



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:56 AM UTC

PDB ID : 8K5A / pdb_00008k5a
EMDB ID : EMD-36899
Title : The cryo-EM map of open TIEA-TEC complex
Authors : Zhang, K.N.; Liu, Y.; Chen, M.; Wang, Y.; Lin, W.; Li, M.; Zhang, X.; Gao, Y.; Gong, Q.; Chen, H.; Steve, M.; Li, S.; Zhang, K.; Liu, B.
Deposited on : 2023-07-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

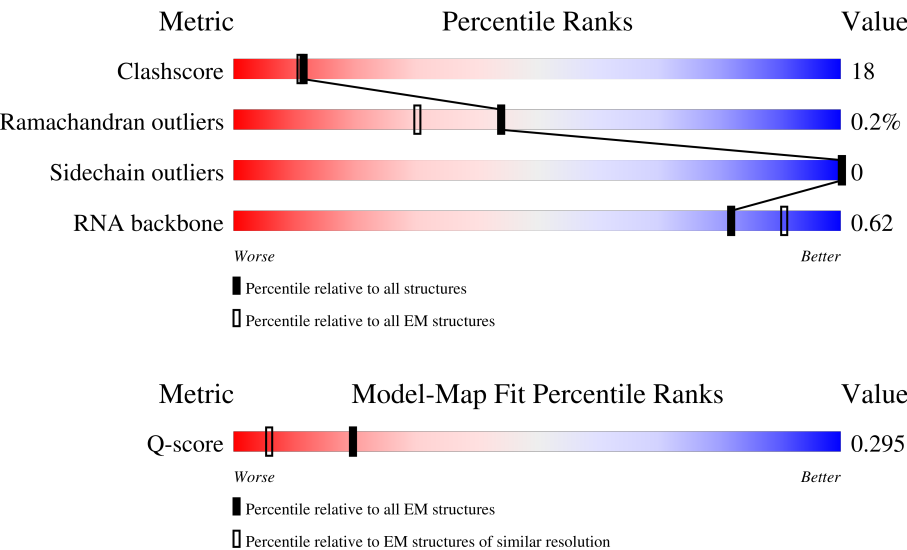
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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

Mol	Chain	Length	Quality of chain
1	A	231	6% 66% 33%
1	B	231	13% 56% 42% .
2	C	1340	13% 62% 38%

Continued on next page...

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Mol	Chain	Length	Quality of chain
3	D	1363	
4	E	76	
5	G	129	
6	H	29	
7	I	29	
8	J	10	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27505 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	A	230	Total	C	N	O	S	0	0
			1788	1112	317	353	6		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1352	Total	C	N	O	S	0	0
			10494	6587	1869	1988	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			606	368	115	122	1		

- Molecule 5 is a protein called 15 kDa RNA polymerase-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	129	Total	C	N	O	S	0	0
			1031	637	188	200	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	29	Total	C	N	O	P	0	0
			583	279	99	177	28		

- Molecule 7 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	22	Total	C	N	O	P	0	0
			448	214	89	125	20		

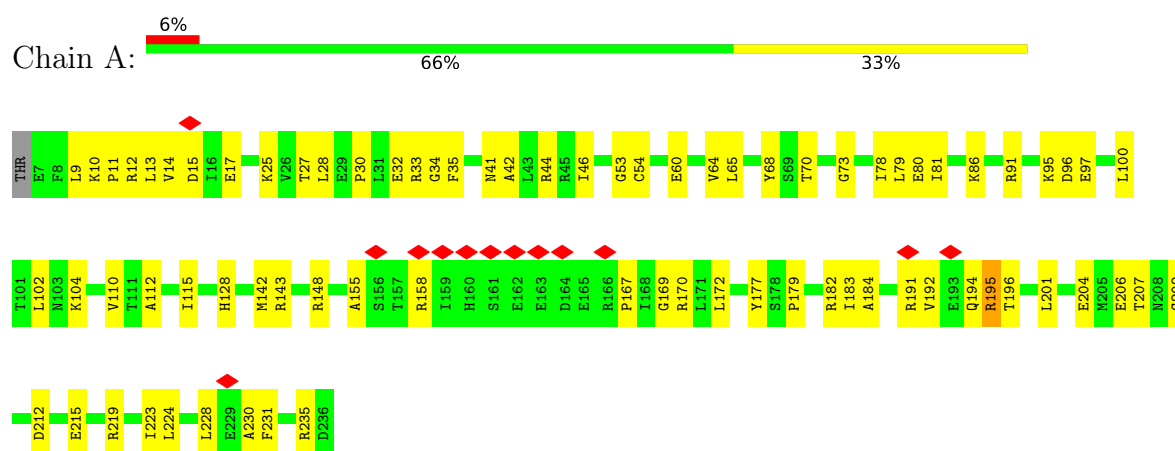
- Molecule 8 is a RNA chain called RNA (5'-R(*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	10	Total	C	N	O	P	0	0
			218	98	45	66	9		

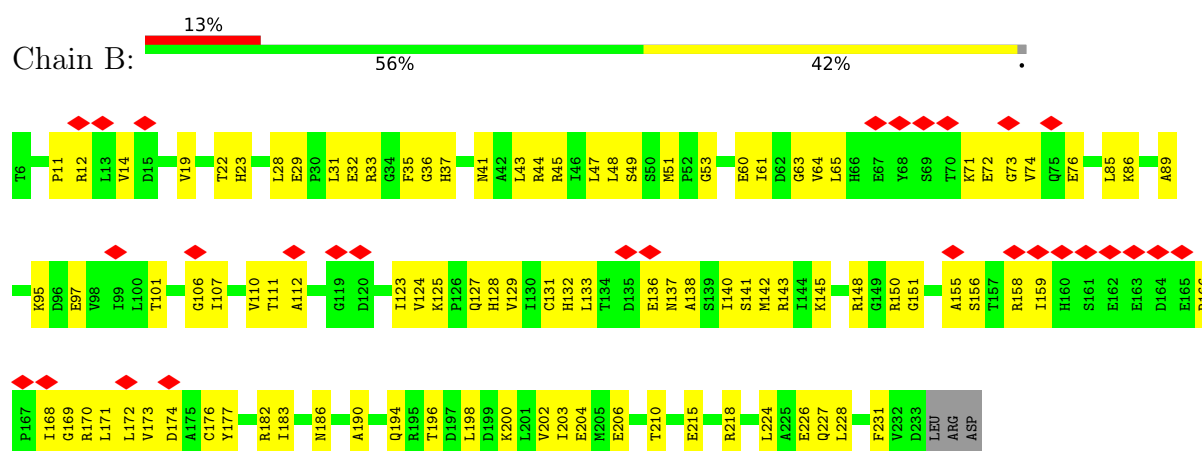
3 Residue-property plots

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.

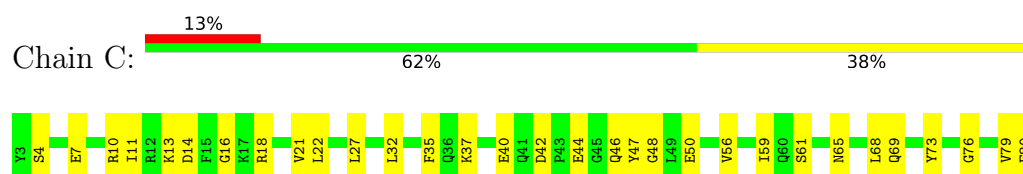
- Molecule 1: DNA-directed RNA polymerase subunit alpha



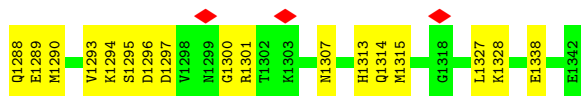
- Molecule 1: DNA-directed RNA polymerase subunit alpha



