



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2025 – 03:15 PM EDT

PDB ID : 8T0L  
EMDB ID : EMD-40943  
Title : E. coli Sw2/Snf2 ATPase RapA bound to both ADP-AlF3 and reconstituted E. coli RNA polymerase post-termination complex on negatively-supercoiled DNA  
Authors : Brewer, J.J.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2023-06-01  
Resolution : 3.62 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
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) : 2.41.4

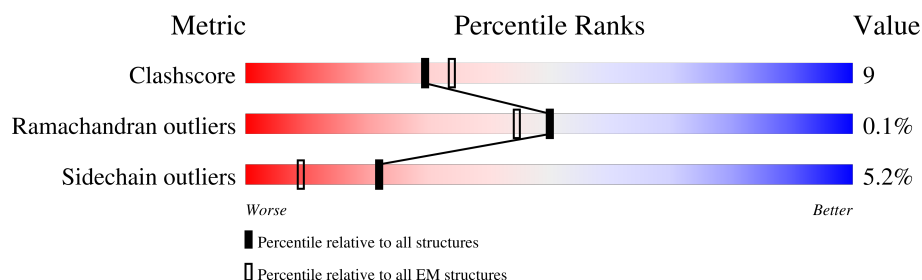
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.62 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	G	232	
1	H	232	
2	I	1340	
3	J	1358	
4	K	72	
5	F	966	
6	A	23	
7	B	23	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	AF3	F	1001	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 33530 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	223	Total	C	N	O	S	0	0
			1706	1068	298	334	6		
1	H	218	Total	C	N	O	S	0	0
			1667	1043	291	327	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	235	ALA	-	expression tag	UNP C3SR67
H	235	ALA	-	expression tag	UNP C3SR67

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	1333	Total	C	N	O	S	0	0
			10366	6514	1848	1954	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	262	ALA	THR	conflict	UNP A0A369F490

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	72	Total	C	N	O	S	0	0
			577	352	110	114	1		

- Molecule 5 is a protein called RNA polymerase-associated protein RapA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	966	Total	C	N	O	S	0	0
			7670	4800	1370	1471	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	144	ALA	TYR	conflict	UNP B7MAI2
F	413	ALA	THR	conflict	UNP B7MAI2
F	428	ALA	PHE	conflict	UNP B7MAI2
F	596	ALA	ARG	conflict	UNP B7MAI2
F	640	ALA	ARG	conflict	UNP B7MAI2
F	685	ALA	ARG	conflict	UNP B7MAI2
F	714	ALA	ASN	conflict	UNP B7MAI2
F	725	ALA	ILE	conflict	UNP B7MAI2

- Molecule 6 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	23	Total	C	N	O	P	0	0
			483	230	115	115	23		

- Molecule 7 is a DNA chain called DNA (5'-D(P\*TP\*CP\*TP\*GP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*AP\*TP\*TP\*CP\*AP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	23	Total	C	N	O	P	0	0
			460	230	46	161	23		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

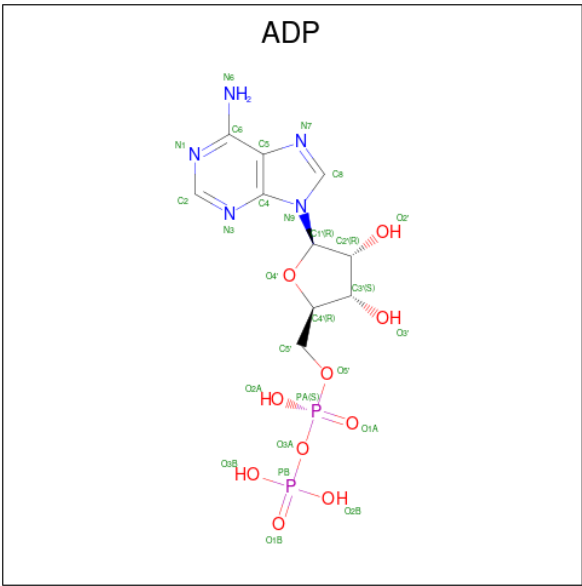
Mol	Chain	Residues	Atoms		AltConf
8	J	1	Total	Mg	0
			1	1	

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	J	2	Total	Zn	0
			2	2	

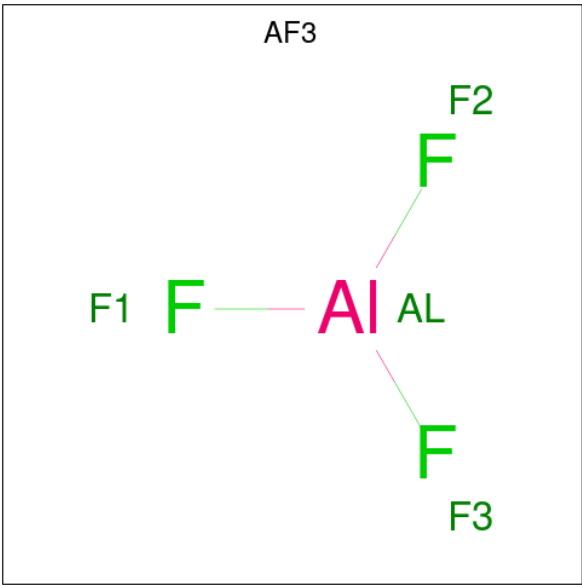
- Molecule 10 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).




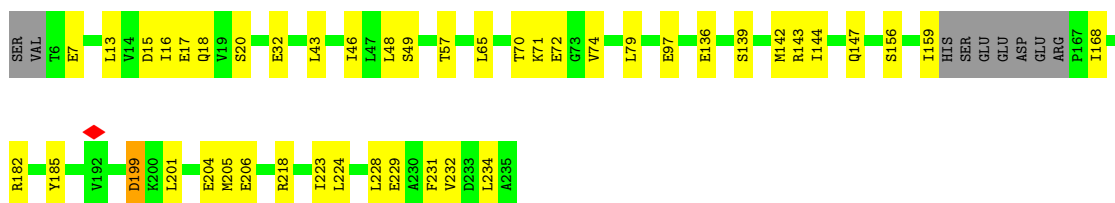
Mol	Chain	Residues	Atoms			AltConf
11	F	1	Total	Al	F	0
			4	1	3	

### 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.

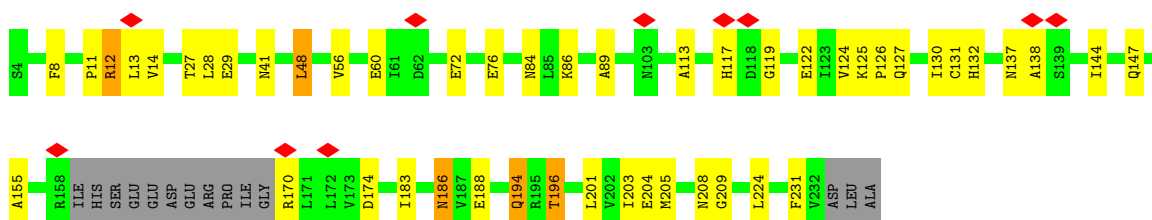
- Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain G: 



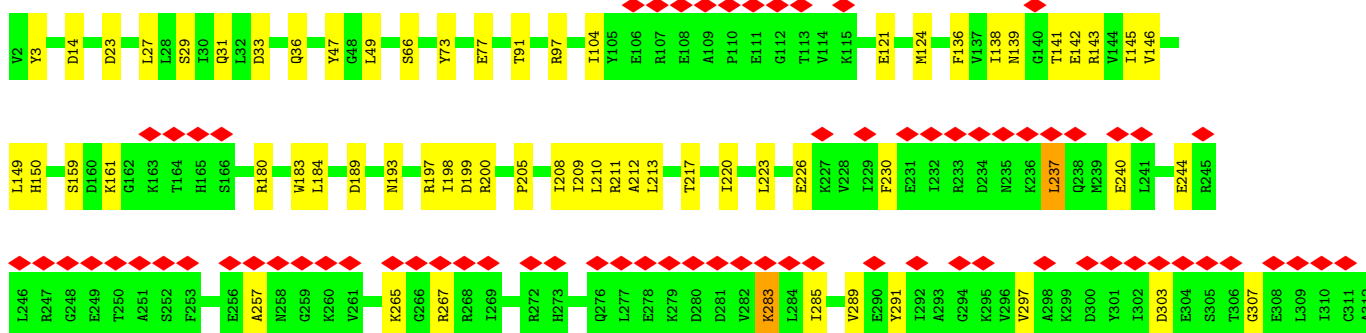
- Molecule 1: DNA-directed RNA polymerase subunit alpha

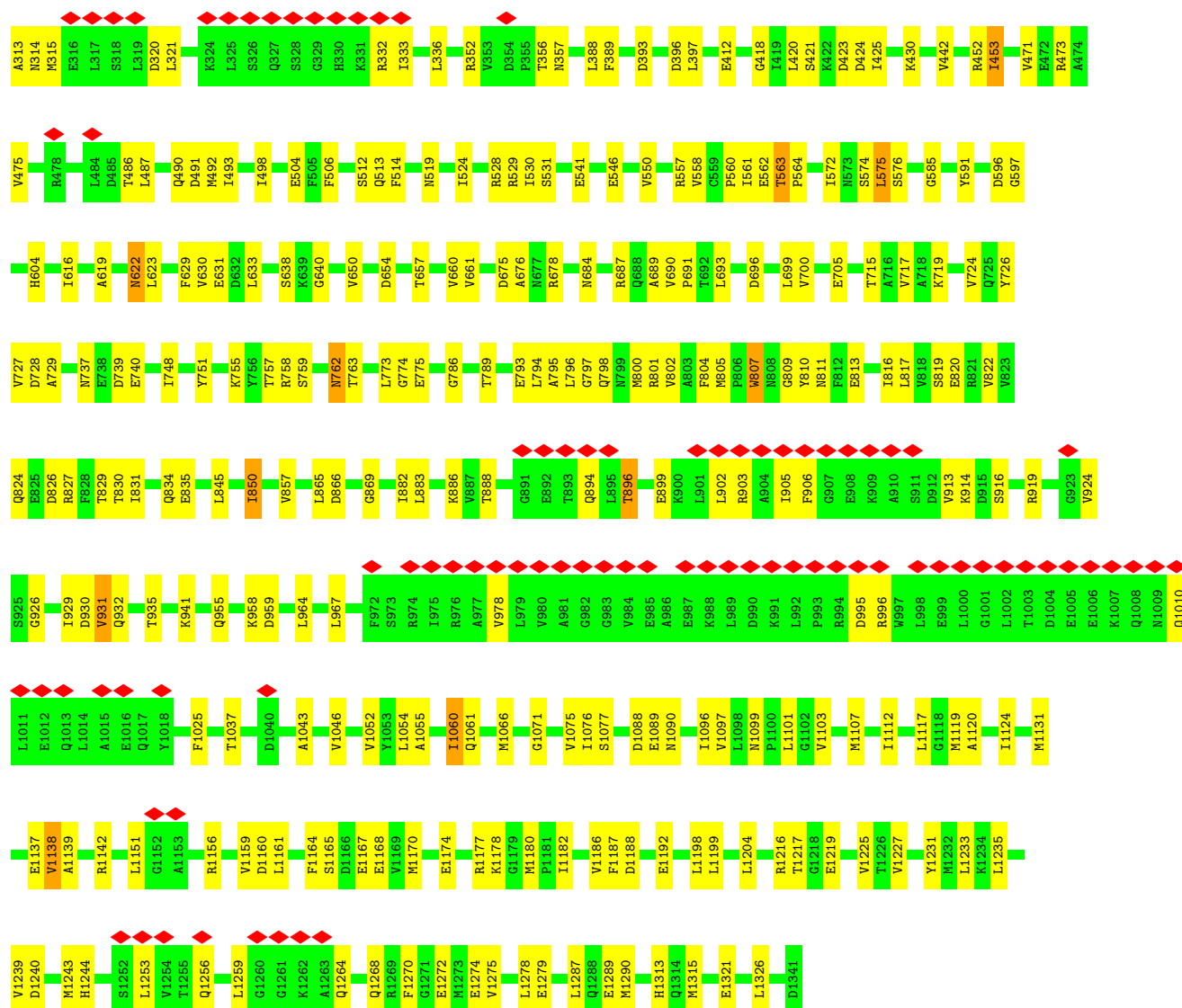
Chain H: 



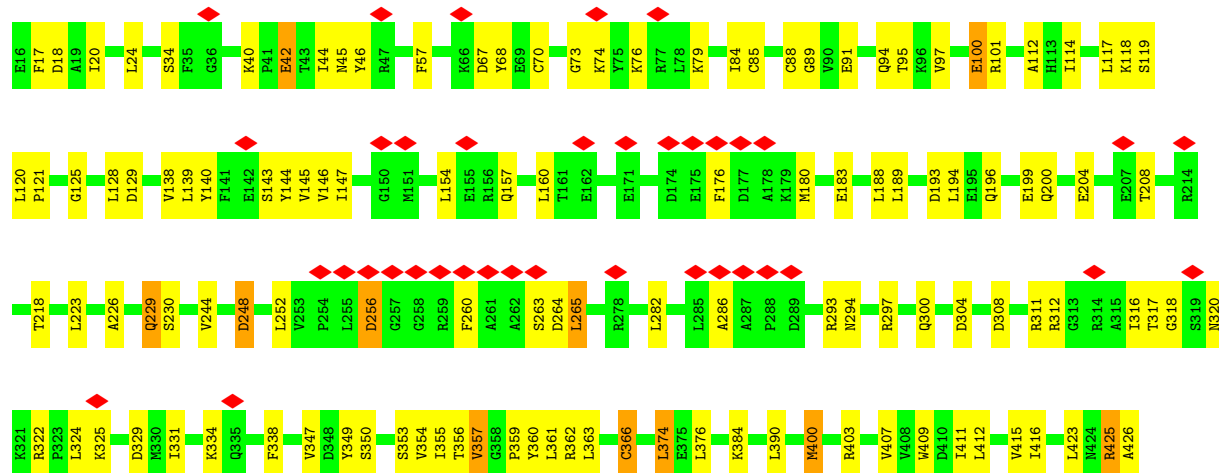
- Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I: 

