



Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 11:26 am GMT

PDB ID : 8Q91
EMDB ID : EMD-18267
Title : Structure of the human 20S U5 snRNP core
Authors : Schneider, S.; Galej, W.P.
Deposited on : 2023-08-19
Resolution : 3.10 Å(reported)

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

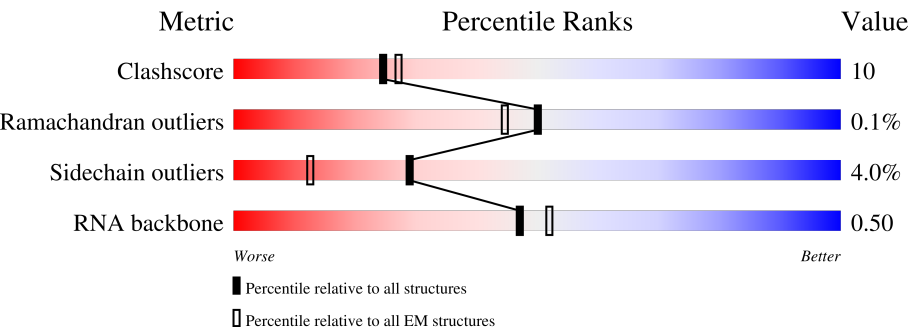
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	F	341	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>33%7%59%</div></div>
2	A	2335	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>50%18%30%</div></div>
3	5	117	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>28%45%13%11%</div></div>
4	E	941	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>6%94%</div></div>
5	D	820	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>5%93%</div></div>
6	C	972	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>69%17%13%</div></div>
7	B	2136	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>99%</div></div>

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Mol	Chain	Length	Quality of chain
8	m	86	<div><div></div><div>10%</div><div>85%</div><div>15%</div></div>
9	n	76	<div><div></div><div>22%</div><div>97%</div><div>.</div></div>
10	i	119	<div><div></div><div>68%</div><div>32%</div></div>
11	j	118	<div><div></div><div>16%</div><div>83%</div><div>17%</div></div>
12	k	126	<div><div></div><div>67%</div><div>33%</div></div>
13	h	240	<div><div></div><div>30%</div><div>70%</div></div>
14	l	92	<div><div></div><div>5%</div><div>83%</div><div>.</div><div>16%</div></div>

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 26706 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 CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	140	Total	C	N	O	S	0	0
			887	552	165	169	1		

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1627	Total	C	N	O	S	0	0
			13247	8535	2321	2333	58		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 4 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	60	Total	C	N	O	0	0
			300	180	60	60		

- Molecule 5 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	54	Total	C	N	O	0	0
			455	294	78	83		

- Molecule 6 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	847	Total	C	N	O	S	0	0
			6629	4238	1108	1250	33		

- Molecule 7 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	27	Total	C	N	O	S	0	0
			201	123	38	39	1		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	m	73	Total	C	N	O	0	0
			356	210	73	73		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	74	Total	C	N	O	0	0
			364	215	74	75		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	81	Total	C	N	O	0	0
			401	239	81	81		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	j	98	Total	C	N	O	0	0
			487	291	98	98		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	k	84	Total	C	N	O	0	0
			414	246	84	84		

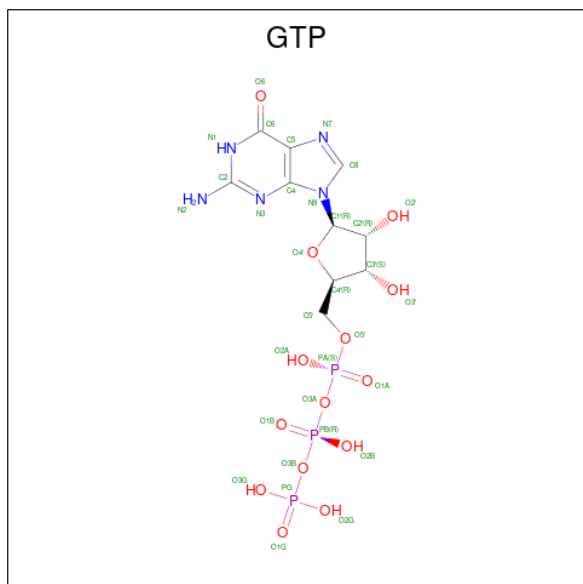
- Molecule 13 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1	77	Total	C	N	O	0	0
			381	227	77	77		

- Molecule 15 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).







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

- Molecule 6: 116 kDa U5 small nuclear ribonucleoprotein component



NET	ASP	THR	ASP	ASP	LEU	TYR	ASP	ASP	GLU	PHE	GLY	ASN	TYR	ILE	GLY	PRO	GLU	LEU	ASP	ASP	SER	ASP	ASP	GLU	ASP	ASP	ASP	ASP	GLU	GLY	ARG	GLU	THR	LYS	ASP	ASP	LEU	LEU	GLU	GLU	NET	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	VAL	VAL	GLY	GLY	ASP	ASP	HIS	HIS	ASP	ASP	ASP	ASP	PRO	PRO	GLY	GLY	NET	GLU	VAL	VAL	VAL	VAL	LEU	LEU	HIS
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GLU	ASP	LYS	TYR	TYR	PRO	THR	ALA	GLU	VAL	VAL	TYR	GLY	PRO	GLU	VAL	GLU	THR	ILE	VAL	GLN	GLU	GLU	ASP	THR	GLN	PRO	LEU	THR	GLU	PRO	ILE	ILE	LYS	PRO	VAL	LYS	THR	LYS	PHE	THR	LEU	M105	E106	Q107	T108	L109	P110		M116		L122		T133		H137	L138
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H140	G141	K142	T143	C144	F145	V146	D147	C148	L149	I150	R158	K159	R160	Y161	D162	G163	D164	L165	C166	Y167	T168	D169	I170	T173	E174	R177	G178	I181	K182	V186	D192	K196	S212	D213	E214	V215	T216	L219	D230	E233	M236	T239	L242
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R262	E266	E296	N297	L298	L299	P302	L303	L304	G305	N306	V307	G308	S312	Q313	L320	F323	N335	E338	R342	L343	W344	K352	T357	K358	K359	T362	S363	V370	L373	L374	S391	R394	L399	G400	I401	E406	E407	L418
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H433	H434	C434	V435	H436	H437	I438	K446	K447	P448	I449	G455	S459	M465	P473	T479	S483	F490	S498	E512	E520	C525	W531	V534	A535	R536	V537	H538	R543	K561	T562	N571	E572	E573	K589	M603	Y614	P615	S616	L617
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K620	V621	E622	V628	R645	I 651	D657	S670	C674	F675	A676	I685	T686	M687	L692	L696	A697	E701	K713	L714	G715	E716	Q719	T720	K721	Y722	D723	W724	L727	A728	A729	R730	S731	I732	W733	A734	F735	D738	I744	D747	P751	V756
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F770	F775	C780	D793	I808	V815	V816	Y817	S818	M822	E829	P830	V836	V846	I863	T870	A877	F881	L887	S897	V907	P925	H928	K941	S944	E945	D946	V947	K951	PHE	PHE	ASP	ASP	PAR	MET	LEU	LEU	GU
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LE	AI	LY	GI	AS	VA	VA	LE	AS	TY	PH	ME
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- Molecule 7: U5 small nuclear ribonucleoprotein 200 kDa helicase



MET	ALA	ASP	ASP	THR	ALA	ARG	SER	LEU	GLN	TYR	GLU	TYR	LYS	ALA	ALA	ASN	SER	ASN	LEU	VAL	LEU	GLN	ALA	ASP	ARG	SER	LEU	ILE	ASP	ARG	THR	ARG	ARG	ASP	GLU	P36	E39	V40	L41	S42	L47	E48	C49	T50	R51	M52	G53	D54	Q57	O62	MET	GLN	GLU	GLU	ARG
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ALA	LYS	ARG	ARG	LYS	ASP	ASP	ARG	HIS	ASP	ASP	LYS	LYS	LYS	GLY	THR	THR	LEU	LEU	SER	GLU	GLY	ILE	ASP	GLU	GLU	MET	VAL	GLY	ILE	ILE	THR	THR	LYS	PRO	LYS	THR	LYS	THR	GLU	GLU	VAL	LEU	LEU	SER	PHE	ILE	ILE	GLN	ALA	ALA	LEU	LEU	GLY	ASP	GLN	PRO
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ARG	ASP	ILE	LEU	CYS	GLY	ALA	ALA	ASP	GLU	VAL	LEU	ALA	VAL	LEU	LYS	GLU	GLY	LYS	LEU	ASP	ARG	LYS	GLU	ASP	LEU	LEU	LEU	GLY	GLN	THR	ASP	ASP	THR	ARG	TVR	HIS	VAL	VAL	VAL	ASN	ASN	LEU	GLY	LYS	ILE	THR	ASP	THR	TVR	GLY	GLY	ASP	LYS	ASP	GLU	ILE
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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	76918	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 ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.051	Depositor
Minimum map value	-0.392	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	526.6296, 526.6296, 526.6296	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0449, 1.0449, 1.0449	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTP

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	F	0.29	0/896	0.57	0/1224
2	A	0.27	0/13608	0.53	2/18483 (0.0%)
3	5	0.24	0/2444	0.89	6/3798 (0.2%)
4	E	0.22	0/298	0.35	0/414
5	D	0.31	0/464	0.56	0/620
6	C	0.28	0/6777	0.51	2/9214 (0.0%)
7	B	0.31	0/202	0.66	0/268
8	m	0.29	0/355	0.57	0/490
9	n	0.24	0/363	0.50	0/501
10	i	0.34	0/400	0.51	0/556
11	j	0.24	0/485	0.51	0/674
12	k	0.27	0/413	0.49	0/573
13	h	0.26	0/358	0.51	0/495
14	l	0.25	0/380	0.62	1/528 (0.2%)
All	All	0.27	0/27443	0.57	11/37838 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	57	G	O4'-C1'-N9	7.73	114.38	108.20
3	5	23	C	C2-N1-C1'	7.18	126.70	118.80
3	5	23	C	N1-C2-O2	6.71	122.92	118.90
2	A	1692	MET	CA-CB-CG	6.02	123.54	113.30
3	5	23	C	N3-C2-O2	-6.01	117.69	121.90
2	A	1070	ASP	CB-CG-OD1	5.91	123.61	118.30
6	C	144	CYS	N-CA-CB	5.48	120.47	110.60
14	l	15	VAL	C-N-CA	5.42	135.25	121.70
6	C	793	ASP	CB-CG-OD1	5.38	123.14	118.30
3	5	58	U	O5'-P-OP2	-5.11	101.11	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	5	23	C	C6-N1-C2	-5.08	118.27	120.30

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	F	887	0	714	27	0
2	A	13247	0	12877	324	0
3	5	2192	0	1111	43	0
4	E	300	0	132	0	0
5	D	455	0	450	13	0
6	C	6629	0	6607	113	0
7	B	201	0	214	10	0
8	m	356	0	156	0	0
9	n	364	0	160	0	0
10	i	401	0	165	0	0
11	j	487	0	199	0	0
12	k	414	0	185	0	0
13	h	360	0	149	0	0
14	l	381	0	159	0	0
15	C	32	0	12	1	0
All	All	26706	0	23290	496	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 10.

