	ASP	PHE	GLN	PRO	LEU	THR	GLY	ALA	GLY	SER	ARG	LEU	ALA	VAL	VAL	LYS	PHE	THR	THR	MET	ARG	GLY	GLY	PRO	CYS	VAL	LEU	ARG	ILE	ALA	PRO	ALA	PHE	SER	SER	MET	SER	ASN	LYS	TYR	PRO	GLY	GLN	ALA	VAL	PHE	LEU	GLU	VAL	ASP
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VAL	HIS	GLN	CYS	GLY	THR	ALA	THR	ASN	ILE	SER	ALA	THR	PRO	PHE	LEU	PHE	PHE	ASN	ARG	LYS	VAL	ARG	ILE	ASP	GLN	TYR	GLN	GLY	ALA	CYS	ASP	ALA	VAL	GLY	LEU	LEU	GLU	GLU	LYS	ILE	LYS	GLN	SER	ASN	ASP	PRO	GLY	PRO	SER	ASN	GLU	ASP	THR	ASP	T117	D118	I119	P120
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L126	F129	I130	N131	L138	D153	L157	L166	I167	T168	V169	A170	K176	P185	D186	Q189	E222	Y235	Q239	T245	G253	E254	R259	I260	R280	E287	S288	H289
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• Molecule 20: PSMD5



MET	ALA	ALA	GLN	ALA	LEU	ALA	LEU	ARG	GLU	VAL	ALA	ARG	LEU	GLU	PRO	ALA	LEU	GLU	GLU	ARG	LEU	ALA	HIS	SER	VAL	LEU	GLN	ALA	V32	P33	L34	N35	E36	L49	E55	N56	H57	R58	E59	K60	T61	T62	L63	C64	V65	S66	I67	R70	L71	L72	E76	P77
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V80	L84	D87	P95	D96	K100	I101	L102	D115	I120	L126	I127	K128	Y132	N138	L139	S140	V141	Q156	L159	E164	L168	L171	I180	R184	V185	Y186	I189	S199	T204	T205	L208	V209	T210	Q211	L212	L213	R214	E215
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L222	S233	L234	Q242	I250	P264	Y269	L270	P271	S285	P286	Q287	Q288	E291	R292	Y293	E298	K299	V300	I304	V314	D317	G320	I321	L322	G323	S324	N325	V326	Q333	T337	L342	I346	Q349	S350	A353	P354	L357	L362	D363
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S367	F372	P373	E374	Q375	T377	D378	D379	L380	M383	W387	R393	R400	P406	K416	T419	F437	V438	E439	Y440	V441	V442	E458	L459	V460	K461	A462	L463	A464	M465	I469	A470	E471	I472	F473	G474	M475	P476	M477	Y478	L479	R480	L481	R482	T483	T497
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T498	E501	G502	A503	GLU
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	54253	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	100000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.194	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	349.92, 349.92, 349.92	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.38	0/2878	0.69	0/3884
2	B	0.40	0/2989	0.73	0/4028
3	C	0.50	0/2949	0.82	0/3964
4	D	0.52	0/2982	0.77	0/4027
5	E	0.45	0/3071	0.76	0/4131
6	F	0.39	0/2967	0.68	0/3997
7	U	0.34	0/6589	0.71	0/8922
8	V	0.25	0/3803	0.58	0/5134
9	W	0.33	0/3612	0.69	0/4858
10	X	0.36	0/855	0.57	0/1150
11	Y	0.37	0/3173	0.69	0/4273
12	Z	0.31	0/2333	0.59	0/3162
13	a	0.26	0/3061	0.56	0/4144
14	b	0.52	0/1469	0.79	0/1989
15	c	0.34	0/2315	0.68	0/3129
16	d	0.26	0/2212	0.60	0/2988
17	e	0.26	0/338	0.58	0/450
18	f	0.28	0/5776	0.59	0/7791
19	g	0.25	0/1410	0.55	0/1902
20	z	0.29	0/3768	0.56	0/5111
All	All	0.36	0/58550	0.67	0/79034

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 ⓘ

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	2833	0	2894	42	0
2	B	2948	0	3012	57	0
3	C	2912	0	3023	62	0
4	D	2935	0	2982	64	0
5	E	3025	0	3101	59	0
6	F	2930	0	3023	31	0
7	U	6472	0	6494	98	0
8	V	3731	0	3780	43	0
9	W	3564	0	3685	37	0
10	X	844	0	886	10	0
11	Y	3115	0	3120	32	0
12	Z	2290	0	2320	39	0
13	a	3003	0	3016	22	0
14	b	1449	0	1497	43	0
15	c	2272	0	2288	42	0
16	d	2166	0	2196	19	0
17	e	334	0	294	5	0
18	f	5695	0	5718	63	0
19	g	1383	0	1331	15	0
20	z	3704	0	3762	42	0
21	A	27	0	12	3	0
21	F	27	0	12	1	0
22	C	31	0	12	0	0
22	D	31	0	12	4	0
22	E	31	0	12	0	0
23	C	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
24	c	1	0	0	0	0
All	All	57756	0	58482	751	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 6.