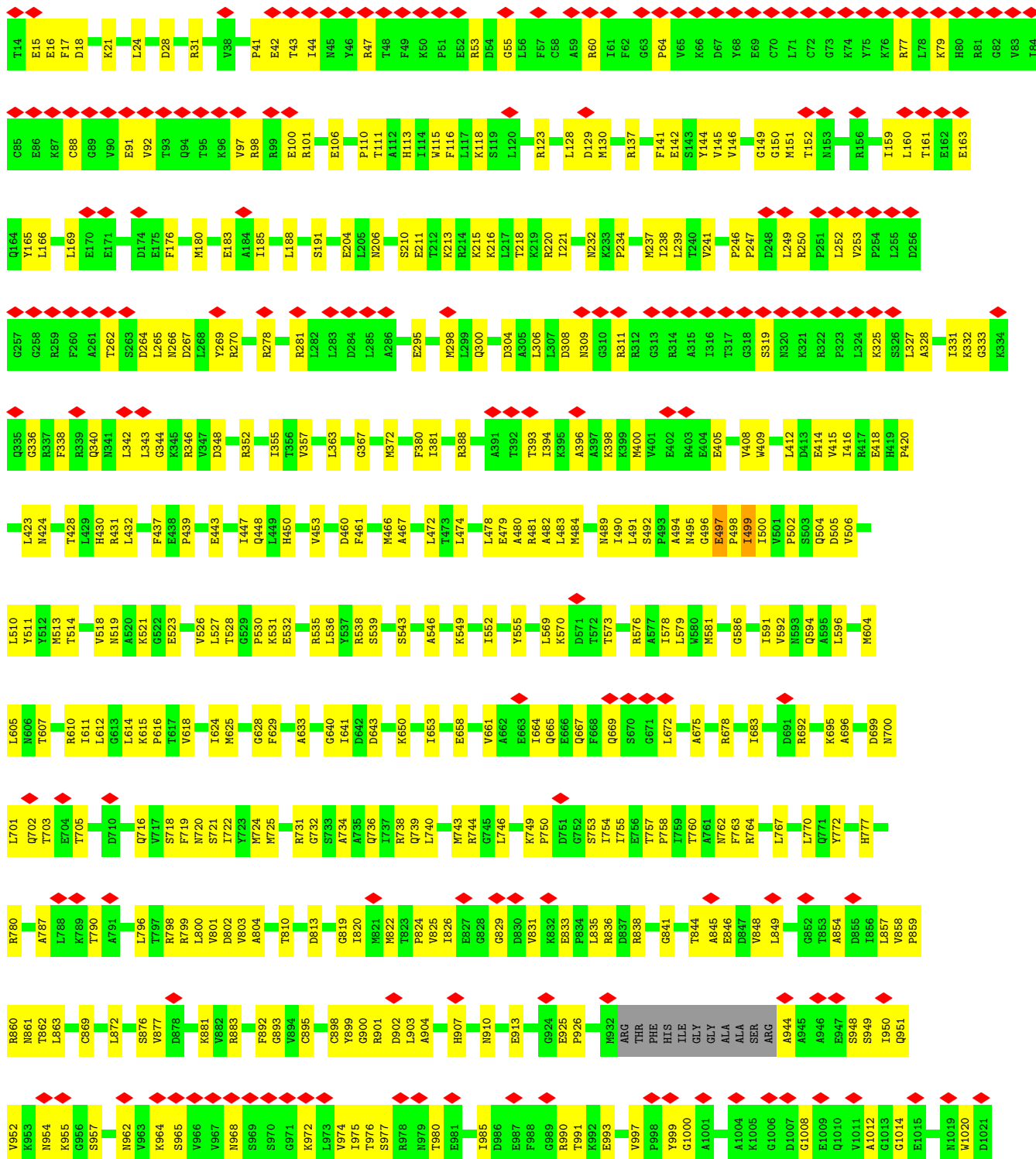
- Molecule 2: DNA-directed RNA polymerase subunit beta