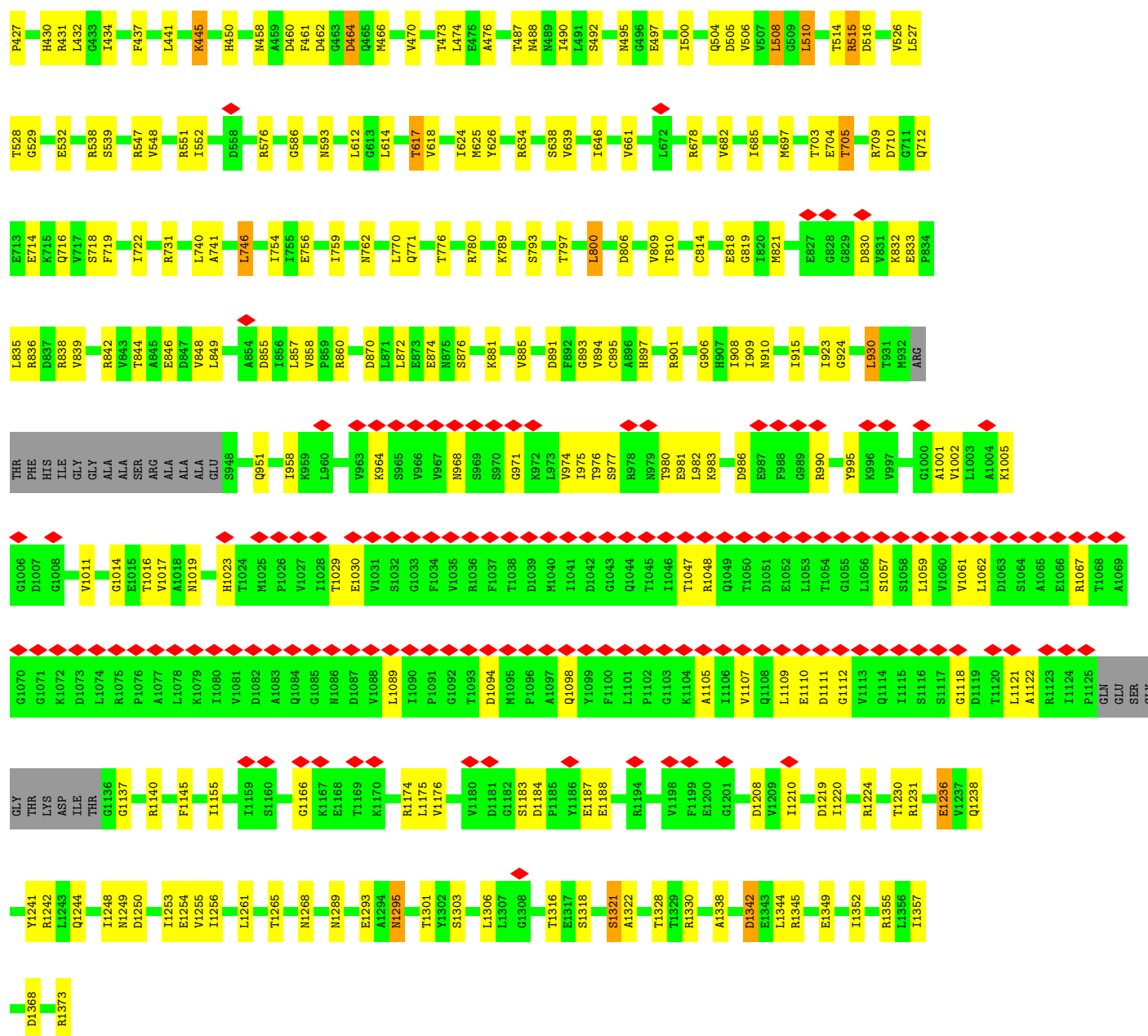




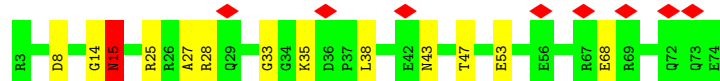
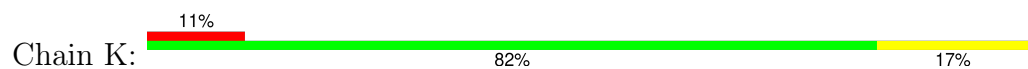
• Molecule 3: DNA-directed RNA polymerase subunit beta'



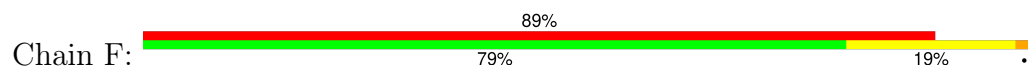




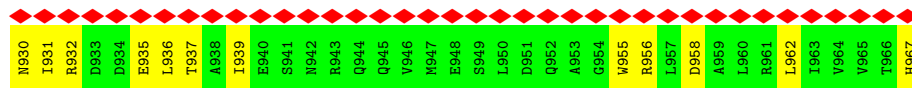
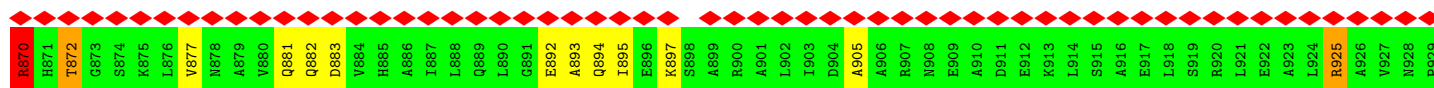
- Molecule 4: DNA-directed RNA polymerase subunit omega



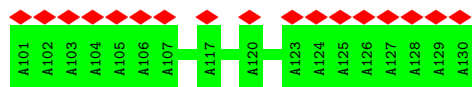
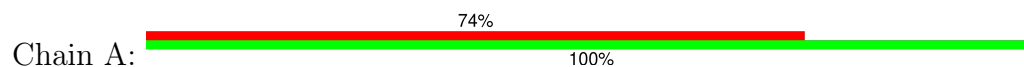
- Molecule 5: RNA polymerase-associated protein RapA



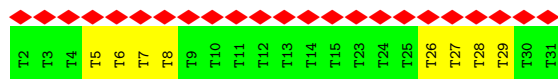
P810	P811	G812	T813	L814	L815	V816	E817	L818	I819	Y820	V821	V822	F763	A824	Q825	A826	P827	K828	Q829	L830	Q831	L832	N833	R834	F835	L836	P837	P838	T839	P840	V841	R842	M843	L844	L845	D846	K847	N848	G849	N850	N851	L852	A853	A854	Q855	V856	E857	F858	E859	T860	F861	N862	R863	Q864	L865	N866	A867	V868	N869		
D750	F751	F752	G753	L754	S755	E756	D757	T758	I759	T760	I761	F762	F763	D764	R765	E766	V767	A768	L769	A770	R771	E772	D773	A774	Q775	F776	I777	T778	W779	E780	H781	F782	L783	I784	R785	N786	G787	L788	D789	L790	I791	L792	S793	G794	D795	T796	G797	T798	S799	T800	L801	S802	L803	Q804	K805	N806	K807	V808	L809		
E690	I691	H692	S693	M694	G695	G696	E697	K698	A699	Q700	A701	L702	A703	E704	S705	T706	E707	E708	Q709	D710	D711	D712	T713	A714	L715	I716	A717	F718	R719	M720	N721	L722	L723	D724	A725	I726	G727	I728	N729	H730	P611	D732	V612	L613	E614	E615	T616	A617	Q618	S619	V620	L621	V622	R623	W624	Y625	H626	E627	G628	L629	
R570	N571	F572	Q573	F574	A575	S576	H577	M578	V579	M580	F581	D582	L583	P584	F585	N586	D588	L589	L590	E591	Q592	R593	I594	O595	A596	L597	D598	R599	I600	O601	Q602	A603	H604	D605	L606	Q607	I608	H609	V610	P611	V612	L613	E614	E615	T616	A617	Q618	S619	V620	L621	V622	R623	W624	Y625	H626	E627	G628	L629			
K449	V450	S451	Q452	L453	M454	G455	A456	R457	K458	S459	A460	E461	D462	R463	A464	R465	D466	M467	L468	Y469	P470	E471	R472	L473	V474	Q475	E476	F477	E478	G479	D480	N481	A482	T483	V484	M485	N486	F487	D488	P489	R490	V491	E492	M493	L494	M495	Q496	Y497	L498	T499	S500	H501	R502	S503	Q504	K505	V506	L507	V508		
A389	N390	S391	D392	S393	E394	D395	A396	Q397	S398	A399	R400	Q401	E402	L403	V404	S405	M406	L407	M408	D409	R410	H411	G412	A413	S414	R415	V416	L417	F418	R419	N420	T421	R422	N423	G424	V425	K426	Q427	A428	P429	K430	R431	E432	L433	H434	T435	L436	K437	L438	P439	S500	L440	P441	T442	Q443	Y444	Q445	T446	A447	T448	
R329	L330	L331	D332	P333	N334	R335	F336	H337	D338	F339	A340	Q341	F342	V343	E344	E345	Q346	K347	N348	Y349	R350	P351	V352	A353	D354	A355	V356	A357	N358	L359	L360	A361	G362	N363	K364	L365	S366	N367	D368	E369	L370	N371	M372	L373	G374	E375	N376	L377	G378	E379	Q380	D381	S323	H324	F325	P384	A326	L385	L386	Q387	A388
H64	D65	H92	G66	W67	Q68	Q70	V71	E72	E73	V74	K75	E76	E77	M78	G79	L80	L81	T82	Y83	G84	G85	T86	R87	L88	D89	T90	E91	E92	S93	G94	V95	A96	L97	R98	E99	V100	F101	L102	D103	S104	K105	L106	V107	F108	S109	K110	P111	Q112	D113	R114	L115	F116	A117	G118	Q119	I120	D121	R122	M123		
D124	R125	F126	A127	L128	L129	Y130	R131	A132	R133	K134	Y135	S136	S137	E138	Q139	F140	R141	M142	P143	A144	S145	G146	L147	R148	Q149	Q150	R151	L152	S153	L154	H157	Q158	L159	N160	A162	H163	D164	V165	G166	R167	R168	H169	A170	P171	R172	V173	L174	L175	A176	D177	E178	V179	G180	L181	Q182	K183					
T190	L191	H192	Q193	Q194	L195	S197	G198	A199	A200	E201	R202	V203	V207	P208	E209	T210	L211	V215	L216	V217	L220	R221	R222	F223	N224	L225	R226	F227	D232	E233	R234	Y235	A236	E237	Q239	H240	F246	E249	Q250	L251	V252	I253	L256	D257	R260	R261	S262	K263													
L266	E271	A272	E273	W274	D275	L276	L277	V278	V279	D280	E281	A282	H283	H284	L285	V286	W287	S288	E289	D290	A291	P292	S293	R294	D295	V296	Q297	A298	I299	E300	Q301	L302	A303	E304	H305	V306	P307	G308	V309	L310	L311	L312	T313	A314	T315	P316	E317	Q318	L319	G320	M321	Q322	S323	H324	F325	A326	R327	L328			
R329	L330	L331	D332	P333	N334	R335	F336	H337	D338	F339	A340	Q341	F342	V343	E344	E345	Q346	K347	N348	Y349	R350	P351	V352	A353	D354	A355	V356	A357	N358	L359	L360	A361	G362	N363	K364	L365	S366	N367	D368	E369	L370	N371	M372	L373	G374	E375	N376	L377	G378	E379	Q380	D381	S323	H324	F325	P384	A326	L385	L386	Q387	A388



• Molecule 6: DNA (29-MER)



• Molecule 7: DNA (5'-D(P\*TP\*CP\*TP\*GP\*AP\*AP\*TP\*TP\*TP\*AP\*AP\*AP\*TP\*TP\*CP\*A  
P\*GP\*A)-3')



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100010	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 ( $e^-/\text{\AA}^2$ )	55.9	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.838	Depositor
Minimum map value	-1.797	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.186	Depositor
Map size ( $\text{\AA}$ )	275.456, 275.456, 275.456	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.076, 1.076, 1.076	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, MG, ZN, AF3

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	G	0.32	0/1726	0.56	0/2340
1	H	0.29	0/1686	0.54	0/2287
2	I	0.35	0/10736	0.55	0/14487
3	J	0.33	0/10523	0.57	0/14207
4	K	0.25	0/579	0.57	0/779
5	F	0.26	0/7812	0.53	0/10586
6	A	0.55	0/550	0.75	0/843
7	B	0.75	0/504	1.30	0/774
All	All	0.33	0/34116	0.58	0/46303

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	1
5	F	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	870	ARG	Peptide
3	J	76	LYS	Peptide

## 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	G	1706	0	1734	24	0
1	H	1667	0	1693	32	0
2	I	10567	0	10585	210	0
3	J	10366	0	10587	224	0
4	K	577	0	588	7	0
5	F	7670	0	7534	123	0
6	A	483	0	255	0	0
7	B	460	0	278	6	0
8	J	1	0	0	0	0
9	J	2	0	0	0	0
10	F	27	0	12	6	0
11	F	4	0	0	3	0
All	All	33530	0	33266	599	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 9.

All (599) 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)
3:J:460:ASP:OD2	3:J:462:ASP:OD1	1.58	1.22
2:I:826:ASP:OD1	2:I:829:THR:OG1	1.99	0.81
2:I:684:ASN:OD1	2:I:687:ARG:NH2	2.14	0.80
3:J:806:ASP:OD1	3:J:1345:ARG:NH1	2.15	0.80
5:F:727:GLY:O	5:F:743:SER:OG	2.00	0.78
1:G:71:LYS:NZ	1:G:139:SER:O	2.16	0.78
2:I:813:GLU:OE1	3:J:504:GLN:NE2	2.17	0.77
5:F:11:SER:OG	5:F:14:GLU:O	2.03	0.77
5:F:8:ARG:O	5:F:52:ARG:NH1	2.18	0.77
3:J:347:VAL:O	3:J:350:SER:OG	2.03	0.76
1:H:41:ASN:ND2	2:I:1217:THR:O	2.18	0.76
1:H:122:GLU:N	1:H:122:GLU:OE1	2.19	0.76
5:F:34:PHE:O	5:F:38:GLY:N	2.19	0.75
3:J:977:SER:OG	3:J:980:THR:OG1	2.04	0.75
2:I:97:ARG:NH2	2:I:121:GLU:O	2.19	0.75