All (751) 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)
14:b:140:ILE:HG21	14:b:153:LEU:HB3	1.67	0.75
12:Z:195:VAL:HG21	13:a:375:LEU:HD11	1.69	0.74
4:D:231:VAL:HG13	5:E:262:ASN:HD21	1.56	0.70
10:X:354:ILE:HG22	10:X:356:LEU:HB2	1.74	0.69
7:U:749:GLN:HA	7:U:755:THR:HA	1.75	0.68
6:F:370:SER:HB2	6:F:375:VAL:HG21	1.75	0.67
14:b:140:ILE:HD11	14:b:156:PHE:CD2	2.30	0.67
7:U:646:PRO:HB3	7:U:680:VAL:HG11	1.78	0.66
14:b:140:ILE:HD11	14:b:156:PHE:HD2	1.61	0.66
3:C:99:VAL:HG12	3:C:123:LEU:HD12	1.79	0.65
4:D:181:VAL:HG11	4:D:261:ILE:HD13	1.77	0.65
3:C:326:LEU:HD22	3:C:345:ARG:HG2	1.78	0.65
12:Z:40:LEU:HB3	12:Z:89:GLU:HB3	1.79	0.65
7:U:675:MET:HE3	7:U:683:VAL:HG13	1.78	0.65
7:U:627:PHE:HE1	7:U:749:GLN:HB3	1.61	0.64
1:A:84:LYS:HB2	2:B:98:LYS:HZ1	1.63	0.64
3:C:99:VAL:HA	3:C:123:LEU:HB2	1.79	0.63
6:F:97:LEU:HB3	6:F:121:CYS:HB3	1.81	0.63
7:U:685:GLN:HB3	7:U:726:ALA:HA	1.80	0.63
3:C:188:LEU:HD23	3:C:315:ILE:HG13	1.81	0.63
3:C:326:LEU:CD2	3:C:345:ARG:HG2	2.29	0.63
5:E:226:GLN:HB3	5:E:272:ARG:HD3	1.81	0.63
1:A:95:VAL:HB	2:B:130:GLU:HB2	1.79	0.62
2:B:102:LEU:HD22	2:B:138:PHE:HZ	1.64	0.62
1:A:238:ILE:HD12	1:A:272:ILE:HG12	1.81	0.62
7:U:221:ILE:HD11	7:U:252:LEU:HD23	1.81	0.62
18:f:76:GLU:C	18:f:78:LEU:H	2.08	0.61
2:B:259:TYR:HB2	2:B:262:ASP:HB2	1.82	0.61
2:B:227:PRO:HD2	2:B:353:PHE:HB2	1.81	0.61
4:D:168:GLY:HA3	4:D:344:ILE:HD13	1.81	0.61
3:C:254:ILE:HG13	3:C:269:VAL:HB	1.82	0.61
15:c:125:VAL:HG22	19:g:287:GLU:HB3	1.81	0.61
13:a:353:LEU:HD23	13:a:356:TRP:HE1	1.66	0.60
5:E:223:ARG:HB2	5:E:270:LEU:HD13	1.83	0.60
9:W:32:ALA:HB1	9:W:73:MET:HG3	1.83	0.60
18:f:759:LEU:H	18:f:809:ILE:HD12	1.67	0.60
2:B:232:LYS:HB3	2:B:353:PHE:HE2	1.66	0.60
3:C:108:VAL:HG22	3:C:126:ILE:HD12	1.83	0.60
1:A:346:PRO:HG2	1:A:351:ARG:HH21	1.66	0.60
18:f:240:VAL:HG13	18:f:257:ARG:HE	1.66	0.60
4:D:179:GLU:HG3	4:D:329:ARG:HH22	1.67	0.60
8:V:96:ARG:HD2	8:V:98:LEU:HD21	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HD21	1:A:222:LYS:HD2	1.83	0.60
1:A:394:MET:HE3	2:B:349:ARG:HH22	1.66	0.60
16:d:171:LEU:HD21	16:d:191:LEU:HD13	1.83	0.60
20:z:464:ALA:HB2	20:z:481:LEU:HD11	1.84	0.60
11:Y:240:VAL:HB	11:Y:260:LEU:HD21	1.84	0.60
16:d:223:ASN:O	16:d:227:LYS:HB2	2.01	0.60
1:A:178:GLY:H	21:A:501:ADP:HN62	1.50	0.59
8:V:68:ASP:O	8:V:72:LEU:HB2	2.02	0.59
4:D:163:MET:HG3	4:D:165:ALA:H	1.68	0.59
8:V:72:LEU:O	8:V:76:LYS:HB2	2.02	0.59
7:U:649:ARG:HB3	7:U:675:MET:HE1	1.85	0.59
11:Y:297:ARG:HA	11:Y:300:ARG:HE	1.66	0.59
4:D:130:VAL:HG12	4:D:142:VAL:HA	1.84	0.59
14:b:140:ILE:HD12	14:b:157:VAL:HG23	1.85	0.59
3:C:304:ALA:HA	3:C:307:ARG:HG2	1.85	0.59
3:C:371:LEU:HD11	4:D:190:LEU:HG	1.85	0.59
1:A:122:VAL:HB	6:F:88:TYR:HB2	1.85	0.58
2:B:123:VAL:HG21	2:B:152:LEU:HD21	1.85	0.58
14:b:29:GLN:HA	14:b:179:LEU:HD23	1.84	0.58
18:f:453:SER:HA	18:f:488:ALA:HA	1.85	0.58
7:U:692:ALA:HB1	7:U:736:ILE:HB	1.85	0.58
3:C:251:ILE:H	3:C:293:MET:HE1	1.68	0.58
4:D:265:ASP:HB2	5:E:262:ASN:HD22	1.69	0.58
7:U:885:MET:HG2	7:U:887:ALA:H	1.67	0.58
6:F:311:LEU:HD23	6:F:314:LEU:HD12	1.85	0.58
11:Y:17:LEU:HD13	11:Y:150:PHE:HB3	1.85	0.58
4:D:254:ALA:HB2	4:D:262:ILE:HD11	1.86	0.58
8:V:51:ALA:HB2	8:V:61:GLU:HB2	1.85	0.58
2:B:64:LYS:HG2	2:B:67:ARG:HH21	1.69	0.58
4:D:170:MET:HB3	4:D:173:GLN:HB2	1.86	0.58
7:U:381:THR:HG22	7:U:412:HIS:HA	1.86	0.58
13:a:56:LEU:HB2	13:a:86:GLN:HG3	1.86	0.58
3:C:162:LYS:O	3:C:166:GLU:HG3	2.04	0.57
11:Y:104:MET:HE1	11:Y:127:THR:HB	1.85	0.57
18:f:493:ASN:HD21	18:f:527:VAL:HG22	1.68	0.57
7:U:667:GLU:HA	7:U:670:ASN:HB2	1.85	0.57
18:f:294:MET:HE1	18:f:321:MET:HA	1.87	0.57
4:D:208:PRO:HB2	5:E:291:ARG:HG3	1.87	0.57
4:D:256:GLU:HG3	4:D:257:ASN:N	2.20	0.57
5:E:152:PRO:HB2	5:E:274:LYS:HE3	1.85	0.57
7:U:656:LEU:HD11	7:U:671:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:GLY:HA3	2:B:360:THR:HG22	1.85	0.57
12:Z:192:THR:HG21	13:a:376:THR:HG23	1.86	0.57
15:c:115:HIS:HB3	15:c:118:PHE:HB2	1.86	0.57
5:E:171:LEU:HB3	5:E:298:LYS:HA	1.87	0.56
12:Z:70:LEU:HD11	12:Z:108:ILE:HG23	1.86	0.56
3:C:358:GLU:HA	4:D:324:PRO:HG2	1.86	0.56
9:W:231:ILE:HG23	9:W:243:ILE:HG23	1.87	0.56
12:Z:260:VAL:HA	15:c:292:MET:HE1	1.86	0.56
1:A:212:VAL:HG12	1:A:318:LEU:HD22	1.88	0.56
3:C:375:ARG:HH22	3:C:379:THR:HG23	1.71	0.56
7:U:213:PHE:HA	7:U:216:VAL:HB	1.87	0.56
8:V:147:PHE:HB2	8:V:150:ARG:HB3	1.88	0.56
12:Z:172:VAL:HG11	15:c:220:LEU:HD23	1.88	0.56
3:C:69:GLN:HG3	4:D:136:SER:HA	1.86	0.56
2:B:107:MET:HE1	2:B:151:LEU:HB3	1.87	0.56
2:B:109:VAL:HG11	2:B:163:LEU:HD22	1.86	0.56
9:W:68:VAL:HG13	9:W:107:GLN:HB2	1.88	0.56
5:E:194:ASN:ND2	5:E:227:PRO:HG2	2.21	0.55
11:Y:17:LEU:HD23	11:Y:213:LEU:HD22	1.87	0.55
18:f:125:ILE:HD13	18:f:129:LEU:HG	1.88	0.55
5:E:196:LEU:HG	5:E:230:ILE:HD12	1.87	0.55
16:d:204:ARG:HB3	16:d:207:GLU:HB2	1.87	0.55
8:V:452:ASN:HB3	8:V:457:TYR:HB2	1.89	0.55
20:z:57:HIS:HB3	20:z:60:LYS:HB2	1.89	0.55
4:D:187:HIS:HB3	4:D:190:LEU:HB3	1.89	0.55
14:b:134:GLU:HA	19:g:138:LEU:HB3	1.88	0.55
18:f:711:SER:HA	18:f:749:ALA:HB2	1.87	0.55
7:U:676:THR:O	7:U:684:ARG:HG2	2.07	0.55
9:W:395:ASN:HA	9:W:398:VAL:HG22	1.87	0.55
5:E:169:GLY:HA3	5:E:275:MET:HE2	1.87	0.55
18:f:691:PRO:HA	18:f:694:LEU:HB2	1.89	0.55
2:B:200:SER:HA	2:B:349:ARG:CZ	2.37	0.54
11:Y:234:PRO:O	11:Y:238:GLU:HG2	2.07	0.54
20:z:333:GLN:HB2	20:z:383:MET:HE3	1.90	0.54
20:z:469:ILE:HD11	20:z:477:ASN:HD22	1.72	0.54
8:V:100:MET:HG3	8:V:102:PRO:HD2	1.89	0.54
18:f:714:SER:HB3	18:f:753:ALA:HB2	1.89	0.54
6:F:312:GLU:O	6:F:316:GLN:HB3	2.07	0.54
11:Y:268:TYR:HA	11:Y:271:PHE:HB3	1.88	0.54
18:f:761:MET:HE3	18:f:809:ILE:HG13	1.90	0.54
19:g:189:GLN:HG3	19:g:259:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HB3	2:B:79:ILE:HG21	1.90	0.54
4:D:103:VAL:HG11	4:D:132:LEU:HD21	1.88	0.54
7:U:483:LEU:HD22	7:U:781:LEU:HD13	1.89	0.54
11:Y:164:ALA:HA	11:Y:167:LEU:HB3	1.89	0.54
5:E:365:GLU:O	5:E:369:LYS:HG2	2.08	0.54
18:f:659:LEU:HA	18:f:663:GLY:HA3	1.88	0.54
2:B:226:GLY:HA3	2:B:353:PHE:HB2	1.88	0.54
3:C:157:GLN:HA	3:C:160:GLU:HG2	1.89	0.54
7:U:504:ASP:HB3	19:g:235:TYR:HD2	1.73	0.54
7:U:759:SER:HA	7:U:782:ALA:HA	1.90	0.54
16:d:174:TYR:HA	16:d:178:TYR:HB2	1.89	0.54
3:C:303:SER:O	3:C:307:ARG:HG2	2.08	0.54
4:D:257:ASN:O	4:D:258:ALA:C	2.50	0.54
7:U:372:ALA:HB2	7:U:731:ILE:HG22	1.90	0.54
7:U:541:HIS:CD2	15:c:62:VAL:HG12	2.43	0.54
8:V:94:VAL:HG13	8:V:142:GLU:HB2	1.90	0.54
5:E:186:ALA:O	5:E:190:GLN:HG2	2.08	0.54
7:U:556:MET:HE1	7:U:563:ALA:HB3	1.90	0.54
7:U:579:ARG:HG3	7:U:614:VAL:HG21	1.90	0.54
19:g:176:LYS:HG2	19:g:239:GLN:HA	1.90	0.54
20:z:186:TYR:HA	20:z:189:ILE:HD12	1.90	0.54
20:z:460:VAL:HG12	20:z:481:LEU:HD13	1.89	0.54
1:A:182:GLU:O	1:A:186:LYS:HG2	2.08	0.53
12:Z:65:ASP:HB3	12:Z:103:LYS:HB2	1.89	0.53
12:Z:194:GLN:HE21	15:c:297:VAL:HG13	1.73	0.53
14:b:4:GLU:HA	14:b:106:LYS:H	1.73	0.53
14:b:62:THR:HG21	14:b:71:ILE:HG12	1.90	0.53
9:W:196:VAL:HG13	9:W:198:ASP:H	1.72	0.53
10:X:394:ASP:HB3	10:X:397:TYR:HB2	1.90	0.53
14:b:72:LEU:O	14:b:76:HIS:HB2	2.09	0.53
4:D:97:ASP:CG	4:D:98:GLN:H	2.15	0.53
9:W:39:ARG:HB3	9:W:42:GLU:HB2	1.90	0.53
9:W:240:TYR:HA	9:W:243:ILE:HD12	1.90	0.53
11:Y:221:THR:HG22	11:Y:256:VAL:HG21	1.90	0.53
20:z:271:PRO:HB2	20:z:314:VAL:HG11	1.91	0.53
4:D:121:ARG:HA	4:D:124:LEU:HD23	1.91	0.53
6:F:272:PHE:HD2	6:F:316:GLN:HG3	1.74	0.53
8:V:179:LYS:HE3	8:V:212:TYR:HA	1.91	0.53
8:V:296:LYS:HA	8:V:299:GLN:HG2	1.91	0.53
14:b:52:ILE:HG22	14:b:60:VAL:HA	1.90	0.53
16:d:233:GLU:HG3	16:d:237:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLN:HG2	2:B:182:GLU:H	1.72	0.53
2:B:287:ILE:HG23	2:B:337:LEU:HD11	1.90	0.53
4:D:354:LEU:HD11	4:D:358:VAL:HG11	1.90	0.53
6:F:283:ILE:HB	6:F:328:VAL:HG12	1.92	0.52
11:Y:50:MET:HE3	11:Y:115:GLY:HA3	1.92	0.52
18:f:388:ASP:HB3	18:f:391:LEU:HB2	1.91	0.52
6:F:137:ILE:HG23	6:F:160:ILE:HD12	1.91	0.52
14:b:140:ILE:HD13	14:b:153:LEU:HD22	1.90	0.52
18:f:213:GLN:HG3	18:f:246:SER:HB2	1.92	0.52
20:z:171:LEU:HD22	20:z:185:VAL:HG13	1.91	0.52
5:E:182:LEU:HA	5:E:185:ARG:HD2	1.92	0.52
2:B:106:PRO:HG3	3:C:120:SER:HA	1.92	0.52
2:B:392:GLY:HA2	2:B:395:ILE:HD12	1.90	0.52
2:B:407:LEU:HD12	3:C:178:LEU:HD22	1.91	0.52
5:E:199:VAL:HG12	5:E:201:SER:H	1.74	0.52
9:W:363:ILE:HD11	9:W:382:LEU:HD11	1.90	0.52
7:U:802:TYR:HE2	7:U:880:ASN:HA	1.74	0.52
16:d:305:LYS:HD2	16:d:306:ARG:HB2	1.91	0.52
19:g:168:THR:HG22	19:g:245:THR:HA	1.90	0.52
2:B:287:ILE:HG22	2:B:331:THR:HG21	1.92	0.52
4:D:231:VAL:HG13	5:E:262:ASN:ND2	2.24	0.52
8:V:72:LEU:O	8:V:76:LYS:CB	2.58	0.52
3:C:269:VAL:HG11	4:D:287:ARG:NH1	2.25	0.52
12:Z:259:VAL:HA	12:Z:262:LEU:HD12	1.91	0.52
15:c:100:LYS:HG3	15:c:105:PRO:HB3	1.90	0.52
15:c:114:SER:HB2	15:c:147:PRO:HD3	1.92	0.52
19:g:185:PRO:HD2	19:g:259:ARG:HH12	1.74	0.52
20:z:477:ASN:HA	20:z:480:ARG:HB2	1.91	0.52
7:U:24:LEU:HD11	7:U:60:ALA:HA	1.92	0.51
7:U:491:GLN:HA	7:U:494:TYR:HB3	1.92	0.51
7:U:762:GLY:HA3	7:U:782:ALA:HB2	1.92	0.51
1:A:252:GLU:HA	1:A:255:ARG:HB2	1.92	0.51
2:B:300:GLY:HA2	2:B:303:ARG:HB2	1.92	0.51
12:Z:81:MET:HE2	15:c:95:MET:HE1	1.91	0.51
14:b:117:VAL:H	14:b:149:ASN:HD21	1.56	0.51
17:e:49:GLU:HG2	17:e:53:SER:HB2	1.91	0.51
8:V:148:ARG:HG3	8:V:149:PRO:HD3	1.93	0.51
13:a:245:VAL:HG21	13:a:300:ALA:HA	1.92	0.51
2:B:152:LEU:HD12	2:B:157:HIS:HB3	1.93	0.51
6:F:247:THR:HG21	6:F:278:LYS:HG3	1.92	0.51
7:U:401:LYS:HE3	7:U:437:TYR:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:8:ILE:HA	7:U:11:LEU:HD13	1.92	0.51
9:W:166:LEU:HD13	9:W:189:GLN:HG2	1.93	0.51
14:b:7:MET:HG2	14:b:97:LEU:HD12	1.91	0.51
6:F:232:GLY:HA2	21:F:501:ADP:H3'	1.93	0.51
20:z:304:ILE:HG21	20:z:342:LEU:HD21	1.93	0.51
3:C:72:TYR:CE1	3:C:118:ASN:HA	2.46	0.51
5:E:142:ILE:HG22	5:E:183:LEU:HD11	1.91	0.51
7:U:368:ALA:HB3	7:U:731:ILE:HD12	1.93	0.51
2:B:74:MET:HE1	18:f:650:GLN:HG3	1.93	0.51
3:C:192:PRO:HD2	4:D:323:ARG:HH21	1.76	0.51
3:C:300:ILE:HA	4:D:274:ARG:HH21	1.76	0.51
16:d:148:LEU:HD13	16:d:167:TYR:HD1	1.75	0.51
18:f:191:ILE:HG22	18:f:231:LEU:HD11	1.92	0.51
4:D:231:VAL:HB	4:D:234:GLU:HB3	1.93	0.51
8:V:172:VAL:HA	8:V:175:MET:HE3	1.92	0.51
11:Y:149:LEU:HD21	11:Y:186:LEU:HD23	1.93	0.51
11:Y:316:LEU:HD12	11:Y:352:GLU:HA	1.93	0.51
14:b:129:LYS:HA	14:b:132:LYS:HB3	1.93	0.51
1:A:277:ILE:HA	1:A:280:ILE:HB	1.91	0.51
7:U:684:ARG:O	7:U:688:LEU:HG	2.11	0.51
3:C:140:VAL:HB	3:C:213:ARG:HD2	1.93	0.50
5:E:146:ARG:HH22	5:E:190:GLN:HG3	1.76	0.50
12:Z:172:VAL:HG22	15:c:217:LEU:HD11	1.92	0.50
13:a:109:GLU:HA	13:a:112:ILE:HD12	1.92	0.50
5:E:182:LEU:HD12	5:E:185:ARG:HD2	1.92	0.50
8:V:350:GLN:HB2	8:V:353:LEU:HB2	1.93	0.50
9:W:187:LEU:HD21	9:W:222:LEU:HB3	1.93	0.50
15:c:80:THR:HB	15:c:85:GLU:HG3	1.94	0.50
18:f:118:ASN:HB3	18:f:130:ALA:HB1	1.91	0.50
18:f:594:LEU:O	18:f:598:CYS:HB2	2.12	0.50
20:z:354:PRO:HD2	20:z:357:LEU:HD12	1.92	0.50
2:B:334:ILE:HD12	2:B:337:LEU:HG	1.92	0.50
4:D:284:GLU:HA	4:D:287:ARG:HE	1.76	0.50
1:A:299:MET:HA	1:A:302:LEU:HD23	1.93	0.50
5:E:100:LEU:HG	5:E:107:ILE:HG13	1.94	0.50
7:U:479:LEU:HB2	7:U:511:ALA:HB1	1.92	0.50
15:c:89:PRO:HA	15:c:92:GLN:HE21	1.77	0.50
15:c:216:MET:HA	15:c:219:ASN:HD22	1.76	0.50
20:z:156:GLN:HA	20:z:159:LEU:HD12	1.92	0.50
20:z:204:THR:HG22	20:z:209:VAL:HG11	1.93	0.50
2:B:190:LEU:HD11	2:B:356:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:LEU:HB3	2:B:346:ARG:HH12	1.76	0.50
3:C:209:CYS:HA	3:C:243:PRO:HB2	1.93	0.50
4:D:113:VAL:HB	4:D:138:ALA:HA	1.92	0.50
2:B:104:GLY:O	2:B:107:MET:HG2	2.12	0.50
5:E:236:ASP:HB3	5:E:285:LEU:HD22	1.93	0.50
7:U:645:ASN:HB3	7:U:648:VAL:HG22	1.94	0.50
7:U:338:HIS:HB3	7:U:785:PRO:HG2	1.92	0.50
11:Y:79:ASP:HA	11:Y:82:LYS:HD3	1.94	0.50
12:Z:23:PHE:HB2	12:Z:97:THR:HG21	1.93	0.50
4:D:261:ILE:HA	4:D:306:LYS:O	2.12	0.50
4:D:341:LYS:HE2	4:D:370:ILE:HG22	1.94	0.50
6:F:246:ALA:HB1	6:F:280:PRO:HB2	1.92	0.50
12:Z:194:GLN:HB3	15:c:304:LEU:HD11	1.93	0.50
14:b:171:VAL:HG21	14:b:188:ILE:HD11	1.94	0.50
8:V:94:VAL:HG21	8:V:138:PRO:HG3	1.94	0.50
15:c:301:ALA:O	15:c:305:ASP:HB2	2.12	0.50
7:U:202:VAL:HG13	7:U:206:MET:HE3	1.94	0.49
5:E:188:ALA:O	5:E:192:ASP:N	2.43	0.49
2:B:260:LEU:HD12	2:B:304:GLU:HB2	1.95	0.49
3:C:310:ARG:N	3:C:310:ARG:HD3	2.28	0.49
5:E:381:GLU:HG2	6:F:343:LEU:HB3	1.95	0.49
15:c:242:GLU:HA	15:c:245:VAL:HG12	1.95	0.49
18:f:190:GLU:HB2	18:f:193:PRO:HD2	1.94	0.49
6:F:281:SER:HB2	6:F:326:VAL:HA	1.94	0.49
7:U:685:GLN:HG2	7:U:686:GLY:N	2.28	0.49
8:V:135:LEU:HG	8:V:178:SER:HB2	1.94	0.49
8:V:369:THR:HB	17:e:52:PHE:HZ	1.78	0.49
10:X:344:ARG:HG3	10:X:386:ILE:HG13	1.94	0.49
14:b:142:ASN:HB2	14:b:172:THR:HA	1.94	0.49
15:c:84:VAL:HG21	19:g:280:ARG:HG3	1.94	0.49
4:D:243:GLY:O	4:D:246:MET:HG2	2.13	0.49
5:E:359:HIS:HB2	5:E:361:PHE:HD2	1.78	0.49
7:U:142:LEU:HD11	7:U:166:THR:HG22	1.94	0.49
7:U:685:GLN:HB2	7:U:729:GLY:HA3	1.95	0.49
8:V:467:TYR:HE2	12:Z:251:LEU:HG	1.77	0.49
9:W:254:PRO:HA	9:W:257:GLN:HB2	1.95	0.49
13:a:8:LEU:HD13	13:a:26:GLU:HA	1.94	0.49
14:b:143:PHE:CD2	14:b:179:LEU:HD22	2.48	0.49
9:W:256:ILE:HA	9:W:259:GLU:HG2	1.95	0.49
4:D:172:ILE:O	4:D:175:GLN:HG2	2.13	0.49
5:E:226:GLN:HB2	5:E:227:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:427:LEU:HD21	7:U:439:GLU:HA	1.94	0.49
7:U:895:PRO:HB2	7:U:898:CYS:HB2	1.93	0.49
9:W:73:MET:HA	9:W:76:GLU:HB2	1.95	0.49
1:A:368:ILE:HB	20:z:222:LEU:HD22	1.95	0.49
7:U:772:TRP:CD1	7:U:775:LEU:HG	2.47	0.49
11:Y:247:LEU:HA	11:Y:250:LEU:HG	1.95	0.49
2:B:222:VAL:HG22	2:B:349:ARG:HD3	1.94	0.48
7:U:772:TRP:HB3	7:U:775:LEU:HB2	1.93	0.48
13:a:28:LEU:HA	13:a:31:LYS:HG2	1.95	0.48
13:a:225:LEU:HB3	13:a:234:ILE:HD11	1.93	0.48
16:d:281:LYS:HB2	16:d:315:TYR:HB3	1.95	0.48
18:f:52:LEU:HG	18:f:53:GLN:HG3	1.93	0.48
18:f:673:ARG:HA	18:f:709:THR:HG23	1.94	0.48
20:z:353:ALA:HB1	20:z:357:LEU:HB2	1.95	0.48
4:D:97:ASP:OD1	4:D:98:GLN:N	2.46	0.48
18:f:232:TYR:HE2	18:f:263:PRO:HG2	1.78	0.48
4:D:211:GLY:H	22:D:501:AGS:H5'1	1.78	0.48
16:d:224:VAL:HG12	16:d:252:PRO:HB3	1.96	0.48
18:f:156:HIS:O	18:f:160:ARG:HB2	2.14	0.48
4:D:261:ILE:HB	4:D:308:ILE:HG22	1.96	0.48
18:f:76:GLU:C	18:f:78:LEU:N	2.70	0.48
7:U:468:ALA:HB1	7:U:474:ARG:HG2	1.96	0.48
9:W:109:CYS:HA	9:W:112:VAL:HG12	1.96	0.48
9:W:112:VAL:HB	9:W:124:LEU:HD23	1.96	0.48
11:Y:141:VAL:HA	11:Y:144:LEU:HD12	1.95	0.48
2:B:190:LEU:HB3	2:B:235:LEU:HD11	1.96	0.48
12:Z:263:ALA:HB3	15:c:292:MET:HE3	1.95	0.48
14:b:142:ASN:ND2	14:b:150:THR:HA	2.29	0.48
15:c:88:ASP:HB2	15:c:91:PHE:HB2	1.96	0.48
1:A:102:ILE:HD11	1:A:110:LYS:HD2	1.96	0.47
2:B:150:VAL:HA	2:B:163:LEU:H	1.79	0.47
10:X:365:LEU:HD13	10:X:385:LEU:HD22	1.96	0.47
14:b:112:PHE:HE1	14:b:141:ILE:HD12	1.79	0.47
18:f:407:MET:HE1	18:f:440:ILE:HG13	1.96	0.47
19:g:157:LEU:HB3	19:g:260:ILE:HB	1.96	0.47
2:B:170:LEU:HD13	2:B:266:LEU:HD11	1.96	0.47
4:D:199:PRO:HG2	4:D:329:ARG:HH21	1.79	0.47
7:U:883:ARG:HH22	7:U:885:MET:HE1	1.79	0.47
8:V:488:ASN:O	8:V:492:LYS:HB2	2.14	0.47
12:Z:106:ILE:HD12	12:Z:153:LYS:HG2	1.95	0.47
12:Z:235:ASN:HA	13:a:289:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:c:267:PRO:HA	15:c:270:LEU:HD12	1.97	0.47
3:C:377:HIS:CE1	3:C:379:THR:HG22	2.50	0.47
1:A:192:GLU:HA	1:A:195:LEU:HD12	1.96	0.47
1:A:201:PHE:HB3	1:A:206:ILE:HG23	1.96	0.47
12:Z:198:LEU:HD23	15:c:229:LEU:HD11	1.96	0.47
3:C:338:LEU:HD22	3:C:342:ILE:HD13	1.96	0.47
7:U:543:LYS:HZ1	7:U:772:TRP:HE3	1.59	0.47
11:Y:127:THR:HG21	11:Y:140:ILE:HG13	1.95	0.47
2:B:60:LEU:HD11	18:f:181:ARG:HA	1.97	0.47
2:B:282:VAL:HB	2:B:327:VAL:HG22	1.97	0.47
7:U:155:LEU:HD11	7:U:188:MET:HE1	1.96	0.47
18:f:72:ARG:HH12	18:f:83:ARG:HB2	1.79	0.47
1:A:122:VAL:HG21	6:F:164:LEU:HD21	1.97	0.47
3:C:168:PRO:HA	3:C:172:PRO:HA	1.96	0.47
7:U:437:TYR:HD1	7:U:472:ILE:HG21	1.80	0.47
7:U:787:CYS:HB2	7:U:789:ILE:HG13	1.96	0.47
8:V:290:TYR:HD1	8:V:309:MET:HE1	1.79	0.47
12:Z:15:VAL:HG13	12:Z:53:SER:HB2	1.96	0.47
15:c:305:ASP:HA	15:c:308:VAL:HG22	1.96	0.47
2:B:102:LEU:HD22	2:B:138:PHE:CZ	2.46	0.47
4:D:239:TYR:HA	20:z:501:GLU:O	2.15	0.47
7:U:481:LEU:HD21	7:U:493:VAL:HB	1.96	0.47
5:E:180:LYS:HG2	5:E:301:ILE:HG13	1.96	0.47
6:F:95:GLU:HA	6:F:147:PRO:HG3	1.97	0.47
13:a:273:GLN:HG3	13:a:300:ALA:HB1	1.96	0.47
14:b:33:VAL:HG11	14:b:75:LEU:HD23	1.96	0.47
14:b:112:PHE:CE1	14:b:141:ILE:HD12	2.49	0.47
5:E:61:LEU:HD11	5:E:72:LYS:HB2	1.96	0.47
8:V:30:PRO:HG3	8:V:83:GLU:HG3	1.96	0.47
8:V:97:ALA:H	8:V:107:ARG:HG3	1.80	0.47
11:Y:329:PHE:HB2	17:e:66:LYS:HE3	1.97	0.47
12:Z:34:ARG:HD3	12:Z:102:HIS:CD2	2.50	0.47
18:f:715:HIS:HA	18:f:752:HIS:HD2	1.79	0.47
7:U:769:PHE:HB3	7:U:776:SER:HB3	1.97	0.46
3:C:86:LEU:HD11	3:C:94:LYS:HB2	1.97	0.46
5:E:216:ARG:HA	5:E:263:GLN:HE22	1.81	0.46
7:U:389:ASN:HD21	7:U:392:TRP:HB3	1.80	0.46
8:V:136:GLU:HA	8:V:139:MET:HG2	1.96	0.46
13:a:131:THR:O	13:a:135:ILE:HG12	2.16	0.46
13:a:232:TRP:HB3	13:a:255:TRP:CE2	2.51	0.46
19:g:138:LEU:HD12	19:g:166:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:120:ILE:HG23	20:z:126:LEU:HD23	1.96	0.46
20:z:211:GLN:HA	20:z:214:ARG:HB3	1.96	0.46
4:D:214:MET:HE2	4:D:214:MET:HB3	1.88	0.46
18:f:75:LEU:C	18:f:77:GLU:H	2.23	0.46
18:f:651:GLY:HA2	18:f:654:VAL:HG12	1.96	0.46
2:B:192:ASN:HD22	2:B:354:PRO:HD3	1.80	0.46
4:D:168:GLY:HA2	4:D:347:THR:HG21	1.97	0.46
8:V:209:LYS:HZ3	8:V:234:ARG:HB3	1.80	0.46
12:Z:190:ARG:HB2	15:c:297:VAL:HG21	1.96	0.46
16:d:98:LEU:HB3	16:d:150:ILE:HD13	1.97	0.46
3:C:304:ALA:CA	3:C:307:ARG:HG2	2.45	0.46
7:U:322:THR:HA	7:U:325:MET:HG2	1.97	0.46
7:U:790:GLY:HA2	7:U:912:ILE:HG13	1.97	0.46
6:F:169:ASP:HB3	6:F:172:VAL:HG23	1.97	0.46
7:U:140:ARG:O	7:U:144:ASP:HB2	2.16	0.46
9:W:146:THR:HA	9:W:149:LEU:HB2	1.97	0.46
4:D:133:HIS:HB3	4:D:137:ASN:N	2.30	0.46
9:W:272:LEU:HD23	9:W:340:VAL:HB	1.98	0.46
12:Z:65:ASP:HB2	12:Z:103:LYS:HD2	1.98	0.46
14:b:173:VAL:HG11	14:b:182:ALA:HB1	1.98	0.46
7:U:646:PRO:HB3	7:U:680:VAL:HG21	1.98	0.46
15:c:87:VAL:HG21	15:c:133:PHE:CZ	2.51	0.46
15:c:122:LEU:HD22	15:c:126:ASP:HB3	1.96	0.46
8:V:305:ALA:O	8:V:309:MET:HB2	2.16	0.46
9:W:433:ASN:HA	9:W:436:MET:HG3	1.98	0.46
1:A:84:LYS:HB2	2:B:98:LYS:NZ	2.31	0.45
9:W:132:THR:HB	9:W:138:VAL:HG21	1.98	0.45
13:a:282:PHE:HB2	13:a:336:VAL:HG11	1.97	0.45