All (496) 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)
2:A:885:LEU:HD21	2:A:922:LEU:HD21	1.53	0.89
2:A:813:THR:HG21	2:A:996:LEU:HD11	1.59	0.84
2:A:1237:MET:HG2	2:A:1284:LEU:HD13	1.66	0.78
2:A:975:VAL:HG11	2:A:1153:VAL:HG21	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:829:GLU:HG3	6:C:907:VAL:HG22	1.66	0.77
2:A:1366:PRO:HD2	2:A:1474:MET:HE3	1.67	0.76
2:A:1314:VAL:HG13	2:A:1478:LEU:HD23	1.67	0.76
2:A:1368:LEU:HD11	2:A:1467:LEU:HD23	1.67	0.76
2:A:200:ASP:OD1	2:A:240:ARG:NH2	2.19	0.75
5:D:243:LYS:HG3	5:D:244:SER:H	1.52	0.75
2:A:1032:ARG:HD3	2:A:1445:TYR:HE2	1.50	0.74
2:A:1622:MET:O	2:A:1687:TYR:OH	2.05	0.74
2:A:1171:GLU:OE2	2:A:1171:GLU:N	2.18	0.73
2:A:1622:MET:SD	2:A:1622:MET:N	2.62	0.73
2:A:292:ASP:OD2	2:A:1130:ASN:ND2	2.22	0.72
2:A:370:PRO:HG2	6:C:304:LEU:HD21	1.69	0.72
6:C:406:GLU:OE1	6:C:406:GLU:N	2.22	0.72
2:A:530:LEU:HG	2:A:535:ARG:HG3	1.71	0.72
2:A:1701:VAL:HA	2:A:1716:GLY:HA3	1.70	0.72
2:A:585:VAL:HG11	2:A:637:TRP:CZ2	2.25	0.72
2:A:1573:LEU:HA	2:A:1576:ILE:HG22	1.72	0.72
5:D:243:LYS:HG3	5:D:244:SER:N	2.05	0.71
2:A:329:LEU:HB3	6:C:177:ARG:HD3	1.72	0.71
1:F:164:LEU:O	1:F:198:ARG:NH2	2.23	0.70
2:A:974:ASN:OD1	2:A:1100:ARG:NH1	2.25	0.70
3:5:19:A:N3	3:5:21:A:N6	2.40	0.69
2:A:1543:ASN:O	2:A:1563:HIS:ND1	2.25	0.69
2:A:1576:ILE:HG23	2:A:1577:PHE:HD1	1.57	0.69
2:A:1626:CYS:SG	2:A:1627:ALA:N	2.66	0.69
2:A:1289:VAL:HG21	7:B:42:SER:HA	1.72	0.69
2:A:776:LEU:HA	2:A:779:LEU:HD12	1.74	0.68
6:C:147:ASP:HA	6:C:150:ILE:HB	1.75	0.68
2:A:1544:ARG:HG3	2:A:1672:ASP:OD2	1.93	0.68
6:C:846:VAL:HG22	6:C:887:LEU:HD11	1.75	0.68
2:A:549:GLU:HB3	2:A:591:MET:HG2	1.75	0.68
2:A:1493:THR:HA	2:A:1747:ILE:HD11	1.75	0.68
2:A:1660:TYR:OH	2:A:1717:ASN:O	2.09	0.67
1:F:117:ASP:OD2	2:A:541:GLY:N	2.27	0.66
2:A:877:ALA:O	2:A:881:ILE:HG12	1.96	0.65
2:A:1032:ARG:HD3	2:A:1445:TYR:CE2	2.32	0.65
5:D:275:GLU:OE1	5:D:275:GLU:N	2.30	0.65
2:A:1069:ASN:OD1	2:A:1075:GLN:NE2	2.28	0.65
2:A:171:ASP:OD2	2:A:523:ASN:ND2	2.30	0.64
6:C:159:LYS:NZ	6:C:160:ARG:O	2.29	0.64
2:A:341:LYS:O	5:D:301:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1625:SER:OG	2:A:1663:ASP:OD2	2.14	0.64
2:A:1631:LEU:HD12	2:A:1660:TYR:HB3	1.80	0.64
6:C:436:GLN:OE1	6:C:437:HIS:NE2	2.30	0.64
2:A:855:ARG:HH12	2:A:857:ASN:HB3	1.62	0.64
2:A:992:LEU:HD13	2:A:996:LEU:HD23	1.80	0.64
6:C:137:HIS:O	6:C:142:LYS:NZ	2.31	0.64
2:A:881:ILE:HD12	2:A:918:THR:HA	1.80	0.63
2:A:1474:MET:HE2	2:A:1474:MET:HA	1.78	0.63
2:A:1411:SER:HA	2:A:1414:ARG:HD3	1.80	0.63
1:F:102:ASP:OD1	1:F:106:ASN:N	2.28	0.63
1:F:105:GLY:HA3	2:A:1532:ARG:HD2	1.79	0.63
2:A:1737:ASN:HB3	2:A:1740:LEU:HB2	1.80	0.63
1:F:168:ARG:H	1:F:222:ARG:HD3	1.64	0.62
2:A:143:GLN:NE2	2:A:207:PHE:O	2.27	0.62
2:A:1544:ARG:HG2	2:A:1546:ASN:H	1.64	0.62
2:A:813:THR:HG21	2:A:996:LEU:CD1	2.30	0.62
6:C:215:VAL:HG11	6:C:242:LEU:HD22	1.82	0.62
1:F:120:LEU:HD22	2:A:539:ARG:HD2	1.82	0.62
2:A:1712:HIS:HB3	2:A:1734:MET:HE1	1.81	0.61
6:C:143:THR:O	6:C:144:CYS:C	2.39	0.61
2:A:474:ARG:NH2	3:5:14:U:OP2	2.33	0.61
2:A:1555:LEU:HD11	2:A:1574:ILE:HD11	1.82	0.61
6:C:685:ILE:HD11	6:C:808:ILE:HD11	1.83	0.61
2:A:856:LEU:O	2:A:861:ARG:NH2	2.34	0.60
6:C:144:CYS:HB3	6:C:312:SER:HB2	1.83	0.60
6:C:335:ASN:ND2	6:C:338:GLU:OE1	2.34	0.60
2:A:1687:TYR:O	2:A:1693:SER:OG	2.20	0.60
6:C:697:ALA:O	6:C:701:GLU:HG2	2.01	0.60
2:A:1342:TRP:CZ2	2:A:1353:PHE:HB2	2.36	0.60
2:A:309:ARG:NH1	5:D:285:ASP:OD2	2.29	0.59
2:A:1434:LYS:O	2:A:1439:ARG:NH2	2.28	0.59
6:C:473:PRO:HB2	6:C:571:ASN:HD21	1.67	0.59
2:A:1342:TRP:CE2	2:A:1353:PHE:HB2	2.38	0.59
2:A:1427:ARG:HD3	2:A:1428:HIS:H	1.68	0.59
6:C:512:GLU:OE1	6:C:562:THR:OG1	2.21	0.59
2:A:772:CYS:O	2:A:776:LEU:HG	2.03	0.58
2:A:881:ILE:HG23	2:A:918:THR:HG23	1.85	0.58
6:C:407:GLU:OE1	6:C:418:LEU:HD21	2.03	0.58
6:C:170:ILE:HG22	6:C:536:ARG:HE	1.68	0.58
6:C:473:PRO:O	6:C:498:SER:OG	2.20	0.58
2:A:608:LEU:HD13	2:A:632:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:585:VAL:HG11	2:A:637:TRP:HZ2	1.69	0.58
2:A:1082:ALA:O	2:A:1083:HIS:ND1	2.37	0.58
2:A:304:ILE:HG21	5:D:250:ILE:HD13	1.86	0.58
6:C:140:HIS:NE2	6:C:233:GLU:OE1	2.36	0.58
2:A:1536:LEU:O	2:A:1539:SER:OG	2.18	0.57
6:C:144:CYS:O	6:C:148:CYS:N	2.29	0.57
2:A:507:LEU:HD11	2:A:652:LEU:HD11	1.86	0.57
2:A:1703:ILE:HG12	2:A:1714:ALA:HB2	1.86	0.57
5:D:285:ASP:OD1	5:D:287:ASN:N	2.37	0.57
6:C:169:ASP:HB3	6:C:174:GLU:HB3	1.87	0.57
2:A:1444:GLN:HG3	2:A:1445:TYR:HD1	1.69	0.57
3:5:67:A:H2'	3:5:68:C:C6	2.39	0.57
5:D:282:THR:HG22	5:D:283:SER:H	1.69	0.57
2:A:252:ASP:OD1	2:A:252:ASP:N	2.38	0.57
2:A:147:MET:O	2:A:151:MET:HG3	2.04	0.57
2:A:1218:ASN:HB3	2:A:1221:THR:HG22	1.86	0.57
5:D:245:LYS:H	5:D:245:LYS:HD2	1.69	0.57
2:A:856:LEU:HD13	2:A:860:GLN:HB3	1.87	0.56
2:A:1676:ILE:HD13	2:A:1706:ASP:HB2	1.87	0.56
3:5:57:G:O2'	3:5:58:U:O5'	2.16	0.56
2:A:899:MET:HB2	2:A:906:VAL:HG13	1.86	0.56
2:A:1607:GLU:N	2:A:1632:PHE:O	2.37	0.56
2:A:1610:GLN:NE2	2:A:1612:GLU:OE1	2.37	0.56
2:A:1410:ASP:OD1	2:A:1410:ASP:N	2.34	0.56
3:5:17:U:H2'	3:5:18:C:C6	2.40	0.56
2:A:1474:MET:HA	2:A:1474:MET:CE	2.34	0.56
2:A:1090:ARG:NH1	2:A:1091:TYR:O	2.38	0.56
2:A:544:PHE:HA	2:A:651:TRP:CH2	2.41	0.56
3:5:111:A:H2'	3:5:112:A:C8	2.41	0.56
2:A:776:LEU:O	2:A:780:THR:HG23	2.06	0.55
2:A:1560:ILE:HG21	2:A:1573:LEU:HD13	1.88	0.55
2:A:1307:MET:CE	2:A:1307:MET:H	2.19	0.55
6:C:455:GLY:O	6:C:459:SER:OG	2.23	0.55
6:C:573:GLU:OE1	6:C:573:GLU:N	2.31	0.55
1:F:117:ASP:HB3	1:F:120:LEU:HB3	1.87	0.55
2:A:1076:ASP:OD1	2:A:1077:ILE:N	2.40	0.55
2:A:1597:PHE:HE1	2:A:1604:LEU:HD12	1.72	0.55
6:C:394:ARG:NH1	6:C:394:ARG:HB3	2.22	0.55
1:F:209:MET:CE	1:F:214:ASN:HB3	2.38	0.54
2:A:531:THR:O	2:A:535:ARG:N	2.40	0.54
2:A:827:PHE:HD2	2:A:1005:ILE:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1093:ASP:N	2:A:1093:ASP:OD1	2.40	0.54
2:A:1747:ILE:HD12	2:A:1748:ARG:N	2.23	0.54
6:C:479:THR:HA	6:C:562:THR:HG22	1.90	0.54
2:A:494:LEU:HD21	2:A:562:VAL:HG21	1.89	0.54
2:A:899:MET:HB2	2:A:906:VAL:CG1	2.38	0.54
2:A:1630:LEU:HD21	2:A:1696:PRO:HG3	1.90	0.54
6:C:159:LYS:HG3	6:C:164:ASP:HA	1.89	0.54
2:A:1579:ALA:O	2:A:1584:LYS:NZ	2.40	0.54
2:A:1311:PHE:HE1	2:A:1315:VAL:HG21	1.72	0.54
6:C:173:THR:O	6:C:177:ARG:HG2	2.08	0.54
2:A:996:LEU:HB3	2:A:1043:TYR:HE2	1.71	0.54
1:F:123:ILE:O	1:F:127:LYS:N	2.40	0.53
2:A:156:ARG:NH1	2:A:157:ASP:OD1	2.41	0.53
1:F:71:VAL:HG23	2:A:1575:GLN:HB2	1.90	0.53
2:A:1127:GLY:O	2:A:1170:TRP:NE1	2.34	0.53
3:5:47:A:O2'	3:5:48:A:O5'	2.26	0.53
2:A:939:TRP:NE1	2:A:1049:ASP:OD2	2.40	0.53
6:C:724:TRP:HZ3	6:C:732:ILE:HD11	1.73	0.53
2:A:1333:VAL:HG23	7:B:40:VAL:HG13	1.89	0.53
2:A:805:GLU:O	2:A:809:VAL:HG12	2.08	0.53
2:A:950:LEU:HD12	2:A:1379:PHE:CD1	2.43	0.53
2:A:1002:ASP:OD2	2:A:1004:ASN:ND2	2.42	0.53
1:F:90:PHE:CD1	2:A:1574:ILE:HG13	2.44	0.53
2:A:1334:LEU:HD13	2:A:1364:LEU:HD23	1.91	0.53
2:A:946:GLU:OE1	2:A:951:LEU:HD23	2.08	0.53
2:A:67:ARG:HD3	2:A:179:ALA:HB2	1.91	0.52
2:A:1586:HIS:NE2	2:A:1628:ASP:OD2	2.41	0.52
2:A:1031:ILE:HB	2:A:1034:LEU:HG	1.91	0.52
6:C:945:GLU:OE2	6:C:946:ASP:HB2	2.10	0.52
2:A:1313:PRO:HG2	2:A:1335:ILE:HD12	1.91	0.52
6:C:133:THR:HG21	6:C:219:LEU:HD23	1.92	0.52
2:A:1019:TYR:O	2:A:1021:ASP:N	2.42	0.52
2:A:1368:LEU:HD11	2:A:1467:LEU:CD2	2.37	0.52
2:A:940:ILE:HD11	2:A:1046:LEU:HB2	1.92	0.52
3:5:69:A:H2'	3:5:70:A:O4'	2.09	0.52
3:5:109:G:H2'	3:5:110:C:C6	2.44	0.52
6:C:177:ARG:HG3	6:C:177:ARG:HH11	1.73	0.52
2:A:1612:GLU:HG2	2:A:1627:ALA:HB3	1.90	0.52
2:A:1661:TRP:NE1	2:A:1697:SER:O	2.42	0.52
2:A:436:PRO:HG2	2:A:439:GLN:HG3	1.92	0.52
6:C:692:LEU:HD22	6:C:696:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:549:GLU:CB	2:A:591:MET:HG2	2.39	0.52