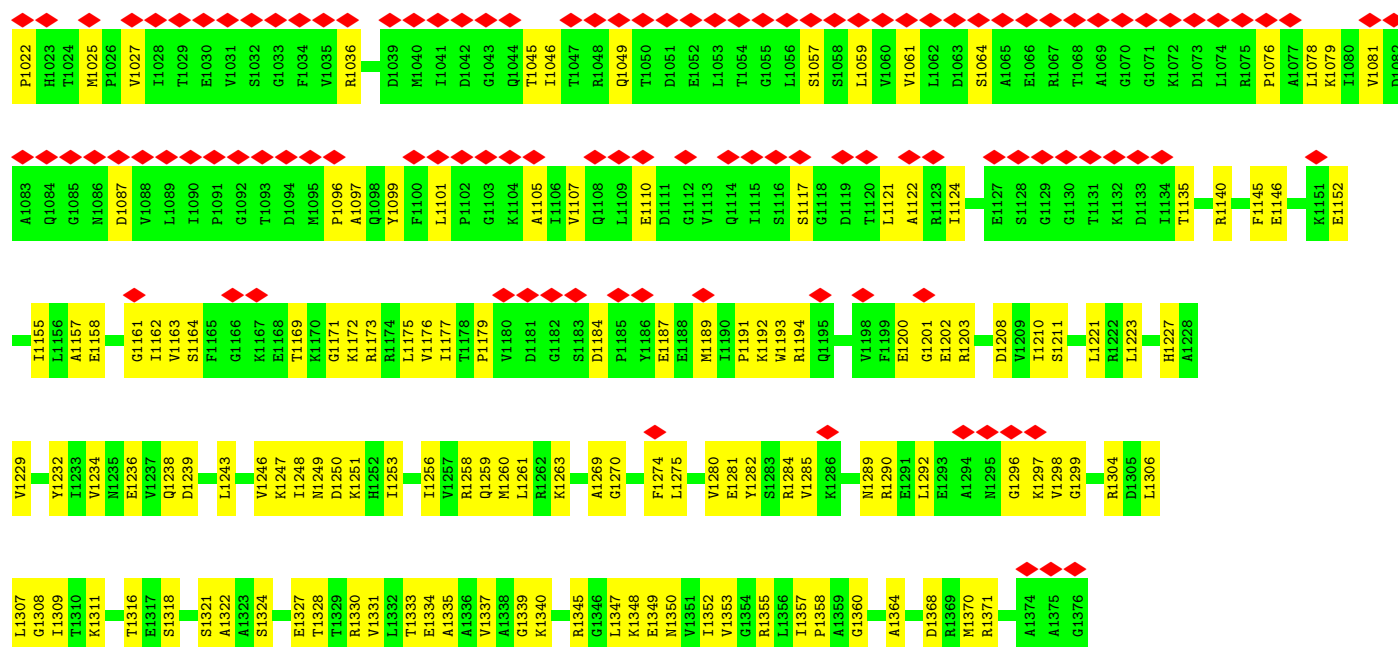


G1218	E1137	K1048	T843	K755	M653	I561	R470	V364	K299	L237	Q86
E1219	V1138	I1049	R644	Y756	D654	E562	V471	Y367	D300	Q238	I87
Q1220	A1139	Y1053	G846	T757	V655	E565	E472	R368	Y301	M239	R88
R1223	L1054	L1054	G847	S759	T657	E566	V475	M369	I302	E240	G89
F1224	R1058	R1058	E848	C764	Q659	N568	R478	R370	E304	L241	S93
V1225	R1059	R1059	E849	I765	V660	S574	L479	P372	S305	V242	A94
T1226	P1062	P1062	E850	P769	V663	N582	D483	G373	G307	E243	P95
V1227	M1066	M1066	E851	S772	A665	E588	L484	P375	E308	E244	L96
Y1229	K1073	K1073	E852	E775	E672	E589	D486	P376	L309	R246	R97
M1230	I1076	I1076	E853	D790	D675	Y691	L487	N387	I310	R247	R98
M1232	S1077	S1077	E854	G792	A676	R592	M488	F389	C311	G248	K100
Y1231	P1081	P1081	E855	G793	R678	D596	Q490	D393	A313	E249	I104
M1232	I1082	I1082	E856	E794	R681	G597	D491	D396	E316	E251	Y105
M1233	M1085	M1085	E857	L794	V690	V598	M492	L397	N314	S252	R107
K1234	Y1087	Y1087	E858	L796	P691	T600	P497	M403	M315	D254	E108
H1237	P1086	P1086	E859	N799	T692	D601	F505	K404	E318	E256	A109
L1238	S1077	S1077	E860	R800	L693	Y605	S512	R407	L319	I255	P110
V1239	P1081	P1081	E861	G802	R694	L606	S512	R407	D320	A257	T113
D1240	I1082	I1082	E862	E803	R694	S607	S512	R407	L321	R260	V114
M1243	M1085	M1085	E863	F804	R694	E610	D516	E412	L322	V261	K115
H1244	Y1087	Y1087	E864	N808	V700	E611	Q517	E412	A323	V262	K118
A1245	N1090	N1090	E865	N809	V701	E612	N518	E412	K324	V263	E119
R1246	G1091	G1091	E866	N810	V702	E613	N519	E412	L325	E264	Q120
S1250	D1095	D1095	E867	N811	V703	E614	P520	E412	S326	I209	E121
Y1251	P1096	P1096	E868	F812	M704	E615	S522	E412	Q327	L209	E122
S1252	I1097	I1097	E869	E813	R705	E616	S522	E412	G329	L210	E123
L1253	V1097	V1097	E870	D814	R706	E617	S522	E412	G330	G266	M124
V1254	L1098	L1098	E871	S815	R707	E618	S522	E412	K331	R267	G125
V1255	N1099	N1099	E872	L816	V708	E619	S522	E412	R332	R268	E126
Q1256	P1100	P1100	E873	R817	V709	E620	S522	E412	L333	I269	M129
F1187	G1102	G1102	E874	E818	R710	E621	S522	E412	E334	T270	G134
D1188	Y1103	Y1103	E875	S819	R711	E622	S522	E412	L335	A271	T135
K1191	P1104	P1104	E876	L820	R712	E623	S522	E412	T336	R272	F136
I1195	S1105	S1105	E877	R821	R713	E624	S522	E412	L337	R275	I138
K1196	M1107	M1107	E878	E822	R714	E625	S522	E412	F337	Q276	N139
E1197	N1108	N1108	E879	D826	R715	E626	S522	E412	N339	L277	G140
L1198	I1109	I1109	E880	R827	R716	E627	S522	E412	D340	E278	E142
L1199	G1110	G1110	E881	R828	R717	E628	S522	E412	L341	K279	R143
L1200	Q1111	Q1111	E882	F829	R718	E629	S522	E412	D342	D280	D160
G1201	I1112	I1112	E883	T829	R719	E630	S522	E412	H343	D281	K161
Q1204	E1114	E1114	E884	Q834	R720	E631	S522	E412	P345	D282	G162
P1206	L1117	L1117	E885	R835	R721	E632	S522	E412	Y346	K283	K163
T1206	M1118	M1118	E886	L836	R722	E633	S522	E412	I347	L284	T164
Q1209	A1120	A1120	E887	V839	R723	E634	S522	E412	L351	I285	H165
V1275	K1122	K1122	E888	R840	R724	E635	S522	E412	V352	E286	S166
V1276	L1128	L1128	E889	R841	R725	E636	S522	E412	D354	R287	S167
A1280	M1129	M1129	E890	R842	R726	E637	S522	E412	L357	P288	G168
Y1281	G1130	G1130	E891	R843	R727	E638	S522	E412	N357	V289	
G1282	I1130	I1130	E892	R844	R728	E639	S522	E412	D358	E290	
A1284	T1217	T1217	E893	R845	R729	E640	S522	E412	R359	I292	
Y1285	L1047	L1047	E894	R846	R730	E641	S522	E412	L363	A293	
			E895	R847	R731	E642	S522	E412		K295	
			E896	R848	R732	E643	S522	E412		V296	
			E897	R849	R733	E644	S522	E412			
			E898	R850	R734	E645	S522	E412			
			E899	R851	R735	E646	S522	E412			
			E900	R852	R736	E647	S522	E412			
			E901	R853	R737	E648	S522	E412			
			E902	R854	R738	E649	S522	E412			
			E903	R855	R739	E650	S522	E412			
			E904	R856	R740	E651	S522	E412			
			E905	R857	R741	E652	S522	E412			
			E906	R858	R742	E653	S522	E412			
			E907	R859	R743	E654	S522	E412			
			E908	R860	R744	E655	S522	E412			
			E909	R861	R745	E656	S522	E412			
			E910	R862	R746	E657	S522	E412			
			E911	R863	R747	E658	S522	E412			
			E912	R864	R748	E659	S522	E412			
			E913	R865	R749	E660	S522	E412			
			E914	R866	R750	E661	S522	E412			
			E915	R867	R751	E662	S522	E412			
			E916	R868	R752	E663	S522	E412			
			E917	R869	R753	E664	S522	E412			
			E918	R870	R754	E665	S522	E412			
			E919	R871	R755	E666	S522	E412			
			E920	R872	R756	E667	S522	E412			
			E921	R873	R757	E668	S522	E412			
			E922	R874	R758	E669	S522	E412			
			E923	R875	R759	E670	S522	E412			
			E924	R876	R760	E671	S522	E412			
			E925	R877	R761	E672	S522	E412			
			E926	R878	R762	E673	S522	E412			
			E927	R879	R763	E674	S522	E412			
			E928	R880	R764	E675	S522	E412			
			E929	R881	R765	E676	S522	E412			
			E930	R882	R766	E677	S522	E412			
			E931	R883	R767	E678	S522	E412			
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			E940	R892	R776	E687	S522	E412			
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			E942	R894	R778	E689	S522	E412			
			E943	R895	R779	E690	S522	E412			
			E944	R896	R780	E691	S522	E412			
			E945	R897	R781	E692	S522	E412			
			E946	R898	R782	E693	S522	E412			
			E947	R899	R783	E694	S522	E412			
			E948	R900	R784	E695	S522	E412			
			E949	R901	R785	E696	S522	E412			
			E950	R902	R786	E697	S522	E412			
			E951	R903	R787	E698	S522	E412			
			E952	R904	R788	E699	S522	E412			
			E953	R905	R789	E700	S522	E412			
			E954	R906	R790	E701	S522	E412			
			E955	R907	R791	E702	S522	E412			
			E956	R908	R792	E703	S522	E412			
			E957	R909	R793	E704	S522	E412			
			E958	R910	R794	E705	S522	E412			
			E959	R911	R795	E706	S522	E412			
			E960	R912	R796	E707	S522	E412			
			E961	R913	R797	E708	S522	E412			
			E962	R914	R798	E709	S522	E412			
			E963	R915	R799	E710	S522	E412			
			E964	R916	R800	E711	S522	E412			
			E965	R917	R801	E712	S522	E412			
			E966	R918	R802	E713	S522	E412			
			E967	R919	R803	E714	S522	E412			
			E968	R920	R804	E715	S522	E412			
			E969	R921	R805	E716	S522	E412			
			E970	R922	R806	E717	S522	E412			
			E971	R923	R807	E718	S522	E412			
			E972	R924	R808	E719	S522	E412			
			E973	R925	R809	E720	S522	E412			
			E974	R926	R810	E721	S522	E412			
			E975	R927	R811	E722	S522	E412			
			E976	R928	R812	E723	S522	E412			
			E977	R929	R813	E724	S522	E412			
			E978	R930	R814	E725	S522	E412			
			E979	R931	R815	E726	S522	E412			
			E980	R932	R816	E727	S522	E412			
			E981	R933	R817	E728	S522	E412			
			E982	R934	R818	E729	S522	E412			
			E983	R935	R819	E730	S522	E412			
			E984	R936	R820	E731	S522	E412			
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			E986	R938	R822	E733	S522	E412			

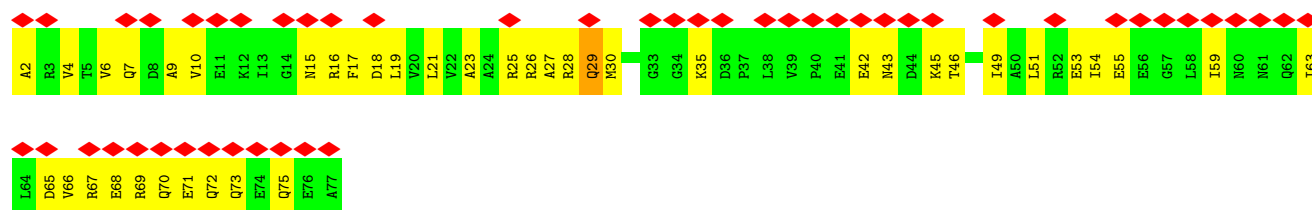


● Molecule 3: DNA-directed RNA polymerase subunit beta'

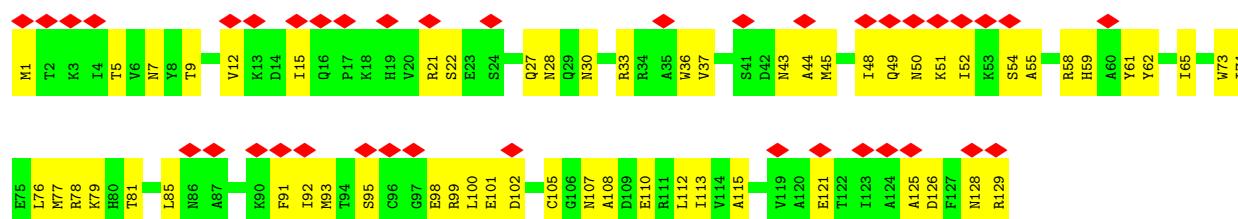




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: 15 kDa RNA polymerase-binding protein



• Molecule 6: DNA (29-MER)



• Molecule 7: DNA (29-MER)



● Molecule 8: RNA (5'-R(*CP*GP*GP*AP*GP*AP*GP*GP*UP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	225078	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.108	Depositor
Minimum map value	-0.669	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.20	0/1810	0.45	0/2451
1	B	0.20	0/1789	0.50	0/2425
2	C	0.20	0/10739	0.43	2/14489 (0.0%)
3	D	0.19	0/10652	0.47	3/14382 (0.0%)
4	E	0.26	0/608	0.87	2/817 (0.2%)
5	G	0.17	0/1046	0.54	1/1411 (0.1%)
6	H	0.15	0/650	0.31	0/1000
7	I	0.16	0/503	0.31	0/773
8	J	0.08	0/245	0.19	0/382
All	All	0.20	0/28042	0.46	8/38130 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	29	GLN	CA-C-N	-6.72	110.30	121.92
4	E	29	GLN	C-N-CA	-6.72	110.30	121.92
5	G	12	VAL	N-CA-C	-6.58	106.59	112.90
2	C	1162	SER	N-CA-C	-6.24	106.63	114.56
3	D	499	ILE	N-CA-C	-5.69	107.44	112.90
3	D	47	ARG	N-CA-C	-5.50	107.21	114.31
3	D	1191	PRO	CA-N-CD	-5.47	104.34	112.00
2	C	625	GLU	CB-CA-C	-5.15	110.23	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1810	70	0
1	B	1767	0	1789	96	0
2	C	10570	0	10582	393	0
3	D	10494	0	10712	409	0
4	E	606	0	612	46	0
5	G	1031	0	1026	47	0
6	H	583	0	329	9	0
7	I	448	0	249	10	0
8	J	218	0	111	6	0
All	All	27505	0	27220	963	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 18.