14:b:157:VAL:HG11	14:b:170:LEU:HB2	1.98	0.45
1:A:151:ILE:HG13	1:A:153:LEU:H	1.81	0.45
1:A:159:PRO:O	1:A:160:THR:C	2.59	0.45
1:A:354:ILE:HG12	21:A:501:ADP:C6	2.51	0.45
2:B:383:LEU:HD22	2:B:423:LYS:HG3	1.98	0.45
7:U:432:SER:HB3	7:U:435:SER:HB3	1.98	0.45
10:X:414:LEU:HD22	12:Z:276:ILE:HG13	1.99	0.45
13:a:201:GLY:HA3	13:a:233:LEU:HD21	1.98	0.45
18:f:714:SER:HB2	18:f:749:ALA:HB1	1.98	0.45
7:U:556:MET:HG3	7:U:589:ALA:HB2	1.98	0.45
14:b:161:ASN:HB3	14:b:168:SER:H	1.82	0.45
18:f:138:GLU:HB3	18:f:189:LYS:HG3	1.99	0.45
18:f:426:LEU:HD11	18:f:460:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:CYS:HB3	1:A:270:CYS:HA	1.98	0.45
3:C:163:GLU:HA	3:C:167:LEU:HB2	1.97	0.45
3:C:385:MET:HA	3:C:388:ALA:HB3	1.98	0.45
7:U:497:LEU:HB2	7:U:516:LEU:HD13	1.98	0.45
9:W:120:ILE:HG13	9:W:121:LYS:H	1.81	0.45
15:c:146:ASP:H	15:c:156:VAL:HG23	1.81	0.45
6:F:399:VAL:HG13	6:F:423:GLY:HA3	1.99	0.45
7:U:113:VAL:HG12	7:U:158:ARG:NH1	2.32	0.45
7:U:372:ALA:O	7:U:376:MET:HB2	2.16	0.45
9:W:166:LEU:HD12	9:W:192:LEU:HD22	1.98	0.45
11:Y:280:GLN:HG2	17:e:60:LEU:HD13	1.99	0.45
14:b:24:THR:HG23	14:b:27:GLN:H	1.82	0.45
3:C:364:THR:HA	4:D:196:ILE:HD12	1.97	0.45
7:U:514:LEU:HD13	7:U:550:VAL:HG13	1.98	0.45
10:X:407:MET:HE1	12:Z:266:ILE:HA	1.98	0.45
14:b:142:ASN:HD21	14:b:150:THR:HA	1.81	0.45
18:f:586:PRO:HA	18:f:589:SER:HB2	1.99	0.45
19:g:126:LEU:HA	19:g:129:PHE:HD2	1.82	0.45
3:C:306:LEU:HA	3:C:311:ILE:HG21	1.98	0.45
5:E:229:ILE:CG2	5:E:274:LYS:HB2	2.46	0.45
5:E:371:VAL:O	5:E:372:ARG:HB2	2.17	0.45
7:U:90:VAL:HG12	7:U:101:ILE:HD11	1.98	0.45
13:a:374:ILE:HD11	16:d:340:ILE:HG23	1.98	0.45
18:f:72:ARG:HB3	18:f:73:PRO:HD3	1.99	0.45
2:B:139:VAL:HB	2:B:144:LEU:HD11	1.98	0.45
12:Z:172:VAL:O	12:Z:176:LEU:HG	2.17	0.45
12:Z:259:VAL:HG12	15:c:291:LEU:HD21	1.98	0.45
1:A:75:PRO:HA	1:A:78:TRP:CD1	2.52	0.45
1:A:329:PRO:HA	1:A:332:MET:HE3	1.99	0.45
2:B:224:LEU:HD13	2:B:328:ILE:HG23	1.99	0.45
4:D:87:LEU:HD22	4:D:133:HIS:HA	1.99	0.45
8:V:296:LYS:HD3	8:V:304:GLU:HG2	1.99	0.45
9:W:125:ILE:HG22	9:W:145:LEU:HD13	1.98	0.45
18:f:261:ARG:HA	18:f:269:ALA:HB2	1.97	0.45
1:A:209:PRO:HB3	1:A:338:ASP:HB2	1.98	0.45
1:A:238:ILE:HG21	1:A:260:LEU:HD21	1.99	0.45
3:C:100:ASP:HB2	3:C:124:HIS:HA	1.98	0.45
2:B:335:GLU:HB2	20:z:406:PRO:HG2	1.99	0.44
5:E:309:ARG:HA	5:E:312:ILE:HG22	1.98	0.44
6:F:96:LEU:HD21	6:F:145:LEU:HB3	1.99	0.44
14:b:143:PHE:HD2	14:b:179:LEU:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:VAL:HG21	3:C:116:LEU:HD11	1.99	0.44
3:C:237:MET:HA	3:C:240:GLU:HG3	1.99	0.44
4:D:204:MET:HE2	4:D:310:ALA:HB2	1.99	0.44
4:D:236:VAL:HG21	5:E:208:ILE:HG13	2.00	0.44
11:Y:275:LEU:HD11	11:Y:296:VAL:HG23	1.99	0.44
15:c:80:THR:O	15:c:86:ALA:HB2	2.17	0.44
20:z:128:LYS:HE3	20:z:132:TYR:HE2	1.82	0.44
20:z:471:GLU:HG3	20:z:472:ILE:HG13	2.00	0.44
8:V:289:LEU:HA	8:V:292:THR:HG22	2.00	0.44
9:W:101:VAL:HA	9:W:104:MET:HG2	1.99	0.44
11:Y:84:LEU:HB3	11:Y:107:LYS:HD3	1.99	0.44
20:z:208:LEU:O	20:z:211:GLN:HG2	2.17	0.44
20:z:497:THR:HG22	20:z:498:THR:H	1.82	0.44
1:A:194:PRO:HB2	1:A:316:LYS:HD2	2.00	0.44
3:C:254:ILE:HG12	3:C:273:MET:HE3	1.97	0.44
7:U:213:PHE:HB3	7:U:248:ILE:HG21	1.99	0.44
8:V:306:ARG:HD2	8:V:336:GLU:HG2	2.00	0.44
14:b:130:ARG:HA	14:b:133:LYS:HE2	1.99	0.44
20:z:180:ILE:HG22	20:z:184:ARG:HE	1.82	0.44
20:z:317:ASP:O	20:z:321:ILE:HG12	2.18	0.44
5:E:58:GLY:HA2	5:E:73:ALA:HA	1.98	0.44
5:E:135:ILE:HD13	5:E:183:LEU:HD22	1.98	0.44
11:Y:244:ALA:HA	11:Y:247:LEU:HD13	1.99	0.44
16:d:212:LEU:HD11	16:d:220:ILE:HD12	1.99	0.44
19:g:131:ASN:HB3	19:g:170:ALA:HB3	2.00	0.44
6:F:361:ALA:O	6:F:365:ILE:HG12	2.17	0.44
7:U:802:TYR:HB2	7:U:878:LEU:HB2	1.98	0.44
12:Z:12:HIS:HB2	12:Z:15:VAL:HG23	2.00	0.44
14:b:74:LYS:HD2	14:b:74:LYS:HA	1.86	0.44
6:F:422:GLU:HA	6:F:425:LEU:HG	1.98	0.44
7:U:118:LEU:HA	7:U:119:PRO:HD3	1.84	0.44
11:Y:315:THR:HG23	11:Y:318:TYR:H	1.81	0.44
1:A:277:ILE:HD13	1:A:319:MET:HB3	2.00	0.44
2:B:412:MET:H	18:f:51:GLN:HA	1.81	0.44
5:E:148:VAL:HG11	5:E:297:ARG:HG3	1.98	0.44
5:E:172:LEU:HB3	5:E:180:LYS:HD2	2.00	0.44
8:V:65:ARG:HA	8:V:68:ASP:HB2	2.00	0.44
9:W:186:ILE:HD12	9:W:208:LYS:HD3	1.98	0.44
13:a:163:TYR:HA	13:a:166:ILE:HG12	1.99	0.44
2:B:205:LEU:HD22	2:B:324:ASP:HB3	1.99	0.44
3:C:287:LYS:C	3:C:289:ILE:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:133:HIS:HB3	4:D:137:ASN:H	1.82	0.44
4:D:210:CYS:HB3	4:D:333:PHE:HB3	1.99	0.44
5:E:312:ILE:HD12	5:E:312:ILE:HA	1.84	0.44
7:U:436:ALA:HA	7:U:439:GLU:HG2	2.00	0.44
13:a:245:VAL:HG22	13:a:272:ILE:HG13	1.99	0.44
18:f:597:VAL:HG11	18:f:635:LYS:HB3	1.99	0.44
5:E:275:MET:HE1	5:E:295:LEU:HD12	2.00	0.43
5:E:310:LEU:HG	5:E:328:TYR:HE2	1.83	0.43
7:U:213:PHE:H	7:U:244:MET:HE2	1.82	0.43
9:W:187:LEU:HA	9:W:190:MET:HB2	2.00	0.43
18:f:602:GLY:HA2	18:f:639:LYS:HG3	2.00	0.43
3:C:196:LYS:HB2	3:C:196:LYS:HE3	1.82	0.43
4:D:207:PRO:HG2	4:D:335:LEU:HG	1.99	0.43
8:V:495:ARG:HD3	8:V:495:ARG:HA	1.71	0.43
20:z:441:VAL:HG13	20:z:459:LEU:HB3	2.00	0.43
7:U:8:ILE:HD13	7:U:26:LYS:HB3	2.00	0.43
8:V:33:GLN:HA	8:V:36:GLU:HG2	2.00	0.43
16:d:91:ALA:HA	16:d:94:MET:SD	2.57	0.43
18:f:138:GLU:HG2	18:f:189:LYS:HE2	2.00	0.43
20:z:84:LEU:HB3	20:z:87:ASP:HB2	2.00	0.43
20:z:168:LEU:HD11	20:z:208:LEU:HD12	2.01	0.43
20:z:346:ILE:HA	20:z:349:GLN:HB2	1.99	0.43
6:F:153:VAL:HG22	6:F:160:ILE:HG12	2.00	0.43
11:Y:148:GLY:HA3	11:Y:156:LEU:HB2	1.99	0.43
15:c:58:LEU:HA	15:c:108:VAL:HA	2.00	0.43
1:A:178:GLY:N	21:A:501:ADP:HN62	2.14	0.43
4:D:173:GLN:HG2	4:D:333:PHE:CD1	2.54	0.43
7:U:788:VAL:HG23	7:U:909:GLY:HA2	2.00	0.43
8:V:227:VAL:HG22	8:V:231:LEU:HG	2.00	0.43
16:d:268:ARG:HH22	16:d:291:LEU:C	2.26	0.43
1:A:56:LEU:HG	2:B:72:LEU:HD22	2.00	0.43
2:B:59:ARG:HH21	18:f:185:LEU:HD22	1.82	0.43
2:B:59:ARG:HH22	18:f:189:LYS:HB2	1.84	0.43
3:C:127:LEU:HD22	4:D:96:VAL:HG21	2.01	0.43
3:C:253:SER:HB2	4:D:287:ARG:HG2	2.01	0.43
3:C:362:VAL:HG22	3:C:390:VAL:HG11	2.00	0.43
4:D:329:ARG:HB3	4:D:331:ILE:HG13	2.00	0.43
5:E:352:MET:HE1	6:F:212:PHE:HE2	1.84	0.43
7:U:680:VAL:HB	7:U:683:VAL:HB	2.01	0.43
8:V:285:TRP:HB3	8:V:315:LYS:HD3	2.01	0.43
18:f:643:PRO:O	18:f:646:MET:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:72:LEU:HD22	20:z:80:VAL:HG22	2.00	0.43
3:C:304:ALA:HA	3:C:307:ARG:CG	2.48	0.43
3:C:366:ALA:HB1	3:C:378:VAL:HG11	2.00	0.43
7:U:596:ASN:HA	7:U:599:ILE:HG12	2.00	0.43
10:X:368:MET:HG2	10:X:373:LYS:HB2	2.00	0.43
12:Z:39:LEU:HB3	12:Z:92:VAL:HG23	2.01	0.43
15:c:125:VAL:HB	19:g:289:HIS:CE1	2.54	0.43
16:d:148:LEU:HB3	16:d:171:LEU:HD13	2.00	0.43
3:C:276:LEU:HD23	3:C:280:LEU:HD23	2.01	0.43
5:E:208:ILE:HD13	5:E:252:GLU:HB2	1.99	0.43
7:U:518:LEU:HD21	7:U:554:LEU:HD22	2.00	0.43
7:U:691:SER:O	7:U:695:MET:HG2	2.18	0.43
18:f:300:ARG:HA	18:f:492:SER:HA	2.00	0.43
18:f:486:GLY:HA2	18:f:525:ILE:HD11	2.01	0.43
20:z:419:THR:HA	20:z:462:ALA:HB1	2.01	0.43
3:C:44:ARG:HG3	8:V:494:MET:HB2	2.01	0.43
5:E:274:LYS:HA	5:E:274:LYS:HD3	1.78	0.43
16:d:197:LEU:HD11	16:d:263:LEU:HD22	2.00	0.43
18:f:716:ASP:HB2	18:f:753:ALA:HA	2.00	0.43
3:C:189:TYR:CZ	3:C:316:GLU:HB2	2.54	0.43
20:z:65:VAL:HG13	20:z:102:LEU:HB2	2.01	0.43
20:z:100:LYS:HD3	20:z:141:VAL:HG11	2.00	0.43
7:U:170:SER:HB2	7:U:176:MET:SD	2.59	0.42
8:V:321:ALA:HA	8:V:326:GLN:HE22	1.84	0.42
18:f:54:ASP:HB2	18:f:57:GLU:H	1.84	0.42
18:f:348:ILE:HG23	18:f:723:TYR:HE1	1.84	0.42
1:A:201:PHE:HE1	6:F:408:LEU:HD13	1.84	0.42
3:C:325:ARG:HA	3:C:328:ILE:HD12	2.02	0.42
4:D:290:LEU:HD23	4:D:293:LEU:HD21	2.01	0.42
7:U:685:GLN:HA	7:U:688:LEU:HD12	2.01	0.42
13:a:361:LYS:HB3	13:a:365:MET:HE1	2.01	0.42
18:f:564:LEU:HD22	18:f:776:LEU:HG	2.01	0.42
3:C:86:LEU:HA	3:C:96:VAL:HA	2.01	0.42
3:C:284:GLU:O	3:C:285:ALA:C	2.61	0.42
8:V:84:LYS:HA	8:V:125:ASN:HB2	2.01	0.42
9:W:72:LYS:HA	9:W:75:TYR:CZ	2.53	0.42
9:W:408:ARG:HB2	10:X:345:VAL:HA	2.00	0.42
9:W:438:LEU:HD11	12:Z:229:GLN:HG2	2.01	0.42
13:a:90:PRO:HA	13:a:93:ALA:HB3	2.02	0.42
15:c:150:SER:HB2	15:c:156:VAL:HG22	2.01	0.42
18:f:784:ASP:HB3	18:f:798:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:459:LEU:HD12	20:z:462:ALA:HB3	2.01	0.42
11:Y:59:LYS:HD2	11:Y:59:LYS:HA	1.89	0.42
11:Y:202:LEU:HD13	11:Y:239:LYS:HD3	2.02	0.42
14:b:26:LEU:H	14:b:26:LEU:HD22	1.85	0.42
15:c:87:VAL:HG21	15:c:133:PHE:HZ	1.84	0.42
18:f:71:TYR:CE2	18:f:78:LEU:HD21	2.54	0.42
2:B:59:ARG:HH11	18:f:139:CYS:HB2	1.84	0.42
3:C:59:LEU:HD23	3:C:59:LEU:HA	1.92	0.42
5:E:217:GLU:HA	5:E:220:ASN:HB2	2.01	0.42
7:U:374:SER:HA	7:U:411:ILE:HG13	2.01	0.42
7:U:649:ARG:HH21	7:U:680:VAL:CG2	2.32	0.42
8:V:410:ILE:HG21	8:V:422:ILE:HG13	2.01	0.42
9:W:293:ASP:HB3	9:W:296:LEU:HB2	2.02	0.42
11:Y:148:GLY:HA2	11:Y:153:ASP:HB2	2.02	0.42
12:Z:101:LEU:HG	12:Z:123:ILE:HD11	2.01	0.42
14:b:107:MET:HG2	14:b:136:VAL:HG22	2.00	0.42
18:f:542:ILE:HG13	18:f:588:ARG:HE	1.84	0.42
3:C:233:GLU:O	3:C:237:MET:HG2	2.20	0.42
3:C:357:ALA:HB1	4:D:324:PRO:O	2.19	0.42
4:D:256:GLU:HG3	4:D:257:ASN:H	1.85	0.42
5:E:70:ILE:HG22	5:E:80:VAL:HG22	2.02	0.42
5:E:257:LEU:O	5:E:261:LEU:HG	2.20	0.42
6:F:325:GLN:HG2	6:F:326:VAL:HG23	2.02	0.42
7:U:738:ASP:HB2	7:U:742:HIS:CD2	2.55	0.42
14:b:131:LEU:HD22	14:b:136:VAL:HG11	2.02	0.42
20:z:49:LEU:HD21	20:z:67:ILE:HG22	2.02	0.42
1:A:173:THR:HG22	1:A:176:ASP:HB2	2.01	0.42
7:U:133:ILE:HA	7:U:136:LYS:HE2	2.02	0.42
11:Y:387:ILE:HG12	12:Z:276:ILE:HD13	2.02	0.42
2:B:102:LEU:HD23	2:B:160:ILE:HG21	2.01	0.42
2:B:197:ILE:HD11	2:B:224:LEU:HD11	2.01	0.42
2:B:357:ASP:OD1	2:B:360:THR:HG23	2.20	0.42
4:D:211:GLY:N	22:D:501:AGS:O2B	2.53	0.42
4:D:216:ALA:HB1	5:E:267:PHE:CZ	2.55	0.42
7:U:249:CYS:HA	7:U:252:LEU:HD12	2.02	0.42
12:Z:16:LEU:HD22	15:c:216:MET:HE3	2.00	0.42
14:b:56:ASN:HD21	14:b:82:GLY:HA3	1.85	0.42
18:f:233:LEU:HD12	18:f:264:GLU:HG3	2.01	0.42
20:z:138:ASN:HB3	20:z:141:VAL:HB	2.01	0.42
1:A:351:ARG:HD3	1:A:385:ILE:HD11	2.01	0.42
2:B:103:ARG:HG3	2:B:160:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:139:SER:HA	5:E:142:ILE:HG12	2.01	0.42
5:E:335:SER:HA	5:E:371:VAL:HG13	2.02	0.42
5:E:367:PHE:O	5:E:371:VAL:HG23	2.20	0.42
8:V:50:GLU:HB3	8:V:61:GLU:HG3	2.01	0.42
9:W:268:LYS:HE3	9:W:268:LYS:HB2	1.84	0.42
9:W:297:GLU:HG3	9:W:303:LYS:HZ2	1.84	0.42
10:X:356:LEU:HG	10:X:357:SER:H	1.84	0.42
12:Z:78:MET:HA	12:Z:81:MET:SD	2.60	0.42
14:b:4:GLU:HB3	14:b:106:LYS:HB2	2.02	0.42
3:C:146:SER:HB2	3:C:201:ARG:HD2	2.01	0.42
7:U:779:LEU:HD12	7:U:782:ALA:HB3	2.02	0.42
8:V:263:LEU:HG	8:V:266:GLN:HB3	2.02	0.42
9:W:449:GLU:HG2	12:Z:211:TYR:OH	2.20	0.42
12:Z:61:ASP:HB2	12:Z:67:VAL:HB	2.02	0.42
14:b:140:ILE:HD13	14:b:153:LEU:HB3	2.02	0.42
17:e:63:HIS:HB3	17:e:67:MET:HE3	2.01	0.42
2:B:365:PHE:CE2	2:B:384:ILE:HG12	2.55	0.41
14:b:47:ASN:O	14:b:66:PRO:HA	2.20	0.41
18:f:466:LEU:HA	18:f:469:TYR:HB3	2.02	0.41
18:f:516:GLY:HA3	18:f:557:TRP:HE3	1.85	0.41
3:C:160:GLU:HB2	3:C:313:ARG:HH12	1.86	0.41
5:E:364:GLN:O	5:E:368:MET:HG2	2.20	0.41
7:U:94:SER:HB3	7:U:97:VAL:HG12	2.01	0.41
7:U:678:ASP:O	7:U:684:ARG:NE	2.52	0.41
7:U:886:PRO:HA	7:U:889:LEU:HB2	2.01	0.41
12:Z:15:VAL:HG21	12:Z:50:VAL:HG12	2.02	0.41
15:c:192:LEU:HG	15:c:196:LEU:HD23	2.01	0.41
5:E:171:LEU:HA	5:E:277:MET:HB2	2.02	0.41
7:U:557:TYR:CG	7:U:588:MET:HE3	2.55	0.41
10:X:415:TYR:HE1	11:Y:383:LEU:HB2	1.84	0.41
14:b:12:ASN:H	14:b:55:ALA:HB2	1.85	0.41
15:c:123:SER:HB3	19:g:289:HIS:CE1	2.56	0.41
18:f:292:LYS:HZ2	18:f:879:ARG:HB2	1.84	0.41
20:z:76:GLU:HA	20:z:77:PRO:HD3	1.96	0.41
2:B:122:ILE:HD11	2:B:130:GLU:HB3	2.02	0.41
2:B:423:LYS:HD2	2:B:427:LEU:HD11	2.02	0.41
4:D:61:ILE:HD13	4:D:61:ILE:HA	1.89	0.41
7:U:396:ALA:HB1	7:U:400:ALA:HB3	2.02	0.41
7:U:622:LEU:HD23	7:U:625:ILE:HD12	2.01	0.41
7:U:703:CYS:HA	7:U:704:PRO:HD3	1.93	0.41
12:Z:8:LYS:HB3	12:Z:47:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:51:LEU:HD21	14:b:75:LEU:HD13	2.02	0.41
15:c:33:ILE:HD12	15:c:69:VAL:HG11	2.01	0.41
1:A:261:PHE:HE1	1:A:272:ILE:HG21	1.85	0.41
4:D:211:GLY:N	22:D:501:AGS:H5'1	2.35	0.41
5:E:5:ARG:HG3	6:F:38:THR:HG22	2.02	0.41
7:U:368:ALA:HB1	7:U:731:ILE:HB	2.03	0.41
7:U:649:ARG:HH21	7:U:680:VAL:HG21	1.86	0.41
18:f:461:PRO:HG2	18:f:463:LEU:HD13	2.01	0.41
18:f:683:GLU:O	18:f:687:ARG:HB2	2.21	0.41
20:z:250:ILE:HG22	20:z:293:TYR:HE2	1.86	0.41
20:z:285:SER:HB3	20:z:288:GLN:HB3	2.02	0.41
1:A:296:GLN:O	1:A:300:LEU:HG	2.21	0.41
5:E:141:GLN:HG2	5:E:301:ILE:HD13	2.02	0.41
5:E:326:ILE:HG22	5:E:328:TYR:HB3	2.02	0.41
7:U:465:LEU:HB3	7:U:496:LEU:HD21	2.03	0.41
8:V:368:ARG:HA	8:V:409:MET:HE1	2.03	0.41
14:b:22:LEU:HB2	14:b:23:PRO:HD3	2.03	0.41
15:c:192:LEU:HA	15:c:196:LEU:HB3	2.02	0.41
15:c:274:ASN:HA	15:c:277:LYS:HB3	2.01	0.41
16:d:113:GLY:HA2	16:d:154:TRP:HE1	1.85	0.41
18:f:634:LYS:HA	18:f:637:LYS:HE2	2.02	0.41
4:D:144:PRO:HA	4:D:145:PRO:HD3	1.95	0.41
4:D:212:LYS:HB3	4:D:310:ALA:HB1	2.01	0.41
7:U:756:HIS:HB3	7:U:759:SER:OG	2.20	0.41
9:W:393:LEU:HD21	9:W:413:ILE:HG21	2.02	0.41
14:b:87:CYS:HA	14:b:90:ILE:HG22	2.02	0.41
15:c:231:LEU:HB3	15:c:232:GLN:H	1.72	0.41
5:E:242:ARG:HA	5:E:254:GLN:HG2	2.01	0.41
7:U:377:HIS:HB2	7:U:411:ILE:HG12	2.03	0.41
7:U:791:LEU:HB2	7:U:913:ILE:HG13	2.03	0.41
8:V:225:ASP:HB3	8:V:261:TYR:HE2	1.86	0.41
14:b:32:ALA:HB1	14:b:183:LEU:HD22	2.02	0.41
1:A:164:MET:HE2	1:A:263:MET:HB3	2.02	0.41
3:C:139:MET:HE3	3:C:210:THR:HB	2.02	0.41
4:D:209:GLY:HA2	22:D:501:AGS:H5'2	2.03	0.41
5:E:140:GLU:HA	5:E:143:ARG:HG2	2.03	0.41
5:E:342:ASP:O	5:E:346:VAL:HG23	2.20	0.41
6:F:224:LEU:HB2	6:F:348:LEU:HG	2.02	0.41
7:U:348:THR:HG22	7:U:376:MET:HE3	2.02	0.41
7:U:401:LYS:HE3	7:U:401:LYS:HB2	1.90	0.41
11:Y:307:LEU:HD12	11:Y:307:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:141:ILE:HD13	14:b:183:LEU:HD11	2.03	0.41
15:c:134:GLU:HB2	15:c:138:GLU:HA	2.02	0.41
16:d:212:LEU:HD12	16:d:215:LEU:HD22	2.03	0.41
18:f:667:GLY:HA2	18:f:671:ALA:HB3	2.02	0.41
3:C:168:PRO:O	3:C:172:PRO:HG3	2.22	0.41
3:C:319:PRO:HA	3:C:320:PRO:HD3	1.89	0.41
6:F:86:LEU:O	6:F:87:PRO:C	2.64	0.41
8:V:348:PHE:HB2	8:V:357:LEU:HD13	2.03	0.41
9:W:75:TYR:HA	9:W:79:GLU:HB2	2.03	0.41
9:W:407:ASP:HB3	9:W:412:ILE:HB	2.02	0.41
12:Z:206:LEU:HD22	12:Z:209:ARG:HH22	1.85	0.41
20:z:208:LEU:O	20:z:212:LEU:HG	2.21	0.41
1:A:125:LEU:HD12	1:A:129:VAL:HG23	2.04	0.40
6:F:62:VAL:O	6:F:66:LEU:HB2	2.22	0.40
6:F:251:LEU:HD12	6:F:256:LEU:HD21	2.02	0.40
15:c:262:GLU:HA	15:c:270:LEU:HD11	2.02	0.40
19:g:119:ILE:HA	19:g:120:PRO:HD3	1.94	0.40
20:z:208:LEU:O	20:z:209:VAL:C	2.63	0.40
2:B:105:THR:OG1	2:B:106:PRO:HD3	2.22	0.40
3:C:285:ALA:O	3:C:286:THR:C	2.64	0.40
3:C:329:LEU:HG	3:C:344:LEU:HD22	2.03	0.40
4:D:346:SER:HA	4:D:349:THR:HG22	2.03	0.40
6:F:267:LEU:HD12	6:F:267:LEU:HA	1.89	0.40
12:Z:275:LEU:HD21	12:Z:279:LYS:HE2	2.02	0.40
13:a:217:LEU:HD23	13:a:217:LEU:HA	1.90	0.40
13:a:371:ALA:O	13:a:375:LEU:HB2	2.22	0.40
16:d:109:LEU:HD21	16:d:158:ARG:HG3	2.02	0.40
18:f:173:LEU:HD23	18:f:173:LEU:HA	1.92	0.40
1:A:333:ARG:HB2	1:A:336:ARG:HD2	2.03	0.40
5:E:181:THR:HG22	5:E:231:PHE:HZ	1.86	0.40
7:U:173:VAL:HA	7:U:176:MET:HE2	2.03	0.40
7:U:629:THR:HB	7:U:632:GLN:HB2	2.02	0.40
9:W:438:LEU:HD12	9:W:438:LEU:HA	1.91	0.40
1:A:289:ALA:HB3	1:A:292:ASP:HB2	2.03	0.40
3:C:287:LYS:HB3	3:C:289:ILE:HG23	2.03	0.40
7:U:446:LEU:HD13	7:U:457:ILE:HD11	2.04	0.40
8:V:366:ALA:HA	8:V:369:THR:HG22	2.03	0.40
9:W:79:GLU:OE2	9:W:83:LEU:HB2	2.21	0.40
11:Y:236:LEU:O	11:Y:240:VAL:HG22	2.22	0.40
14:b:135:LYS:HD2	14:b:135:LYS:HA	1.89	0.40
15:c:121:TRP:HB3	15:c:191:ALA:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:z:383:MET:HE2	20:z:387:TRP:CH2	2.56	0.40
1:A:397:ILE:HG23	2:B:202:GLU:HG3	2.03	0.40
4:D:215:LEU:HA	4:D:215:LEU:HD13	1.87	0.40
4:D:237:GLN:HE21	4:D:246:MET:HE1	1.85	0.40
4:D:261:ILE:HD12	4:D:308:ILE:HG21	2.02	0.40
5:E:60:VAL:HA	5:E:71:VAL:HG12	2.03	0.40
5:E:196:LEU:N	5:E:196:LEU:HD23	2.36	0.40
6:F:192:ASP:HA	6:F:195:ILE:HD12	2.04	0.40
7:U:182:LYS:HB3	7:U:182:LYS:HE2	1.88	0.40
11:Y:48:ASN:HB3	11:Y:113:ARG:HH21	1.85	0.40
11:Y:164:ALA:O	11:Y:165:LYS:C	2.64	0.40
18:f:272:LEU:HD23	18:f:272:LEU:HA	1.91	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	357/433 (82%)	315 (88%)	42 (12%)	0	100	100
2	B	371/440 (84%)	326 (88%)	45 (12%)	0	100	100
3	C	366/406 (90%)	330 (90%)	36 (10%)	0	100	100
4	D	367/418 (88%)	339 (92%)	28 (8%)	0	100	100
5	E	378/389 (97%)	356 (94%)	22 (6%)	0	100	100
6	F	370/439 (84%)	345 (93%)	25 (7%)	0	100	100
7	U	825/953 (87%)	756 (92%)	69 (8%)	0	100	100
8	V	459/534 (86%)	428 (93%)	31 (7%)	0	100	100
9	W	435/456 (95%)	406 (93%)	29 (7%)	0	100	100
10	X	103/422 (24%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	Y	376/389 (97%)	346 (92%)	30 (8%)	0	100	100
12	Z	285/324 (88%)	275 (96%)	10 (4%)	0	100	100
13	a	372/376 (99%)	361 (97%)	11 (3%)	0	100	100
14	b	187/377 (50%)	165 (88%)	22 (12%)	0	100	100
15	c	287/310 (93%)	268 (93%)	19 (7%)	0	100	100
16	d	263/350 (75%)	244 (93%)	19 (7%)	0	100	100
17	e	36/70 (51%)	30 (83%)	6 (17%)	0	100	100
18	f	716/908 (79%)	650 (91%)	66 (9%)	0	100	100
19	g	171/289 (59%)	158 (92%)	13 (8%)	0	100	100
20	z	470/504 (93%)	443 (94%)	27 (6%)	0	100	100
All	All	7194/8787 (82%)	6642 (92%)	552 (8%)	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	310/372 (83%)	308 (99%)	2 (1%)	78	81
2	B	331/385 (86%)	327 (99%)	4 (1%)	63	73
3	C	321/352 (91%)	317 (99%)	4 (1%)	63	73
4	D	322/366 (88%)	317 (98%)	5 (2%)	55	70
5	E	333/341 (98%)	331 (99%)	2 (1%)	78	81
6	F	323/379 (85%)	321 (99%)	2 (1%)	78	81
7	U	707/816 (87%)	702 (99%)	5 (1%)	76	79
8	V	400/460 (87%)	400 (100%)	0	100	100
9	W	402/416 (97%)	401 (100%)	1 (0%)	87	87
10	X	97/362 (27%)	97 (100%)	0	100	100
11	Y	334/344 (97%)	334 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	258/295 (88%)	258 (100%)	0	100	100
13	a	334/336 (99%)	334 (100%)	0	100	100
14	b	167/312 (54%)	166 (99%)	1 (1%)	78	81
15	c	253/268 (94%)	249 (98%)	4 (2%)	55	70
16	d	235/294 (80%)	235 (100%)	0	100	100
17	e	38/63 (60%)	38 (100%)	0	100	100
18	f	620/763 (81%)	620 (100%)	0	100	100
19	g	157/253 (62%)	157 (100%)	0	100	100
20	z	417/441 (95%)	414 (99%)	3 (1%)	76	79
All	All	6359/7618 (84%)	6326 (100%)	33 (0%)	78	82