2:A:1094:ARG:HH22	2:A:1190:CYS:H	1.58	0.52
6:C:780:CYS:O	6:C:941:LYS:NZ	2.43	0.52
6:C:391:SER:O	6:C:391:SER:OG	2.25	0.51
2:A:425:PRO:HB2	2:A:428:LYS:HB2	1.92	0.51
2:A:1368:LEU:HG	2:A:1372:ILE:HD11	1.92	0.51
1:F:176:ARG:NE	2:A:59:GLU:HB3	2.26	0.51
2:A:1017:ILE:HD11	2:A:1026:ASN:HB2	1.92	0.51
2:A:1391:LEU:O	2:A:1394:GLN:HG3	2.11	0.51
2:A:1607:GLU:HB2	2:A:1634:SER:HB3	1.93	0.51
2:A:379:GLU:OE1	2:A:379:GLU:N	2.42	0.51
2:A:923:ASP:OD2	2:A:1439:ARG:NH1	2.32	0.51
2:A:1641:ARG:HG2	2:A:1642:PRO:HD2	1.92	0.51
7:B:62:GLN:N	7:B:62:GLN:OE1	2.43	0.51
6:C:147:ASP:C	6:C:149:LEU:H	2.14	0.51
2:A:946:GLU:HG3	2:A:950:LEU:HD22	1.93	0.51
2:A:1061:MET:HE1	2:A:1088:PHE:HB3	1.93	0.51
2:A:1188:ASN:HD21	2:A:1233:ASP:CG	2.15	0.51
2:A:1447:VAL:HG12	2:A:1449:LYS:H	1.76	0.51
2:A:134:TRP:HZ2	3:5:58:U:OP2	1.94	0.50
2:A:919:ASP:OD2	2:A:1012:LYS:NZ	2.41	0.50
2:A:1678:ARG:HH12	2:A:1681:ARG:HD3	1.77	0.50
2:A:837:LYS:O	2:A:841:LEU:HG	2.11	0.50
2:A:1465:TRP:HD1	2:A:1467:LEU:HD11	1.76	0.50
6:C:147:ASP:C	6:C:149:LEU:N	2.62	0.50
2:A:1504:GLU:N	2:A:1504:GLU:OE1	2.45	0.50
2:A:1559:GLY:HA2	2:A:1622:MET:HE1	1.94	0.50
2:A:420:ARG:NH1	3:5:57:G:H5"	2.27	0.50
2:A:1257:THR:HG21	2:A:1320:LYS:HE3	1.93	0.50
2:A:1322:LEU:HD12	2:A:1498:TRP:CZ2	2.45	0.50
2:A:1482:GLU:CD	2:A:1483:GLY:N	2.65	0.50
2:A:461:HIS:HD2	3:5:27:U:H3	1.59	0.50
2:A:1129:ASN:ND2	2:A:1173:SER:O	2.43	0.50
2:A:1193:GLU:HB3	2:A:1231:ARG:HB2	1.94	0.50
6:C:692:LEU:HD21	6:C:744:ILE:HD12	1.94	0.50
2:A:106:MET:HE2	2:A:578:LEU:HD13	1.93	0.50
2:A:1013:ASN:HA	2:A:1031:ILE:HG12	1.94	0.50
2:A:1283:GLU:N	2:A:1283:GLU:OE1	2.45	0.50
6:C:620:LYS:NZ	6:C:622:GLU:OE1	2.45	0.50
2:A:841:LEU:HD21	2:A:1429:THR:HG22	1.93	0.49
2:A:865:GLY:O	2:A:868:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:145:PHE:HA	6:C:148:CYS:HB2	1.93	0.49
2:A:318:TYR:O	6:C:645:ARG:NH1	2.45	0.49
2:A:815:HIS:HA	2:A:818:GLU:OE1	2.11	0.49
2:A:1641:ARG:HH21	2:A:1651:VAL:HG22	1.76	0.49
3:5:17:U:H3	3:5:60:G:H1	1.59	0.49
2:A:1392:LYS:O	2:A:1395:GLU:HG3	2.12	0.49
3:5:56:C:H2'	3:5:57:G:H5'	1.94	0.49
3:5:65:G:O6	3:5:66:A:N6	2.46	0.49
2:A:142:SER:HA	2:A:242:ALA:HB2	1.94	0.49
2:A:419:ARG:NH2	2:A:423:ASP:O	2.46	0.49
2:A:829:PRO:HD2	2:A:832:TYR:CD2	2.46	0.49
2:A:1576:ILE:HG23	2:A:1577:PHE:CD1	2.43	0.49
6:C:158:ARG:HH12	6:C:160:ARG:CG	2.26	0.49
2:A:779:LEU:HA	2:A:782:LEU:HD12	1.94	0.49
2:A:1728:GLN:O	2:A:1732:LYS:HG2	2.12	0.49
1:F:209:MET:HE1	1:F:214:ASN:HB3	1.94	0.49
2:A:530:LEU:HG	2:A:535:ARG:CG	2.42	0.49
3:5:36:C:O2	3:5:44:A:N6	2.46	0.49
2:A:1629:ILE:HB	2:A:1662:ILE:HB	1.94	0.49
2:A:1318:THR:HB	2:A:1324:GLY:HA3	1.95	0.49
6:C:561:LYS:NZ	6:C:615:PRO:O	2.43	0.49
2:A:1061:MET:CE	2:A:1088:PHE:HB3	2.43	0.48
2:A:778:ARG:O	2:A:782:LEU:HG	2.12	0.48
2:A:1560:ILE:HD13	2:A:1573:LEU:HD13	1.95	0.48
3:5:37:G:N7	3:5:38:C:O2'	2.44	0.48
6:C:148:CYS:SG	6:C:312:SER:HB2	2.53	0.48
2:A:469:LYS:NZ	3:5:59:G:N7	2.59	0.48
2:A:1300:LYS:HG2	2:A:1311:PHE:CD2	2.48	0.48
1:F:71:VAL:HG22	2:A:1574:ILE:HG22	1.94	0.48
2:A:1597:PHE:HZ	2:A:1719:PHE:HZ	1.59	0.48
6:C:362:THR:OG1	6:C:363:SER:N	2.47	0.48
1:F:174:ALA:HA	1:F:177:ARG:HG2	1.96	0.48
2:A:1125:ILE:HD13	2:A:1147:VAL:HG11	1.95	0.48
2:A:1393:ARG:O	2:A:1397:ILE:HG13	2.13	0.48
6:C:674:CYS:SG	6:C:818:SER:HB2	2.53	0.48
2:A:651:TRP:NE1	2:A:655:LEU:HD22	2.28	0.48
2:A:867:ILE:HD12	2:A:868:GLU:N	2.29	0.48
6:C:177:ARG:HG3	6:C:177:ARG:NH1	2.28	0.48
6:C:720:THR:HG23	6:C:721:LYS:HD3	1.96	0.48
2:A:976:MET:HG2	2:A:1187:PHE:HB3	1.96	0.48
2:A:1368:LEU:HD12	2:A:1368:LEU:HA	1.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:603:MET:HB2	6:C:651:ILE:HD11	1.95	0.48
2:A:944:ASP:OD2	2:A:1435:GLY:N	2.40	0.48
2:A:1672:ASP:OD1	2:A:1673:SER:HB3	2.14	0.48
3:5:12:U:H3	3:5:65:G:H1	1.60	0.48
6:C:357:THR:OG1	6:C:359:LYS:O	2.32	0.48
2:A:136:ILE:HG22	2:A:138:PRO:HD2	1.96	0.47
2:A:1013:ASN:O	2:A:1026:ASN:ND2	2.39	0.47
6:C:696:LEU:HD13	6:C:722:TYR:CE2	2.49	0.47
2:A:979:SER:OG	2:A:980:ARG:N	2.47	0.47
2:A:1090:ARG:HG2	2:A:1091:TYR:O	2.14	0.47
2:A:1621:LYS:HD3	2:A:1624:SER:OG	2.14	0.47
6:C:212:SER:O	6:C:216:THR:HG23	2.13	0.47
2:A:274:PRO:HA	5:D:282:THR:HG22	1.96	0.47
3:5:63:A:H2'	3:5:64:G:H8	1.79	0.47
6:C:483:SER:HB2	6:C:490:PHE:CE2	2.49	0.47
2:A:288:LEU:O	2:A:1136:ARG:NH2	2.48	0.47
6:C:110:PRO:HD2	6:C:537:TYR:CE2	2.50	0.47
6:C:236:MET:O	6:C:239:THR:OG1	2.29	0.47
2:A:1137:ASP:OD1	2:A:1137:ASP:N	2.48	0.47
2:A:1342:TRP:CG	2:A:1482:GLU:OE1	2.68	0.47
2:A:1544:ARG:HH21	2:A:1671:TYR:HB3	1.79	0.47
2:A:1625:SER:OG	2:A:1626:CYS:N	2.47	0.47
6:C:146:VAL:CG1	6:C:186:VAL:HG21	2.45	0.47
6:C:213:ASP:OD1	6:C:213:ASP:N	2.47	0.47
6:C:320:LEU:HD21	6:C:344:TRP:HB2	1.97	0.47
6:C:534:VAL:HG12	6:C:535:ALA:H	1.79	0.47
2:A:913:PRO:HA	2:A:916:LYS:HB2	1.96	0.47
2:A:1606:ILE:HG12	2:A:1637:TRP:HZ2	1.80	0.47
6:C:449:ILE:HD12	6:C:465:MET:HE3	1.97	0.47
6:C:670:SER:HB2	6:C:822:MET:HB2	1.97	0.47
2:A:1209:HIS:O	7:B:51:ARG:NH1	2.48	0.47
2:A:1433:ASP:HB3	2:A:1460:HIS:HE1	1.79	0.47
2:A:344:ASP:HB3	2:A:346:ASP:OD1	2.14	0.47
2:A:488:ASP:OD1	2:A:489:TRP:N	2.48	0.47
2:A:1653:ASP:HB3	2:A:1655:THR:HG22	1.97	0.47
6:C:727:LEU:O	6:C:731:SER:OG	2.20	0.47
2:A:260:LEU:HD21	2:A:454:TYR:CZ	2.50	0.46
2:A:997:LEU:O	2:A:1001:VAL:HG12	2.14	0.46
6:C:146:VAL:HG11	6:C:186:VAL:HG21	1.96	0.46
2:A:1474:MET:HE2	2:A:1474:MET:CA	2.45	0.46
6:C:167:TYR:HA	6:C:536:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:687:MET:HE1	6:C:816:VAL:HG22	1.98	0.46
6:C:830:PRO:HG2	6:C:877:ALA:HB3	1.97	0.46
2:A:1103:ALA:O	2:A:1107:ARG:HG3	2.14	0.46
2:A:1559:GLY:HA2	2:A:1622:MET:CE	2.44	0.46
2:A:1660:TYR:OH	2:A:1701:VAL:HB	2.15	0.46
2:A:1066:GLN:OE1	2:A:1066:GLN:N	2.48	0.46
2:A:511:LYS:HB2	2:A:513:LEU:CD2	2.45	0.46
1:F:116:ARG:CZ	2:A:542:ASN:HD21	2.28	0.46
2:A:908:VAL:HG11	2:A:1448:LEU:CD2	2.46	0.46
2:A:1330:MET:HE2	2:A:1330:MET:HA	1.98	0.46
2:A:1426:ASP:OD2	2:A:1459:ARG:NH1	2.46	0.46
2:A:1615:HIS:ND1	2:A:1617:ARG:HG3	2.30	0.46
3:5:12:U:H2'	3:5:13:C:C6	2.51	0.46
2:A:164:MET:HG2	2:A:569:VAL:HG11	1.98	0.46
2:A:1560:ILE:HG12	2:A:1668:TRP:CD1	2.51	0.46
2:A:1581:LEU:HD12	2:A:1746:ARG:HH11	1.81	0.46
3:5:49:A:H2'	3:5:50:G:H8	1.81	0.46
2:A:214:ARG:HG3	2:A:225:TYR:CD1	2.51	0.46
2:A:828:PRO:HG3	2:A:925:TYR:CE2	2.51	0.46
2:A:1179:SER:O	2:A:1201:ARG:NH1	2.38	0.46
6:C:144:CYS:O	6:C:145:PHE:C	2.54	0.46
2:A:864:LEU:O	2:A:867:ILE:HD12	2.16	0.45
2:A:896:ILE:HD12	2:A:896:ILE:O	2.16	0.45
2:A:1064:PRO:HB2	2:A:1066:GLN:OE1	2.16	0.45
2:A:1202:THR:O	2:A:1202:THR:HG22	2.16	0.45
3:5:66:A:HO2'	3:5:67:A:H8	1.62	0.45
1:F:178:LEU:HD21	1:F:198:ARG:HB3	1.98	0.45
2:A:993:LEU:O	2:A:997:LEU:HG	2.16	0.45
2:A:1365:ILE:HG13	2:A:1474:MET:HE1	1.99	0.45
2:A:1537:TRP:HD1	2:A:1538:TRP:NE1	2.15	0.45
2:A:1559:GLY:HA3	2:A:1582:TRP:CH2	2.51	0.45
3:5:63:A:H2'	3:5:64:G:C8	2.52	0.45
3:5:96:A:O2'	3:5:97:G:OP1	2.29	0.45
1:F:169:GLU:OE2	1:F:177:ARG:HD3	2.17	0.45
3:5:16:U:H2'	3:5:17:U:C6	2.52	0.45
2:A:948:PRO:O	2:A:951:LEU:HB2	2.17	0.45
2:A:1600:GLU:HG2	2:A:1725:LEU:HD13	1.98	0.45
6:C:139:HIS:HE1	6:C:178:GLY:O	2.00	0.45
2:A:1374:PRO:HG3	7:B:52:MET:HB3	1.99	0.45
2:A:1567:PRO:O	2:A:1571:ILE:HG22	2.18	0.45
2:A:1644:LEU:HD11	2:A:1678:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:148:CYS:SG	6:C:312:SER:O	2.75	0.45
1:F:102:ASP:HB3	1:F:108:PHE:CE2	2.52	0.44
2:A:395:THR:HG22	2:A:396:ASP:H	1.81	0.44
3:5:23:C:H5''	3:5:24:G:H2'	1.98	0.44
2:A:809:VAL:O	2:A:813:THR:HG22	2.16	0.44
2:A:1624:SER:CB	2:A:1692:MET:HG3	2.47	0.44
1:F:171:VAL:HG23	1:F:202:LEU:HD11	1.99	0.44
2:A:336:ASN:O	6:C:262:ARG:NH2	2.50	0.44
2:A:598:LEU:HD12	2:A:598:LEU:HA	1.75	0.44