All (963) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HA	1:A:158:ARG:HH12	1.24	0.99
1:A:231:PHE:HE1	1:B:28:LEU:HD13	1.37	0.89
1:A:104:LYS:HD3	1:A:110:VAL:HG22	1.56	0.88
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.59	0.84
1:A:158:ARG:HH21	1:A:172:LEU:HB3	1.43	0.83
3:D:530:PRO:HG2	3:D:581:MET:HE2	1.60	0.81
1:B:11:PRO:HB2	1:B:28:LEU:HD21	1.61	0.80
2:C:1120:ALA:HB2	2:C:1199:LEU:HD22	1.63	0.80
2:C:37:LYS:HE3	2:C:47:TYR:HB2	1.63	0.80
3:D:1308:GLY:H	3:D:1311:LYS:HE2	1.47	0.79
3:D:220:ARG:HH22	5:G:21:ARG:HH22	1.30	0.79
3:D:803:VAL:HG11	3:D:1309:ILE:HD12	1.63	0.79
2:C:93:SER:HB2	2:C:126:GLU:HG2	1.66	0.78
2:C:588:GLU:HG3	2:C:605:TYR:HB3	1.65	0.78
2:C:101:ARG:HB3	2:C:118:LYS:HD3	1.66	0.77
3:D:110:PRO:HD2	3:D:183:GLU:HG2	1.64	0.77
3:D:739:GLN:HB2	3:D:744:ARG:HB3	1.66	0.77
2:C:1313:HIS:HB2	3:D:474:LEU:HD22	1.66	0.77
5:G:1:MET:HE2	5:G:51:LYS:HG3	1.66	0.77
1:A:10:LYS:HZ3	1:B:226:GLU:HG2	1.50	0.77
1:B:33:ARG:HE	2:C:1081:PRO:HG3	1.51	0.76
1:A:41:ASN:HD22	2:C:1218:GLY:HA3	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:15:ILE:HA	5:G:113:ILE:HD12	1.66	0.76
3:D:216:LYS:HD3	5:G:27:GLN:HB3	1.66	0.75
1:A:207:THR:HG23	1:A:209:GLY:H	1.51	0.75
1:A:54:CYS:SG	1:A:148:ARG:NH1	2.60	0.75
3:D:527:LEU:HD21	3:D:536:LEU:HD22	1.69	0.75
2:C:820:GLU:HG2	2:C:824:GLN:HE21	1.52	0.74
2:C:425:ILE:HG22	2:C:429:MET:HE2	1.69	0.74
2:C:561:ILE:HG21	3:D:772:TYR:HE2	1.50	0.74
1:A:155:ALA:HA	1:A:158:ARG:NH1	2.01	0.74
3:D:876:SER:HB3	3:D:990:ARG:HD2	1.69	0.74
1:B:37:HIS:CE1	2:C:1216:ARG:HG3	2.23	0.74
2:C:934:PHE:HB2	2:C:1049:ILE:HB	1.70	0.73
3:D:380:PHE:HZ	3:D:472:LEU:HB2	1.53	0.73
4:E:26:ARG:HG3	4:E:30:MET:HE1	1.71	0.73
2:C:314:ASN:O	2:C:352:ARG:NH1	2.21	0.73
1:A:191:ARG:HH22	1:A:196:THR:HA	1.51	0.73
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.54	0.73
3:D:16:GLU:HA	3:D:1355:ARG:HE	1.54	0.73
1:A:95:LYS:HD3	1:A:97:GLU:H	1.53	0.72
2:C:672:GLU:HB2	3:D:767:LEU:H	1.56	0.71
2:C:821:ARG:HB2	2:C:1082:ILE:HD13	1.72	0.71
1:A:231:PHE:CE2	1:B:43:LEU:HD11	2.26	0.71
1:B:182:ARG:HH22	3:D:581:MET:HE1	1.55	0.71
2:C:32:LEU:HA	2:C:130:MET:HE1	1.73	0.71
2:C:813:GLU:OE2	3:D:504:GLN:NE2	2.23	0.70
2:C:521:LEU:HD21	2:C:664:GLY:HA2	1.72	0.70
1:A:41:ASN:ND2	2:C:1217:THR:O	2.24	0.70
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.73	0.70
4:E:27:ALA:HA	4:E:30:MET:SD	2.32	0.70
4:E:72:GLN:HA	4:E:75:GLN:HG3	1.73	0.70
3:D:1078:LEU:HG	3:D:1101:LEU:HD11	1.72	0.70
3:D:1169:THR:H	3:D:1173:ARG:HA	1.57	0.70
1:B:125:LYS:NZ	1:B:127:GLN:O	2.25	0.70
2:C:890:LYS:H	2:C:913:VAL:HA	1.57	0.69
2:C:517:GLN:HG2	2:C:759:SER:HB2	1.74	0.69
3:D:699:ASP:O	3:D:702:GLN:NE2	2.25	0.69
3:D:24:LEU:HD13	3:D:237:MET:HB3	1.74	0.69
1:B:158:ARG:NH2	1:B:173:VAL:O	2.25	0.69
3:D:490:ILE:HG13	3:D:491:LEU:HD12	1.73	0.69
3:D:591:ILE:HB	3:D:604:MET:HG2	1.75	0.69
1:A:42:ALA:O	1:A:46:ILE:HG12	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:758:ARG:HD3	2:C:835:GLU:HG3	1.75	0.69
1:B:95:LYS:NZ	1:B:97:GLU:O	2.23	0.69
5:G:126:ASP:O	5:G:129:ARG:NH1	2.18	0.68
2:C:262:TYR:OH	2:C:276:GLN:NE2	2.26	0.68
3:D:300:GLN:NE2	3:D:304:ASP:OD1	2.26	0.68
2:C:84:GLU:HA	2:C:87:ILE:HG12	1.75	0.68
3:D:836:ARG:NH1	3:D:869:CYS:SG	2.66	0.68
5:G:99:ARG:NH1	5:G:100:LEU:O	2.27	0.68
1:B:145:LYS:HE3	1:B:170:ARG:HH22	1.57	0.68
3:D:113:HIS:HD2	3:D:115:TRP:H	1.40	0.67
3:D:665:GLN:O	3:D:669:GLN:NE2	2.27	0.67
3:D:483:LEU:O	3:D:489:ASN:ND2	2.26	0.67
5:G:107:ASN:HB3	5:G:110:GLU:HG2	1.77	0.67
5:G:21:ARG:NH2	5:G:28:ASN:O	2.27	0.67
2:C:59:ILE:HG21	2:C:475:VAL:HG13	1.77	0.66
2:C:249:GLU:HG2	2:C:339:ASN:HB3	1.77	0.66
3:D:381:ILE:HD11	3:D:412:LEU:HD13	1.77	0.66
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.77	0.66
2:C:801:ARG:HB3	2:C:1095:ASP:H	1.60	0.66
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.77	0.66
3:D:944:ALA:N	3:D:949:SER:HG	1.93	0.66
5:G:1:MET:HE1	5:G:50:ASN:HB2	1.78	0.66
1:B:194:GLN:OE1	3:D:409:TRP:NE1	2.25	0.66
3:D:901:ARG:NH1	3:D:902:ASP:OD1	2.29	0.66
3:D:555:TYR:HB2	3:D:586:GLY:H	1.60	0.66
2:C:276:GLN:HG2	2:C:279:LYS:HE3	1.78	0.66
2:C:367:TYR:OH	2:C:371:ARG:NH2	2.29	0.66
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.78	0.65
3:D:650:LYS:HE2	3:D:762:ASN:HD21	1.60	0.65
7:I:4:DC:H2''	7:I:5:DT:H5'	1.78	0.65
2:C:1142:ARG:NH2	2:C:1165:SER:O	2.28	0.65
3:D:705:THR:HG21	3:D:719:PHE:HB2	1.76	0.65
2:C:296:VAL:HG22	2:C:316:GLU:HG3	1.79	0.65
2:C:516:ASP:OD2	2:C:522:SER:OG	2.12	0.65
2:C:1107:MET:SD	3:D:739:GLN:NE2	2.68	0.65
1:A:182:ARG:HB2	1:A:206:GLU:HB2	1.77	0.65
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.77	0.65
3:D:267:ASP:OD2	7:I:6:DA:N6	2.30	0.65
3:D:902:ASP:OD2	3:D:1249:ASN:ND2	2.31	0.64
2:C:492:MET:N	2:C:492:MET:SD	2.71	0.64