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	302	LEU
2	B	102	LEU
2	B	105	THR
2	B	199	GLU
2	B	201	VAL
3	C	94	LYS
3	C	114	VAL
3	C	376	VAL
3	C	377	HIS
4	D	113	VAL
4	D	142	VAL
4	D	215	LEU
4	D	253	LEU
4	D	267	ILE
5	E	198	VAL
5	E	229	ILE
6	F	97	LEU
6	F	366	MET
7	U	685	GLN
7	U	737	LEU
7	U	744	VAL
7	U	749	GLN
7	U	755	THR
9	W	76	GLU

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Mol	Chain	Res	Type
14	b	10	VAL
15	c	63	ASP
15	c	65	TYR
15	c	90	VAL
15	c	298	GLN
20	z	205	THR
20	z	210	THR
20	z	215	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	103	ASN
2	B	192	ASN
2	B	207	HIS
3	C	40	GLN
3	C	102	ASN
3	C	278	ASN
3	C	296	ASN
3	C	343	ASN
3	C	377	HIS
3	C	392	GLN
4	D	48	GLN
4	D	76	GLN
4	D	127	ASN
4	D	135	HIS
4	D	137	ASN
4	D	173	GLN
4	D	294	ASN
4	D	301	GLN
5	E	262	ASN
5	E	263	GLN
6	F	64	HIS
6	F	67	GLN
6	F	154	ASN
6	F	208	HIS
6	F	315	ASN
6	F	316	GLN
7	U	18	GLN
7	U	32	ASN
7	U	145	HIS