2:A:1482:GLU:OE1	2:A:1482:GLU:C	2.56	0.44
6:C:192:ASP:N	6:C:196:LYS:O	2.49	0.44
7:B:41:LEU:HD23	7:B:41:LEU:HA	1.76	0.44
2:A:1365:ILE:HG13	2:A:1474:MET:CE	2.47	0.44
6:C:534:VAL:HG12	6:C:535:ALA:N	2.33	0.44
2:A:835:ASP:OD1	2:A:836:THR:N	2.51	0.44
2:A:1076:ASP:OD1	2:A:1078:ALA:N	2.30	0.44
2:A:1589:ILE:HA	2:A:1733:ILE:HD11	1.99	0.44
2:A:1552:GLN:HG2	2:A:1563:HIS:CD2	2.52	0.44
6:C:614:TYR:HB2	6:C:617:LEU:HB2	1.98	0.44
6:C:230:ASP:HB3	6:C:233:GLU:HB2	1.99	0.44
6:C:733:TRP:NE1	6:C:747:ASP:OD2	2.51	0.44
2:A:1276:GLU:OE1	2:A:1375:TRP:N	2.50	0.44
2:A:1585:ILE:HD13	2:A:1739:ALA:HB1	2.00	0.44
3:5:34:U:H2'	3:5:35:U:C6	2.53	0.44
2:A:329:LEU:HB3	6:C:177:ARG:CD	2.43	0.43
2:A:962:LEU:HB2	2:A:965:VAL:HB	2.00	0.43
3:5:110:C:H2'	3:5:111:A:H8	1.83	0.43
5:D:254:TYR:OH	6:C:657:ASP:OD2	2.34	0.43
6:C:713:LYS:O	6:C:716:GLU:HG2	2.18	0.43
6:C:724:TRP:CZ3	6:C:732:ILE:HD11	2.51	0.43
2:A:260:LEU:HD21	2:A:454:TYR:CE2	2.53	0.43
2:A:922:LEU:HD13	2:A:922:LEU:HA	1.86	0.43
2:A:934:ARG:HB3	2:A:934:ARG:CZ	2.49	0.43
2:A:1049:ASP:OD1	2:A:1090:ARG:HD3	2.17	0.43
2:A:1469:ASN:HB2	7:B:57:GLN:HG2	2.01	0.43
6:C:715:GLY:HA2	6:C:729:ALA:HB1	1.99	0.43
2:A:1346:THR:OG1	2:A:1348:VAL:HG12	2.18	0.43
6:C:158:ARG:HD3	6:C:158:ARG:O	2.19	0.43
1:F:102:ASP:OD1	1:F:105:GLY:N	2.52	0.43
2:A:428:LYS:HA	2:A:431:TYR:CE2	2.54	0.43
2:A:1382:SER:HA	2:A:1415:GLY:HA2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1427:ARG:NH1	2:A:1428:HIS:HB2	2.34	0.43
2:A:1730:MET:O	2:A:1733:ILE:HG22	2.18	0.43
3:5:8:G:C2'	3:5:9:G:H5'	2.49	0.43
3:5:113:G:H2'	3:5:114:G:H8	1.83	0.43
2:A:996:LEU:HB3	2:A:1043:TYR:CE2	2.52	0.43
2:A:1639:VAL:HG11	2:A:1699:THR:HG21	2.00	0.43
3:5:17:U:H2'	3:5:18:C:H6	1.83	0.43
6:C:109:LEU:CD2	6:C:116:MET:HG3	2.48	0.43
2:A:1448:LEU:HD23	2:A:1448:LEU:HA	1.78	0.43
2:A:1559:GLY:HA3	2:A:1582:TRP:CZ2	2.54	0.43
3:5:9:G:H8	3:5:9:G:OP2	2.01	0.43
3:5:94:U:HO2'	3:5:95:G:P	2.41	0.43
6:C:181:ILE:HG22	6:C:182:LYS:HG3	2.01	0.43
6:C:818:SER:O	6:C:822:MET:HG2	2.19	0.43
1:F:164:LEU:HB3	1:F:202:LEU:HD23	2.00	0.43
2:A:1418:ARG:O	2:A:1421:THR:HG22	2.19	0.43
2:A:196:ASP:HB3	2:A:199:GLU:HG2	2.01	0.42
2:A:422:LEU:H	2:A:422:LEU:HD23	1.82	0.42
2:A:1308:PRO:HB3	2:A:1548:TYR:CE1	2.54	0.42
1:F:164:LEU:HD23	1:F:202:LEU:CA	2.49	0.42
1:F:176:ARG:HE	2:A:59:GLU:HB3	1.83	0.42
2:A:804:GLU:HA	2:A:807:VAL:HG22	2.00	0.42
2:A:1056:HIS:O	2:A:1060:GLU:HG3	2.20	0.42
2:A:638:LEU:HD23	2:A:638:LEU:HA	1.90	0.42
2:A:1010:THR:HA	2:A:1013:ASN:OD1	2.19	0.42
2:A:1180:LYS:O	2:A:1201:ARG:NH2	2.52	0.42
2:A:1322:LEU:HD23	2:A:1484:ILE:HD13	2.01	0.42
2:A:1531:ASN:OD1	2:A:1531:ASN:N	2.52	0.42
5:D:273:VAL:HG23	5:D:273:VAL:O	2.19	0.42
2:A:1615:HIS:HB3	2:A:1617:ARG:NH1	2.34	0.42
6:C:719:GLN:HG2	6:C:724:TRP:O	2.19	0.42
1:F:117:ASP:OD2	2:A:540:PHE:N	2.53	0.42
2:A:876:GLU:OE1	2:A:880:ARG:NH1	2.52	0.42
3:5:60:G:H2'	3:5:61:A:C8	2.54	0.42
2:A:171:ASP:O	2:A:519:ASP:HB2	2.19	0.42
2:A:507:LEU:HD11	2:A:652:LEU:CD1	2.47	0.42
2:A:1310:ARG:NH2	2:A:1336:PRO:HG2	2.34	0.42
3:5:112:A:H2'	3:5:113:G:C8	2.54	0.42
2:A:164:MET:HB3	2:A:164:MET:HE3	1.81	0.42
2:A:934:ARG:HB3	2:A:934:ARG:NH1	2.35	0.42
2:A:1593:LEU:HD12	2:A:1593:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:62:PRO:HA	2:A:63:PRO:HD3	1.97	0.42
2:A:719:CYS:O	2:A:723:ASN:N	2.53	0.42
2:A:810:TYR:O	2:A:814:VAL:HG13	2.20	0.42
2:A:1017:ILE:HD11	2:A:1026:ASN:CB	2.49	0.42
6:C:446:LYS:HB3	6:C:447:PRO:HD3	2.00	0.42
2:A:406:TRP:CZ2	6:C:266:GLU:HG2	2.55	0.42
2:A:462:ARG:NH2	3:5:51:A:OP2	2.53	0.42
3:5:76:A:H2'	3:5:77:G:C8	2.55	0.42
6:C:186:VAL:HG22	6:C:535:ALA:HB2	2.01	0.42
6:C:254:THR:HB	6:C:433:MET:SD	2.60	0.42
2:A:1022:MET:SD	2:A:1023:ASN:N	2.93	0.41
3:5:51:A:H2'	3:5:52:U:C6	2.55	0.41
6:C:738:ASP:OD1	6:C:775:ARG:NH2	2.47	0.41
6:C:836:VAL:HG22	6:C:897:SER:HB3	2.02	0.41
1:F:160:GLY:O	1:F:164:LEU:HB2	2.20	0.41
2:A:320:TYR:OH	6:C:881:PHE:HB3	2.20	0.41
2:A:1639:VAL:HG21	2:A:1699:THR:HG21	2.02	0.41
5:D:285:ASP:O	5:D:291:LYS:HD3	2.20	0.41
6:C:676:ALA:HB3	6:C:815:VAL:HB	2.01	0.41
6:C:946:ASP:OD1	6:C:947:VAL:N	2.51	0.41
2:A:1394:GLN:HA	2:A:1397:ILE:HD11	2.02	0.41
3:5:7:U:C2	3:5:8:G:C8	3.07	0.41
2:A:881:ILE:O	2:A:885:LEU:HD23	2.20	0.41
6:C:687:MET:HE3	6:C:687:MET:HB3	1.81	0.41
2:A:1624:SER:HB3	2:A:1692:MET:HG3	2.01	0.41
6:C:166:CYS:O	6:C:168:THR:N	2.54	0.41
6:C:370:VAL:HA	6:C:374:LEU:HB2	2.02	0.41
2:A:261:LYS:HD2	2:A:328:HIS:HB3	2.03	0.41
2:A:1006:ALA:O	2:A:1010:THR:HG23	2.20	0.41
3:5:29:A:H2'	3:5:30:A:H8	1.86	0.41
6:C:531:TRP:HB3	6:C:538:HIS:HB3	2.01	0.41
6:C:863:ILE:HD11	6:C:870:THR:HG23	2.03	0.41
2:A:1031:ILE:O	2:A:1032:ARG:HG2	2.21	0.41
2:A:1320:LYS:HA	2:A:1324:GLY:O	2.20	0.41
2:A:1393:ARG:HA	2:A:1403:LEU:HD21	2.02	0.41
2:A:1394:GLN:O	2:A:1397:ILE:HD12	2.21	0.41
2:A:1585:ILE:O	2:A:1589:ILE:HG23	2.21	0.41
2:A:1680:ALA:HB2	2:A:1704:ALA:HB3	2.01	0.41
2:A:617:ASN:HB3	2:A:623:LYS:HD2	2.03	0.41
2:A:811:THR:HA	2:A:814:VAL:HG22	2.02	0.41
2:A:1013:ASN:HA	2:A:1031:ILE:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1465:TRP:CD1	2:A:1467:LEU:HD11	2.55	0.41
2:A:1498:TRP:HA	2:A:1501:LEU:HD23	2.02	0.41
6:C:434:CYS:O	6:C:438:ILE:HB	2.20	0.41
6:C:589:LYS:HG3	6:C:628:VAL:HG13	2.02	0.41
2:A:155:LYS:NZ	2:A:624:GLY:O	2.46	0.41
2:A:257:LEU:HD12	2:A:257:LEU:HA	1.93	0.41
2:A:1369:TYR:O	7:B:52:MET:HG3	2.20	0.41
2:A:1412:TRP:CE3	2:A:1412:TRP:HA	2.56	0.41
2:A:1589:ILE:HD12	2:A:1590:VAL:N	2.35	0.41
2:A:1723:LYS:HB3	2:A:1724:PRO:HD3	2.01	0.41
3:5:96:A:H2	3:5:97:G:C4	2.39	0.41
3:5:111:A:H2'	3:5:112:A:H8	1.84	0.41
6:C:299:ILE:O	6:C:306:ASN:ND2	2.54	0.41
6:C:308:CYS:HB2	6:C:433:MET:HE2	2.03	0.41
6:C:399:LEU:HB2	6:C:401:ILE:HD12	2.03	0.41
6:C:925:PRO:HD2	6:C:928:HIS:NE2	2.36	0.41
2:A:946:GLU:HG3	2:A:950:LEU:HB3	2.04	0.40
2:A:994:ASN:HA	2:A:1010:THR:HG21	2.03	0.40
2:A:1345:GLN:OE1	2:A:1711:LEU:HA	2.21	0.40
6:C:147:ASP:O	6:C:149:LEU:N	2.54	0.40
6:C:302:PRO:HG2	6:C:344:TRP:CD2	2.56	0.40
6:C:751:PRO:HA	6:C:756:LYS:HD3	2.02	0.40
2:A:1045:GLY:HA3	2:A:1090:ARG:CZ	2.51	0.40
2:A:1555:LEU:HD21	2:A:1574:ILE:HD12	2.03	0.40
2:A:1645:LEU:HB2	2:A:1714:ALA:H	1.86	0.40
6:C:145:PHE:CA	6:C:148:CYS:HB2	2.51	0.40
1:F:90:PHE:HD1	1:F:90:PHE:HA	1.76	0.40
2:A:441:VAL:HG23	2:A:444:ARG:HH21	1.85	0.40
2:A:820:ARG:NH1	2:A:1063:GLY:O	2.43	0.40
2:A:938:PRO:HB2	2:A:1071:PHE:HA	2.02	0.40
2:A:1016:VAL:HA	2:A:1025:THR:HA	2.03	0.40
7:B:48:GLU:HG2	7:B:49:GLY:N	2.37	0.40
7:B:51:ARG:N	7:B:54:ASP:OD2	2.45	0.40
2:A:295:GLU:HG3	2:A:1144:LYS:HG3	2.03	0.40
2:A:901:LEU:H	2:A:901:LEU:HD22	1.86	0.40
2:A:1276:GLU:CD	2:A:1375:TRP:H	2.24	0.40
2:A:1403:LEU:HD13	2:A:1403:LEU:HA	1.93	0.40
6:C:122:LEU:HD23	6:C:122:LEU:HA	1.93	0.40
6:C:343:LEU:HD13	6:C:373:ILE:HD11	2.04	0.40
2:A:449:LYS:HA	2:A:449:LYS:HD3	1.87	0.40
6:C:313:GLN:HB2	15:C:1001:GTP:C6	2.57	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	F	134/341 (39%)	123 (92%)	10 (8%)	1 (1%)	19	51
2	A	1615/2335 (69%)	1558 (96%)	56 (4%)	1 (0%)	48	79
4	E	56/941 (6%)	56 (100%)	0	0	100	100
5	D	50/820 (6%)	49 (98%)	1 (2%)	0	100	100
6	C	845/972 (87%)	813 (96%)	31 (4%)	1 (0%)	48	79
7	B	25/2136 (1%)	25 (100%)	0	0	100	100
8	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
9	n	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
10	i	79/119 (66%)	73 (92%)	6 (8%)	0	100	100
11	j	94/118 (80%)	84 (89%)	10 (11%)	0	100	100
12	k	82/126 (65%)	78 (95%)	4 (5%)	0	100	100
13	h	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
14	l	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
All	All	3267/8402 (39%)	3130 (96%)	134 (4%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1020	LYS
6	C	148	CYS
1	F	126	VAL