2:C:1289:GLU:HA	2:C:1293:VAL:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:592:ARG:NH2	2:C:599:VAL:O	2.31	0.64
1:A:78:ILE:HD13	1:A:81:ILE:HD12	1.80	0.64
2:C:199:ASP:HA	7:I:15:DT:H3	1.61	0.64
2:C:453:ILE:HD12	2:C:530:ILE:HD12	1.78	0.64
2:C:628:HIS:HB3	2:C:647:ARG:HH22	1.62	0.64
2:C:143:ARG:NH2	2:C:512:SER:O	2.26	0.64
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.80	0.64
2:C:105:TYR:O	2:C:107:ARG:NH1	2.27	0.63
3:D:502:PRO:HB3	3:D:506:VAL:HG13	1.79	0.63
1:A:79:LEU:HD21	2:C:693:LEU:HD11	1.80	0.63
2:C:210:LEU:HD21	2:C:429:MET:HE1	1.79	0.63
3:D:372:MET:HE1	3:D:447:ILE:HD11	1.79	0.63
3:D:506:VAL:HG21	3:D:625:MET:HA	1.79	0.63
1:B:141:SER:OG	1:B:143:ARG:NH1	2.30	0.63
3:D:910:ASN:ND2	4:E:15:ASN:OD1	2.31	0.63
2:C:35:PHE:HE2	2:C:129:LEU:HD12	1.63	0.63
3:D:955:LYS:HE3	3:D:1012:ALA:HA	1.79	0.63
2:C:817:LEU:HD21	2:C:1085:MET:HE1	1.81	0.63
2:C:972:PHE:HA	2:C:975:ILE:HG12	1.80	0.63
3:D:962:ASN:OD1	3:D:964:LYS:NZ	2.32	0.63
3:D:1057:SER:HB3	3:D:1110:GLU:HG2	1.79	0.63
1:B:60:GLU:HB3	1:B:143:ARG:H	1.65	0.62
4:E:46:THR:HA	4:E:49:ILE:HG12	1.80	0.62
2:C:697:LYS:HD2	2:C:1181:PRO:HG3	1.81	0.62
4:E:69:ARG:HA	4:E:72:GLN:OE1	2.00	0.62
1:A:12:ARG:H	1:A:30:PRO:HD2	1.63	0.62
2:C:4:SER:HB3	2:C:7:GLU:HB2	1.82	0.62
3:D:872:LEU:HD12	3:D:877:VAL:HG11	1.82	0.62
3:D:1260:MET:HE3	3:D:1306:LEU:HD22	1.82	0.62
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.82	0.62
3:D:295:GLU:HA	3:D:298:MET:SD	2.40	0.62
3:D:883:ARG:HB3	3:D:898:CYS:HA	1.80	0.62
3:D:128:LEU:HB3	3:D:130:MET:HE1	1.82	0.62
3:D:1221:LEU:HD22	3:D:1306:LEU:HG	1.80	0.62
7:I:1:DG:H2''	7:I:2:DG:H5'	1.81	0.62
1:A:14:VAL:HG22	1:A:15:ASP:H	1.65	0.62
2:C:79:VAL:O	2:C:1035:LYS:NZ	2.29	0.62
2:C:538:LEU:HD12	2:C:542:ARG:HG2	1.82	0.62
2:C:13:LYS:O	2:C:1183:ALA:N	2.23	0.61
2:C:59:ILE:HD12	2:C:472:GLU:HG3	1.81	0.61
2:C:1058:ARG:NH1	2:C:1240:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:VAL:HB	1:B:28:LEU:HD12	1.81	0.61
5:G:48:ILE:HD12	5:G:62:TYR:HE1	1.63	0.61
1:A:231:PHE:HE2	1:B:43:LEU:HD11	1.64	0.61
3:D:215:LYS:NZ	5:G:95:SER:OG	2.26	0.61
3:D:1172:LYS:HB2	3:D:1189:MET:SD	2.41	0.61
3:D:1175:LEU:O	3:D:1187:GLU:HA	2.00	0.61
1:B:85:LEU:HD11	1:B:173:VAL:HG21	1.83	0.61
3:D:591:ILE:HG13	3:D:592:VAL:HG13	1.82	0.61
3:D:527:LEU:HB3	3:D:532:GLU:HB2	1.83	0.61
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.65	0.61
2:C:195:PHE:HB3	2:C:203:LYS:HB2	1.83	0.61
1:B:45:ARG:O	1:B:49:SER:OG	2.15	0.61
3:D:400:MET:HE3	3:D:408:VAL:HG13	1.83	0.61
1:B:196:THR:HB	3:D:443:GLU:HG2	1.83	0.61
3:D:1105:ALA:HA	3:D:1124:ILE:HG13	1.83	0.61
2:C:678:ARG:HG2	2:C:1108:ASN:HB3	1.81	0.60
2:C:1099:ASN:HD21	2:C:1101:LEU:HD12	1.65	0.60
3:D:246:PRO:HB2	3:D:249:LEU:HD13	1.83	0.60
1:B:19:VAL:HB	1:B:23:HIS:HB3	1.82	0.60
2:C:232:ILE:HA	2:C:237:LEU:HD22	1.83	0.60
2:C:538:LEU:HD13	7:I:16:DG:H1'	1.82	0.60
2:C:756:TYR:H	2:C:766:ASN:HB3	1.65	0.60
2:C:256:GLU:HA	2:C:261:VAL:HA	1.82	0.60
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.83	0.60
3:D:505:ASP:HB3	3:D:629:PHE:HE1	1.65	0.60
3:D:1347:LEU:HD13	3:D:1358:PRO:HD2	1.83	0.60
3:D:640:GLY:N	3:D:643:ASP:OD2	2.31	0.60
2:C:678:ARG:HA	2:C:681:MET:HE2	1.82	0.60
2:C:1234:LYS:HE2	2:C:1238:LEU:HD22	1.84	0.60
3:D:829:GLY:HA2	3:D:993:GLU:HG2	1.82	0.60
1:B:33:ARG:NE	2:C:1081:PRO:HG3	2.16	0.60
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.33	0.60
3:D:393:THR:HG23	3:D:396:ALA:H	1.66	0.60
2:C:1164:PHE:HB3	2:C:1168:GLU:HB2	1.83	0.59
4:E:19:LEU:HD11	4:E:54:ILE:HD12	1.82	0.59
3:D:883:ARG:NH2	3:D:895:CYS:SG	2.75	0.59
4:E:6:VAL:HG22	4:E:51:LEU:HD11	1.85	0.59
1:B:86:LYS:HZ1	1:B:174:ASP:HB2	1.67	0.59
2:C:18:ARG:NH2	2:C:620:ASN:O	2.35	0.59
2:C:246:LEU:HB3	2:C:269:ILE:HG21	1.83	0.59
3:D:106:GLU:HA	3:D:241:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:596:LEU:HD13	3:D:604:MET:HE1	1.85	0.59
3:D:1284:ARG:NH2	3:D:1304:ARG:HH21	2.01	0.59
2:C:808:ASN:H	3:D:633:ALA:HB2	1.68	0.59
2:C:1276:TRP:CH2	3:D:798:ARG:HA	2.38	0.59
3:D:363:LEU:HD23	3:D:618:VAL:HG23	1.85	0.59
2:C:979:LEU:HD21	2:C:1000:LEU:HD23	1.85	0.59
5:G:49:GLN:OE1	5:G:62:TYR:OH	2.20	0.59
6:H:2:DG:N2	7:I:28:DC:O2	2.35	0.59
2:C:1101:LEU:HD23	3:D:725:MET:HE3	1.84	0.59
3:D:492:SER:OG	3:D:496:GLY:O	2.21	0.59
3:D:612:LEU:HB3	3:D:616:PRO:HG2	1.85	0.59
3:D:1335:ALA:HA	3:D:1340:LYS:HG3	1.85	0.59
4:E:25:ARG:HH12	4:E:29:GLN:HE22	1.48	0.59
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.85	0.59
2:C:1212:LEU:HD12	2:C:1225:VAL:HG21	1.85	0.59
3:D:111:THR:O	3:D:239:LEU:N	2.36	0.59
3:D:615:LYS:H	4:E:7:GLN:HE22	1.50	0.59
1:A:46:ILE:HD12	1:B:35:PHE:CE1	2.37	0.59
2:C:979:LEU:HD23	2:C:989:LEU:HD12	1.85	0.58
1:B:48:LEU:HD21	3:D:539:SER:HB3	1.85	0.58
2:C:697:LYS:O	2:C:799:ASN:ND2	2.33	0.58
2:C:1244:HIS:CE1	2:C:1268:GLN:HE22	2.20	0.58