*Continued on next page...*

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:562:GLU:OE2	2:I:687:ARG:NH1	2.21	0.74
3:J:901:ARG:NE	3:J:906:GLY:O	2.19	0.74
3:J:951:GLN:OE1	3:J:1016:THR:OG1	2.05	0.73
2:I:801:ARG:NH2	2:I:1088:ASP:OD2	2.22	0.73
5:F:882:GLN:NE2	5:F:883:ASP:OD1	2.21	0.73
2:I:705:GLU:N	2:I:705:GLU:OE1	2.22	0.73
2:I:1142:ARG:NH1	2:I:1161:LEU:O	2.21	0.73
5:F:653:TYR:OH	5:F:661:GLU:O	2.06	0.73
2:I:811:ASN:O	2:I:1099:ASN:ND2	2.22	0.72
2:I:265:LYS:O	2:I:267:ARG:NH1	2.23	0.72
3:J:120:LEU:O	3:J:1330:ARG:NH1	2.22	0.72
3:J:362:ARG:O	3:J:450:HIS:ND1	2.22	0.72
3:J:614:LEU:O	3:J:617:THR:OG1	2.08	0.72
5:F:724:ASP:OD1	5:F:730:GLN:NE2	2.22	0.72
5:F:408:MET:SD	5:F:414:SER:OG	2.47	0.72
1:H:155:ALA:N	1:H:174:ASP:OD1	2.22	0.71
2:I:541:GLU:OE1	2:I:541:GLU:N	2.24	0.71
2:I:678:ARG:NH2	2:I:1071:GLY:O	2.22	0.71
2:I:1137:GLU:O	2:I:1139:ALA:N	2.23	0.71
3:J:1155:ILE:O	3:J:1210:ILE:N	2.22	0.71
5:F:544:ASP:OD1	5:F:570:ARG:NH2	2.23	0.71
1:G:18:GLN:NE2	1:G:20:SER:O	2.24	0.71
2:I:930:ASP:OD2	2:I:932:GLN:NE2	2.23	0.71
5:F:538:MET:O	5:F:543:ARG:NH1	2.24	0.71
3:J:495:ASN:ND2	3:J:497:GLU:OE2	2.24	0.70
3:J:119:SER:OG	3:J:121:PRO:O	2.08	0.70
2:I:237:LEU:HD22	2:I:289:VAL:HG12	1.74	0.70
4:K:33:GLY:O	4:K:35:LYS:NZ	2.16	0.70
5:F:599:ARG:NH1	10:F:1000:ADP:O1B	2.25	0.70
2:I:1253:LEU:O	2:I:1256:GLN:NE2	2.24	0.70
2:I:421:SER:OG	2:I:423:ASP:OD1	2.08	0.70
2:I:902:LEU:O	2:I:906:PHE:N	2.24	0.70
3:J:844:THR:HG23	3:J:860:ARG:O	1.92	0.70
3:J:118:LYS:O	3:J:311:ARG:NH1	2.25	0.70
2:I:217:THR:OG1	2:I:357:ASN:OD1	2.10	0.69
2:I:715:THR:HG23	2:I:717:VAL:HG23	1.74	0.69
2:I:1225:VAL:HG23	3:J:638:SER:HB2	1.75	0.69
3:J:400:MET:SD	3:J:403:ARG:NH1	2.66	0.69
3:J:70:CYS:SG	3:J:73:GLY:N	2.66	0.69
1:G:136:GLU:N	1:G:136:GLU:OE1	2.25	0.68
5:F:281:GLU:O	5:F:284:HIS:ND1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:ARG:NH1	1:H:29:GLU:OE2	2.27	0.68
3:J:460:ASP:CG	3:J:462:ASP:OD1	2.32	0.67
5:F:583:LEU:HD11	5:F:622:VAL:CG2	2.23	0.67
4:K:38:LEU:N	4:K:53:GLU:OE2	2.27	0.67
5:F:583:LEU:HD11	5:F:622:VAL:HG23	1.75	0.67
2:I:29:SER:OG	2:I:33:ASP:OD2	2.13	0.67
3:J:350:SER:O	3:J:376:LEU:HD21	1.94	0.67
2:I:1192:GLU:N	2:I:1192:GLU:OE1	2.28	0.67
3:J:1029:THR:O	3:J:1118:GLY:N	2.27	0.67
5:F:553:GLU:OE1	5:F:554:ASP:N	2.27	0.67
2:I:197:ARG:O	2:I:200:ARG:NH2	2.27	0.66
3:J:789:LYS:NZ	3:J:930:LEU:O	2.16	0.66
2:I:675:ASP:OD1	2:I:676:ALA:N	2.29	0.66
3:J:1318:SER:OG	3:J:1342:ASP:OD1	2.07	0.66
2:I:726:TYR:OH	2:I:728:ASP:OD2	2.13	0.66
5:F:370:LEU:HD13	5:F:386:LEU:HD21	1.77	0.66
2:I:1219:GLU:OE2	3:J:634:ARG:NE	2.29	0.66
3:J:894:VAL:HG11	3:J:915:ILE:HD11	1.78	0.66
2:I:786:GLY:N	2:I:789:THR:OG1	2.29	0.65
3:J:1002:VAL:N	3:J:1019:ASN:O	2.28	0.65
5:F:605:ASP:OD1	5:F:607:GLN:NE2	2.30	0.65
1:H:29:GLU:OE1	1:H:29:GLU:N	2.30	0.65
5:F:159:LEU:HD12	5:F:703:ALA:HB1	1.77	0.65
2:I:226:GLU:N	2:I:226:GLU:OE1	2.30	0.65
5:F:7:GLN:NE2	5:F:79:GLY:O	2.29	0.65
5:F:58:GLY:O	5:F:70:GLN:NE2	2.30	0.65
5:F:585:PHE:HE1	5:F:654:LEU:HD13	1.61	0.65
2:I:793:GLU:N	2:I:793:GLU:OE1	2.30	0.64
2:I:574:SER:OG	2:I:575:LEU:N	2.30	0.64
3:J:746:LEU:HD13	3:J:754:ILE:HD11	1.78	0.64
5:F:877:VAL:HG21	5:F:962:LEU:HD21	1.79	0.64
2:I:834:GLN:OE1	2:I:924:VAL:HG21	1.97	0.64
1:H:131:CYS:SG	1:H:132:HIS:N	2.71	0.64
3:J:1316:THR:HG22	3:J:1318:SER:H	1.62	0.64
5:F:114:ARG:NH2	5:F:797:GLY:O	2.30	0.64
3:J:576:ARG:NH1	3:J:593:ASN:O	2.31	0.64
3:J:697:MET:CE	3:J:741:ALA:HB3	2.28	0.64
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.79	0.64
3:J:497:GLU:N	3:J:497:GLU:OE1	2.31	0.63
3:J:709:ARG:NH2	3:J:712:GLN:OE1	2.31	0.63
5:F:691:ILE:O	5:F:695:GLY:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:125:GLY:O	3:J:129:ASP:N	2.32	0.63
3:J:300:GLN:NE2	3:J:304:ASP:OD1	2.32	0.63
2:I:798:GLN:NE2	2:I:827:ARG:O	2.32	0.63
3:J:697:MET:HE3	3:J:741:ALA:HB3	1.81	0.63
5:F:179:VAL:HG22	5:F:314:ALA:HB1	1.81	0.62
2:I:810:TYR:HB2	2:I:817:LEU:HD21	1.81	0.62
2:I:748:ILE:HD13	2:I:967:LEU:HD13	1.82	0.62
3:J:204:GLU:O	3:J:208:THR:HG23	1.98	0.62
5:F:233:GLU:N	5:F:233:GLU:OE1	2.33	0.62
2:I:883:LEU:HD12	2:I:1052:VAL:HG11	1.81	0.62
2:I:811:ASN:ND2	2:I:1097:VAL:O	2.32	0.62
3:J:487:THR:OG1	3:J:618:VAL:HG21	2.00	0.62
2:I:412:GLU:N	2:I:412:GLU:OE1	2.33	0.62
3:J:1268:ASN:OD1	3:J:1301:THR:OG1	2.18	0.62
2:I:689:ALA:HB2	2:I:1233:LEU:HD23	1.81	0.61
3:J:183:GLU:N	3:J:183:GLU:OE1	2.33	0.61
5:F:502:ARG:O	5:F:558:GLN:NE2	2.33	0.61
2:I:1124:ILE:HG21	2:I:1180:MET:SD	2.40	0.61
1:G:32:GLU:OE1	1:G:32:GLU:N	2.34	0.61
2:I:184:LEU:HD13	2:I:389:PHE:CZ	2.36	0.61
5:F:147:LEU:HD21	5:F:706:ILE:HD13	1.81	0.61
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.82	0.61
5:F:138:GLU:O	5:F:142:MET:N	2.34	0.61
2:I:528:ARG:NH2	2:I:576:SER:O	2.34	0.61
2:I:1174:GLU:OE1	2:I:1177:ARG:NH1	2.33	0.61
5:F:690:GLU:O	5:F:694:ASN:ND2	2.33	0.61
3:J:968:ASN:OD1	3:J:971:GLY:N	2.34	0.61
5:F:123:MET:SD	5:F:867:ALA:N	2.74	0.60
5:F:583:LEU:HD13	5:F:618:GLN:HB3	1.83	0.60
3:J:40:LYS:NZ	3:J:42:GLU:OE2	2.29	0.60
2:I:619:ALA:N	2:I:654:ASP:OD2	2.35	0.60
2:I:886:LYS:NZ	2:I:916:SER:O	2.22	0.60
2:I:724:VAL:HG13	2:I:774:GLY:H	1.67	0.60
2:I:930:ASP:OD1	2:I:931:VAL:N	2.34	0.60
3:J:848:VAL:O	3:J:857:LEU:N	2.31	0.60
2:I:1101:LEU:HD12	3:J:505:ASP:OD1	2.02	0.60
2:I:3:TYR:OH	2:I:1159:VAL:HG12	2.01	0.60
1:H:72:GLU:N	1:H:72:GLU:OE1	2.35	0.60
2:I:845:LEU:HD11	2:I:903:ARG:NH2	2.16	0.60
3:J:374:LEU:HD12	3:J:409:TRP:CZ3	2.37	0.60
5:F:824:ALA:HB2	5:F:836:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:800:MET:O	2:I:802:VAL:HG13	2.02	0.59
2:I:1061:GLN:NE2	2:I:1240:ASP:OD2	2.36	0.59
3:J:1059:LEU:O	3:J:1107:VAL:N	2.34	0.59
3:J:528:THR:HG22	3:J:529:GLY:H	1.66	0.59
3:J:968:ASN:HB3	3:J:974:VAL:HG13	1.84	0.59
2:I:1321:GLU:N	2:I:1321:GLU:OE1	2.34	0.59
5:F:99:GLU:N	5:F:99:GLU:OE1	2.35	0.59
3:J:140:TYR:OH	3:J:312:ARG:NE	2.35	0.59
5:F:756:GLU:N	5:F:756:GLU:OE1	2.35	0.59
5:F:165:VAL:HG22	5:F:415:ARG:NH2	2.18	0.59
3:J:1047:THR:OG1	3:J:1062:LEU:HD11	2.02	0.59
2:I:142:GLU:N	2:I:142:GLU:OE1	2.36	0.59
1:H:48:LEU:HD21	3:J:539:SER:HB3	1.85	0.59
1:G:15:ASP:OD1	1:G:16:ILE:N	2.36	0.58
1:H:127:GLN:N	1:H:127:GLN:OE1	2.34	0.58
2:I:149:LEU:HD12	2:I:452:ARG:O	2.02	0.58
5:F:663:PHE:CZ	5:F:667:ILE:HD11	2.38	0.58
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.85	0.58
2:I:794:LEU:HD23	2:I:796:LEU:HD11	1.85	0.58
2:I:1239:VAL:HG21	3:J:445:LYS:O	2.04	0.58
2:I:257:ALA:HB1	2:I:285:ILE:HG21	1.86	0.58
3:J:355:ILE:HD11	3:J:466:MET:HB2	1.85	0.58
5:F:316:PRO:O	5:F:327:ARG:NH2	2.36	0.58
5:F:585:PHE:CE1	5:F:654:LEU:HD13	2.38	0.58
2:I:796:LEU:N	2:I:1231:TYR:OH	2.36	0.58
1:H:89:ALA:O	1:H:124:VAL:HG12	2.03	0.58
3:J:154:LEU:HD23	3:J:160:LEU:HD21	1.83	0.58
3:J:1105:ALA:HB1	3:J:1122:ALA:HB1	1.85	0.58
3:J:248:ASP:OD1	3:J:248:ASP:N	2.35	0.57
3:J:951:GLN:NE2	3:J:1014:GLY:O	2.36	0.57
3:J:1238:GLN:OE1	3:J:1242:ARG:NH2	2.36	0.57
5:F:183:LYS:N	10:F:1000:ADP:O2A	2.37	0.57
5:F:881:GLN:N	5:F:881:GLN:OE1	2.37	0.57
2:I:690:VAL:HG22	2:I:691:PRO:HD2	1.85	0.57
1:G:13:LEU:HD21	1:G:16:ILE:HD11	1.86	0.57
1:H:205:MET:SD	1:H:205:MET:N	2.77	0.57
3:J:68:TYR:OH	3:J:94:GLN:NE2	2.38	0.57
5:F:663:PHE:CE2	5:F:667:ILE:HD11	2.38	0.57
2:I:638:SER:O	2:I:640:GLY:N	2.38	0.57
3:J:964:LYS:O	3:J:976:THR:OG1	2.21	0.57
5:F:484:TRP:NE1	5:F:518:GLN:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:281:GLU:N	5:F:312:LEU:O	2.38	0.57
5:F:534:PHE:CE1	5:F:560:LEU:HD11	2.40	0.57
3:J:460:ASP:OD2	3:J:462:ASP:CG	2.40	0.56
3:J:915:ILE:HD12	3:J:1255:VAL:HG11	1.88	0.56
2:I:139:ASN:O	2:I:141:THR:HG22	2.06	0.56
2:I:1103:VAL:HG21	2:I:1112:ILE:HD11	1.87	0.56
5:F:408:MET:O	5:F:413:ALA:N	2.34	0.56
2:I:297:VAL:HG13	2:I:313:ALA:HA	1.88	0.56
2:I:883:LEU:HD12	2:I:1052:VAL:HG21	1.86	0.56
3:J:91:GLU:OE1	3:J:101:ARG:NH2	2.39	0.56
3:J:143:SER:N	3:J:180:MET:SD	2.79	0.56
3:J:1188:GLU:OE1	3:J:1188:GLU:N	2.39	0.56
2:I:1225:VAL:HG23	3:J:638:SER:CB	2.36	0.55
3:J:70:CYS:SG	3:J:74:LYS:N	2.79	0.55
1:G:142:MET:SD	1:G:144:ILE:HD11	2.46	0.55
2:I:1117:LEU:HD21	2:I:1182:ILE:HG21	1.89	0.55
3:J:112:ALA:HB1	3:J:117:LEU:HD11	1.86	0.55
5:F:534:PHE:HE1	5:F:560:LEU:HD11	1.70	0.55
1:H:124:VAL:HG13	1:H:125:LYS:HD3	1.87	0.55
2:I:591:TYR:CE1	2:I:616:ILE:HG21	2.41	0.55
2:I:807:TRP:O	2:I:809:GLY:N	2.39	0.55
2:I:189:ASP:OD1	2:I:193:ASN:N	2.37	0.55
1:G:199:ASP:OD1	1:G:199:ASP:N	2.37	0.55
3:J:366:CYS:SG	3:J:423:LEU:HD21	2.46	0.55
5:F:203:VAL:HG22	5:F:251:LEU:HD22	1.89	0.55
3:J:18:ASP:OD2	3:J:1373:ARG:NH2	2.40	0.55
5:F:431:ARG:NH2	5:F:632:PHE:O	2.40	0.55
2:I:1165:SER:O	2:I:1168:GLU:N	2.37	0.55
3:J:756:GLU:OE1	3:J:756:GLU:N	2.38	0.55
5:F:397:GLN:OE1	5:F:397:GLN:N	2.39	0.55
1:G:7:GLU:N	1:G:7:GLU:OE1	2.40	0.54
2:I:143:ARG:NE	2:I:512:SER:O	2.39	0.54
3:J:384:LYS:HG3	3:J:415:VAL:HG12	1.90	0.54
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.89	0.54
2:I:816:ILE:HG22	2:I:817:LEU:O	2.07	0.54
3:J:45:ASN:ND2	5:F:237:GLU:OE2	2.39	0.54
5:F:154:LEU:HB3	5:F:159:LEU:HD11	1.89	0.54
3:J:1261:LEU:HD12	3:J:1261:LEU:O	2.07	0.54
2:I:563:THR:HG21	3:J:780:ARG:NH1	2.22	0.54
3:J:1176:VAL:HG22	3:J:1187:GLU:HB3	1.88	0.54
3:J:57:PHE:CZ	3:J:252:LEU:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:728:ASP:OD1	2:I:729:ALA:N	2.39	0.54
5:F:302:LEU:O	5:F:306:VAL:HG22	2.08	0.54
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.90	0.54
2:I:657:THR:HG21	2:I:1188:ASP:CB	2.37	0.54
2:I:1313:HIS:O	4:K:28:ARG:NH1	2.41	0.54
5:F:108:PHE:O	5:F:956:ARG:NH1	2.41	0.54
1:H:76:GLU:N	1:H:76:GLU:OE1	2.41	0.54
3:J:145:VAL:HG21	3:J:188:LEU:HD11	1.90	0.54
3:J:515:ARG:NH1	3:J:718:SER:O	2.40	0.54
2:I:1120:ALA:HB2	2:I:1199:LEU:HG	1.90	0.53
2:I:978:VAL:HG21	2:I:1010:GLN:NE2	2.22	0.53
3:J:897:HIS:HA	3:J:908:ILE:HD11	1.91	0.53
1:G:72:GLU:OE2	2:I:726:TYR:OH	2.26	0.53
5:F:471:GLU:OE1	5:F:471:GLU:N	2.37	0.53
5:F:511:ALA:N	5:F:582:ASP:OD2	2.41	0.53
3:J:353:SER:OG	3:J:354:VAL:N	2.42	0.53
5:F:586:ASN:ND2	5:F:589:LEU:HD23	2.23	0.53
1:H:147:GLN:N	1:H:147:GLN:OE1	2.42	0.53
2:I:1060:ILE:HD11	2:I:1076:ILE:HD13	1.91	0.53
5:F:128:LEU:HD22	5:F:718:PHE:HE1	1.73	0.53
5:F:276:LEU:HD13	5:F:308:GLY:HA3	1.91	0.53
2:I:560:PRO:O	3:J:780:ARG:NH2	2.42	0.53
10:F:1000:ADP:O1B	11:F:1001:AF3:F1	2.17	0.53
10:F:1000:ADP:O3A	11:F:1001:AF3:F3	2.17	0.53
3:J:256:ASP:N	3:J:256:ASP:OD1	2.42	0.53
3:J:646:ILE:HD12	3:J:762:ASN:ND2	2.24	0.53
3:J:114:ILE:HA	3:J:117:LEU:HD12	1.90	0.53
3:J:1048:ARG:NH2	3:J:1110:GLU:OE2	2.40	0.52
3:J:1109:LEU:HD22	3:J:1121:LEU:CD2	2.39	0.52
3:J:1140:ARG:NH2	3:J:1236:GLU:OE2	2.41	0.52
5:F:150:GLN:O	5:F:765:ARG:NH1	2.41	0.52
3:J:885:VAL:HG21	3:J:1255:VAL:CG1	2.39	0.52
5:F:936:LEU:HD12	5:F:937:THR:N	2.24	0.52
3:J:138:VAL:HG21	3:J:145:VAL:HB	1.91	0.52
3:J:1293:GLU:N	3:J:1293:GLU:OE1	2.43	0.52
1:H:11:PRO:HB2	1:H:28:LEU:HD12	1.91	0.52
2:I:857:VAL:O	5:F:733:ARG:NH2	2.40	0.52
3:J:349:TYR:HB3	3:J:470:VAL:HG22	1.91	0.52
3:J:810:THR:HG22	3:J:893:GLY:HA3	1.90	0.52
2:I:773:LEU:HD23	2:I:774:GLY:N	2.25	0.52
1:H:48:LEU:HD21	3:J:539:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:141:THR:HG21	2:I:514:PHE:HE1	1.75	0.52
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.92	0.52
1:G:223:ILE:HD12	1:H:8:PHE:CE1	2.45	0.51
2:I:303:ASP:O	2:I:307:GLY:N	2.43	0.51
5:F:147:LEU:O	5:F:150:GLN:NE2	2.40	0.51
3:J:317:THR:OG1	3:J:318:GLY:N	2.42	0.51
3:J:705:THR:OG1	3:J:716:GLN:O	2.29	0.51
1:H:208:ASN:OD1	1:H:209:GLY:N	2.44	0.51
3:J:1265:THR:OG1	3:J:1303:SER:OG	2.28	0.51
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.44	0.51
1:G:218:ARG:NE	1:H:231:PHE:O	2.44	0.51
2:I:283:LYS:O	2:I:285:ILE:HG23	2.10	0.51
3:J:846:GLU:OE1	3:J:846:GLU:N	2.43	0.51
3:J:1249:ASN:OD1	3:J:1250:ASP:N	2.44	0.51
5:F:866:ASN:OD1	5:F:866:ASN:N	2.44	0.51
3:J:981:GLU:OE2	3:J:995:TYR:N	2.43	0.51
3:J:1241:TYR:CG	3:J:1248:ILE:HD12	2.46	0.51
10:F:1000:ADP:O3B	11:F:1001:AF3:F2	2.18	0.51
2:I:149:LEU:N	2:I:531:SER:O	2.44	0.51
3:J:128:LEU:HD21	3:J:189:LEU:HD23	1.93	0.51
3:J:363:LEU:HD21	3:J:500:ILE:HD13	1.93	0.50
3:J:412:LEU:HD21	3:J:441:LEU:HD21	1.93	0.50
3:J:833:GLU:OE1	3:J:838:ARG:NH2	2.44	0.50
3:J:1048:ARG:NH2	3:J:1057:SER:OG	2.44	0.50
1:G:182:ARG:NH1	1:G:204:GLU:OE2	2.44	0.50
2:I:320:ASP:OD1	2:I:321:LEU:N	2.42	0.50
2:I:941:LYS:NZ	2:I:1037:THR:O	2.35	0.50
3:J:412:LEU:HD21	3:J:441:LEU:CD2	2.41	0.50
1:G:182:ARG:NH1	2:I:1090:ASN:O	2.45	0.50
3:J:17:PHE:HZ	3:J:20:ILE:HD13	1.77	0.50
5:F:930:ASN:C	5:F:931:ILE:HD12	2.32	0.50
2:I:183:TRP:N	2:I:199:ASP:OD1	2.44	0.50
2:I:198:ILE:HD11	2:I:388:LEU:HD22	1.94	0.50
5:F:277:LEU:O	5:F:310:LEU:N	2.43	0.50
2:I:1120:ALA:HB1	2:I:1198:LEU:HG	1.93	0.50
3:J:809:VAL:HG21	3:J:909:ILE:HD13	1.93	0.50
2:I:198:ILE:HD12	2:I:389:PHE:CZ	2.46	0.50
2:I:159:SER:HB2	2:I:442:VAL:HG21	1.94	0.50
3:J:1005:LYS:H	3:J:1017:VAL:HG23	1.76	0.50
5:F:894:GLN:O	5:F:897:LYS:NZ	2.44	0.50
3:J:112:ALA:N	3:J:300:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:868:VAL:HG22	5:F:869:ASN:H	1.75	0.50
3:J:819:GLY:O	3:J:881:LYS:NZ	2.37	0.49
5:F:564:GLU:OE2	5:F:589:LEU:HD13	2.11	0.49
1:G:13:LEU:CD2	1:G:16:ILE:HD11	2.42	0.49
1:H:186:ASN:OD1	1:H:186:ASN:N	2.45	0.49
2:I:633:LEU:H	2:I:633:LEU:HD23	1.78	0.49
2:I:758:ARG:NH1	2:I:835:GLU:OE1	2.45	0.49
3:J:361:LEU:O	3:J:626:TYR:OH	2.21	0.49
5:F:809:LEU:O	5:F:967:HIS:NE2	2.45	0.49
2:I:240:GLU:N	2:I:240:GLU:OE1	2.42	0.49