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	F	58/281 (21%)	55 (95%)	3 (5%)	19	48
2	A	1384/2108 (66%)	1325 (96%)	59 (4%)	25	55
5	D	48/721 (7%)	43 (90%)	5 (10%)	5	22
6	C	737/866 (85%)	717 (97%)	20 (3%)	40	67
7	B	22/1908 (1%)	19 (86%)	3 (14%)	3	13
All	All	2249/5884 (38%)	2159 (96%)	90 (4%)	29	58

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	90	PHE
1	F	117	ASP
1	F	198	ARG
2	A	60	ASP
2	A	87	VAL
2	A	106	MET
2	A	164	MET
2	A	171	ASP
2	A	181	ASN
2	A	217	ARG
2	A	251	ASP
2	A	294	ASN
2	A	346	ASP
2	A	353	ASP
2	A	395	THR
2	A	414	ARG
2	A	422	LEU
2	A	503	MET
2	A	510	ARG
2	A	513	LEU
2	A	593	ARG
2	A	600	ARG
2	A	604	MET

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Mol	Chain	Res	Type
2	A	652	LEU
2	A	773	LYS
2	A	832	TYR
2	A	869	GLN
2	A	871	TYR
2	A	981	PHE
2	A	984	MET
2	A	1023	ASN
2	A	1024	HIS
2	A	1044	TYR
2	A	1055	LEU
2	A	1070	ASP
2	A	1094	ARG
2	A	1172	ASN
2	A	1210	LYS
2	A	1217	GLN
2	A	1234	ASP
2	A	1249	MET
2	A	1298	ARG
2	A	1307	MET
2	A	1310	ARG
2	A	1311	PHE
2	A	1327	MET
2	A	1330	MET
2	A	1341	ARG
2	A	1410	ASP
2	A	1427	ARG
2	A	1441	ASP
2	A	1482	GLU
2	A	1597	PHE
2	A	1617	ARG
2	A	1622	MET
2	A	1630	LEU
2	A	1635	TYR
2	A	1668	TRP
2	A	1672	ASP
2	A	1686	ASP
2	A	1728	GLN
2	A	1730	MET
5	D	245	LYS
5	D	252	GLU
5	D	253	ARG

Continued on next page...

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Mol	Chain	Res	Type
5	D	279	SER
5	D	280	GLU
6	C	107	GLN
6	C	109	LEU
6	C	147	ASP
6	C	158	ARG
6	C	162	ASP
6	C	296	GLU
6	C	298	LEU
6	C	323	PHE
6	C	342	ARG
6	C	352	LYS
6	C	357	THR
6	C	498	SER
6	C	520	GLU
6	C	525	CYS
6	C	543	ARG
6	C	620	LYS
6	C	730	ARG
6	C	735	PHE
6	C	770	PHE
6	C	944	SER
7	B	39	GLU
7	B	47	LEU
7	B	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	C	139	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	5	101/117 (86%)	34 (33%)	4 (3%)

All (34) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	5	5	U
3	5	6	C
3	5	9	G
3	5	20	G
3	5	21	A
3	5	22	U
3	5	23	C
3	5	24	G
3	5	25	C
3	5	26	A
3	5	28	A
3	5	36	C
3	5	38	C
3	5	47	A
3	5	48	A
3	5	57	G
3	5	58	U
3	5	59	G
3	5	66	A
3	5	67	A
3	5	69	A
3	5	71	C
3	5	75	G
3	5	78	U
3	5	86	C
3	5	94	U
3	5	95	G
3	5	97	G
3	5	98	G
3	5	105	U
3	5	106	U
3	5	107	U
3	5	108	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	57	G
3	5	58	U
3	5	96	A
3	5	105	U

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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GTP	C	1001	-	26,34,34	1.06	3 (11%)	32,54,54	0.75	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
15	GTP	C	1001	-	-	2/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	1001	GTP	C5-C6	-2.73	1.41	1.47
15	C	1001	GTP	C8-N7	-2.18	1.31	1.35
15	C	1001	GTP	C5-C4	-2.03	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

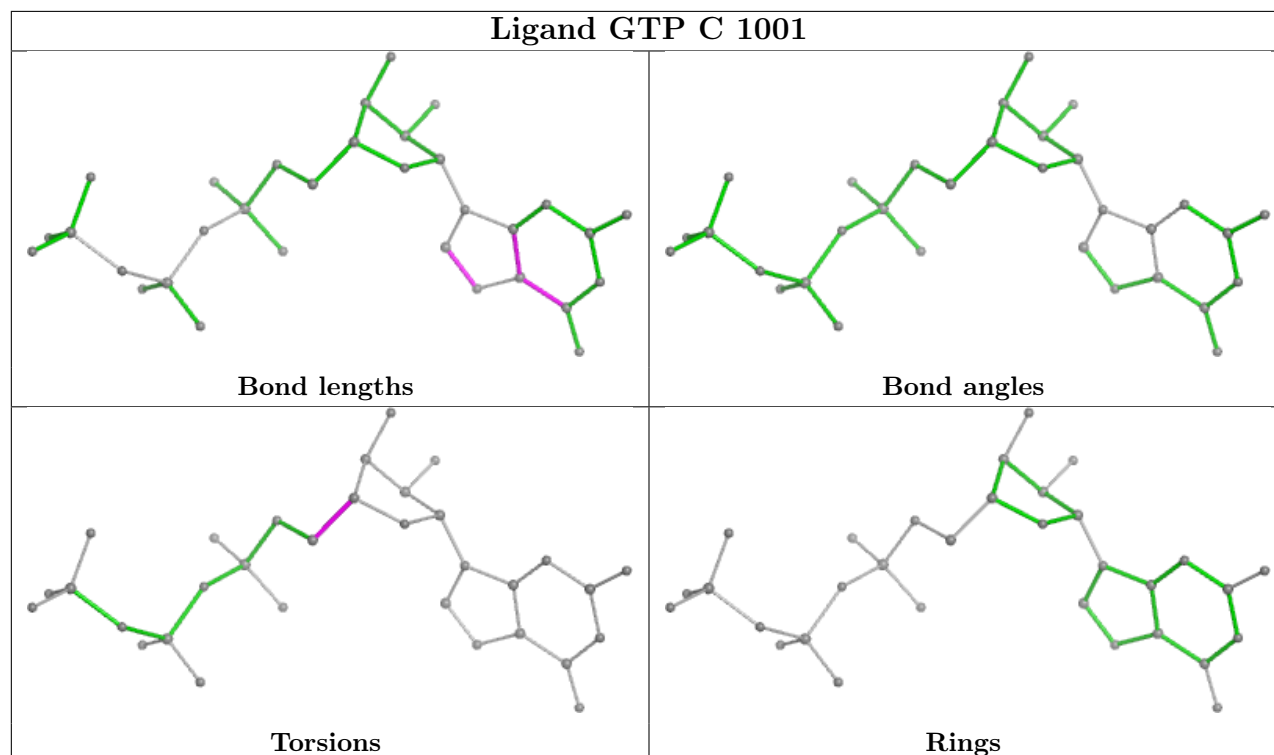
Mol	Chain	Res	Type	Atoms
15	C	1001	GTP	O4'-C4'-C5'-O5'
15	C	1001	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1001	GTP	1	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.



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.

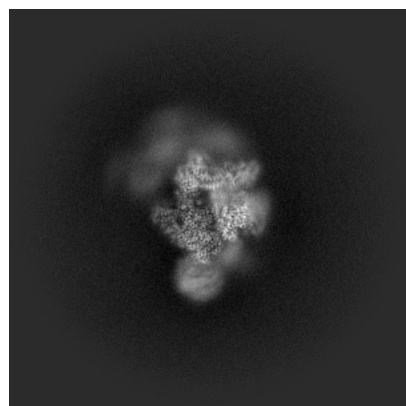
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18267. These allow visual inspection of the internal detail of the map and identification of artifacts.

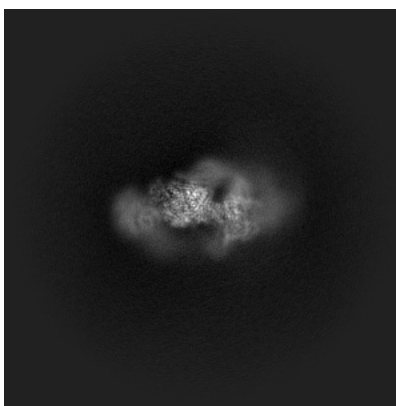
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

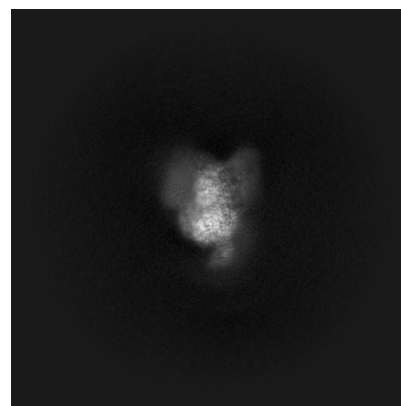
6.1.1 Primary map



X

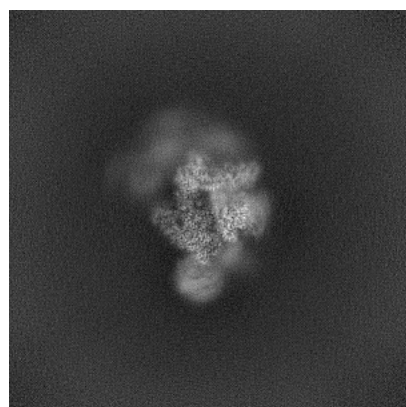


Y

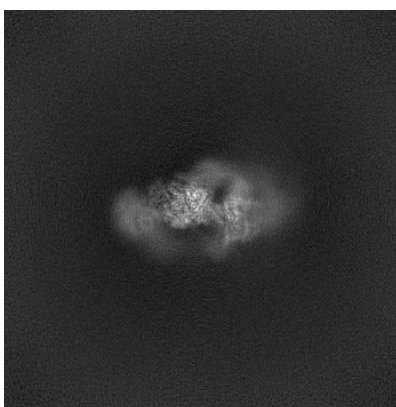


Z

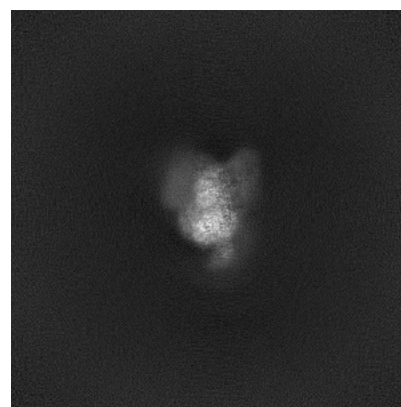
6.1.2 Raw map



X



Y

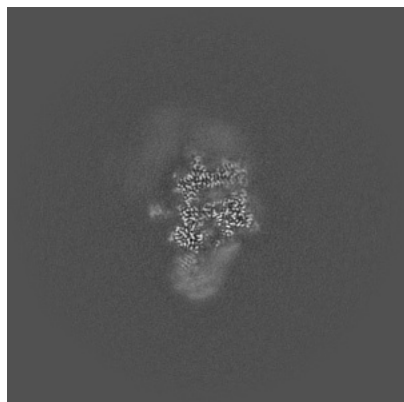


Z

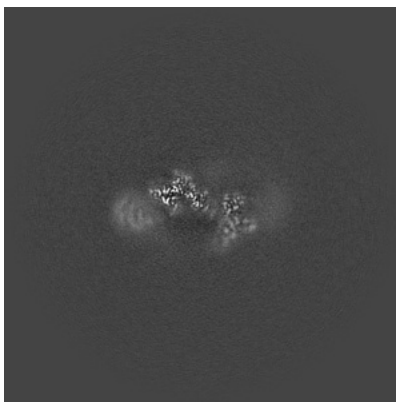
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