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Mol	Chain	Res	Type
7	U	149	GLN
7	U	192	GLN
7	U	227	GLN
7	U	266	GLN
7	U	340	GLN
7	U	525	ASN
7	U	698	GLN
7	U	743	ASN
7	U	801	GLN
7	U	805	ASN
7	U	874	ASN
7	U	876	GLN
8	V	242	HIS
8	V	252	ASN
8	V	266	GLN
8	V	299	GLN
8	V	452	ASN
9	W	107	GLN
9	W	167	GLN
9	W	264	GLN
9	W	281	ASN
10	X	406	ASN
11	Y	77	ASN
12	Z	189	GLN
12	Z	225	GLN
12	Z	243	GLN
13	a	35	HIS
13	a	72	ASN
13	a	86	GLN
13	a	144	ASN
13	a	219	HIS
13	a	244	ASN
13	a	290	GLN
14	b	30	GLN
14	b	94	HIS
14	b	149	ASN
14	b	158	ASN
15	c	128	ASN
15	c	283	HIS
16	d	103	ASN
16	d	314	ASN
18	f	198	HIS

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Mol	Chain	Res	Type
18	f	202	HIS
18	f	238	ASN
18	f	291	GLN
18	f	371	ASN
18	f	457	ASN
18	f	493	ASN
18	f	605	ASN
18	f	757	ASN
18	f	770	HIS
19	g	148	ASN
19	g	187	ASN
19	g	289	HIS
20	z	106	GLN
20	z	333	GLN
20	z	428	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](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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
21	ADP	A	501	-	28,29,29	1.41	5 (17%)	43,45,45	1.98	9 (20%)
22	AGS	E	501	23	32,33,33	0.67	1 (3%)	45,52,52	0.58	0
22	AGS	C	501	23	32,33,33	0.65	1 (3%)	45,52,52	0.53	0
21	ADP	F	501	-	28,29,29	0.45	0	43,45,45	0.49	0
22	AGS	D	501	23	32,33,33	0.68	1 (3%)	45,52,52	0.50	0

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
21	ADP	A	501	-	-	5/16/32/32	0/3/3/3
22	AGS	E	501	23	-	3/21/38/38	0/3/3/3
22	AGS	C	501	23	-	2/21/38/38	0/3/3/3
21	ADP	F	501	-	-	3/16/32/32	0/3/3/3
22	AGS	D	501	23	-	2/21/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	501	ADP	C5-C4	4.56	1.47	1.39
21	A	501	ADP	C5-N7	-2.65	1.34	1.39
21	A	501	ADP	C5-C6	2.41	1.47	1.41
21	A	501	ADP	PA-O3A	2.31	1.62	1.59
22	D	501	AGS	PG-S1G	2.14	1.95	1.90
22	E	501	AGS	PG-S1G	2.13	1.95	1.90
21	A	501	ADP	C8-N7	2.02	1.35	1.31
22	C	501	AGS	PG-S1G	2.02	1.95	1.90

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	501	ADP	C5-C4-N3	-6.59	117.65	126.72
21	A	501	ADP	N3-C4-N9	5.53	136.58	127.17
21	A	501	ADP	C2-N3-C4	3.93	121.43	111.83
21	A	501	ADP	N3-C2-N1	-3.19	123.75	128.58
21	A	501	ADP	C4-C5-N7	-2.88	107.29	110.58
21	A	501	ADP	C3'-C2'-C1'	2.67	106.51	101.46
21	A	501	ADP	C4-N9-C8	2.39	108.24	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	501	ADP	C5'-N7-C8	2.28	107.04	103.45
21	A	501	ADP	C1'-N9-C8	-2.08	122.49	127.09

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	501	ADP	C5'-O5'-PA-O1A
21	A	501	ADP	C5'-O5'-PA-O2A
21	A	501	ADP	C5'-O5'-PA-O3A
22	D	501	AGS	PB-O3A-PA-O5'
22	E	501	AGS	C5'-O5'-PA-O2A
22	E	501	AGS	C5'-O5'-PA-O3A
22	C	501	AGS	O4'-C4'-C5'-O5'
22	C	501	AGS	C3'-C4'-C5'-O5'
21	A	501	ADP	PB-O3A-PA-O1A
22	D	501	AGS	C4'-C5'-O5'-PA
21	F	501	ADP	O4'-C4'-C5'-O5'
21	A	501	ADP	PB-O3A-PA-O5'
21	F	501	ADP	PB-O3A-PA-O1A
21	F	501	ADP	PB-O3A-PA-O2A
22	E	501	AGS	C2'-C1'-N9-C8

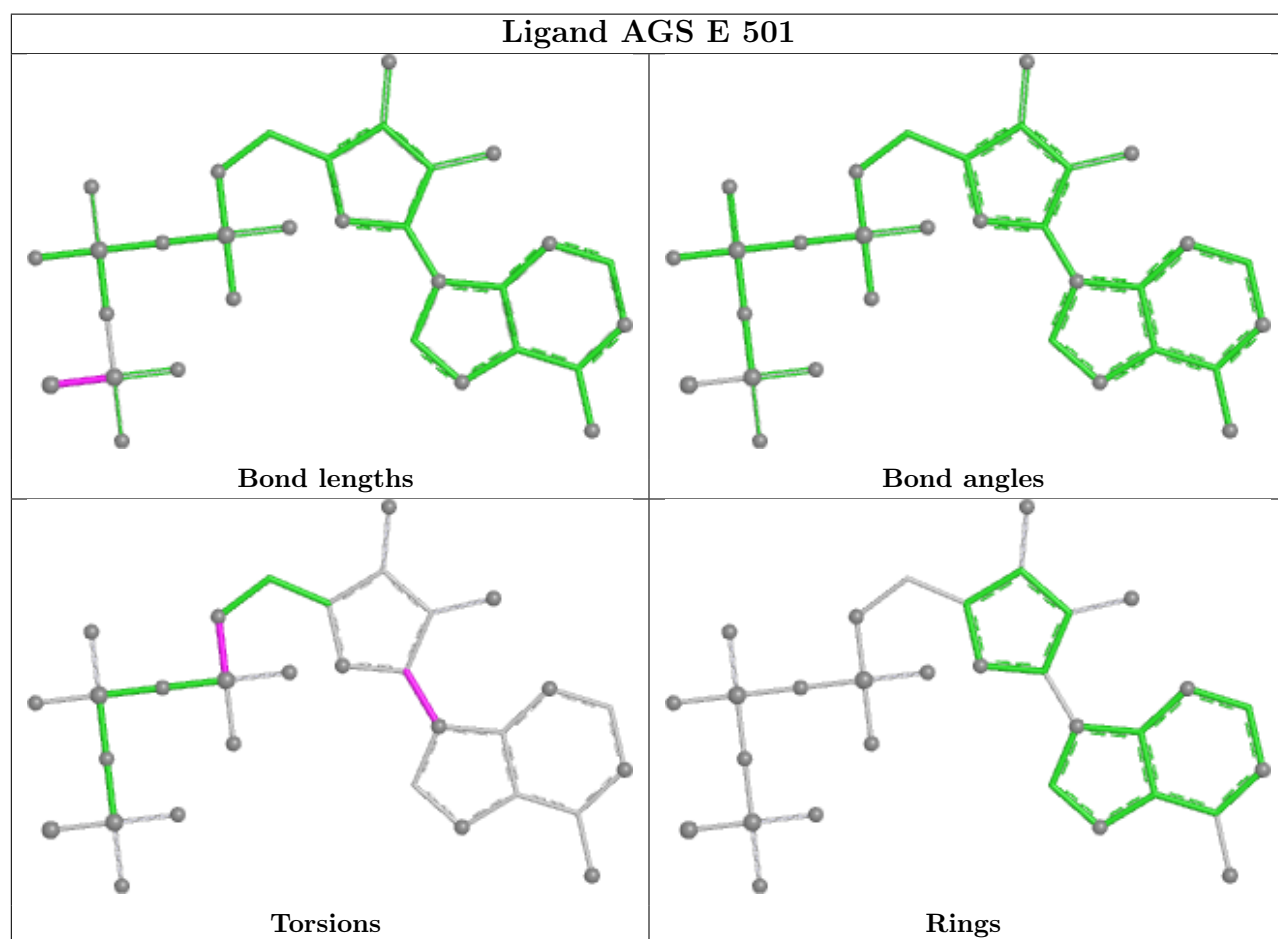
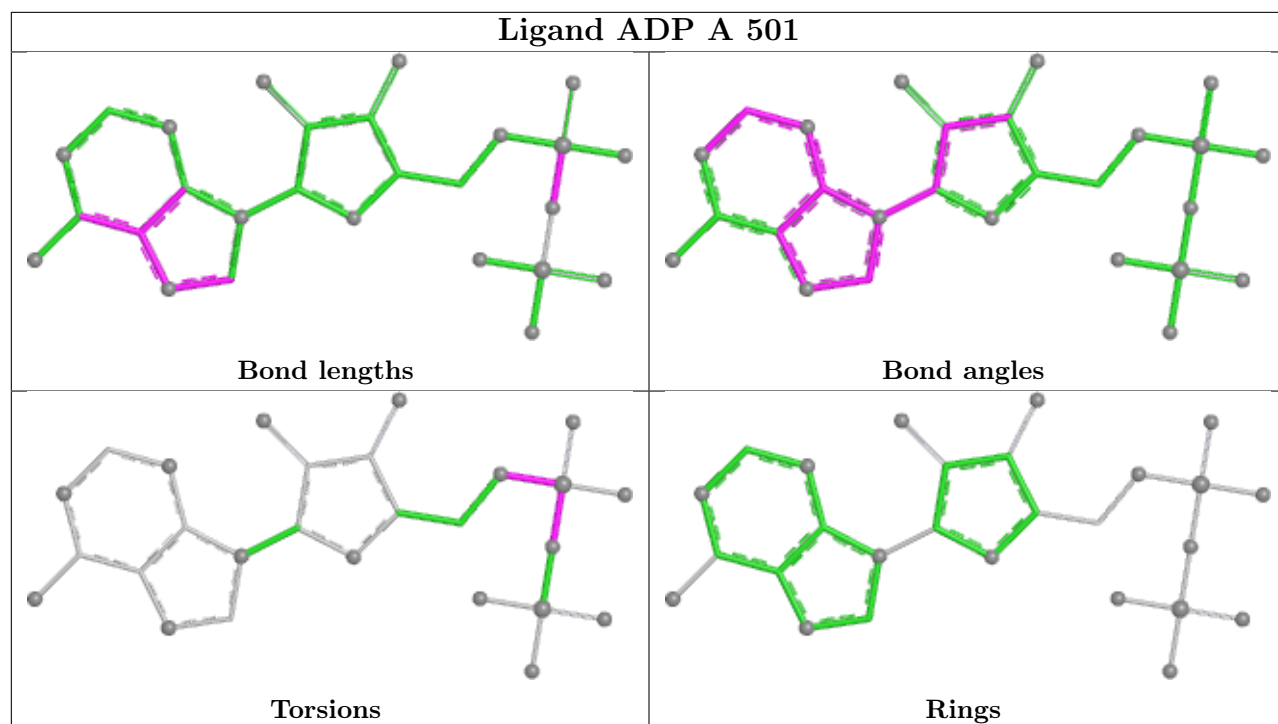
There are no ring outliers.