2:I:209:ILE:O	2:I:213:LEU:HD13	2.12	0.49
2:I:797:GLY:N	2:I:1231:TYR:OH	2.46	0.49
3:J:338:PHE:O	3:J:1352:ILE:HG23	2.13	0.49
3:J:353:SER:OG	3:J:354:VAL:O	2.27	0.49
3:J:872:LEU:O	3:J:876:SER:N	2.44	0.49
3:J:1344:LEU:HD13	3:J:1355:ARG:CD	2.43	0.49
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.48	0.49
3:J:460:ASP:OD1	3:J:460:ASP:N	2.46	0.49
3:J:586:GLY:HA3	3:J:612:LEU:HD11	1.95	0.49
2:I:596:ASP:OD1	2:I:597:GLY:N	2.46	0.49
3:J:426:ALA:HB3	3:J:427:PRO:CD	2.42	0.49
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.95	0.49
2:I:1274:GLU:OE1	2:I:1274:GLU:N	2.43	0.48
2:I:475:VAL:HG22	2:I:492:MET:O	2.13	0.48
3:J:226:ALA:HB1	3:J:1338:ALA:HA	1.94	0.48
3:J:1061:VAL:N	3:J:1105:ALA:O	2.44	0.48
2:I:210:LEU:HD23	2:I:220:ILE:HG23	1.94	0.48
2:I:926:GLY:HA3	2:I:1054:LEU:HD12	1.93	0.48
5:F:892:GLU:OE1	5:F:893:ALA:N	2.46	0.48
3:J:1316:THR:HG21	3:J:1322:ALA:HB2	1.95	0.48
3:J:129:ASP:O	3:J:157:GLN:NE2	2.47	0.48
3:J:263:SER:OG	3:J:264:ASP:N	2.45	0.48
3:J:842:ARG:NH1	3:J:1254:GLU:OE2	2.44	0.48
5:F:256:LEU:HD21	5:F:295:GLU:HB2	1.95	0.48
3:J:836:ARG:NH1	3:J:870:ASP:OD1	2.41	0.48
3:J:923:ILE:HD12	3:J:1248:ILE:HD13	1.96	0.48
5:F:564:GLU:OE1	5:F:593:ARG:NH2	2.41	0.48
2:I:66:SER:CB	2:I:104:ILE:HG22	2.43	0.48
2:I:529:ARG:HH11	2:I:572:ILE:HG22	1.78	0.48
3:J:821:MET:O	3:J:1231:ARG:NH1	2.46	0.48
5:F:192:HIS:NE2	5:F:780:GLU:OE1	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:371:ASN:O	5:F:371:ASN:ND2	2.47	0.48
3:J:746:LEU:HD12	3:J:746:LEU:H	1.79	0.48
2:I:421:SER:OG	2:I:424:ASP:OD1	2.32	0.48
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.96	0.48
3:J:294:ASN:OD1	3:J:297:ARG:NH2	2.46	0.48
2:I:564:PRO:HG2	2:I:572:ILE:HD13	1.95	0.47
2:I:1107:MET:HG2	3:J:740:LEU:HD13	1.96	0.47
2:I:1120:ALA:HB2	2:I:1199:LEU:CD2	2.43	0.47
2:I:739:ASP:OD1	2:I:740:GLU:N	2.47	0.47
2:I:145:ILE:HD12	2:I:145:ILE:N	2.30	0.47
2:I:209:ILE:O	2:I:213:LEU:N	2.48	0.47
2:I:657:THR:HG21	2:I:1188:ASP:HB3	1.96	0.47
3:J:144:TYR:OH	3:J:293:ARG:NH1	2.47	0.47
3:J:199:GLU:OE1	3:J:200:GLN:N	2.48	0.47
5:F:824:ALA:CB	5:F:836:LEU:HD23	2.45	0.47
2:I:820:GLU:O	2:I:824:GLN:N	2.40	0.47
2:I:1117:LEU:HD21	2:I:1182:ILE:CG2	2.44	0.47
2:I:1243:MET:O	2:I:1244:HIS:ND1	2.48	0.47
2:I:184:LEU:HD13	2:I:389:PHE:HZ	1.78	0.47
2:I:831:ILE:HG22	2:I:831:ILE:O	2.14	0.47
3:J:527:LEU:O	3:J:528:THR:OG1	2.31	0.47
5:F:133:ARG:HD3	5:F:821:VAL:HG12	1.96	0.47
2:I:420:LEU:HD13	2:I:425:ILE:HD11	1.96	0.47
2:I:719:LYS:N	2:I:751:TYR:OH	2.48	0.47
3:J:114:ILE:HG21	3:J:308:ASP:OD1	2.15	0.47
3:J:425:ARG:NH1	3:J:464:ASP:OD2	2.48	0.47
3:J:639:VAL:HG23	3:J:722:ILE:HD11	1.97	0.47
2:I:244:GLU:OE1	2:I:244:GLU:N	2.46	0.47
3:J:79:LYS:HA	5:F:13:THR:HG21	1.97	0.47
1:G:156:SER:O	1:G:159:ILE:HG22	2.15	0.47
5:F:128:LEU:HD22	5:F:718:PHE:CE1	2.51	0.46
5:F:144:ALA:O	5:F:193:GLN:NE2	2.48	0.46
5:F:227:PHE:CD2	5:F:253:ILE:HD11	2.50	0.46
1:G:65:LEU:HD11	1:G:168:ILE:HD12	1.97	0.46
2:I:850:ILE:H	2:I:850:ILE:HD12	1.80	0.46
2:I:1186:VAL:HG23	2:I:1187:PHE:N	2.30	0.46
3:J:835:LEU:O	3:J:839:VAL:HG22	2.15	0.46
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.30	0.46
3:J:331:ILE:HG22	3:J:1328:THR:HG21	1.97	0.46
3:J:923:ILE:HD13	3:J:1253:ILE:HD11	1.97	0.46
2:I:1101:LEU:HD21	3:J:508:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:265:LEU:HD22	3:J:265:LEU:H	1.80	0.46
3:J:487:THR:HG1	3:J:618:VAL:HG21	1.79	0.46
1:G:185:TYR:HB2	1:G:201:LEU:HD11	1.98	0.46
3:J:204:GLU:O	3:J:208:THR:N	2.45	0.46
1:H:204:GLU:N	1:H:204:GLU:OE1	2.48	0.46
3:J:797:THR:HG22	3:J:924:GLY:CA	2.44	0.46
3:J:958:ILE:HG23	3:J:982:LEU:CD1	2.46	0.46
3:J:986:ASP:OD1	3:J:990:ARG:N	2.41	0.46
5:F:513:ALA:HB1	5:F:535:HIS:HB2	1.97	0.46
1:G:224:LEU:O	1:G:224:LEU:HD23	2.15	0.46
2:I:865:LEU:HD12	2:I:869:GLY:C	2.36	0.46
2:I:1117:LEU:HD21	2:I:1182:ILE:HB	1.98	0.46
3:J:1176:VAL:HG22	3:J:1187:GLU:CB	2.46	0.46
5:F:328:LEU:HD21	5:F:417:LEU:CD2	2.46	0.46
2:I:1131:MET:SD	2:I:1131:MET:N	2.88	0.46
2:I:1186:VAL:HG23	2:I:1187:PHE:H	1.81	0.46
3:J:146:VAL:HG13	3:J:176:PHE:CE1	2.51	0.46
3:J:450:HIS:NE2	3:J:625:MET:SD	2.89	0.46
2:I:146:VAL:HG23	2:I:529:ARG:HB3	1.98	0.46
2:I:1117:LEU:HD21	2:I:1182:ILE:CB	2.46	0.46
7:B:5:DT:H2''	7:B:6:DT:H71	1.96	0.46
2:I:14:ASP:OD2	2:I:1156:ARG:NH2	2.49	0.45
3:J:329:ASP:N	3:J:329:ASP:OD1	2.50	0.45
3:J:423:LEU:HD22	3:J:437:PHE:CD2	2.51	0.45
2:I:211:ARG:NH1	2:I:356:THR:OG1	2.48	0.45
2:I:453:ILE:HD13	2:I:530:ILE:HD12	1.98	0.45
2:I:805:MET:HB3	2:I:1225:VAL:HG21	1.97	0.45
3:J:117:LEU:HD13	3:J:139:LEU:HD21	1.98	0.45
5:F:99:GLU:HA	5:F:102:LEU:HD23	1.99	0.45
5:F:841:VAL:CG1	5:F:895:ILE:HD11	2.47	0.45
5:F:842:ARG:HE	5:F:853:ALA:HB1	1.81	0.45
1:H:60:GLU:OE1	1:H:170:ARG:N	2.49	0.45
2:I:882:ILE:HD11	2:I:919:ARG:HE	1.80	0.45
3:J:317:THR:OG1	3:J:322:ARG:O	2.11	0.45
2:I:146:VAL:HG11	2:I:513:GLN:OE1	2.16	0.45
3:J:117:LEU:HD13	3:J:139:LEU:CD2	2.46	0.45
3:J:1230:THR:OG1	3:J:1231:ARG:N	2.50	0.45
5:F:798:SER:OG	5:F:799:SER:N	2.50	0.45
2:I:77:GLU:OE1	2:I:77:GLU:N	2.47	0.45
2:I:453:ILE:HG22	2:I:585:GLY:O	2.16	0.45
2:I:888:THR:O	2:I:914:LYS:N	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:229:GLN:OE1	3:J:230:SER:N	2.50	0.45
2:I:561:ILE:CD1	2:I:661:VAL:HG12	2.46	0.45
2:I:690:VAL:HG22	2:I:691:PRO:CD	2.47	0.45
4:K:8:ASP:OD1	4:K:8:ASP:N	2.49	0.45
2:I:762:ASN:OD1	2:I:762:ASN:N	2.50	0.45
3:J:193:ASP:OD1	3:J:193:ASP:N	2.50	0.45
3:J:975:ILE:HG22	3:J:1001:ALA:H	1.82	0.45
3:J:1062:LEU:O	3:J:1067:ARG:NE	2.49	0.45
2:I:800:MET:SD	2:I:822:VAL:HG21	2.57	0.45
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.98	0.45
1:H:113:ALA:N	1:H:126:PRO:O	2.49	0.45
2:I:314:ASN:O	2:I:352:ARG:NH1	2.50	0.45
2:I:802:VAL:HG12	2:I:1096:ILE:HB	1.98	0.45
2:I:696:ASP:O	2:I:795:ALA:HB1	2.17	0.45
5:F:216:LEU:HD21	5:F:227:PHE:O	2.17	0.44
2:I:724:VAL:HG13	2:I:774:GLY:N	2.31	0.44
2:I:794:LEU:CD2	2:I:796:LEU:HD11	2.47	0.44
1:H:84:ASN:ND2	1:H:130:ILE:O	2.50	0.44
2:I:138:ILE:HD12	2:I:506:PHE:HB3	1.98	0.44
3:J:411:ILE:O	3:J:415:VAL:HG13	2.17	0.44
3:J:844:THR:OG1	3:J:846:GLU:O	2.36	0.44
3:J:1295:ASN:OD1	3:J:1295:ASN:N	2.50	0.44
5:F:34:PHE:O	5:F:38:GLY:CA	2.65	0.44
5:F:164:ASP:OD2	5:F:415:ARG:NH2	2.46	0.44
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	2.00	0.44
3:J:923:ILE:CD1	3:J:1248:ILE:HD13	2.48	0.44
5:F:648:ASN:OD1	5:F:652:ASN:ND2	2.49	0.44
1:G:79:LEU:HD23	1:G:79:LEU:O	2.18	0.44
5:F:870:ARG:O	5:F:872:THR:N	2.51	0.44
2:I:557:ARG:O	2:I:558:VAL:HG23	2.18	0.44
2:I:630:VAL:HG13	2:I:631:GLU:CD	2.38	0.44
5:F:877:VAL:CG2	5:F:962:LEU:HD21	2.47	0.44
2:I:727:VAL:HG12	2:I:728:ASP:N	2.32	0.44
3:J:34:SER:O	5:F:28:ARG:NH2	2.51	0.44
3:J:1145:PHE:CE1	3:J:1256:ILE:HG21	2.53	0.44
5:F:202:ARG:NH2	5:F:249:GLU:O	2.50	0.44
5:F:509:ILE:HG22	5:F:562:CYS:HB2	1.98	0.44
2:I:205:PRO:O	2:I:208:ILE:HG22	2.18	0.44
2:I:230:PHE:O	2:I:332:ARG:NE	2.49	0.44
3:J:94:GLN:O	3:J:97:VAL:HG12	2.18	0.44
3:J:316:ILE:HG13	3:J:324:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:49:LEU:HD12	2:I:73:TYR:CE2	2.53	0.43
3:J:703:THR:OG1	3:J:704:GLU:N	2.51	0.43
3:J:363:LEU:HD21	3:J:500:ILE:HG21	2.00	0.43
3:J:416:ILE:O	3:J:416:ILE:HD12	2.18	0.43
1:G:144:ILE:N	1:G:144:ILE:HD12	2.33	0.43
2:I:1275:VAL:HG12	2:I:1279:GLU:OE2	2.18	0.43
5:F:584:PRO:CB	5:F:589:LEU:HD11	2.49	0.43
5:F:585:PHE:O	5:F:625:TYR:OH	2.25	0.43
5:F:120:ILE:HD13	5:F:870:ARG:NH2	2.34	0.43
5:F:450:VAL:O	5:F:450:VAL:HG12	2.17	0.43
1:H:201:LEU:CD2	1:H:203:ILE:HD11	2.48	0.43
2:I:208:ILE:O	2:I:212:ALA:N	2.46	0.43
2:I:622:ASN:OD1	2:I:622:ASN:N	2.51	0.43
2:I:724:VAL:HG13	2:I:724:VAL:O	2.19	0.43
3:J:1219:ASP:OD1	3:J:1220:ILE:N	2.51	0.43
5:F:165:VAL:HB	5:F:190:ILE:HD12	2.00	0.43
2:I:1066:MET:HG3	2:I:1076:ILE:HD11	1.99	0.43
3:J:282:LEU:O	3:J:286:ALA:N	2.51	0.43
3:J:661:VAL:CG1	3:J:685:ILE:HD11	2.49	0.43
3:J:759:ILE:HD12	3:J:771:GLN:HB3	2.00	0.43
3:J:1089:LEU:HD22	3:J:1094:ASP:O	2.19	0.43
3:J:1220:ILE:O	3:J:1224:ARG:N	2.50	0.43
7:B:26:DT:C2'	7:B:27:DT:H71	2.48	0.43
2:I:657:THR:O	2:I:657:THR:OG1	2.37	0.43
3:J:930:LEU:HD12	3:J:1137:GLY:HA2	2.00	0.43
5:F:13:THR:HG23	5:F:793:SER:HB2	1.99	0.43
5:F:207:VAL:HG12	5:F:280:ASP:HB2	2.01	0.43
3:J:1166:GLY:N	3:J:1174:ARG:O	2.51	0.43
5:F:925:ARG:HG2	5:F:931:ILE:HD13	2.01	0.43
1:G:43:LEU:HA	1:G:46:ILE:HG22	1.99	0.43
2:I:1077:SER:HA	3:J:356:THR:HG23	2.01	0.43
3:J:1183:SER:OG	3:J:1184:ASP:N	2.52	0.43
5:F:7:GLN:OE1	5:F:9:TRP:NE1	2.49	0.43
5:F:191:LEU:O	5:F:195:LEU:HD23	2.19	0.43
2:I:124:MET:CE	2:I:498:ILE:HD13	2.49	0.43
2:I:180:ARG:NH1	2:I:393:ASP:O	2.52	0.43
2:I:490:GLN:HA	2:I:493:ILE:HG22	2.00	0.42
2:I:759:SER:OG	2:I:763:THR:N	2.46	0.42
2:I:23:ASP:OD1	2:I:23:ASP:N	2.51	0.42
2:I:257:ALA:CB	2:I:285:ILE:HG21	2.49	0.42
2:I:929:ILE:HD13	2:I:1055:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:509:ILE:HD12	5:F:593:ARG:HD3	2.01	0.42
5:F:584:PRO:HB3	5:F:589:LEU:HD11	2.01	0.42
7:B:28:DT:C2'	7:B:29:DT:H71	2.49	0.42
2:I:223:LEU:O	2:I:430:LYS:NZ	2.46	0.42
3:J:390:LEU:HD13	3:J:407:VAL:HG21	2.01	0.42
5:F:552:GLU:O	5:F:556:GLY:N	2.52	0.42
2:I:1272:GLU:O	2:I:1275:VAL:N	2.52	0.42
3:J:885:VAL:HG21	3:J:1255:VAL:HG13	1.99	0.42
5:F:801:ILE:HD13	5:F:962:LEU:HD23	2.02	0.42
2:I:124:MET:SD	2:I:493:ILE:HD11	2.59	0.42
3:J:490:ILE:CG1	3:J:500:ILE:HD12	2.50	0.42
2:I:491:ASP:N	2:I:491:ASP:OD1	2.50	0.42
2:I:561:ILE:HD12	2:I:661:VAL:HG12	2.01	0.42
3:J:112:ALA:CB	3:J:117:LEU:HD11	2.49	0.42
3:J:718:SER:OG	3:J:719:PHE:N	2.52	0.42
3:J:1111:ASP:OD1	3:J:1112:GLY:N	2.53	0.42
4:K:14:GLY:O	4:K:15:ASN:ND2	2.48	0.42
3:J:849:LEU:HD12	3:J:855:ASP:O	2.19	0.42
7:B:28:DT:H2''	7:B:29:DT:H71	2.02	0.42
1:H:194:GLN:O	1:H:196:THR:OG1	2.32	0.42
3:J:44:ILE:HD13	3:J:260:PHE:CD1	2.55	0.42
3:J:678:ARG:O	3:J:682:VAL:HG23	2.19	0.42
5:F:627:GLU:O	5:F:671:ARG:NH1	2.51	0.42
1:H:84:ASN:OD1	3:J:551:ARG:NH2	2.44	0.42
1:G:229:GLU:HA	1:G:232:VAL:HG23	2.02	0.42
1:H:56:VAL:HG13	1:H:144:ILE:HG23	2.02	0.42
2:I:512:SER:O	2:I:512:SER:OG	2.36	0.42
2:I:905:ILE:O	2:I:905:ILE:HG22	2.19	0.42
3:J:800:LEU:HD12	3:J:1256:ILE:HG12	2.02	0.42
5:F:121:ASP:OD1	5:F:121:ASP:N	2.53	0.42
5:F:935:GLU:O	5:F:939:ILE:HG23	2.20	0.42
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.20	0.41
2:I:297:VAL:HG12	2:I:315:MET:O	2.20	0.41
3:J:67:ASP:OD1	3:J:95:THR:HG22	2.20	0.41
3:J:317:THR:OG1	3:J:320:ASN:O	2.37	0.41
3:J:1061:VAL:HG23	3:J:1107:VAL:CG2	2.50	0.41
5:F:613:LEU:O	5:F:616:THR:HG22	2.20	0.41
5:F:788:LEU:O	5:F:792:LEU:HD23	2.20	0.41
2:I:91:THR:HG22	2:I:138:ILE:O	2.20	0.41
2:I:1259:LEU:HD22	2:I:1264:GLN:HB3	2.03	0.41
3:J:324:LEU:O	3:J:324:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:891:ASP:OD1	3:J:891:ASP:N	2.52	0.41
2:I:180:ARG:O	2:I:396:ASP:N	2.48	0.41
2:I:955:GLN:NE2	2:I:959:ASP:OD2	2.54	0.41
2:I:995:ASP:OD1	2:I:996:ARG:N	2.54	0.41
2:I:1165:SER:O	2:I:1167:GLU:N	2.53	0.41
5:F:435:THR:C	5:F:436:ILE:HD12	2.41	0.41
3:J:374:LEU:HD12	3:J:409:TRP:CH2	2.55	0.41
3:J:473:THR:HG23	3:J:476:ALA:H	1.85	0.41
3:J:1321:SER:OG	3:J:1349:GLU:OE2	2.38	0.41
5:F:120:ILE:HG22	5:F:799:SER:HB3	2.02	0.41
2:I:896:THR:O	2:I:899:GLU:N	2.49	0.41
3:J:85:CYS:O	3:J:89:GLY:N	2.51	0.41
7:B:5:DT:C2'	7:B:6:DT:H71	2.50	0.41
1:H:117:HIS:NE2	1:H:119:GLY:O	2.53	0.41
2:I:1075:VAL:HG22	3:J:461:PHE:O	2.20	0.41
5:F:234:ARG:NH2	5:F:249:GLU:OE2	2.54	0.41
5:F:643:TYR:HH	5:F:647:TYR:HE1	1.69	0.41
1:G:57:THR:HG21	1:G:147:GLN:NE2	2.36	0.41
1:H:137:ASN:OD1	1:H:138:ALA:N	2.54	0.41
2:I:471:VAL:O	2:I:475:VAL:HG23	2.20	0.41
2:I:724:VAL:HG12	2:I:775:GLU:O	2.21	0.41
2:I:804:PHE:O	3:J:638:SER:OG	2.17	0.41
2:I:1119:MET:CE	2:I:1204:LEU:HD13	2.51	0.41
3:J:697:MET:HE2	3:J:741:ALA:HB3	2.00	0.41
3:J:357:VAL:HG12	3:J:359:PRO:HD3	2.02	0.41
3:J:848:VAL:HB	3:J:858:VAL:HG22	2.03	0.41
5:F:571:ASN:OD1	10:F:1000:ADP:O3'	2.35	0.41
2:I:629:PHE:CE1	2:I:650:VAL:HG21	2.56	0.40
2:I:1160:ASP:N	2:I:1160:ASP:OD1	2.54	0.40
2:I:1270:PHE:HZ	2:I:1278:LEU:HD12	1.86	0.40
3:J:84:ILE:N	5:F:42:LEU:O	2.44	0.40
3:J:830:ASP:OD2	3:J:832:LYS:NZ	2.54	0.40
2:I:27:LEU:HD13	2:I:524:ILE:CD1	2.51	0.40
2:I:397:LEU:N	2:I:418:GLY:O	2.48	0.40
2:I:1075:VAL:O	2:I:1075:VAL:HG23	2.21	0.40
3:J:516:ASP:OD2	3:J:547:ARG:NH1	2.53	0.40
3:J:981:GLU:OE1	3:J:983:LYS:NZ	2.38	0.40
1:H:27:THR:C	1:H:28:LEU:HD22	2.41	0.40
1:H:86:LYS:NZ	3:J:532:GLU:OE2	2.54	0.40
2:I:136:PHE:CE1	2:I:145:ILE:HD13	2.55	0.40
2:I:487:LEU:O	2:I:487:LEU:HD12	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:100:GLU:OE1	3:J:101:ARG:N	2.53	0.40
3:J:474:LEU:HD21	4:K:27:ALA:CB	2.51	0.40
3:J:487:THR:HG23	3:J:488:ASN:OD1	2.21	0.40
2:I:1216:ARG:HG3	2:I:1217:THR:HG23	2.04	0.40
3:J:793:SER:O	3:J:797:THR:HG23	2.21	0.40
5:F:625:TYR:O	5:F:630:ASP:N	2.54	0.40
3:J:265:LEU:HD21	3:J:325:LYS:HE2	2.03	0.40
3:J:506:VAL:O	3:J:510:LEU:HD12	2.21	0.40
5:F:459:SER:O	5:F:463:ARG:N	2.47	0.40
7:B:7:DT:H2"	7:B:8:DT:H71	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	219/232 (94%)	197 (90%)	22 (10%)	0	100	100
1	H	214/232 (92%)	195 (91%)	19 (9%)	0	100	100
2	I	1338/1340 (100%)	1186 (89%)	151 (11%)	1 (0%)	48	79
3	J	1327/1358 (98%)	1180 (89%)	147 (11%)	0	100	100
4	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	9	39
5	F	964/966 (100%)	897 (93%)	66 (7%)	1 (0%)	48	79
All	All	4132/4200 (98%)	3719 (90%)	410 (10%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	1138	VAL
4	K	15	ASN
5	F	905	ALA