3:D:42:GLU:H	3:D:55:GLY:HA3	1.68	0.58
2:C:478:ARG:O	2:C:482:GLY:N	2.34	0.58
2:C:548:ARG:O	3:D:780:ARG:NH2	2.32	0.58
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.37	0.58
2:C:1176:LEU:HB3	2:C:1180:MET:HE1	1.85	0.58
3:D:845:ALA:C	3:D:860:ARG:HH22	2.11	0.58
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.39	0.58
3:D:418:GLU:OE2	4:E:45:LYS:N	2.36	0.58
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.85	0.58
2:C:1281:TYR:CG	3:D:484:MET:HE1	2.39	0.58
2:C:1285:TYR:O	2:C:1288:GLN:N	2.36	0.58
2:C:178:PRO:HA	2:C:397:LEU:HD23	1.85	0.58
1:A:41:ASN:ND2	2:C:1218:GLY:HA3	2.18	0.57
1:A:73:GLY:H	2:C:728:ASP:CG	2.12	0.57
2:C:532:ALA:HB1	2:C:538:LEU:HD23	1.84	0.57
3:D:41:PRO:HA	3:D:55:GLY:HA2	1.86	0.57
2:C:14:ASP:OD2	2:C:1156:ARG:NH1	2.37	0.57
2:C:76:GLY:N	2:C:95:PRO:O	2.31	0.57
2:C:549:ASP:OD1	2:C:550:VAL:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.86	0.57
2:C:1103:VAL:HG22	2:C:1111:GLN:HE21	1.69	0.57
3:D:430:HIS:HB3	3:D:925:GLU:HB2	1.86	0.57
3:D:1078:LEU:HD11	3:D:1107:VAL:HG13	1.87	0.57
5:G:93:MET:HE3	5:G:93:MET:HA	1.85	0.57
1:A:32:GLU:OE1	1:A:195:ARG:NH1	2.37	0.57
1:A:46:ILE:HD12	1:B:35:PHE:HE1	1.69	0.57
3:D:813:ASP:OD1	3:D:883:ARG:NH1	2.36	0.57
3:D:150:GLY:H	3:D:176:PHE:HD1	1.53	0.57
3:D:367:GLY:O	3:D:448:GLN:N	2.33	0.57
3:D:423:LEU:HB3	3:D:466:MET:HE2	1.85	0.57
2:C:180:ARG:NH1	2:C:396:ASP:OD2	2.35	0.57
2:C:820:GLU:O	2:C:824:GLN:HG2	2.04	0.57
2:C:1296:ASP:OD1	2:C:1297:ASP:N	2.37	0.57
3:D:206:ASN:HA	5:G:99:ARG:HA	1.86	0.57
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.19	0.57
2:C:611:GLU:OE1	2:C:637:ARG:NH1	2.37	0.56
2:C:835:GLU:HG2	2:C:1053:TYR:CE1	2.40	0.56
5:G:78:ARG:NH1	5:G:79:LYS:HE3	2.20	0.56
3:D:129:ASP:OD2	3:D:220:ARG:NH2	2.35	0.56
3:D:234:PRO:O	3:D:237:MET:HG3	2.05	0.56
2:C:1338:GLU:HB2	3:D:21:LYS:HB3	1.87	0.56
3:D:615:LYS:H	4:E:7:GLN:NE2	2.03	0.56
3:D:802:ASP:OD1	3:D:1348:LYS:NZ	2.39	0.56
2:C:591:TYR:HB2	2:C:606:LEU:HD13	1.87	0.56
3:D:53:ARG:NH2	3:D:88:CYS:SG	2.78	0.56
3:D:734:ALA:O	3:D:738:ARG:HB3	2.06	0.56
3:D:976:THR:HA	3:D:1000:GLY:H	1.70	0.56
1:A:68:TYR:HB3	2:C:756:TYR:CD2	2.41	0.56
1:A:10:LYS:NZ	1:B:226:GLU:HG2	2.21	0.56
1:B:23:HIS:HA	1:B:206:GLU:HG2	1.87	0.55
3:D:836:ARG:HG2	3:D:869:CYS:SG	2.46	0.55
1:A:86:LYS:NZ	2:C:826:ASP:OD1	2.38	0.55
2:C:80:PHE:HB3	2:C:84:GLU:HG2	1.87	0.55
3:D:734:ALA:O	3:D:738:ARG:CB	2.55	0.55
2:C:719:LYS:N	2:C:751:TYR:OH	2.39	0.55
2:C:1151:LEU:HD11	2:C:1197:GLU:HB3	1.88	0.55
2:C:1156:ARG:H	2:C:1156:ARG:HD3	1.71	0.55
4:E:69:ARG:HD2	4:E:70:GLN:N	2.21	0.55
2:C:452:ARG:NH2	2:C:458:GLU:OE2	2.39	0.55
3:D:848:VAL:HG12	3:D:858:VAL:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HB	1:B:131:CYS:HB3	1.88	0.55
2:C:216:THR:HB	2:C:219:GLN:HG2	1.88	0.55
3:D:188:LEU:O	3:D:191:SER:OG	2.18	0.55
3:D:968:ASN:HB2	3:D:1117:SER:HB3	1.88	0.55
3:D:1096:PRO:HD3	3:D:1202:GLU:HB3	1.89	0.55
1:A:17:GLU:HG2	1:A:25:LYS:HB2	1.88	0.55
1:B:44:ARG:NH2	3:D:538:ARG:HB3	2.21	0.55
2:C:568:ASN:ND2	8:J:18:G:OP2	2.33	0.55
2:C:519:ASN:HD21	2:C:796:LEU:HD22	1.72	0.55
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.42	0.55
3:D:64:PRO:HG3	3:D:92:VAL:HA	1.88	0.55
3:D:1261:LEU:HB3	3:D:1306:LEU:HD23	1.89	0.55
3:D:1327:GLU:OE2	3:D:1330:ARG:NH1	2.40	0.55
1:B:29:GLU:HB2	1:B:200:LYS:HG2	1.88	0.55
3:D:1274:PHE:HD2	5:G:95:SER:HB2	1.70	0.55
4:E:26:ARG:NE	4:E:53:GLU:OE2	2.40	0.55
1:B:32:GLU:HG2	1:B:35:PHE:HD2	1.72	0.54
2:C:332:ARG:NH1	2:C:334:GLU:HG3	2.21	0.54
2:C:1307:ASN:HB3	2:C:1314:GLN:HB2	1.89	0.54
3:D:346:ARG:NH2	6:H:17:DC:OP2	2.40	0.54
3:D:521:LYS:O	3:D:543:SER:N	2.36	0.54
2:C:207:THR:HG21	2:C:351:LEU:HG	1.89	0.54
8:J:16:A:H2'	8:J:17:G:H8	1.72	0.54
1:B:65:LEU:HB2	1:B:171:LEU:HD22	1.89	0.54
3:D:1258:ARG:NH2	3:D:1281:GLU:OE2	2.39	0.54
2:C:136:PHE:CE2	2:C:456:VAL:HG21	2.42	0.54
2:C:843:THR:OG1	2:C:846:GLY:O	2.25	0.54
3:D:60:ARG:HG3	3:D:91:GLU:HG3	1.89	0.54
5:G:59:HIS:HA	5:G:62:TYR:CD2	2.42	0.54
1:A:25:LYS:HD3	1:A:204:GLU:HG2	1.89	0.54
2:C:470:ARG:NH2	2:C:497:PRO:O	2.41	0.54
3:D:614:LEU:HB3	4:E:7:GLN:CD	2.32	0.54
3:D:952:VAL:O	3:D:1014:GLY:N	2.39	0.54
2:C:1128:ILE:HD12	2:C:1131:MET:HE3	1.89	0.54
3:D:519:ASN:ND2	3:D:523:GLU:OE1	2.39	0.54
3:D:510:LEU:HA	3:D:513:MET:HG2	1.89	0.54
3:D:804:ALA:HA	3:D:1259:GLN:HG3	1.88	0.54
2:C:238:GLN:NE2	2:C:286:GLU:OE2	2.41	0.54
2:C:729:ALA:O	2:C:755:LYS:NZ	2.41	0.54
2:C:804:PHE:HB2	2:C:1226:THR:OG1	2.07	0.54
2:C:1062:PRO:HA	2:C:1076:ILE:HB	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1315:MET:H	4:E:28:ARG:HH12	1.54	0.54
2:C:801:ARG:O	2:C:1096:ILE:N	2.41	0.54
4:E:9:ALA:HB1	4:E:19:LEU:HD11	1.89	0.54
3:D:400:MET:HE1	3:D:405:GLU:HB2	1.89	0.53
3:D:658:GLU:HA	3:D:661:VAL:HG22	1.89	0.53
1:A:182:ARG:NH2	2:C:1090:ASN:HB3	2.23	0.53