3 monomers are involved in 8 short contacts:

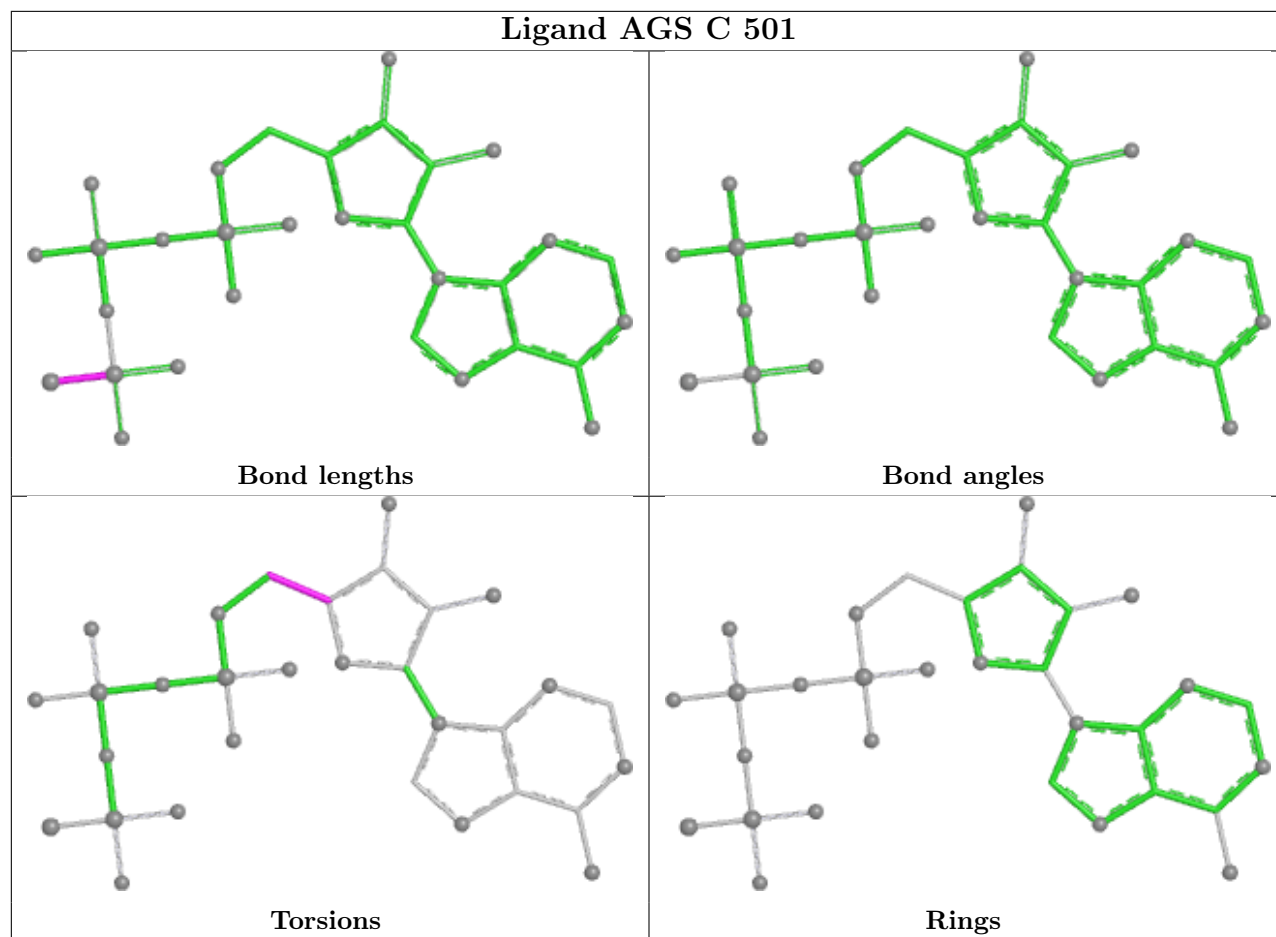
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	501	ADP	3	0
21	F	501	ADP	1	0
22	D	501	AGS	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

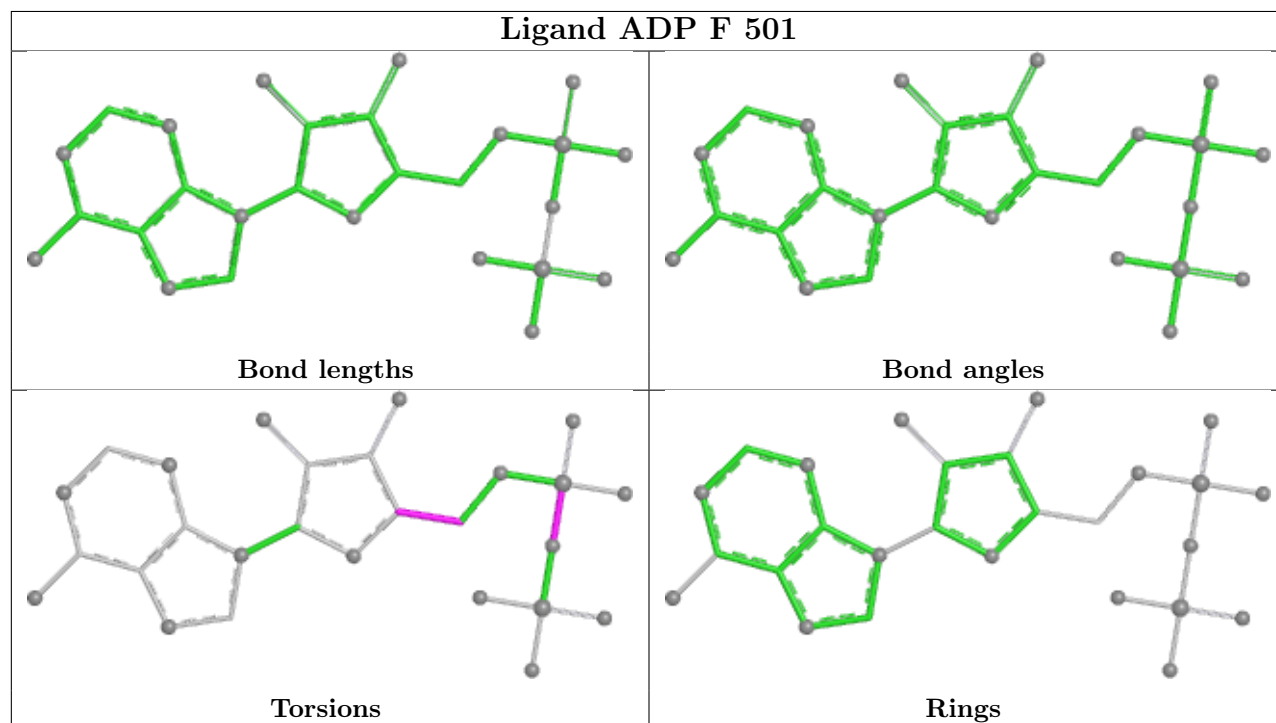
equivalents in the CSD to analyse the geometry.

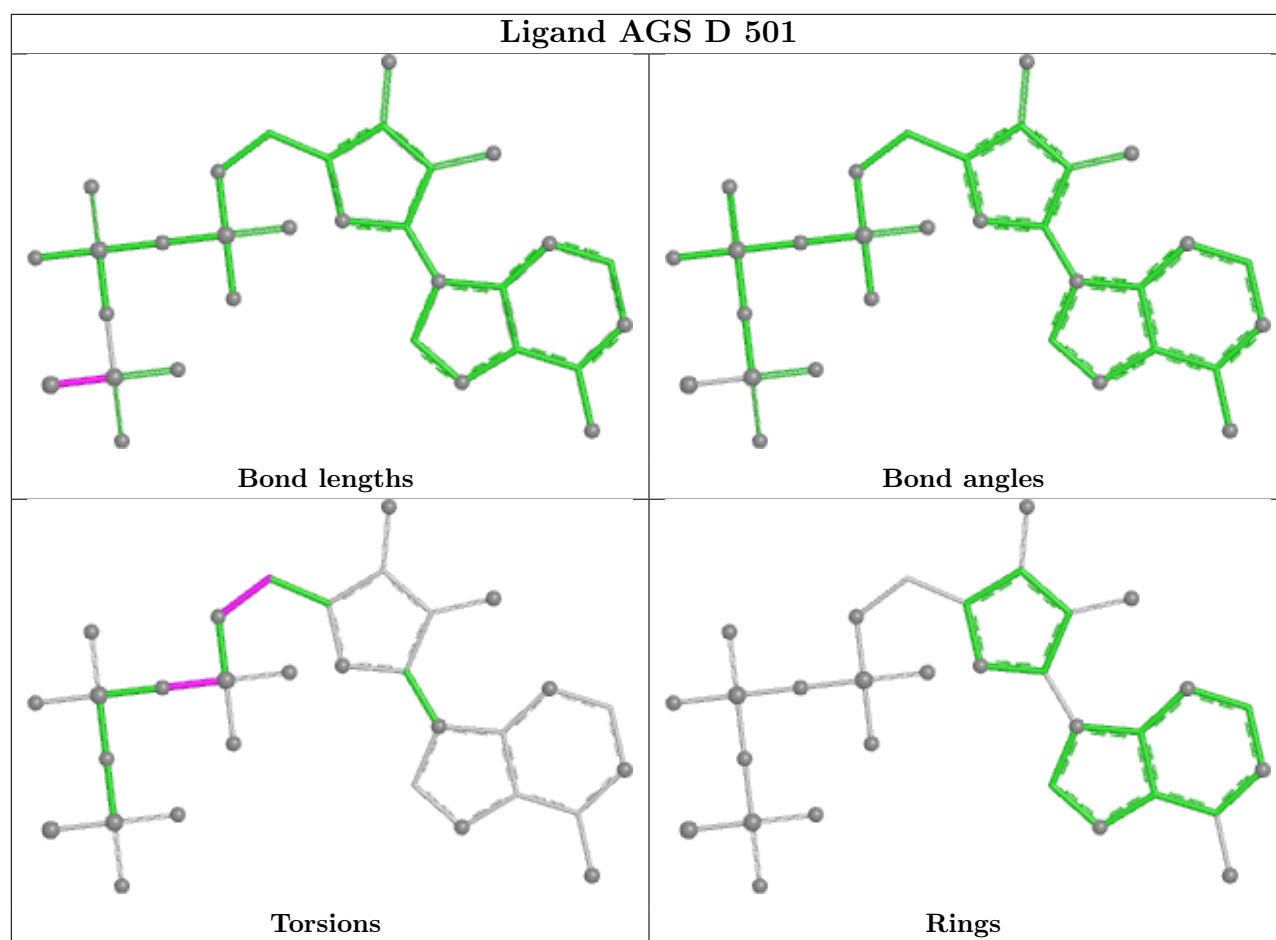


Ligand AGS C 501



Ligand ADP F 501





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.

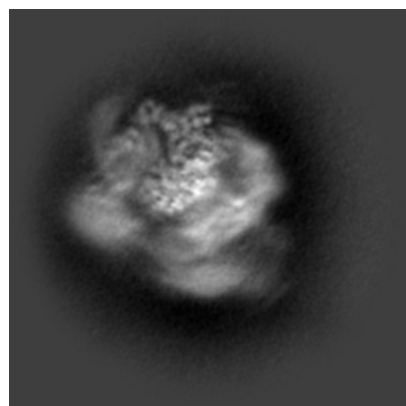
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71810. These allow visual inspection of the internal detail of the map and identification of artifacts.

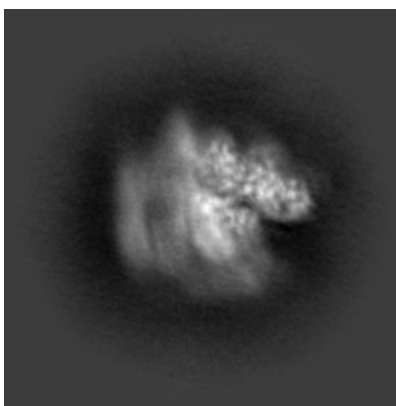
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

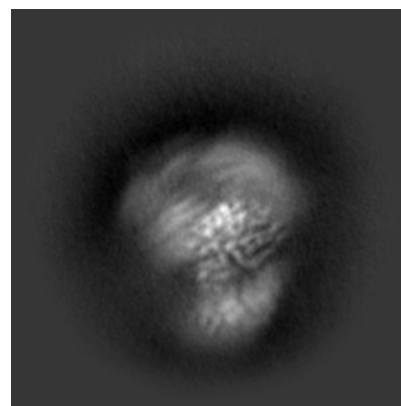
6.1.1 Primary map



X

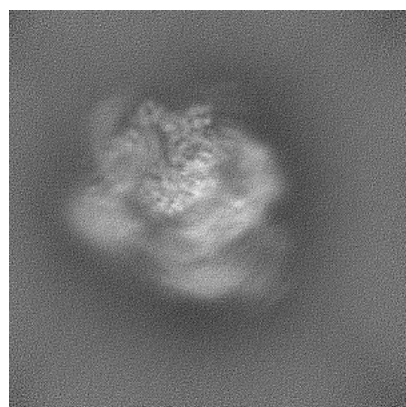


Y

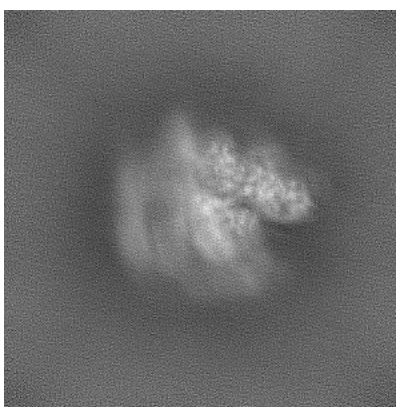


Z

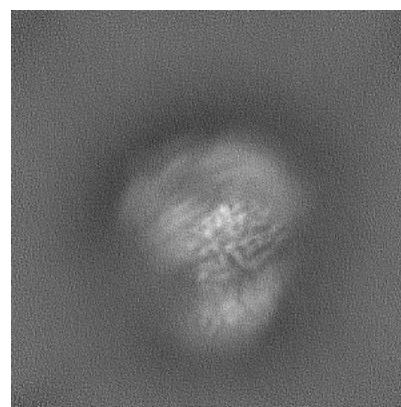
6.1.2 Raw map



X



Y

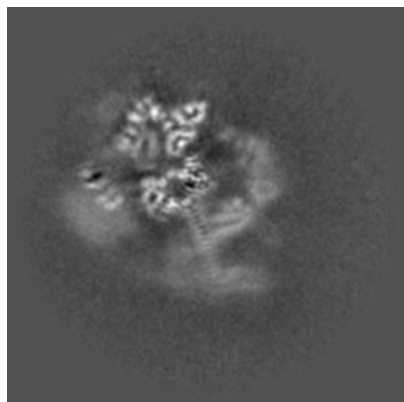


Z

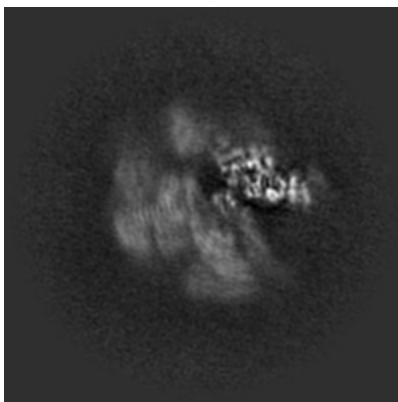
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

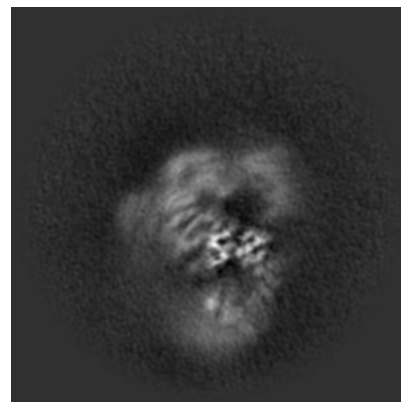
6.2.1 Primary map



X Index: 216

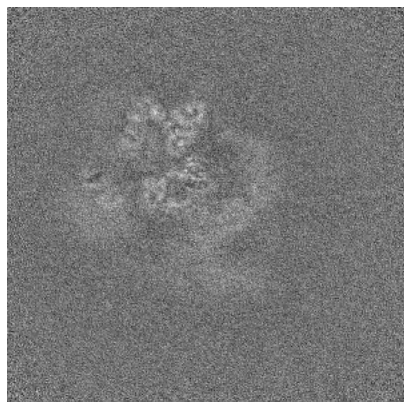


Y Index: 216

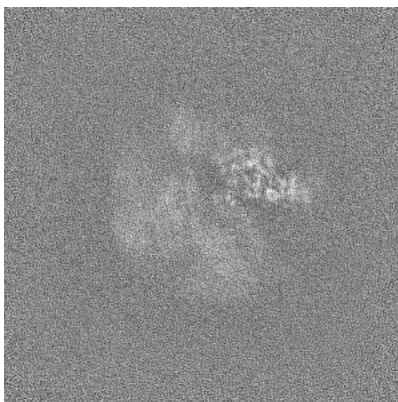


Z Index: 216

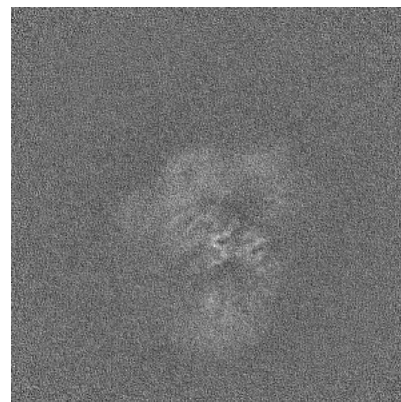
6.2.2 Raw map



X Index: 216



Y Index: 216

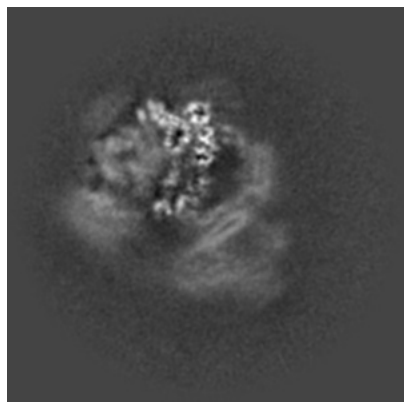


Z Index: 216

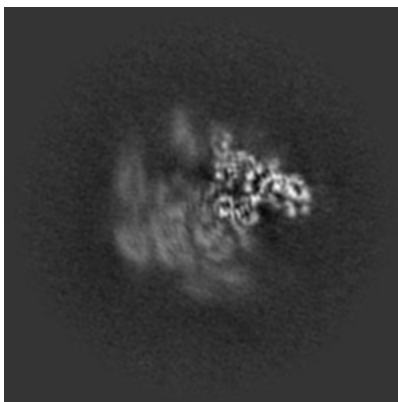
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