### 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	G	187/199 (94%)	174 (93%)	13 (7%)	12	39
1	H	184/199 (92%)	174 (95%)	10 (5%)	18	47
2	I	1155/1155 (100%)	1103 (96%)	52 (4%)	23	52
3	J	1117/1133 (99%)	1049 (94%)	68 (6%)	15	44
4	K	63/63 (100%)	60 (95%)	3 (5%)	21	50
5	F	819/819 (100%)	782 (96%)	37 (4%)	23	52
All	All	3525/3568 (99%)	3342 (95%)	183 (5%)	22	48

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	17	GLU
1	G	48	LEU
1	G	49	SER
1	G	70	THR
1	G	74	VAL
1	G	97	GLU
1	G	143	ARG
1	G	199	ASP
1	G	205	MET
1	G	206	GLU
1	G	228	LEU
1	G	231	PHE
1	G	234	LEU
1	H	12	ARG
1	H	13	LEU
1	H	14	VAL
1	H	48	LEU
1	H	183	ILE
1	H	186	ASN
1	H	188	GLU
1	H	194	GLN
1	H	196	THR

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Mol	Chain	Res	Type
1	H	224	LEU
2	I	31	GLN
2	I	36	GLN
2	I	47	TYR
2	I	150	HIS
2	I	161	LYS
2	I	237	LEU
2	I	283	LYS
2	I	291	TYR
2	I	333	ILE
2	I	336	LEU
2	I	453	ILE
2	I	473	ARG
2	I	486	THR
2	I	504	GLU
2	I	546	GLU
2	I	550	VAL
2	I	563	THR
2	I	575	LEU
2	I	604	HIS
2	I	622	ASN
2	I	623	LEU
2	I	693	LEU
2	I	699	LEU
2	I	737	ASN
2	I	755	LYS
2	I	757	THR
2	I	762	ASN
2	I	807	TRP
2	I	819	SER
2	I	830	THR
2	I	850	ILE
2	I	866	ASP
2	I	894	GLN
2	I	896	THR
2	I	913	VAL
2	I	931	VAL
2	I	935	THR
2	I	958	LYS
2	I	1060	ILE
2	I	1089	GLU
2	I	1138	VAL

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Mol	Chain	Res	Type
2	I	1151	LEU
2	I	1164	PHE
2	I	1170	MET
2	I	1178	LYS
2	I	1227	VAL
2	I	1235	LEU
2	I	1268	GLN
2	I	1289	GLU
2	I	1290	MET
2	I	1315	MET
2	I	1326	LEU
3	J	24	LEU
3	J	42	GLU
3	J	46	TYR
3	J	88	CYS
3	J	100	GLU
3	J	147	ILE
3	J	194	LEU
3	J	196	GLN
3	J	218	THR
3	J	223	LEU
3	J	229	GLN
3	J	244	VAL
3	J	248	ASP
3	J	256	ASP
3	J	265	LEU
3	J	334	LYS
3	J	357	VAL
3	J	360	TYR
3	J	366	CYS
3	J	374	LEU
3	J	400	MET
3	J	425	ARG
3	J	430	HIS
3	J	431	ARG
3	J	432	LEU
3	J	434	ILE
3	J	445	LYS
3	J	458	ASN
3	J	464	ASP
3	J	492	SER
3	J	508	LEU

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Mol	Chain	Res	Type
3	J	510	LEU
3	J	514	THR
3	J	515	ARG
3	J	526	VAL
3	J	538	ARG
3	J	548	VAL
3	J	552	ILE
3	J	617	THR
3	J	624	ILE
3	J	705	THR
3	J	710	ASP
3	J	714	GLU
3	J	731	ARG
3	J	746	LEU
3	J	770	LEU
3	J	800	LEU
3	J	814	CYS
3	J	818	GLU
3	J	874	GLU
3	J	895	CYS
3	J	910	ASN
3	J	930	LEU
3	J	1011	VAL
3	J	1023	HIS
3	J	1030	GLU
3	J	1098	GLN
3	J	1175	LEU
3	J	1208	ASP
3	J	1236	GLU
3	J	1244	GLN
3	J	1289	ASN
3	J	1295	ASN
3	J	1306	LEU
3	J	1321	SER
3	J	1342	ASP
3	J	1357	ILE
3	J	1368	ASP
4	K	15	ASN
4	K	43	ASN
4	K	47	THR
5	F	75	LYS
5	F	99	GLU

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Mol	Chain	Res	Type
5	F	108	PHE
5	F	120	ILE
5	F	121	ASP
5	F	131	ARG
5	F	138	GLU
5	F	142	MET
5	F	147	LEU
5	F	148	ARG
5	F	169	HIS
5	F	178	GLU
5	F	217	VAL
5	F	226	ARG
5	F	227	PHE
5	F	240	HIS
5	F	415	ARG
5	F	458	LYS
5	F	463	ARG
5	F	469	TYR
5	F	553	GLU
5	F	571	ASN
5	F	589	LEU
5	F	590	LEU
5	F	686	ASP
5	F	729	ASN
5	F	745	HIS
5	F	799	SER
5	F	865	LEU
5	F	866	ASN
5	F	869	ASN
5	F	870	ARG
5	F	872	THR
5	F	925	ARG
5	F	932	ARG
5	F	955	TRP
5	F	958	ASP

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

Mol	Chain	Res	Type
5	F	268	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z  > 2$
11	AF3	F	1001	-	0,3,3	-	-	-		
10	ADP	F	1000	-	24,29,29	0.87	0	29,45,45	1.21	2 (6%)

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
10	ADP	F	1000	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	1000	ADP	N3-C2-N1	-4.18	123.00	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	1000	ADP	C4-C5-N7	-2.28	106.92	109.34

There are no chirality outliers.