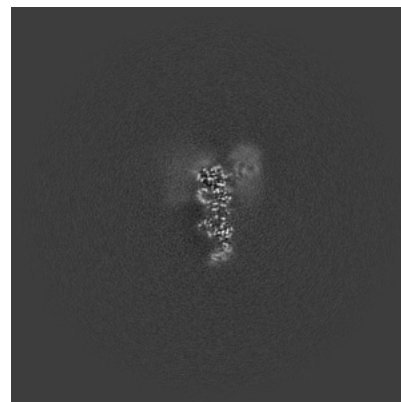
6.2.1 Primary map



X Index: 252

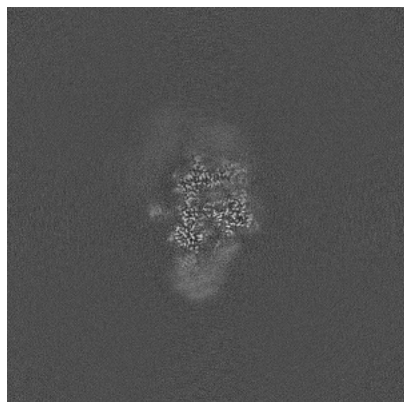


Y Index: 252

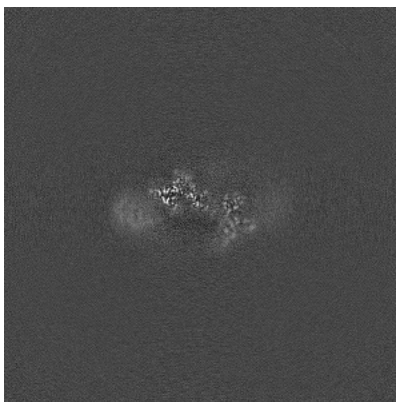


Z Index: 252

6.2.2 Raw map



X Index: 252



Y Index: 252

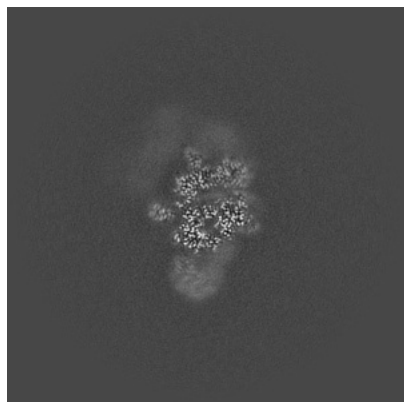


Z Index: 252

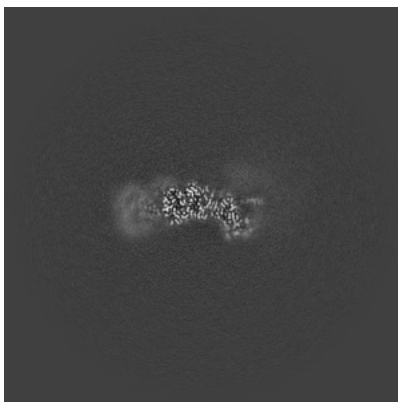
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

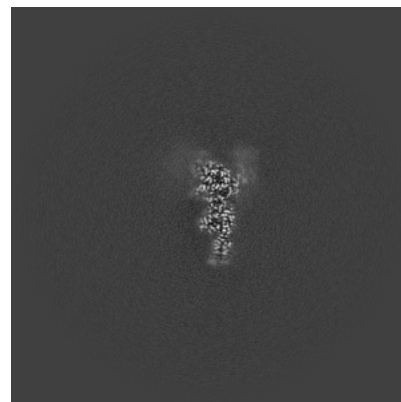
6.3.1 Primary map



X Index: 256

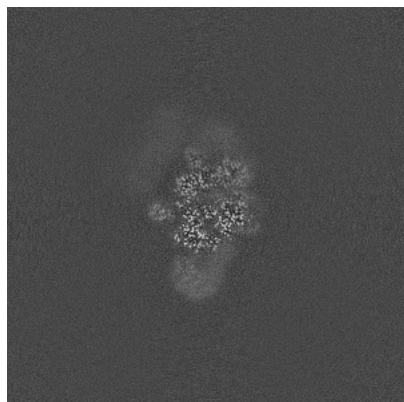


Y Index: 228

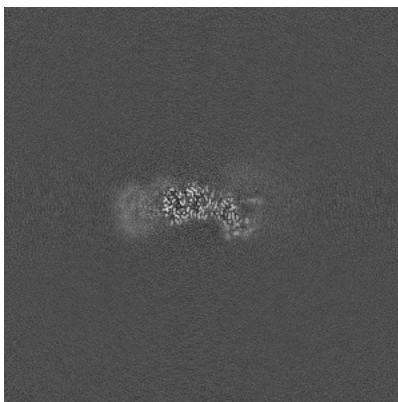


Z Index: 241

6.3.2 Raw map



X Index: 256



Y Index: 228

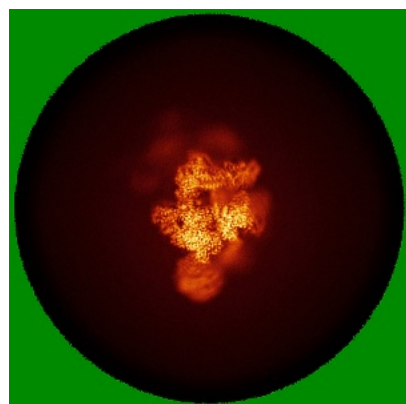


Z Index: 241

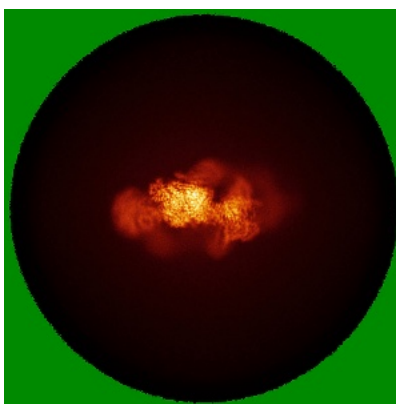
The images above show the largest variance slices of the map in three orthogonal directions.

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

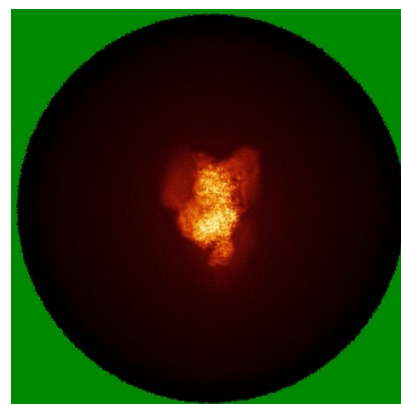
6.4.1 Primary map



X

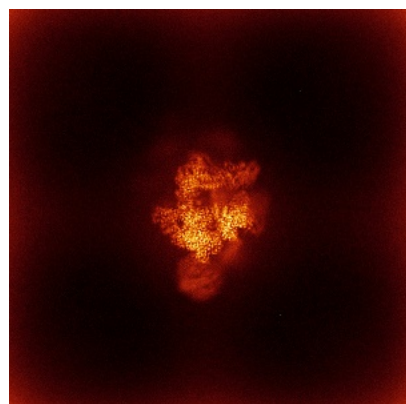


Y

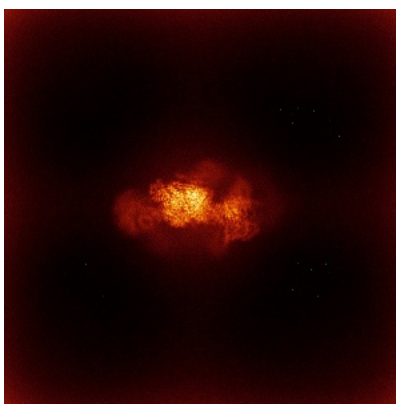


Z

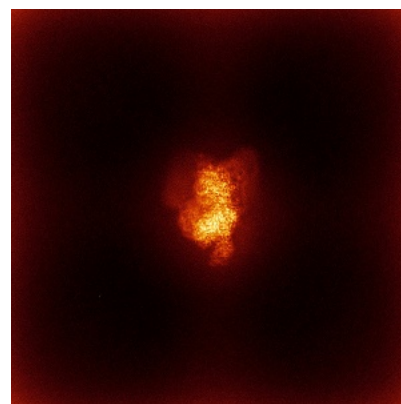
6.4.2 Raw map



X



Y

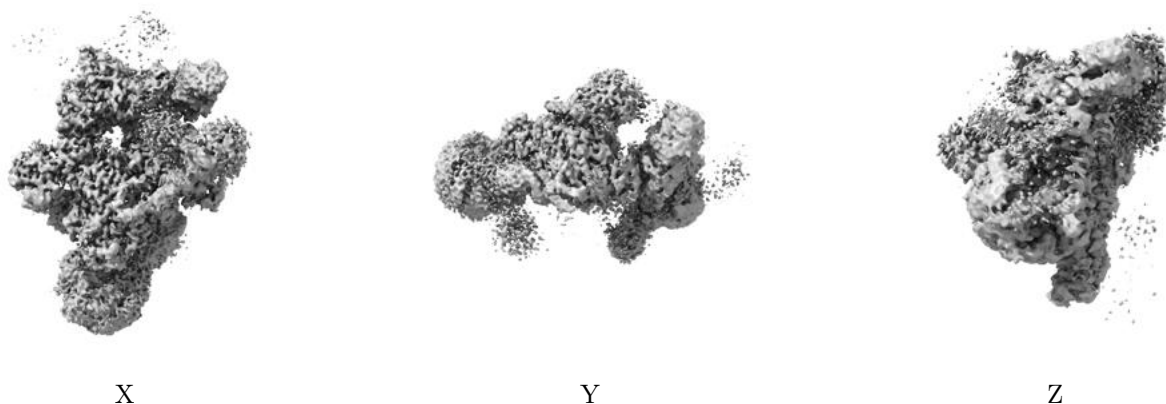


Z

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.

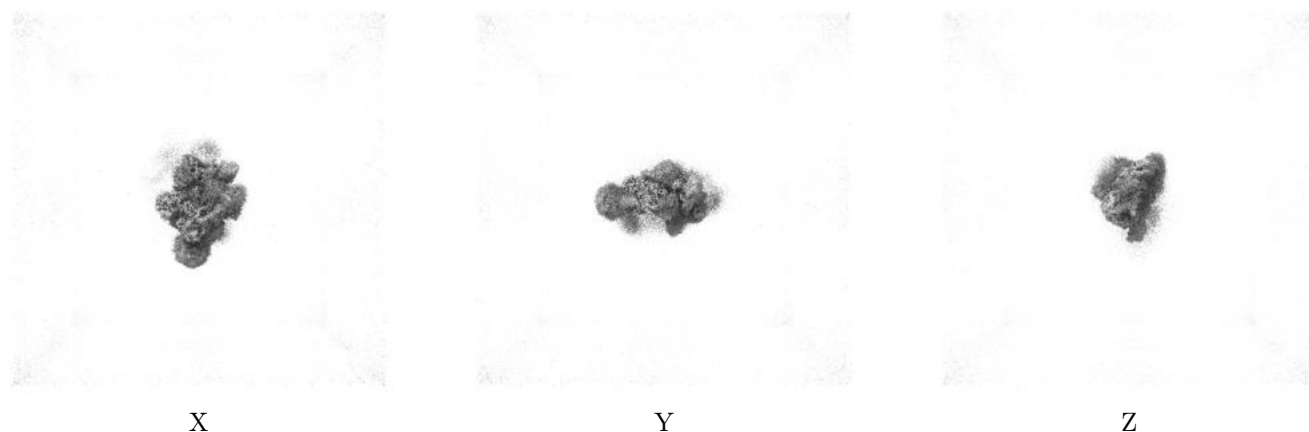
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

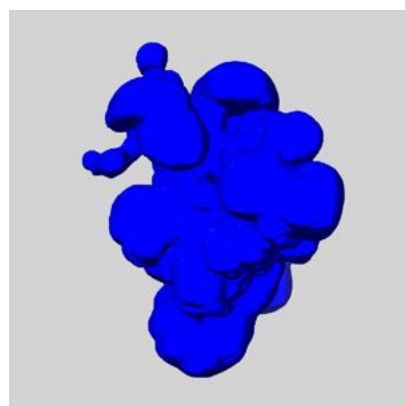
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

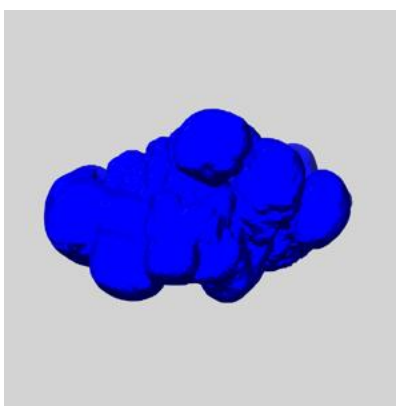
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