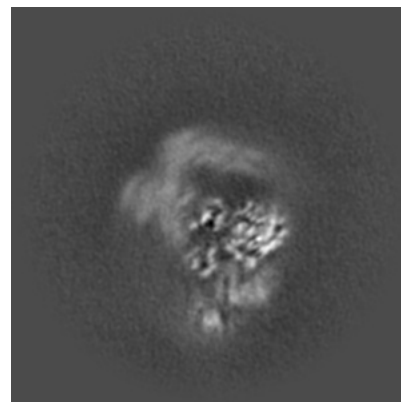
6.3.1 Primary map



X Index: 231

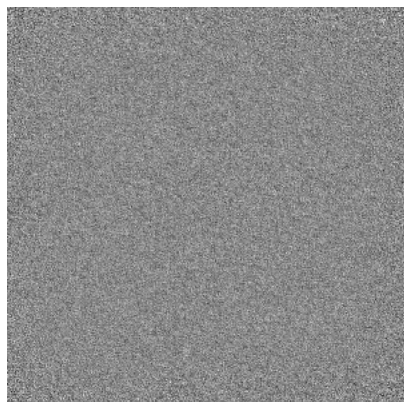


Y Index: 203

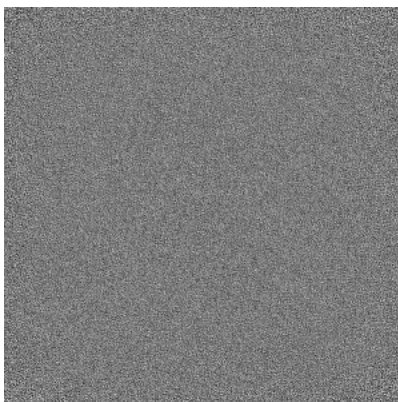


Z Index: 239

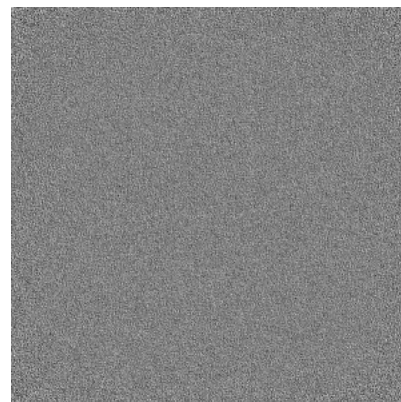
6.3.2 Raw map



X Index: 0



Y Index: 0

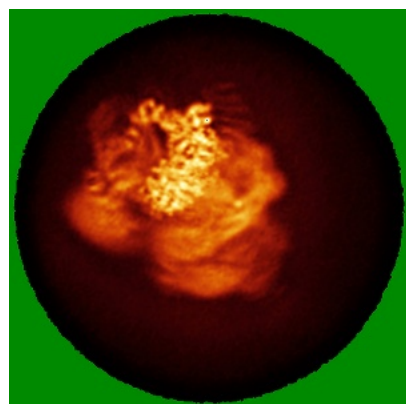


Z Index: 0

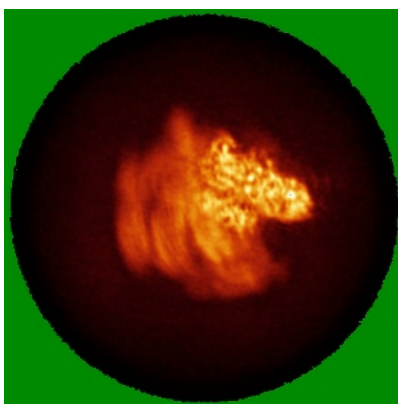
The images above show the largest variance slices of the map in three orthogonal directions.

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

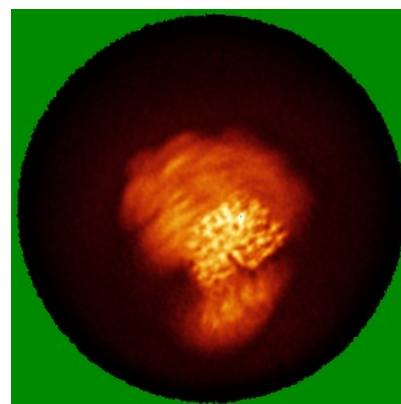
6.4.1 Primary map



X

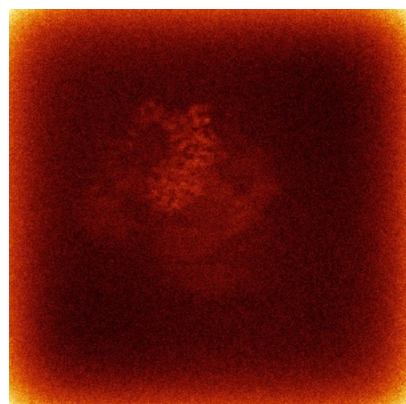


Y

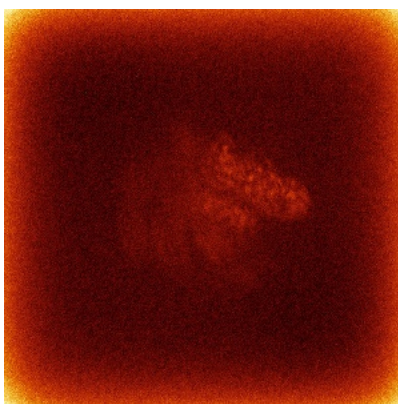


Z

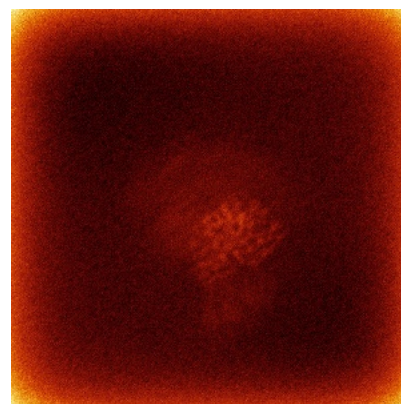
6.4.2 Raw map



X



Y

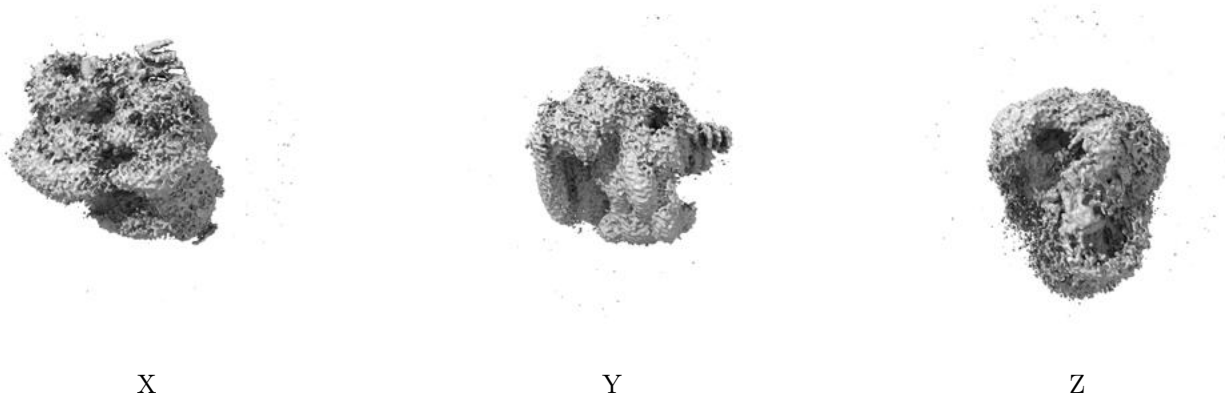


Z

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.

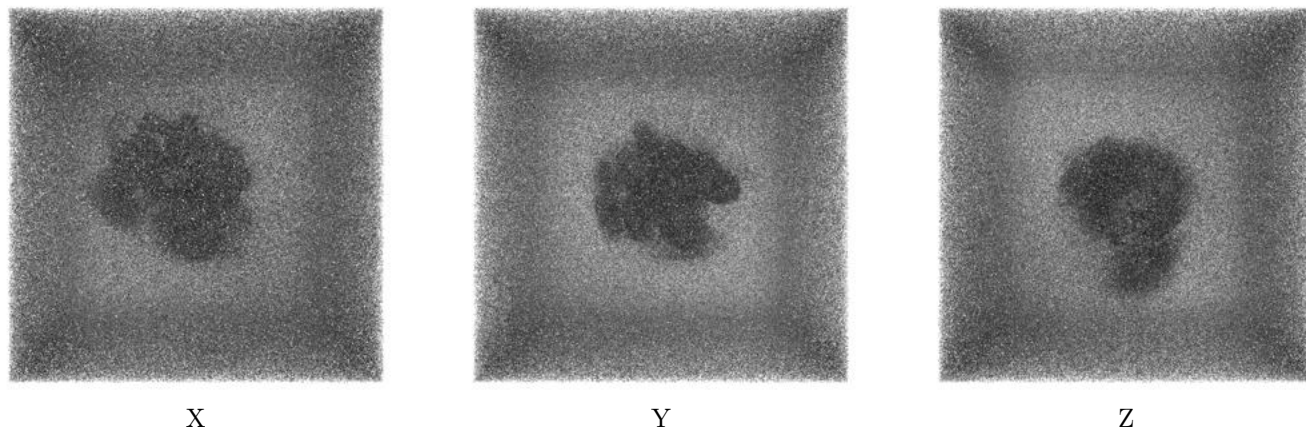
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

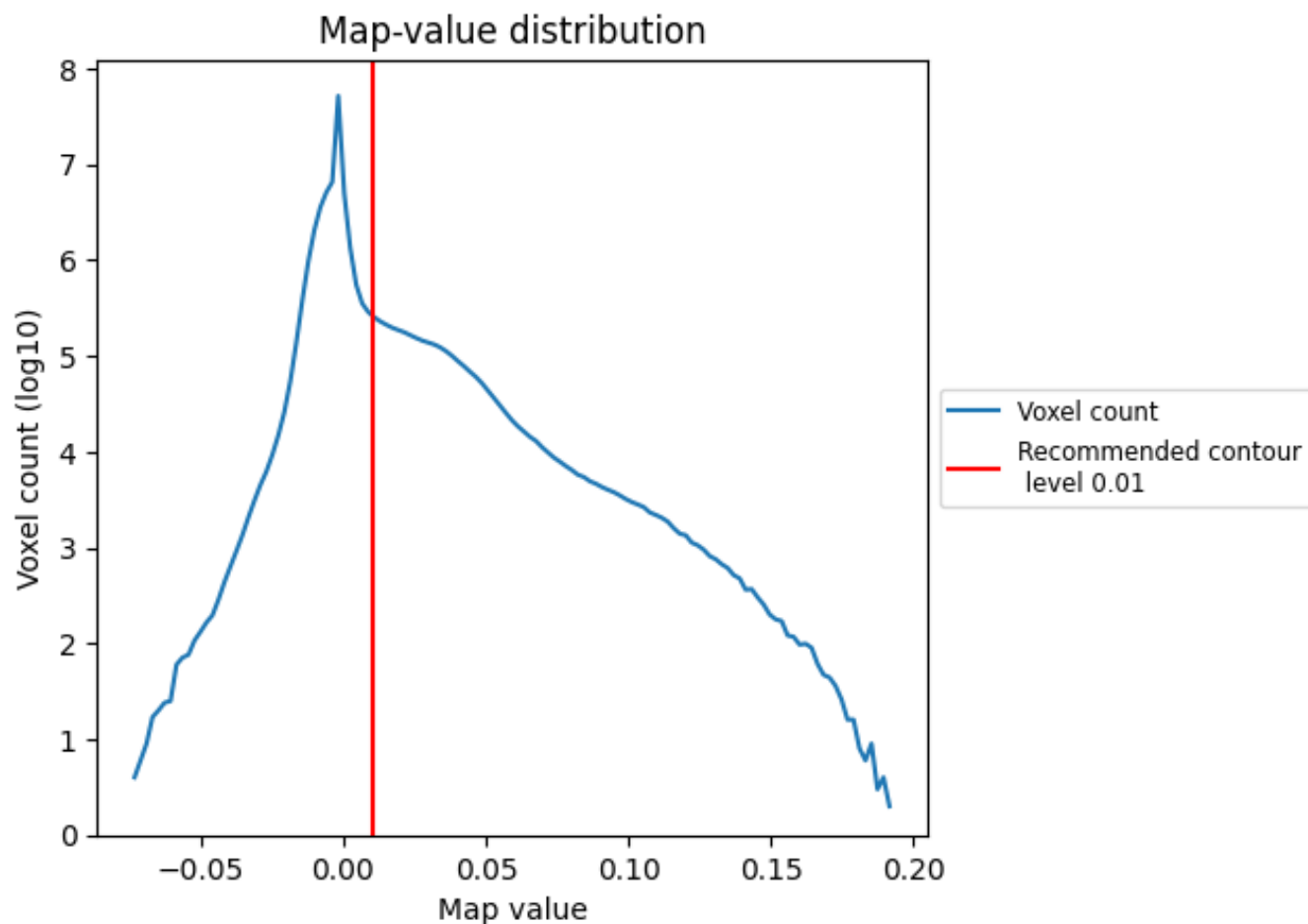
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

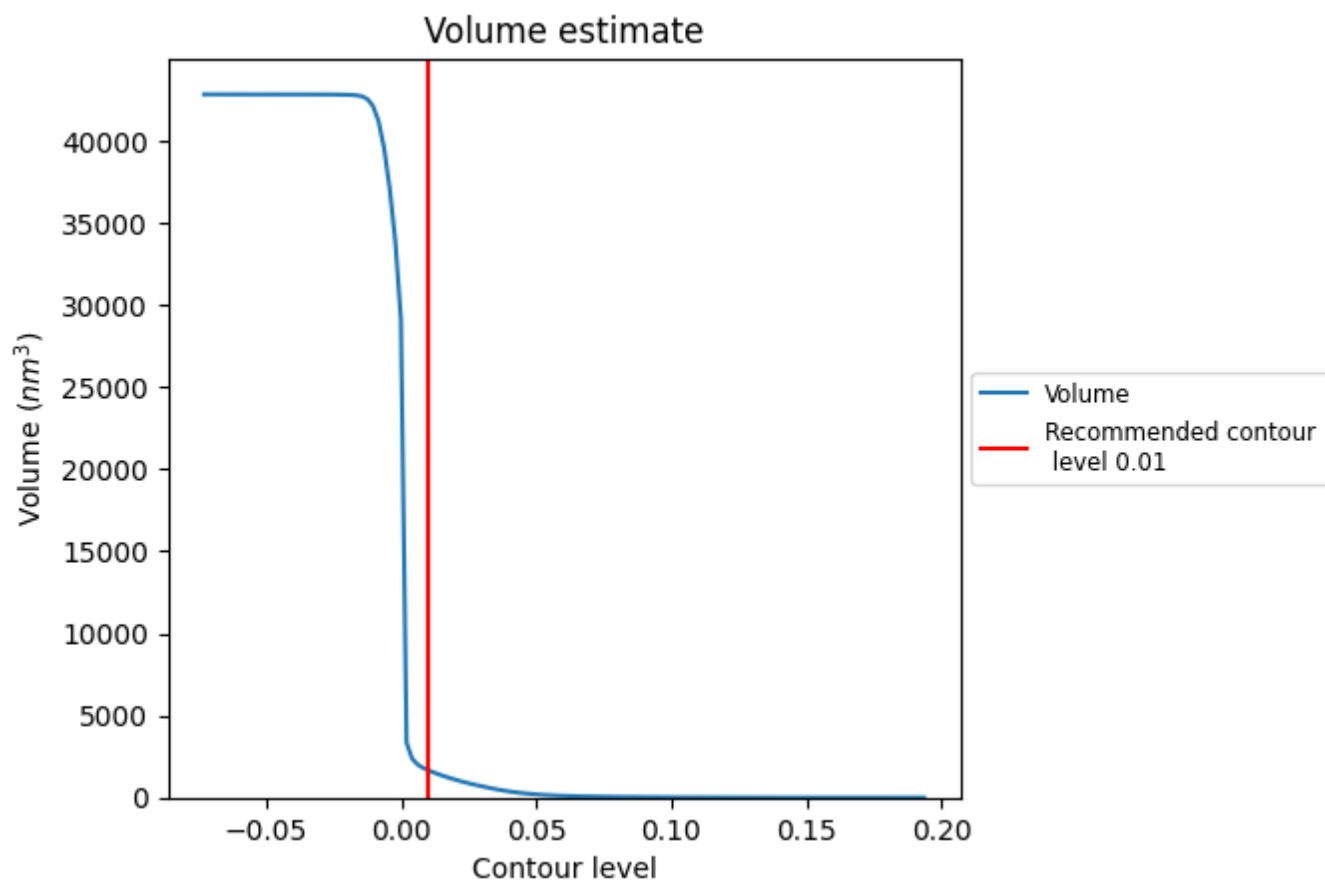
This section contains the results of statistical analysis of the map.

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.