All (3) torsion outliers are listed below:

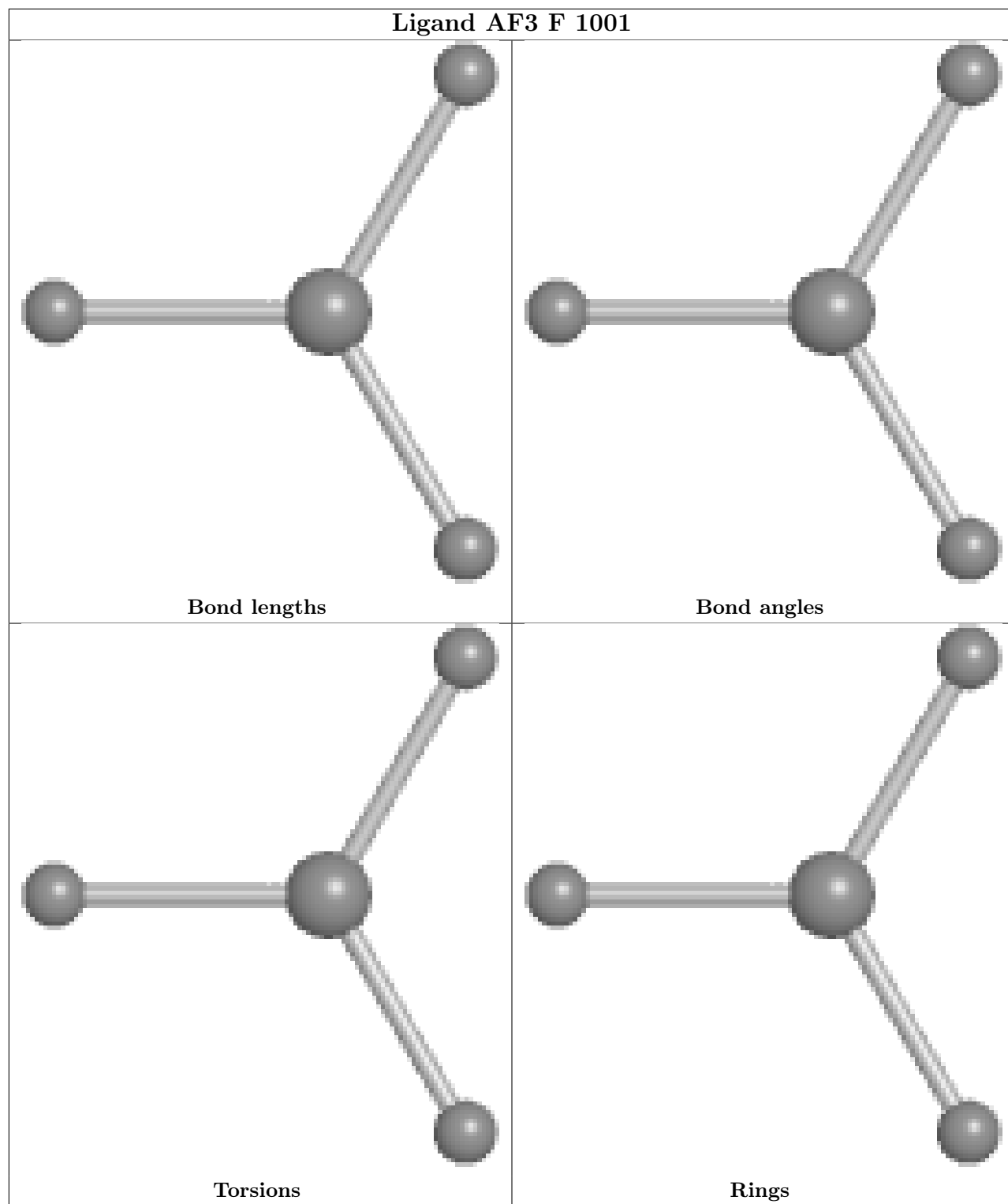
Mol	Chain	Res	Type	Atoms
10	F	1000	ADP	C5'-O5'-PA-O1A
10	F	1000	ADP	C5'-O5'-PA-O3A
10	F	1000	ADP	C5'-O5'-PA-O2A

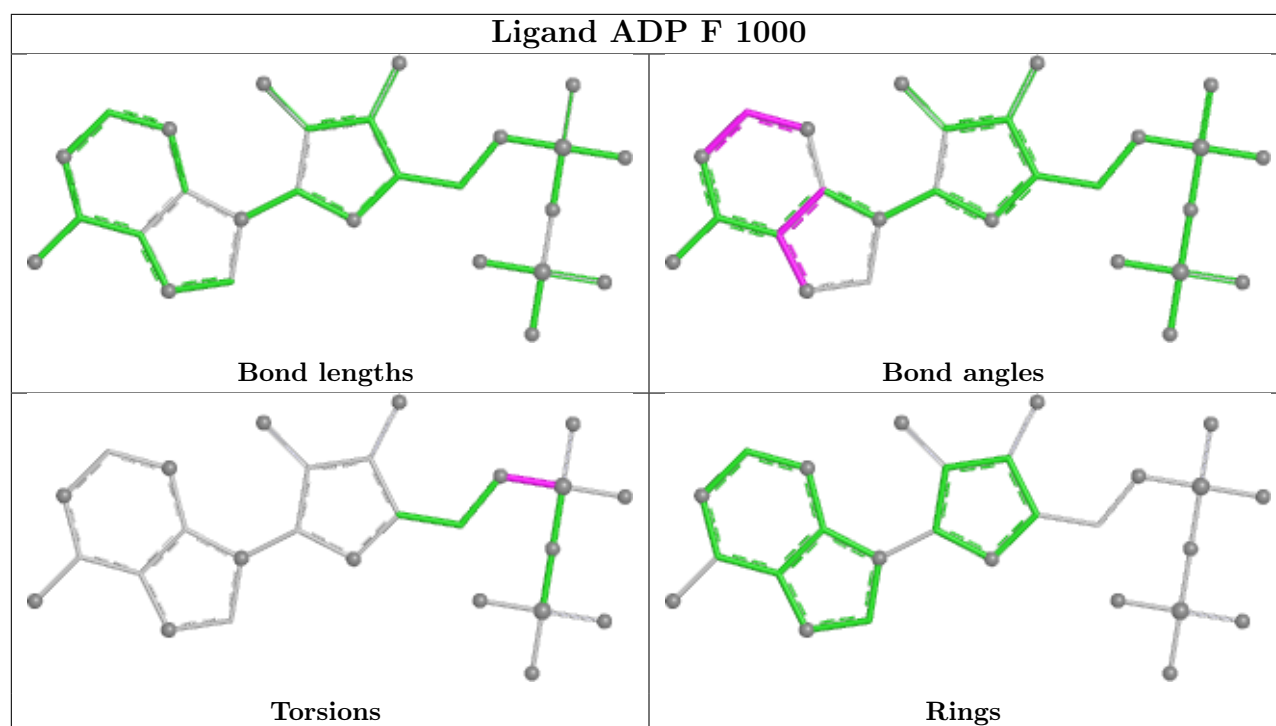
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	1001	AF3	3	0
10	F	1000	ADP	6	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	B	1
6	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	15:DT	O3'	23:DT	P	30.33
1	A	109:DA	O3'	117:DA	P	17.32

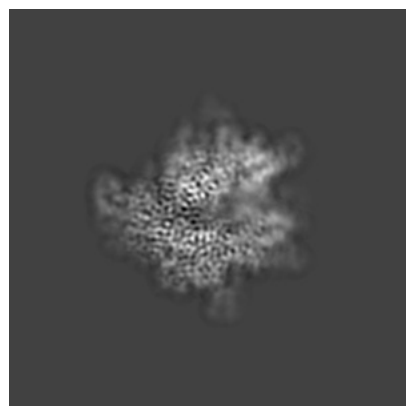
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40943. These allow visual inspection of the internal detail of the map and identification of artifacts.

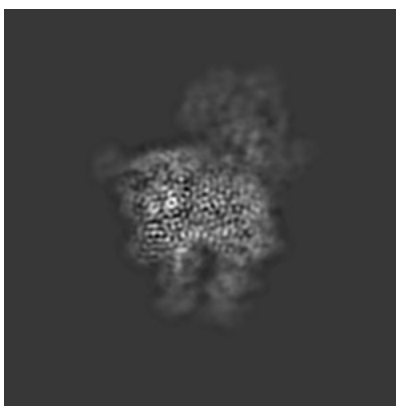
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

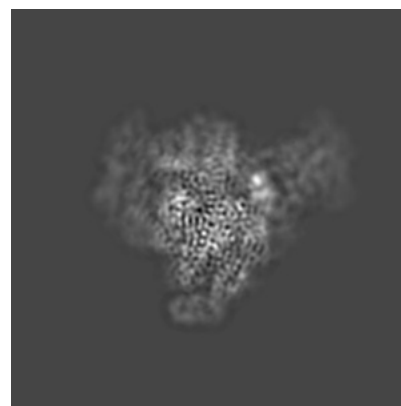
#### 6.1.1 Primary map



X

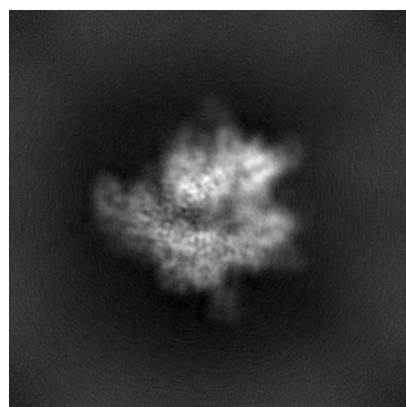


Y

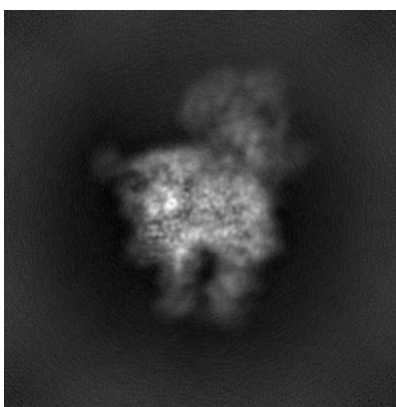


Z

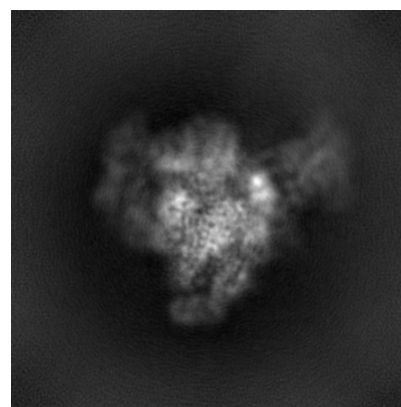
#### 6.1.2 Raw map



X



Y

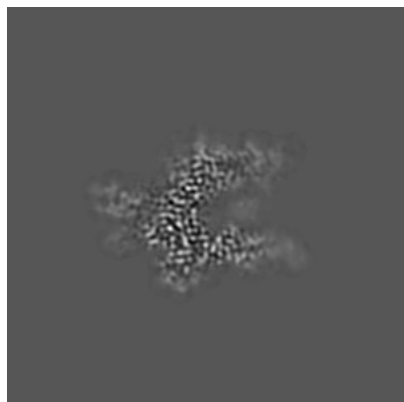


Z

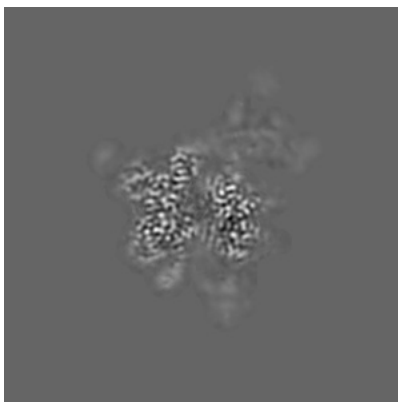
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