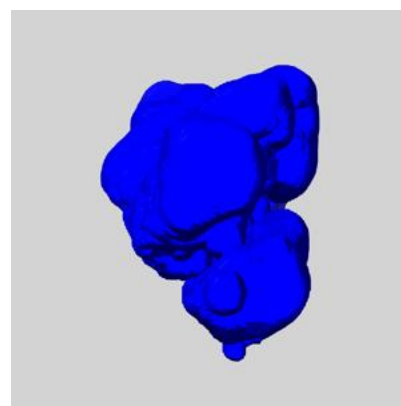
6.6.1 emd_18267_msk_1.map [i](#)



X



Y

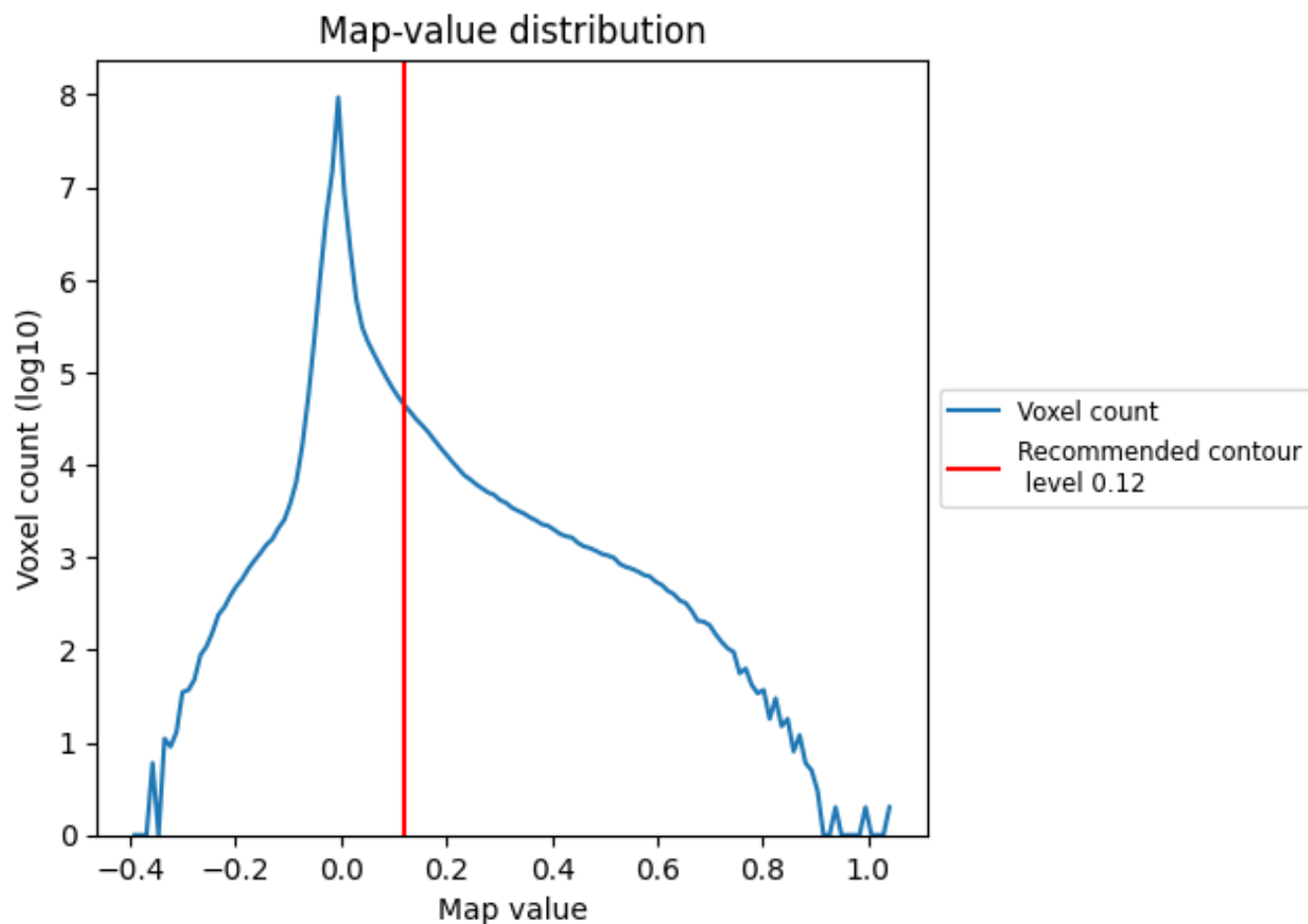


Z

7 Map analysis [i](#)

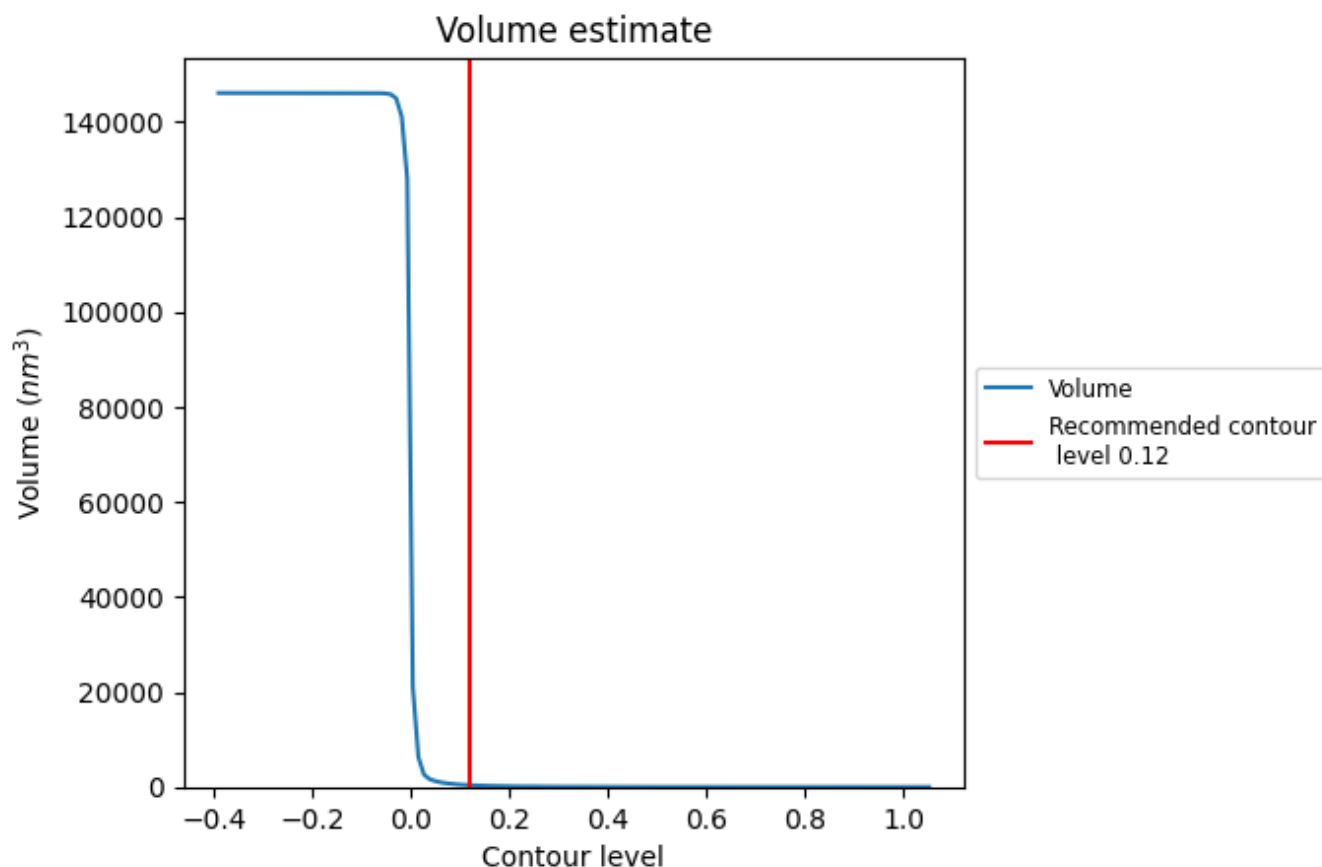
This section contains the results of statistical analysis of the map.

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.

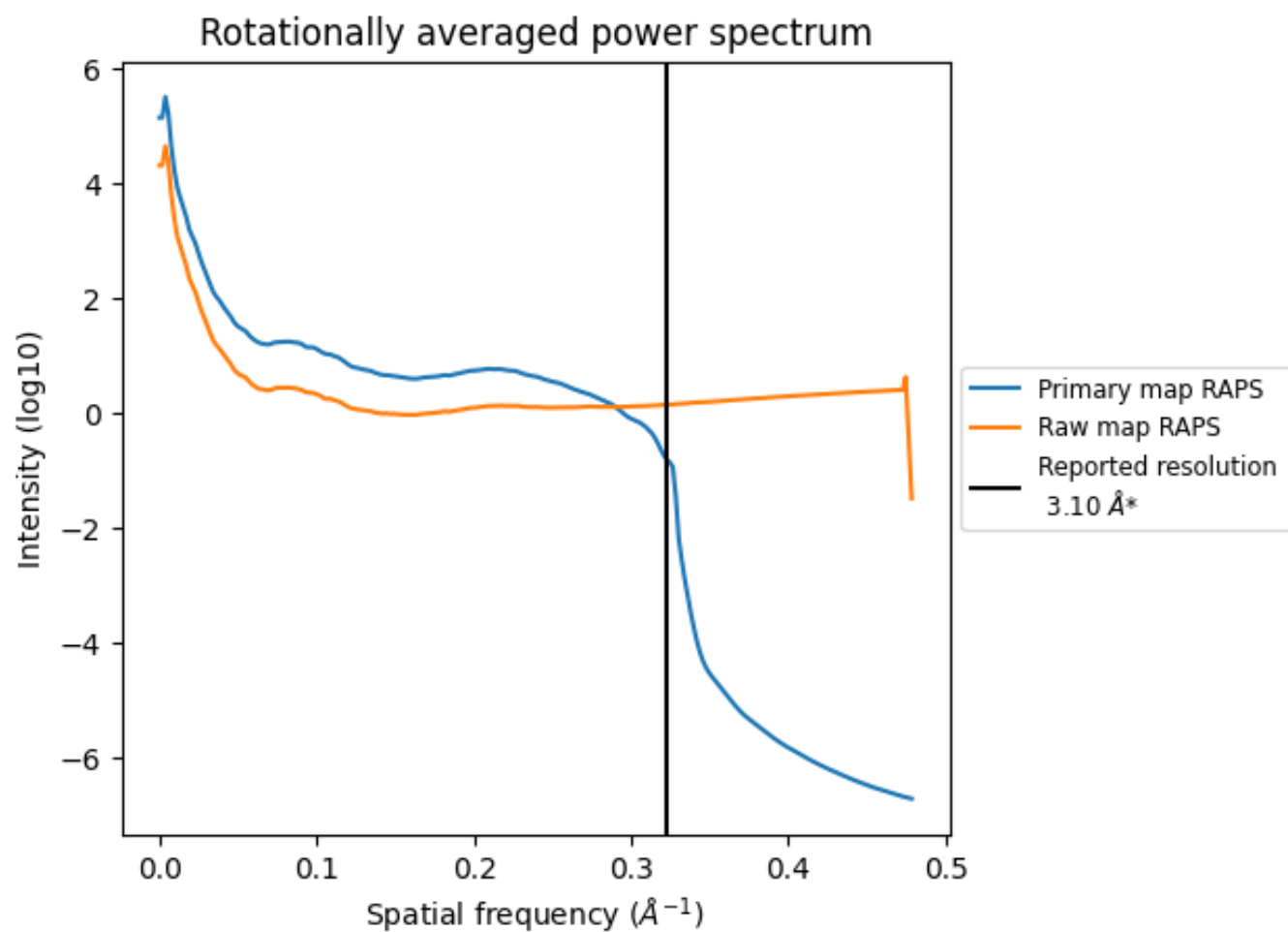
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm^3 ; this corresponds to an approximate mass of 327 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