3:D:910:ASN:HD22	4:E:15:ASN:HA	1.73	0.53
5:G:52:ILE:HB	5:G:58:ARG:HG2	1.90	0.53
2:C:516:ASP:O	2:C:522:SER:OG	2.25	0.53
3:D:484:MET:HE2	3:D:484:MET:HA	1.89	0.53
3:D:926:PRO:HB3	3:D:1246:VAL:HG11	1.88	0.53
3:D:1049:GLN:H	3:D:1059:LEU:HD23	1.72	0.53
2:C:816:ILE:HG12	2:C:1098:LEU:HD23	1.91	0.53
2:C:961:SER:O	2:C:965:GLN:HG2	2.09	0.53
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.90	0.53
3:D:511:TYR:CE1	3:D:724:MET:HG3	2.43	0.53
3:D:667:GLN:HB3	3:D:672:LEU:HB2	1.91	0.53
3:D:824:PRO:HD3	3:D:835:LEU:HD22	1.91	0.53
1:B:65:LEU:HD13	1:B:171:LEU:HD13	1.91	0.53
2:C:551:HIS:H	2:C:554:HIS:CE1	2.26	0.53
3:D:480:ALA:HA	3:D:484:MET:HB2	1.89	0.53
3:D:504:GLN:OE1	3:D:731:ARG:NH1	2.42	0.53
3:D:796:LEU:HA	3:D:799:ARG:HD3	1.90	0.53
5:G:33:ARG:HA	5:G:36:TRP:NE1	2.24	0.53
1:A:155:ALA:HB3	2:C:1059:ARG:HH12	1.74	0.53
2:C:488:MET:HE3	2:C:489:PRO:HD2	1.90	0.53
2:C:699:LEU:O	2:C:1182:ILE:N	2.37	0.53
3:D:1027:VAL:O	3:D:1121:LEU:N	2.39	0.53
3:D:21:LYS:NZ	3:D:1339:GLY:O	2.37	0.52
3:D:137:ARG:NH1	3:D:142:GLU:OE1	2.42	0.52
3:D:549:LYS:HE3	3:D:569:LEU:HG	1.90	0.52
3:D:859:PRO:HG2	3:D:862:THR:HB	1.91	0.52
3:D:1164:SER:HA	3:D:1200:GLU:HG2	1.92	0.52
3:D:437:PHE:CZ	3:D:453:VAL:HG11	2.39	0.52
3:D:950:ILE:HG13	3:D:1020:TRP:HH2	1.75	0.52
2:C:633:LEU:HG	2:C:644:LEU:HD12	1.91	0.52
2:C:701:GLY:O	2:C:1184:THR:N	2.35	0.52
4:E:25:ARG:NH1	4:E:29:GLN:HE22	2.07	0.52
5:G:21:ARG:HG2	5:G:22:SER:H	1.74	0.52
1:B:31:LEU:HD13	1:B:36:GLY:HA2	1.91	0.52
3:D:450:HIS:NE2	3:D:625:MET:HE1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:977:SER:H	3:D:999:TYR:HD1	1.57	0.52
1:A:100:LEU:HD23	1:A:115:ILE:HG21	1.91	0.52
1:B:145:LYS:HE3	1:B:170:ARG:NH2	2.25	0.52
2:C:241:LEU:N	2:C:283:LYS:O	2.33	0.52
2:C:692:THR:OG1	2:C:694:ARG:O	2.28	0.52
1:B:22:THR:O	1:B:206:GLU:HA	2.09	0.52
2:C:104:ILE:HD12	2:C:115:LYS:HD2	1.90	0.52
2:C:1138:VAL:HG12	2:C:1170:MET:HE1	1.90	0.52
3:D:97:VAL:HA	3:D:100:GLU:HG2	1.92	0.52
3:D:432:LEU:HD13	3:D:499:ILE:HG21	1.91	0.52
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.91	0.52
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.92	0.52
2:C:617:ALA:HB2	2:C:650:VAL:HG21	1.91	0.52
3:D:340:GLN:HG3	3:D:1352:ILE:HA	1.89	0.52
3:D:701:LEU:O	3:D:718:SER:OG	2.21	0.52
2:C:1209:GLN:HG2	2:C:1226:THR:HG22	1.92	0.52
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.92	0.52
3:D:474:LEU:HD11	4:E:46:THR:OG1	2.10	0.52
2:C:99:LYS:HB3	2:C:118:LYS:HE2	1.91	0.52
2:C:204:LEU:HD11	2:C:369:MET:HG2	1.91	0.52
2:C:218:GLU:HG2	2:C:299:LYS:HA	1.92	0.52
2:C:325:LEU:HD13	2:C:333:ILE:HD11	1.92	0.52
3:D:702:GLN:NE2	3:D:703:THR:HG22	2.24	0.52
3:D:1145:PHE:O	3:D:1309:ILE:HG12	2.10	0.52
2:C:812:PHE:HB3	3:D:357:VAL:HG21	1.91	0.51
3:D:848:VAL:HG13	3:D:857:LEU:HB3	1.92	0.51
2:C:1290:MET:HG2	2:C:1294:LYS:HZ2	1.76	0.51
3:D:355:ILE:HG13	3:D:461:PHE:CD1	2.45	0.51
4:E:72:GLN:O	4:E:75:GLN:N	2.44	0.51
5:G:81:THR:HG23	5:G:100:LEU:HD11	1.92	0.51
3:D:319:SER:O	8:J:13:G:N2	2.39	0.51
3:D:481:ARG:HH11	4:E:4:VAL:HG13	1.75	0.51
3:D:944:ALA:N	3:D:949:SER:OG	2.43	0.51
1:A:64:VAL:HG11	1:A:78:ILE:HG13	1.92	0.51
2:C:971:LEU:HD23	2:C:974:ARG:HH11	1.74	0.51
2:C:1197:GLU:HA	2:C:1200:LYS:HE2	1.93	0.51
2:C:1237:HIS:NE2	8:J:19:U:O2'	2.40	0.51
1:A:80:GLU:OE1	2:C:694:ARG:NH1	2.44	0.51
2:C:800:MET:HE1	2:C:827:ARG:NE	2.26	0.51
5:G:99:ARG:NH1	5:G:102:ASP:OD1	2.44	0.51
6:H:7:DT:H2''	6:H:8:DC:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:82:VAL:O	2:C:86:GLN:HG2	2.10	0.51
2:C:211:ARG:NH2	2:C:217:THR:OG1	2.24	0.51
2:C:657:THR:HG22	2:C:1187:PHE:HB2	1.92	0.51
3:D:746:LEU:HB3	3:D:754:ILE:HD11	1.93	0.51
1:B:32:GLU:HA	1:B:198:LEU:HD13	1.92	0.51
2:C:176:ILE:HD11	2:C:428:VAL:HG21	1.92	0.51
2:C:332:ARG:HH11	2:C:334:GLU:HG3	1.76	0.51
2:C:995:ASP:OD2	2:C:996:ARG:NH1	2.44	0.51
3:D:116:PHE:HB3	3:D:123:ARG:HB2	1.93	0.51
1:A:158:ARG:H	1:A:158:ARG:HD3	1.75	0.51
3:D:144:TYR:N	3:D:160:LEU:O	2.44	0.51
3:D:965:SER:HB3	3:D:975:ILE:HA	1.93	0.51
1:A:194:GLN:OE1	1:A:195:ARG:HG2	2.11	0.51
3:D:328:ALA:O	3:D:331:ILE:HB	2.10	0.51
3:D:825:VAL:N	3:D:833:GLU:OE2	2.32	0.51
4:E:65:ASP:HA	4:E:68:GLU:HG2	1.92	0.51
1:B:183:ILE:HD11	1:B:203:ILE:HD11	1.93	0.51
2:C:886:LYS:HG2	2:C:916:SER:HB2	1.93	0.51
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.92	0.51
2:C:720:ARG:HH21	2:C:736:VAL:HG21	1.76	0.50
1:B:44:ARG:NH1	3:D:538:ARG:HE	2.10	0.50
1:B:76:GLU:OE1	1:B:132:HIS:N	2.44	0.50
2:C:68:LEU:HD11	2:C:100:LEU:HB3	1.92	0.50
2:C:444:ASP:HB2	2:C:447:HIS:HB2	1.93	0.50
2:C:454:ARG:HG2	2:C:459:MET:HG3	1.92	0.50
3:D:129:ASP:CG	3:D:220:ARG:HH21	2.19	0.50
3:D:1270:GLY:HA2	3:D:1298:VAL:H	1.77	0.50
2:C:253:PHE:HB2	2:C:288:PRO:HD2	1.92	0.50
2:C:971:LEU:O	2:C:975:ILE:HG23	2.11	0.50