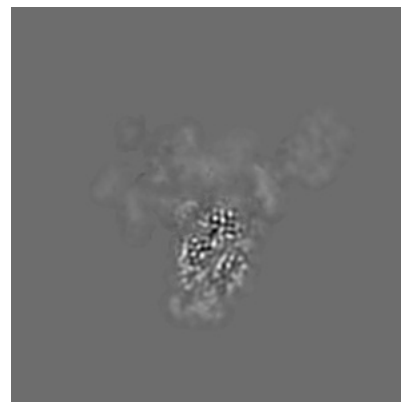
### 6.2.1 Primary map



X Index: 128

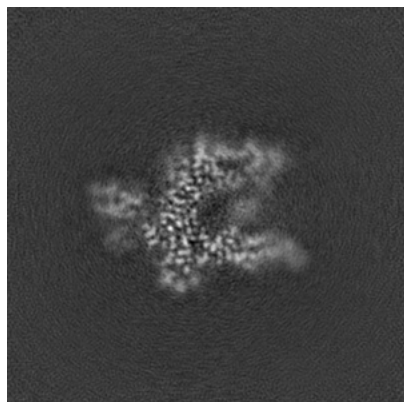


Y Index: 128

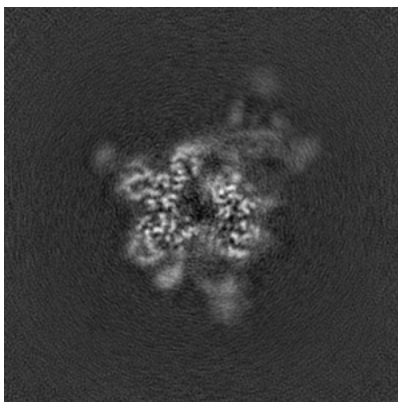


Z Index: 128

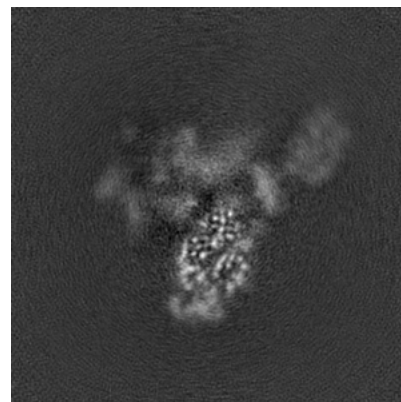
### 6.2.2 Raw map



X Index: 128



Y Index: 128



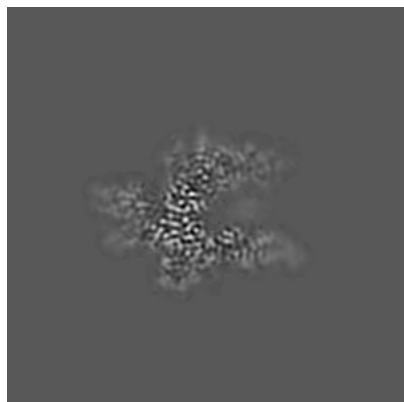
Z Index: 128

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

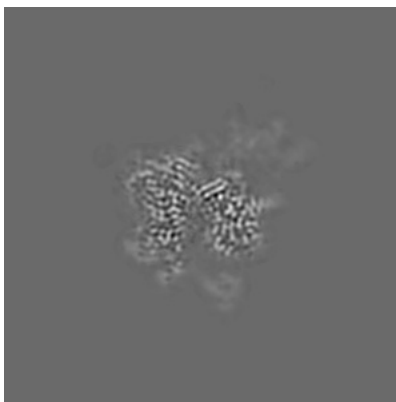


## 6.3 Largest variance slices [i](#)

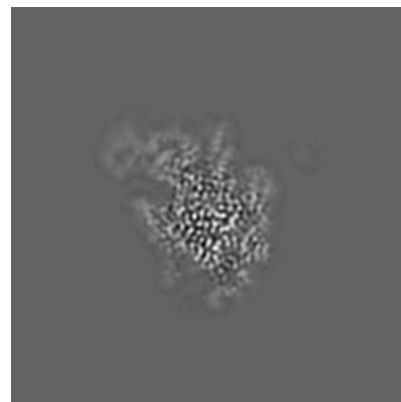
### 6.3.1 Primary map



X Index: 130

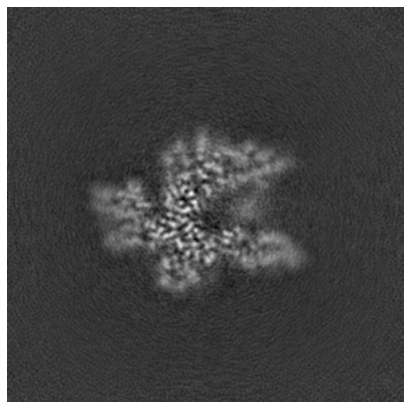


Y Index: 123

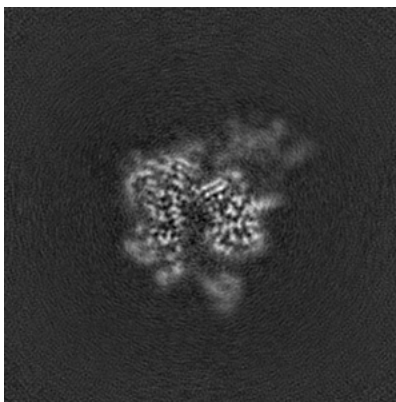


Z Index: 109

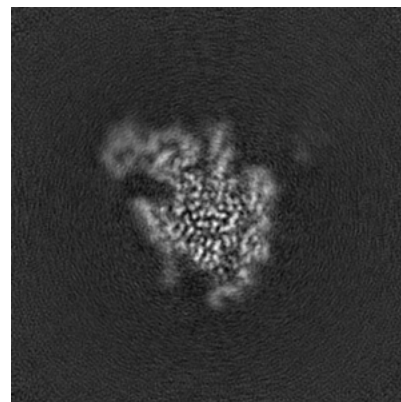
### 6.3.2 Raw map



X Index: 131



Y Index: 123

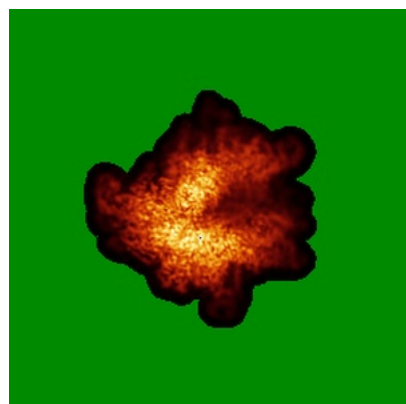


Z Index: 109

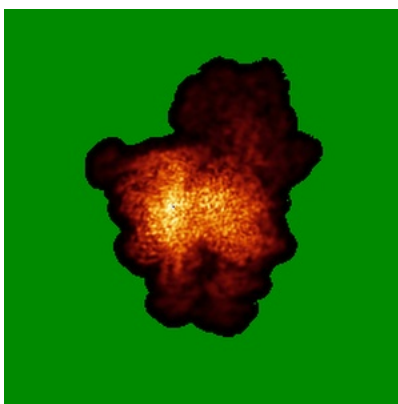
The images above show the largest variance slices of the map in three orthogonal directions.

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

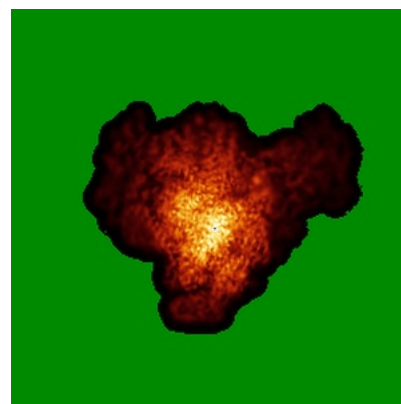
### 6.4.1 Primary map



X

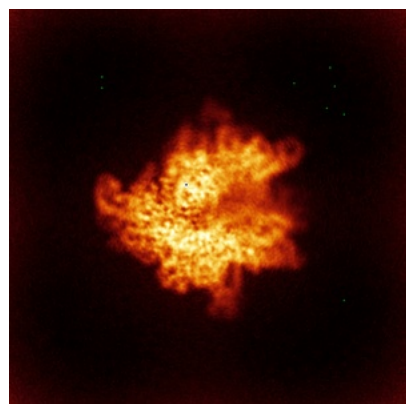


Y

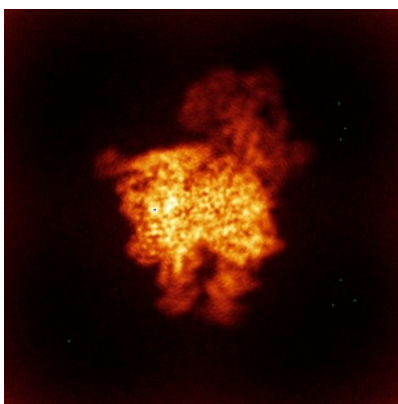


Z

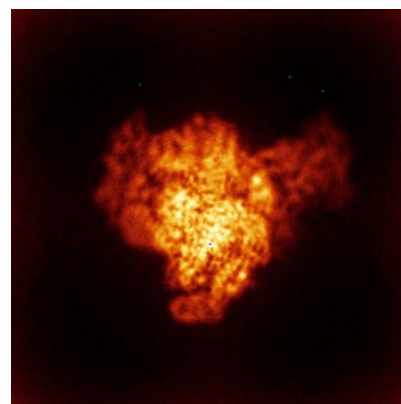
### 6.4.2 Raw map



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 0.186. 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.

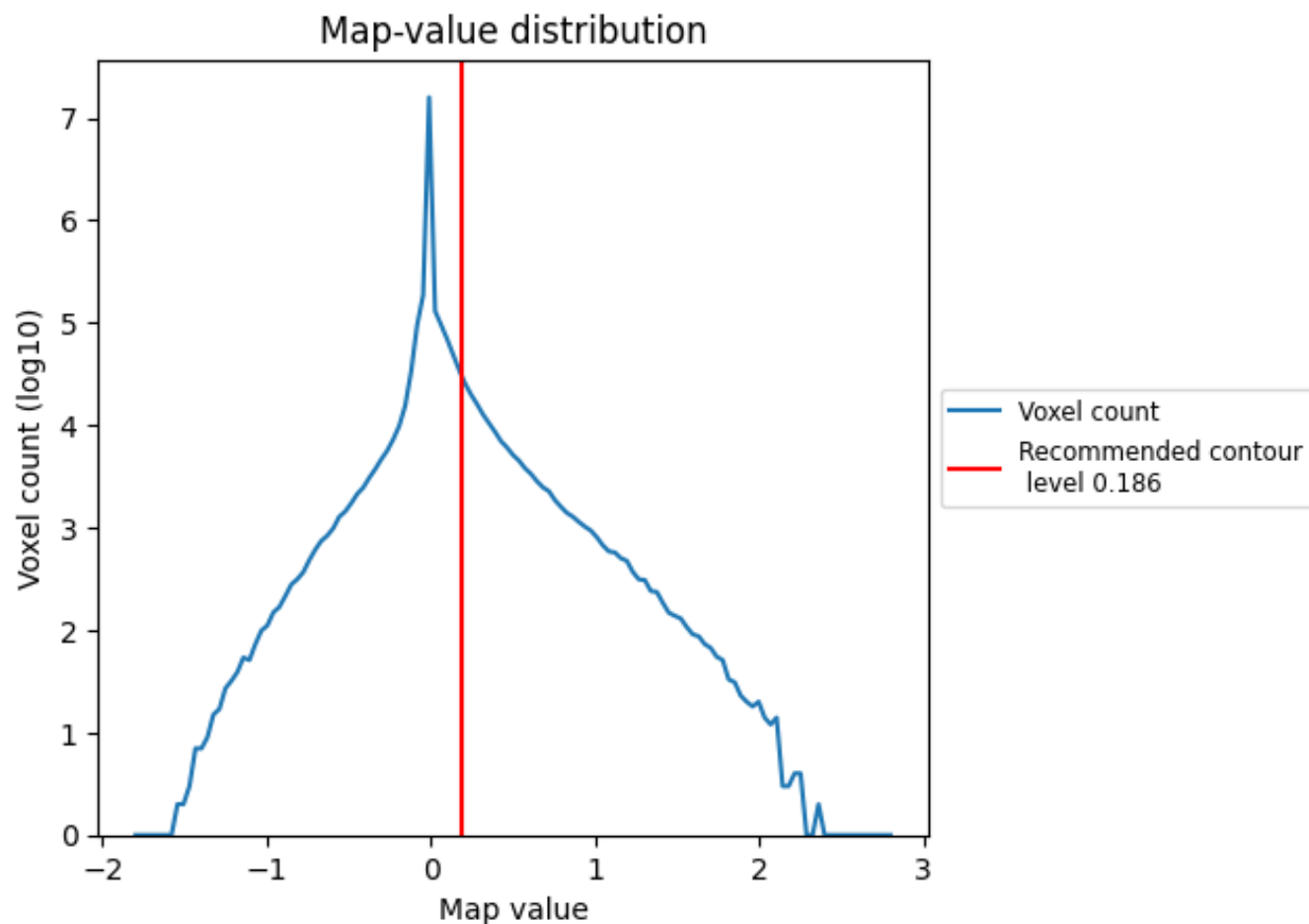
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

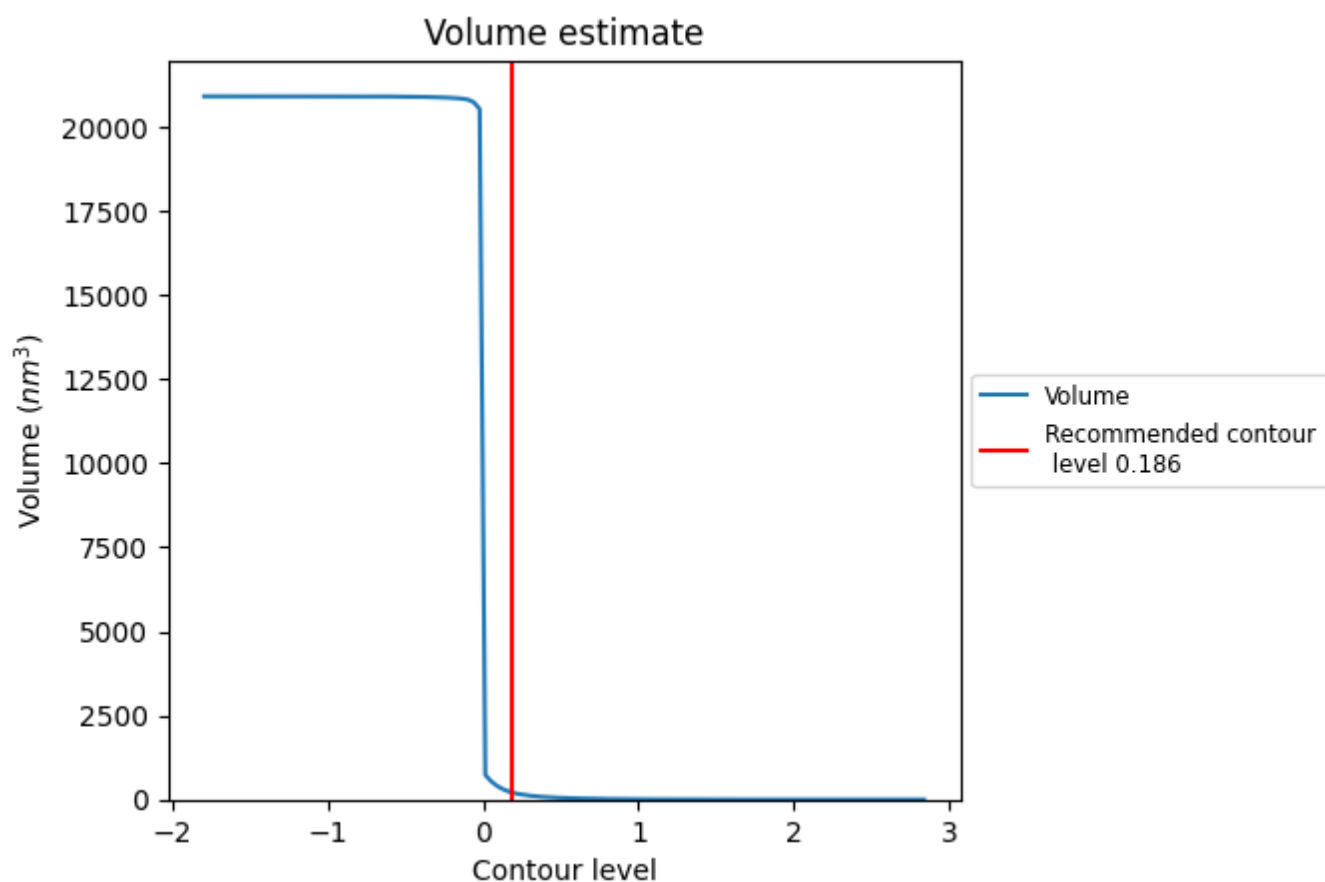
This section contains the results of statistical analysis of the map.