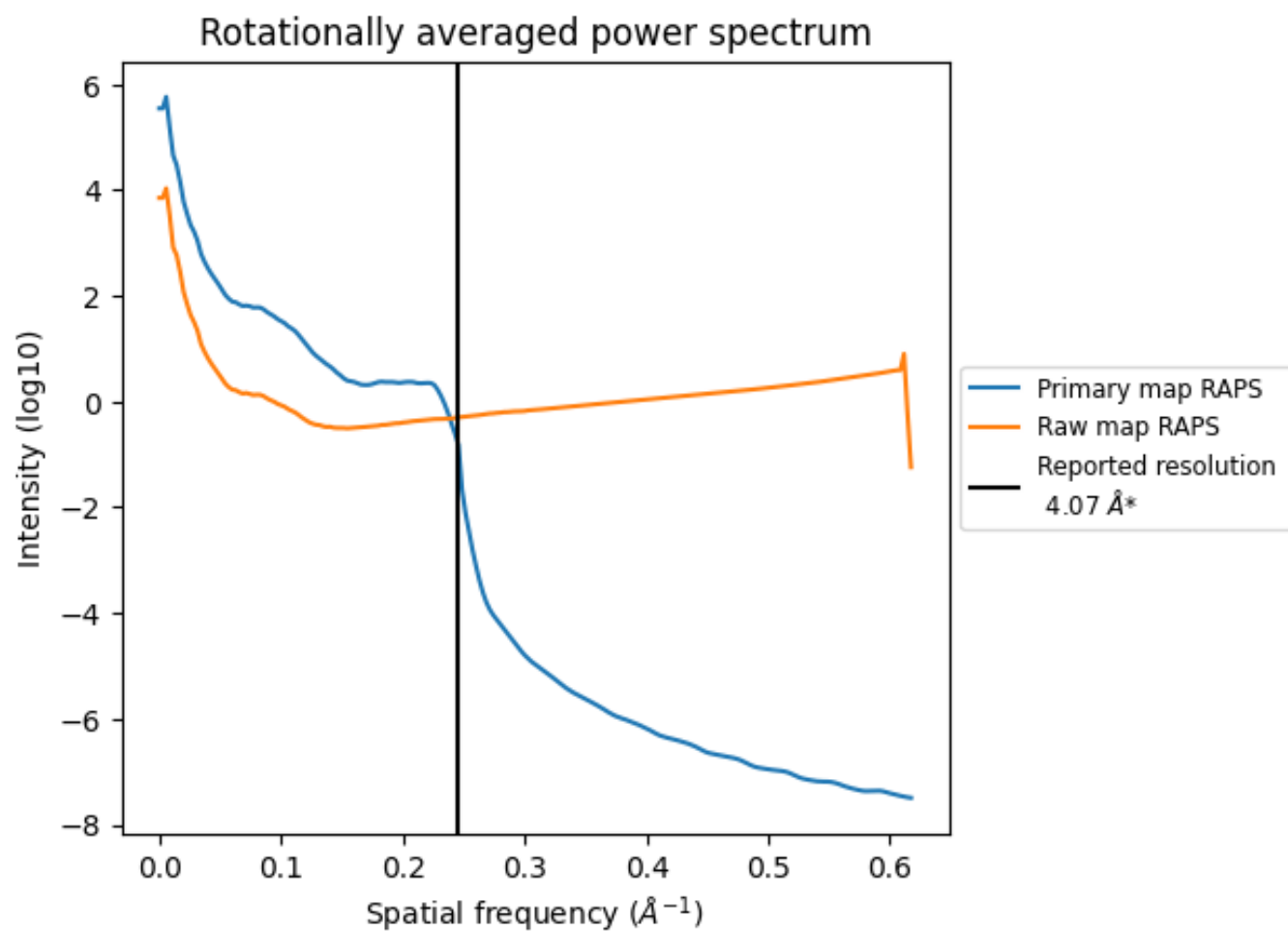
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1654 nm^3 ; this corresponds to an approximate mass of 1494 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 ⓘ

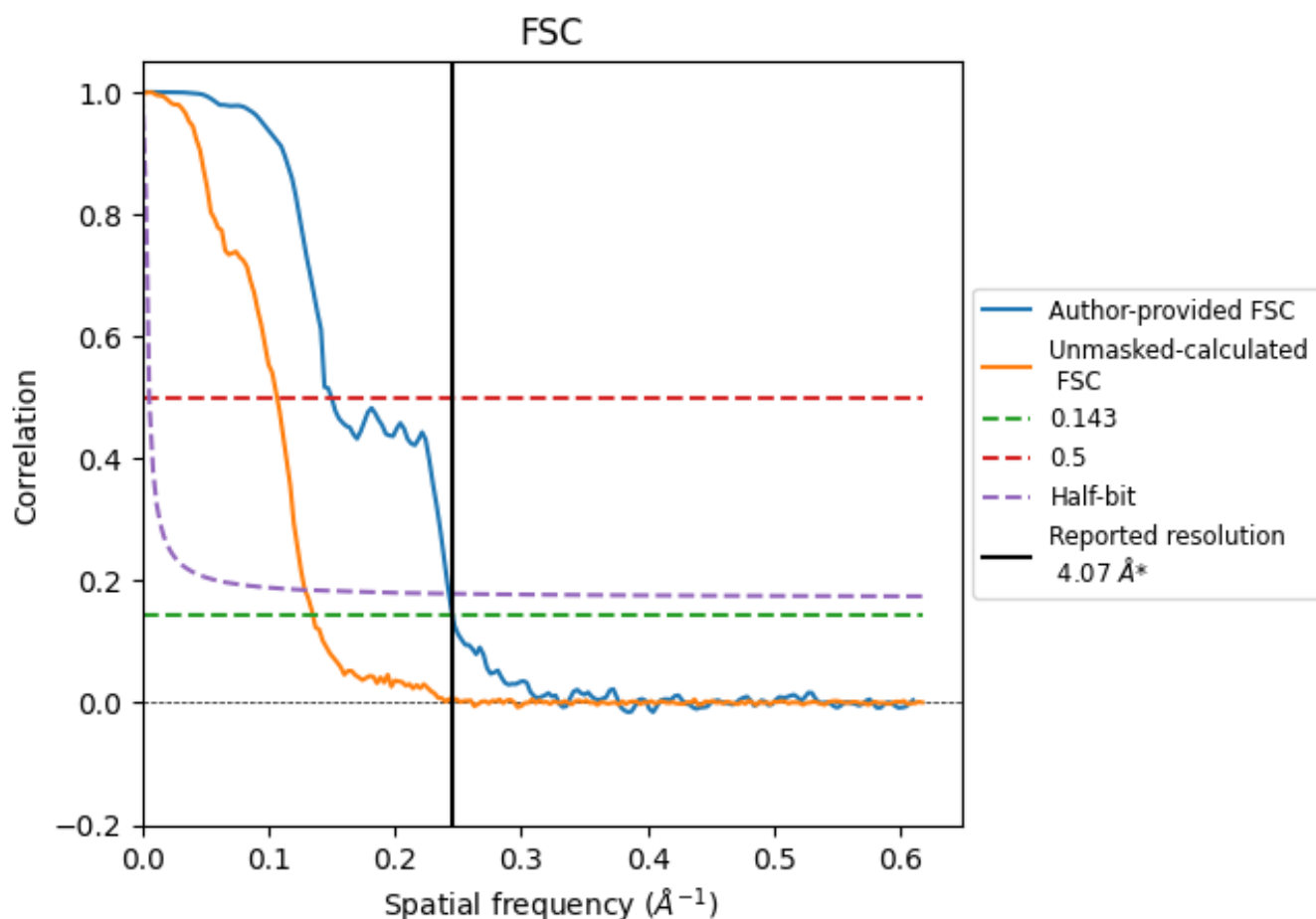


*Reported resolution corresponds to spatial frequency of 0.246 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.246 Å⁻¹

8.2 Resolution estimates [i](#)

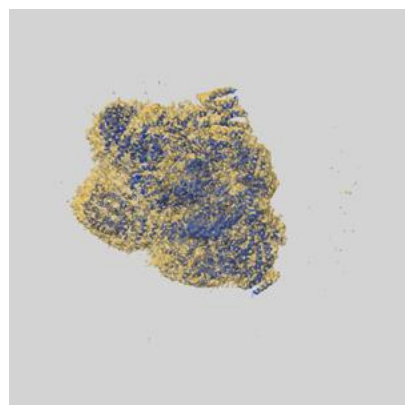
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.07	-	-
Author-provided FSC curve	4.07	6.68	4.12
Unmasked-calculated*	7.40	9.37	7.77

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.40 differs from the reported value 4.07 by more than 10 %

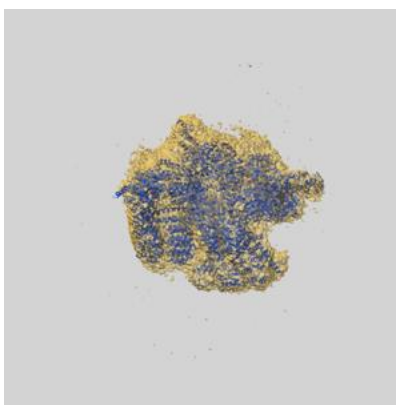
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71810 and PDB model 9PRO. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

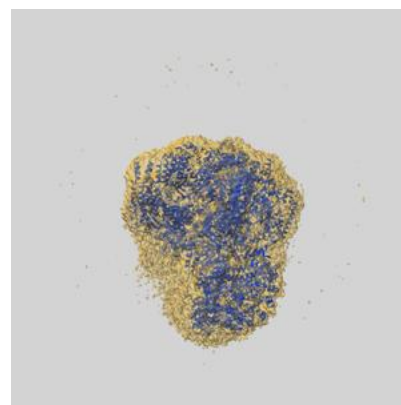
9.1 Map-model overlay [i](#)



X



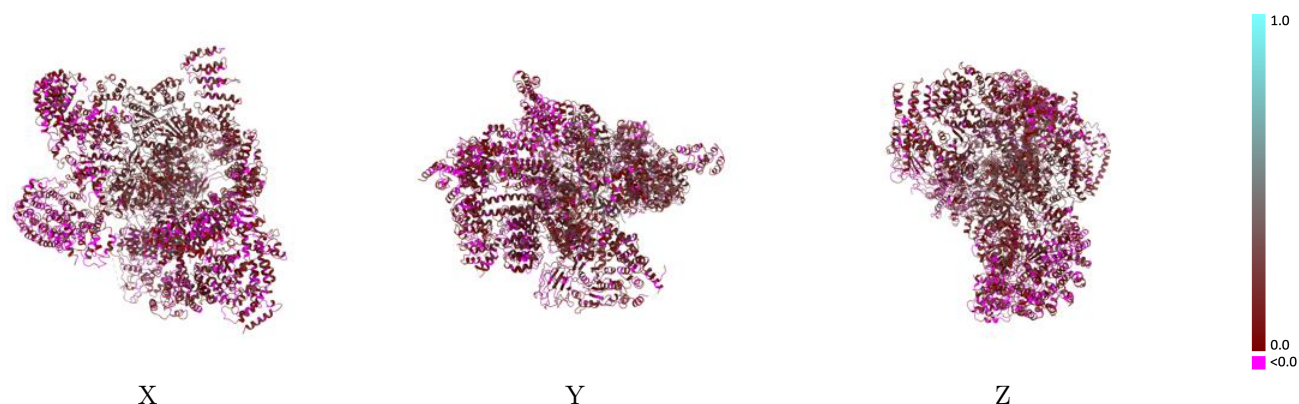
Y



Z

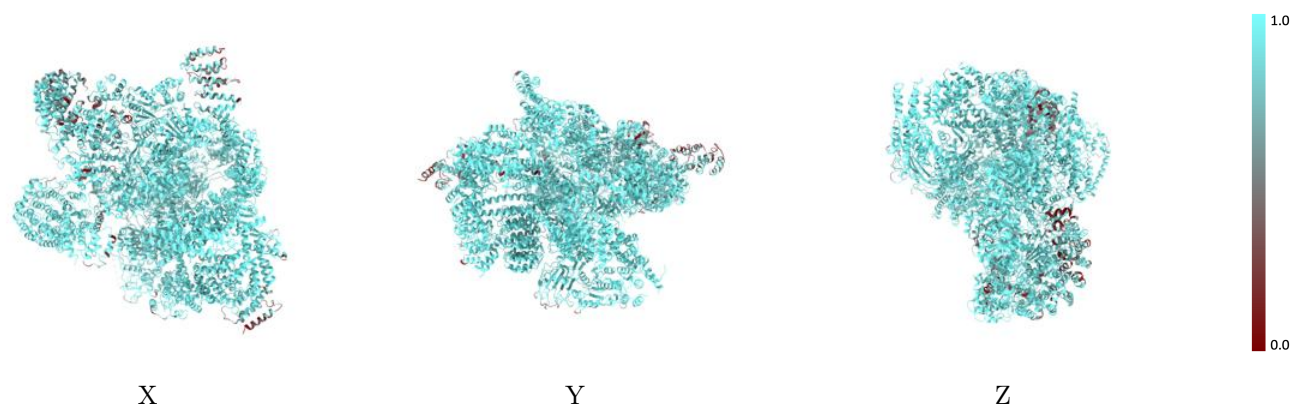
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



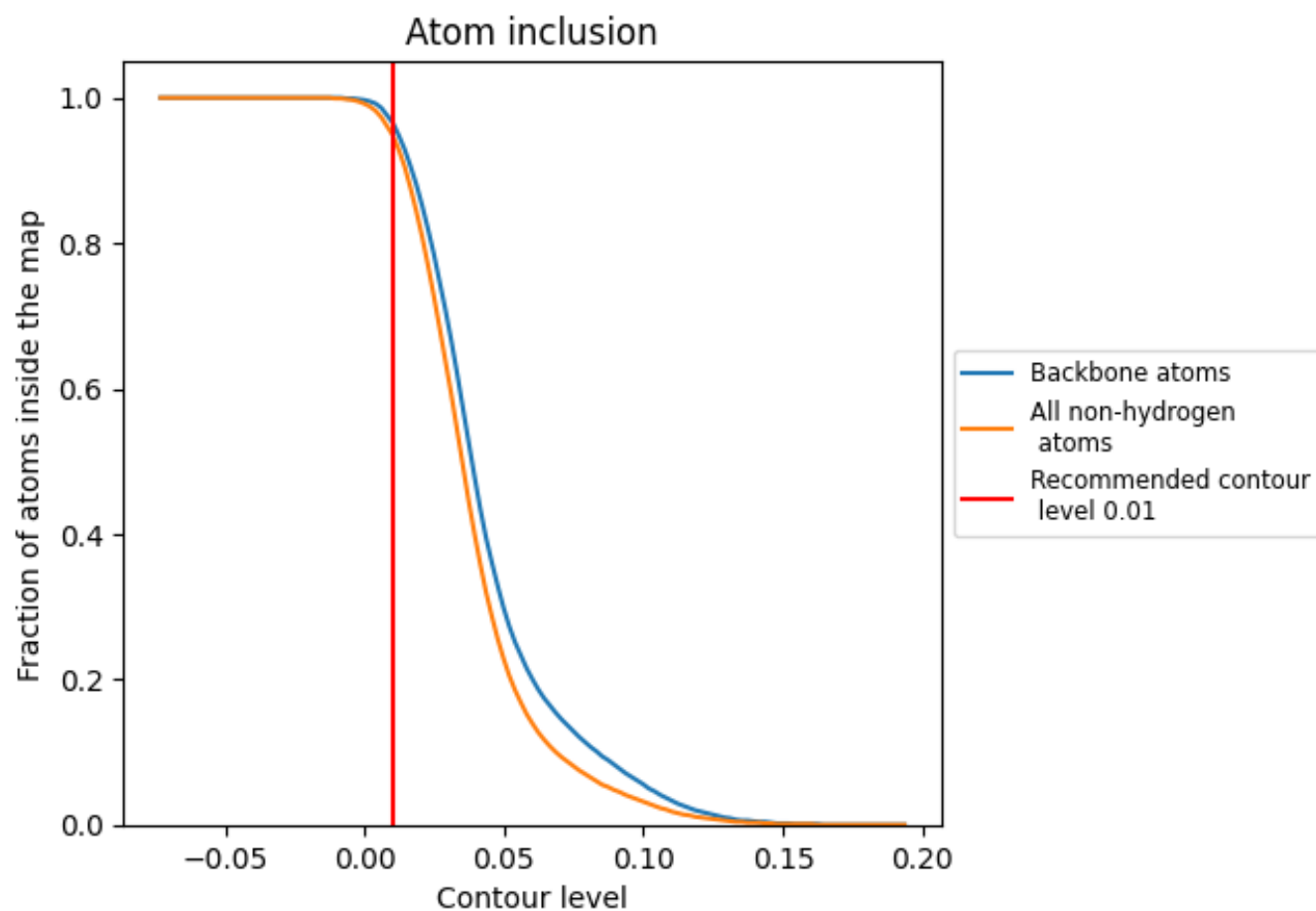
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 95% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.1350
A	 0.8990	 0.1360
B	 0.9200	 0.1210
C	 0.9750	 0.2160
D	 0.9800	 0.2440
E	 0.9790	 0.2510
F	 0.9870	 0.2350
U	 0.9880	 0.0970
V	 0.9840	 0.0990
W	 0.8550	 0.1460
X	 0.9860	 0.1220
Y	 0.9880	 0.0810
Z	 1.0000	 0.1790
a	 0.9930	 0.1500
b	 0.9850	 0.1260
c	 0.9810	 0.1590
d	 0.8590	 0.0870
e	 1.0000	 0.0690
f	 0.9740	 0.0510
g	 0.9380	 0.0770
z	 0.7650	 0.0990