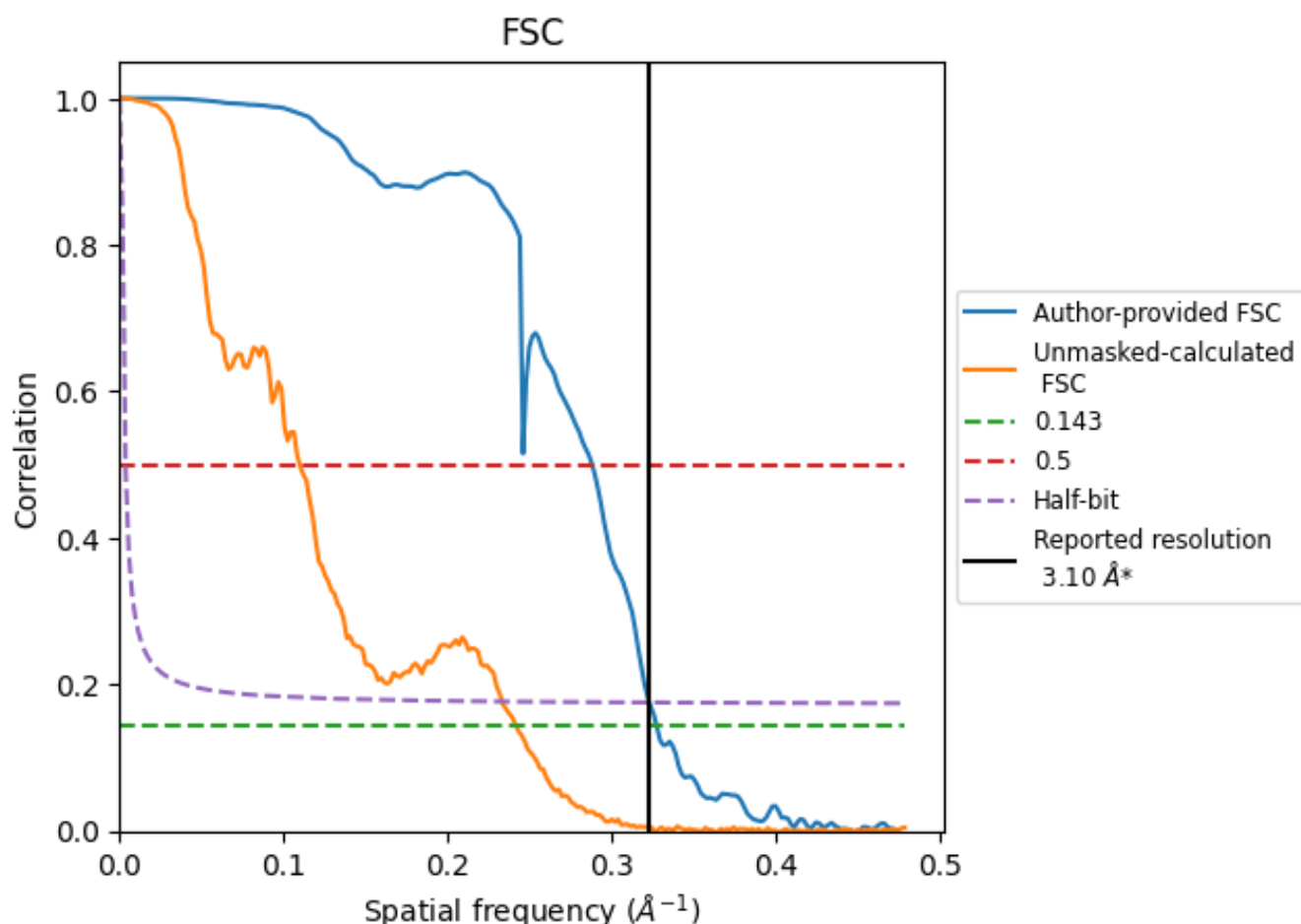


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

8 Fourier-Shell correlation [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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

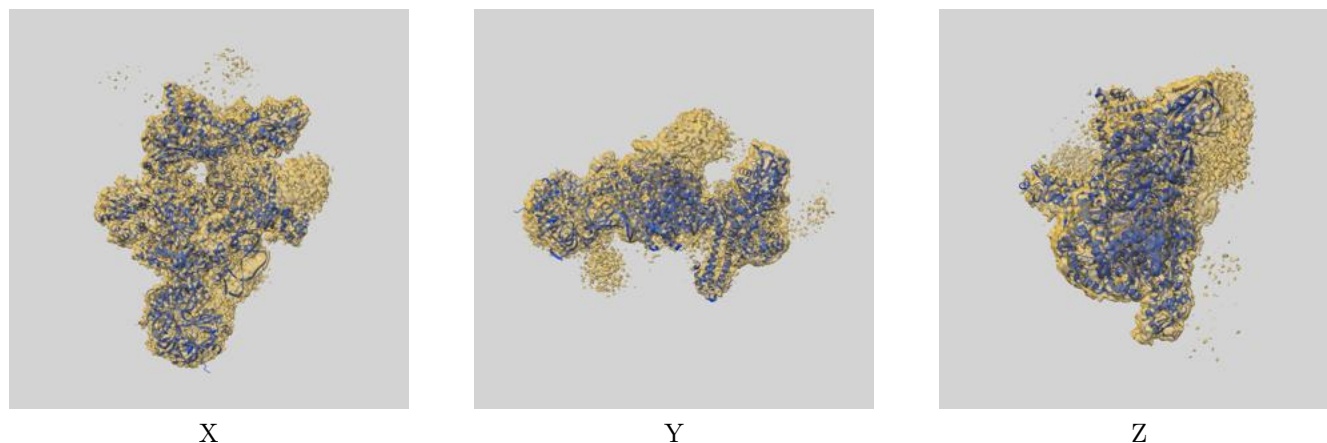
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.47	3.10
Unmasked-calculated*	4.14	9.11	4.29

*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 4.14 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

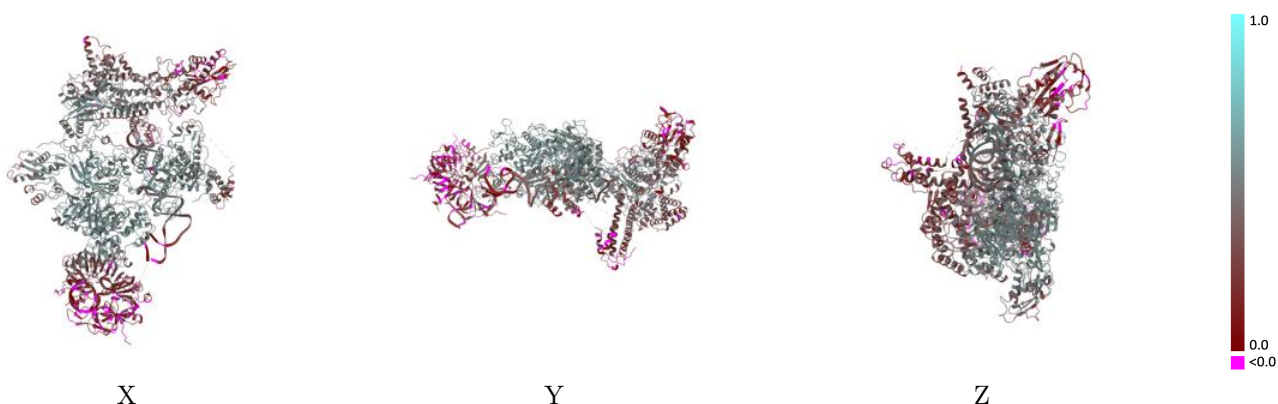
This section contains information regarding the fit between EMDB map EMD-18267 and PDB model 8Q91. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



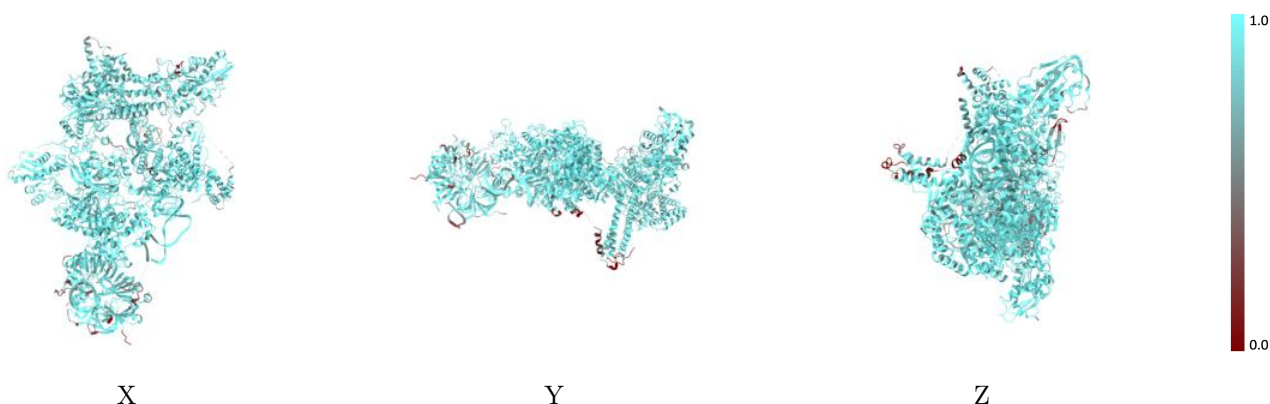
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



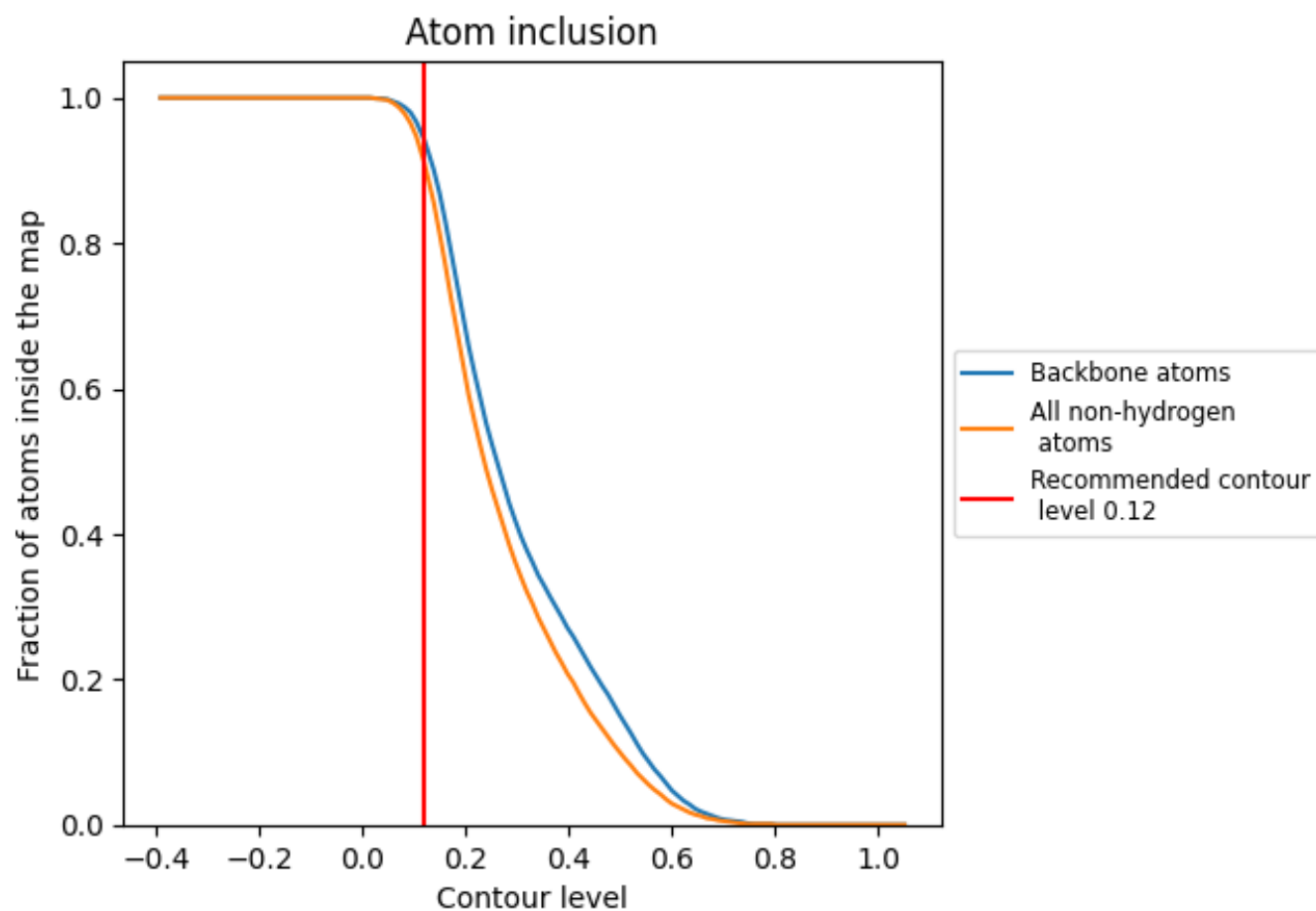
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9100	<div></div> 0.4170
5	<div></div> 0.8850	<div></div> 0.2720
A	<div></div> 0.9190	<div></div> 0.4350
B	<div></div> 0.7870	<div></div> 0.4280
C	<div></div> 0.9590	<div></div> 0.5270
D	<div></div> 0.8880	<div></div> 0.5120
E	<div></div> 0.4570	<div></div> 0.2020
F	<div></div> 0.8490	<div></div> 0.3660
h	<div></div> 0.8940	<div></div> 0.2550
i	<div></div> 0.9250	<div></div> 0.1800
j	<div></div> 0.7700	<div></div> 0.0980
k	<div></div> 0.9350	<div></div> 0.3980
l	<div></div> 0.8920	<div></div> 0.1310
m	<div></div> 0.8480	<div></div> 0.0930
n	<div></div> 0.7450	<div></div> 0.2620

1.0

0.0

<0.0