### 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.

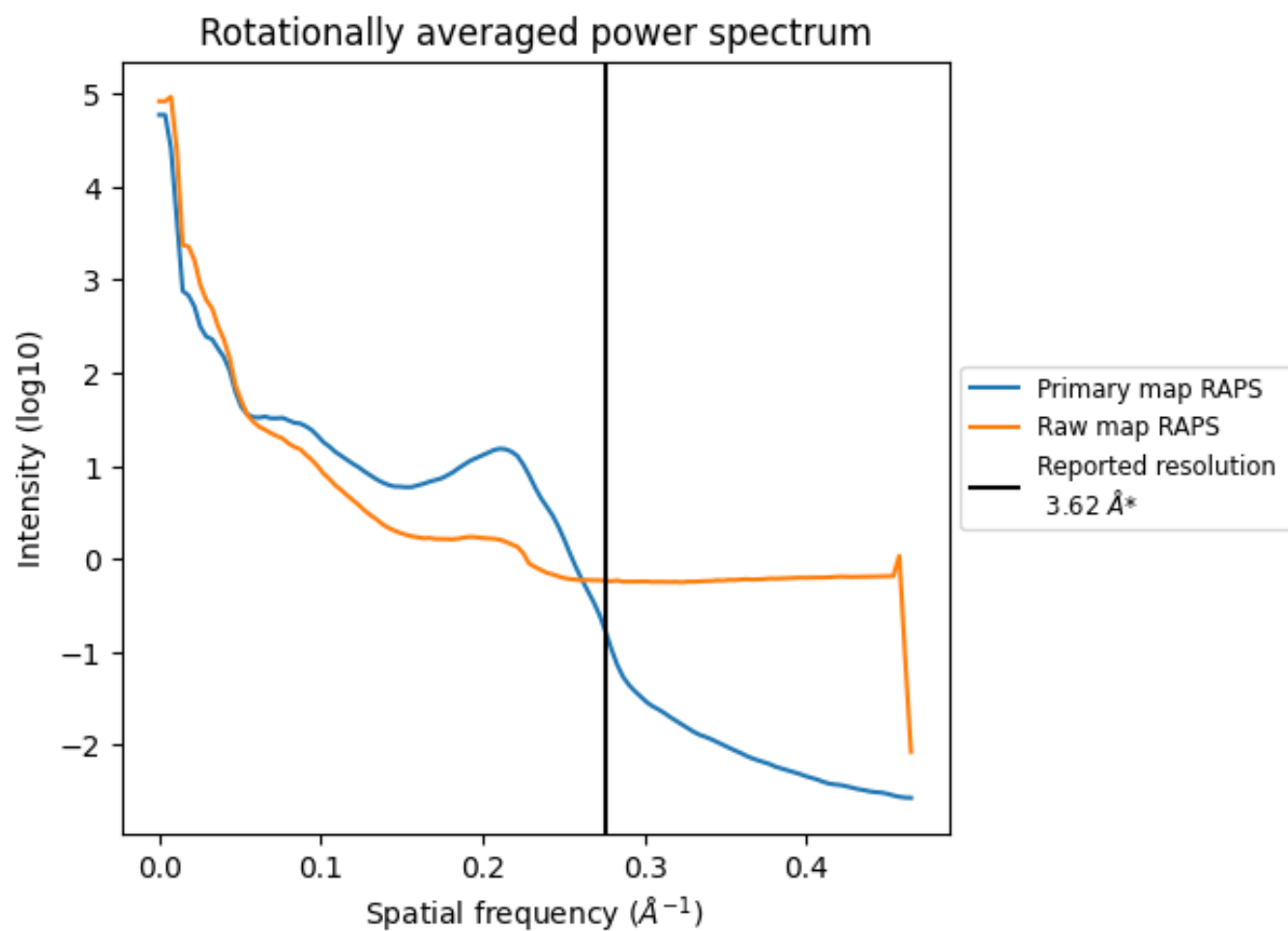
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm<sup>3</sup>; this corresponds to an approximate mass of 190 kDa.

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

### 7.3 Rotationally averaged power spectrum [i](#)

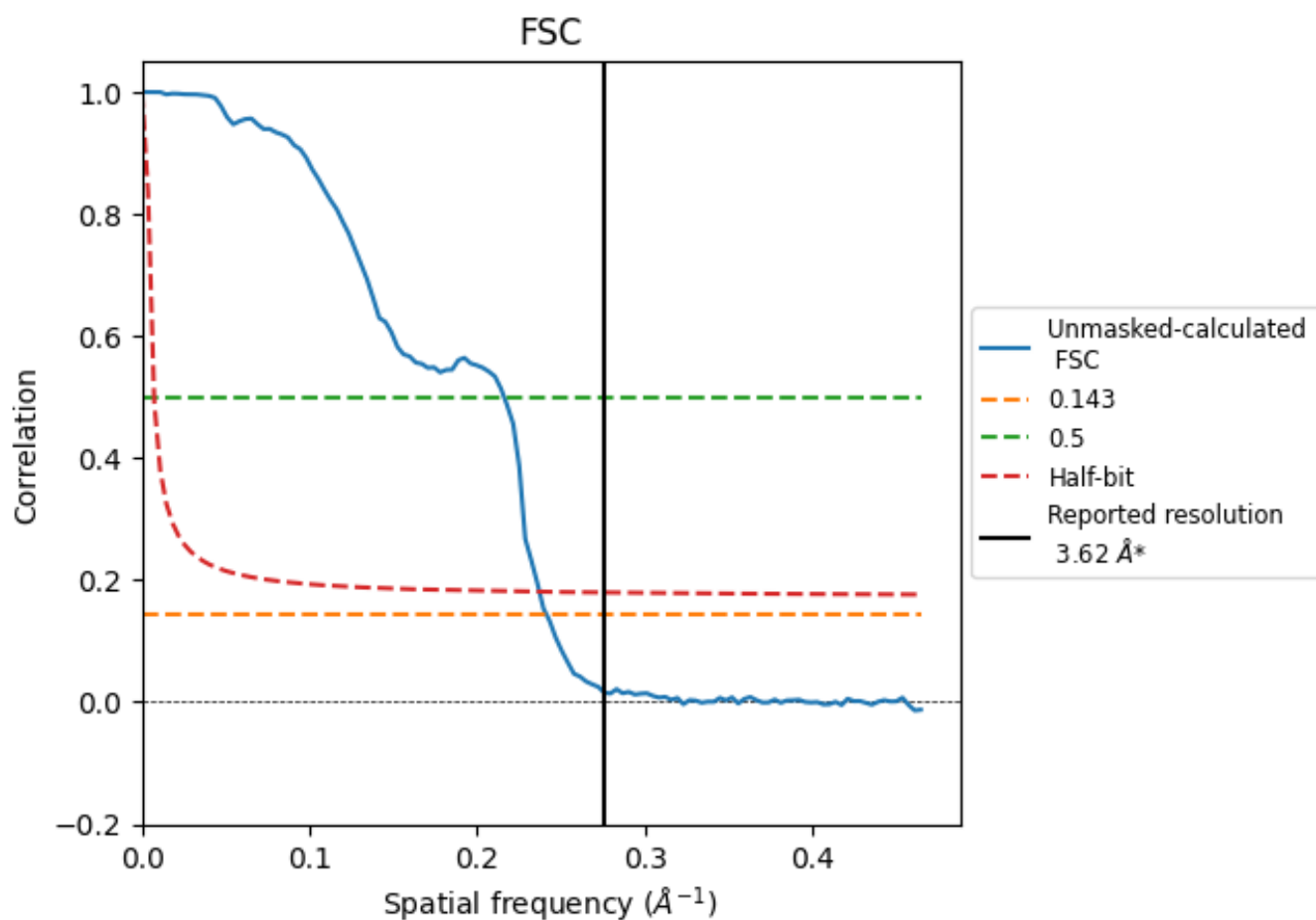


\*Reported resolution corresponds to spatial frequency of  $0.276 \text{ \AA}^{-1}$

## 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  $0.276 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	4.63	4.22

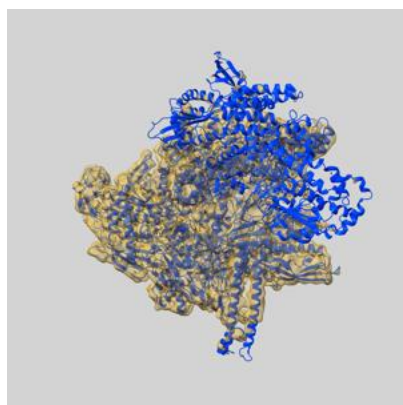
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.62 by more than 10 %



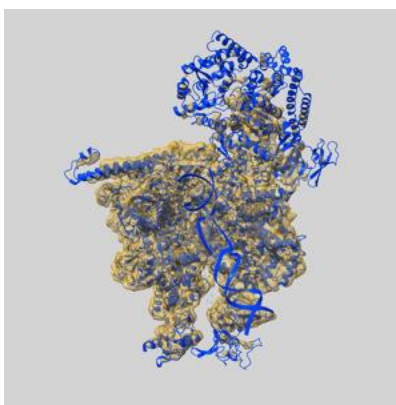
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40943 and PDB model 8T0L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

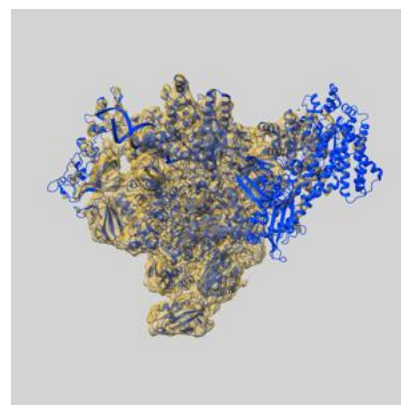
### 9.1 Map-model overlay [i](#)



X



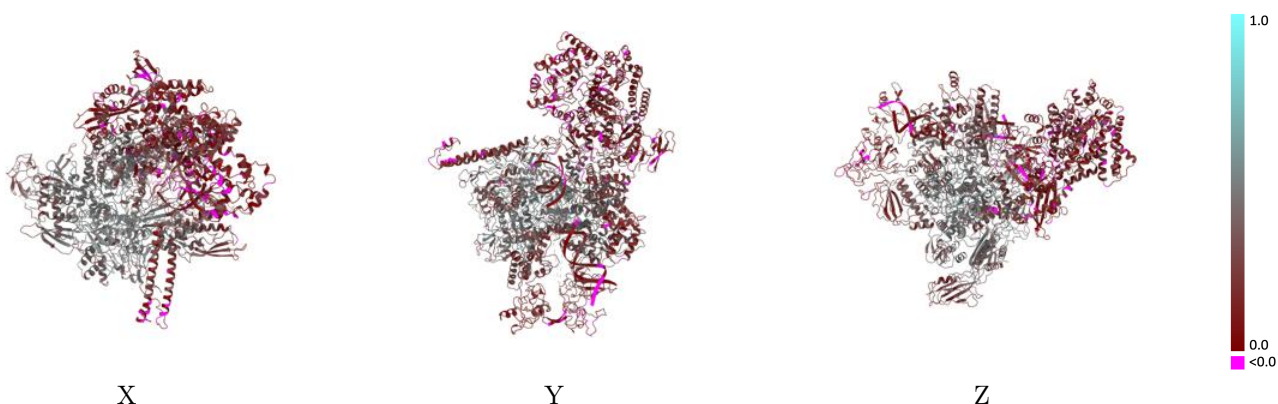
Y



Z

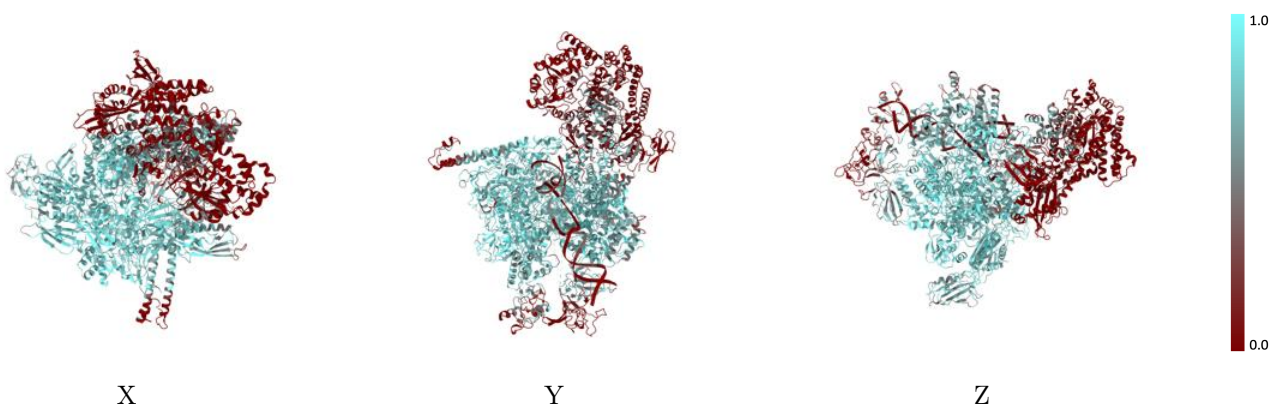
The images above show the 3D surface view of the map at the recommended contour level 0.186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



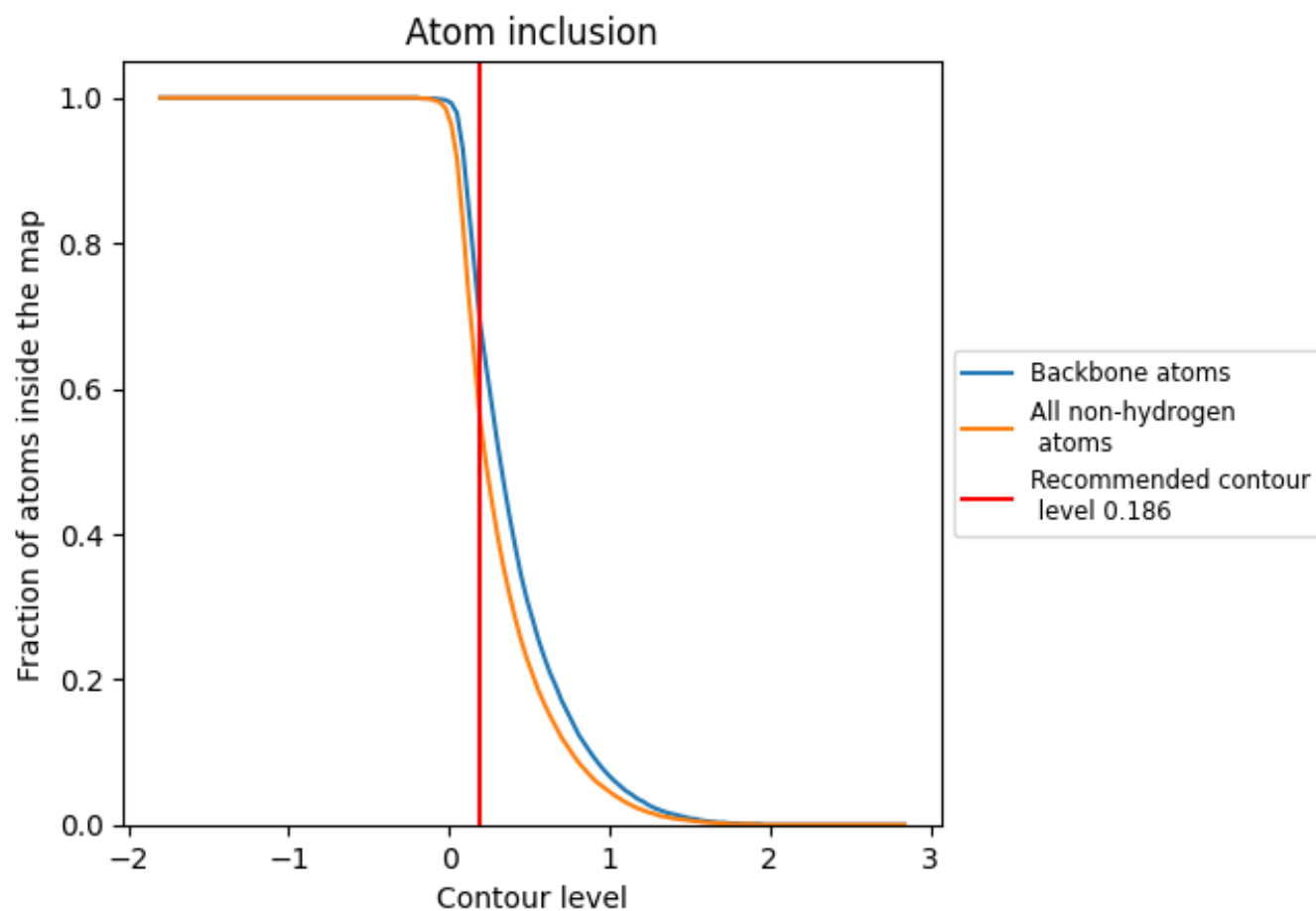
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.186).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 57% 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 (0.186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5730	<div></div> 0.3070
A	<div></div> 0.1950	<div></div> 0.0980
B	<div></div> 0.1000	<div></div> 0.0870
F	<div></div> 0.1100	<div></div> 0.1590
G	<div></div> 0.8340	<div></div> 0.4300
H	<div></div> 0.7320	<div></div> 0.3630
I	<div></div> 0.7380	<div></div> 0.3700
J	<div></div> 0.7140	<div></div> 0.3420
K	<div></div> 0.6650	<div></div> 0.3140

1.0

0.0

<0.0