3:D:610:ARG:HG3	3:D:611:ILE:HG13	1.93	0.50
1:A:60:GLU:HG2	1:A:143:ARG:HH12	1.76	0.50
2:C:230:PHE:CZ	2:C:295:LYS:HG3	2.46	0.50
2:C:834:GLN:HB2	2:C:1054:LEU:HB2	1.92	0.50
1:B:190:ALA:HB2	1:B:200:LYS:HG3	1.94	0.50
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.94	0.50
5:G:9:THR:HB	5:G:121:GLU:HG3	1.94	0.50
2:C:180:ARG:HG2	2:C:396:ASP:HB2	1.93	0.50
6:H:19:DT:H2'	6:H:20:DC:C6	2.46	0.50
2:C:264:GLU:OE1	2:C:267:ARG:NH2	2.44	0.50
2:C:340:ASP:O	2:C:341:LEU:HB2	2.10	0.50
2:C:623:LEU:HD11	2:C:653:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:910:ASN:ND2	4:E:15:ASN:O	2.44	0.50
3:D:1027:VAL:HB	3:D:1122:ALA:H	1.77	0.50
3:D:1253:ILE:O	3:D:1256:ILE:HG22	2.10	0.50
2:C:658:GLN:NE2	2:C:704:MET:SD	2.83	0.50
2:C:880:GLY:N	2:C:920:VAL:O	2.45	0.50
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.45	0.50
3:D:513:MET:HE2	3:D:579:LEU:HB2	1.94	0.50
3:D:552:ILE:HD11	3:D:570:LYS:HG3	1.93	0.50
3:D:1347:LEU:HD12	3:D:1357:ILE:HB	1.93	0.50
2:C:65:ASN:HB3	2:C:105:TYR:HD2	1.77	0.49
2:C:524:ILE:O	2:C:528:ARG:HG3	2.12	0.49
1:B:166:ARG:HB3	1:B:170:ARG:HB2	1.94	0.49
3:D:813:ASP:HA	3:D:895:CYS:SG	2.52	0.49
4:E:6:VAL:HG12	4:E:6:VAL:O	2.12	0.49
2:C:14:ASP:CG	2:C:16:GLY:H	2.21	0.49
2:C:465:ARG:O	2:C:469:VAL:HG23	2.12	0.49
2:C:633:LEU:HD11	2:C:644:LEU:HB3	1.95	0.49
3:D:269:TYR:CE1	3:D:306:LEU:HD11	2.47	0.49
3:D:643:ASP:OD1	3:D:643:ASP:N	2.43	0.49
3:D:899:TYR:CZ	3:D:1251:LYS:HD3	2.47	0.49
4:E:66:VAL:HA	4:E:69:ARG:HG3	1.93	0.49
5:G:5:THR:O	5:G:7:ASN:ND2	2.45	0.49
5:G:61:TYR:CE1	5:G:65:ILE:HD11	2.48	0.49
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.93	0.49
2:C:979:LEU:HD12	2:C:1002:LEU:HD13	1.93	0.49
2:C:1176:LEU:HD13	2:C:1180:MET:HE1	1.94	0.49
3:D:211:GLU:O	3:D:215:LYS:HG2	2.12	0.49
3:D:518:VAL:HG22	3:D:716:GLN:HG2	1.94	0.49
3:D:892:PHE:HA	3:D:1345:ARG:CZ	2.43	0.49
3:D:900:GLY:HA3	3:D:1251:LYS:HZ1	1.77	0.49
5:G:30:ASN:H	5:G:33:ARG:NH1	2.11	0.49
1:B:155:ALA:N	1:B:174:ASP:OD1	2.38	0.49
2:C:104:ILE:HB	2:C:115:LYS:HG2	1.95	0.49
3:D:1064:SER:O	3:D:1192:LYS:HB3	2.10	0.49
2:C:1284:ALA:N	3:D:479:GLU:OE2	2.46	0.49
3:D:749:LYS:N	3:D:753:SER:O	2.38	0.49
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.95	0.49
2:C:1290:MET:HG2	2:C:1294:LYS:NZ	2.26	0.49
3:D:732:GLY:HA2	3:D:736:GLN:OE1	2.13	0.49
2:C:48:GLY:N	2:C:461:GLU:OE2	2.42	0.49
2:C:135:THR:HG21	2:C:142:GLU:OE1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:552:PRO:HB2	2:C:640:GLY:HA3	1.94	0.49
3:D:1135:THR:HG23	3:D:1140:ARG:HH21	1.76	0.49
2:C:367:TYR:OH	2:C:374:GLU:OE2	2.22	0.48
2:C:812:PHE:HB2	3:D:357:VAL:HG11	1.95	0.48
5:G:78:ARG:NH1	5:G:79:LYS:HG2	2.28	0.48
7:I:25:DT:H2"	7:I:26:DA:H8	1.77	0.48
2:C:68:LEU:HD21	2:C:100:LEU:HD13	1.95	0.48
2:C:209:ILE:O	2:C:213:LEU:N	2.45	0.48
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.94	0.48
3:D:502:PRO:HB3	3:D:506:VAL:CG1	2.42	0.48
3:D:913:GLU:H	3:D:1360:GLY:H	1.61	0.48
1:A:102:LEU:HD23	1:A:142:MET:SD	2.53	0.48
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.20	0.48
2:C:561:ILE:HD11	2:C:665:ALA:HB1	1.96	0.48
2:C:871:VAL:HG11	2:C:883:LEU:HD22	1.94	0.48
2:C:1086:PRO:HB2	2:C:1212:LEU:HD13	1.95	0.48
3:D:1172:LYS:HD2	3:D:1193:TRP:HZ3	1.79	0.48
1:B:53:GLY:HA3	1:B:177:TYR:O	2.12	0.48
2:C:758:ARG:NH1	2:C:759:SER:O	2.47	0.48
3:D:16:GLU:HA	3:D:1355:ARG:NE	2.26	0.48
3:D:246:PRO:HD2	3:D:249:LEU:HD22	1.94	0.48
1:B:73:GLY:HA3	1:B:137:ASN:ND2	2.29	0.48
1:B:186:ASN:OD1	1:B:202:VAL:HB	2.14	0.48
2:C:935:THR:N	2:C:1040:ASP:OD1	2.47	0.48
2:C:968:GLU:HG3	2:C:994:ARG:HH12	1.79	0.48
2:C:1295:SER:O	2:C:1301:ARG:NH1	2.46	0.48
2:C:1160:ASP:HA	2:C:1162:SER:H	1.79	0.48
3:D:118:LYS:HD2	3:D:311:ARG:HD2	1.96	0.48
5:G:74:ILE:HA	5:G:77:MET:HG2	1.94	0.48
2:C:27:LEU:HD13	2:C:663:VAL:HG11	1.96	0.48
2:C:211:ARG:CZ	2:C:357:ASN:HA	2.42	0.48
2:C:845:LEU:HB3	2:C:891:GLY:H	1.78	0.48
3:D:250:ARG:HB2	3:D:265:LEU:HD23	1.96	0.48
3:D:355:ILE:HG21	3:D:466:MET:HB2	1.93	0.48
3:D:1027:VAL:HG21	3:D:1099:TYR:CE2	2.49	0.48
4:E:68:GLU:HA	4:E:71:GLU:OE1	2.13	0.48
2:C:339:ASN:H	2:C:345:PRO:HD3	1.78	0.48
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.94	0.48
3:D:43:THR:HB	3:D:270:ARG:HH21	1.77	0.48
3:D:332:LYS:CB	3:D:1328:THR:HG21	2.44	0.48
3:D:414:GLU:HG2	4:E:43:ASN:HD21	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:653:ILE:HD13	3:D:692:ARG:HB3	1.96	0.48
1:B:182:ARG:NH2	3:D:581:MET:HE1	2.24	0.48
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.94	0.48
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.95	0.48
3:D:1025:MET:SD	3:D:1124:ILE:HB	2.54	0.48
5:G:30:ASN:H	5:G:33:ARG:HH11	1.60	0.48
7:I:25:DT:H2"	7:I:26:DA:C8	2.49	0.48
3:D:820:ILE:O	3:D:881:LYS:HA	2.13	0.48
3:D:1269:ALA:O	3:D:1298:VAL:HB	2.14	0.48
2:C:205:PRO:HG2	2:C:354:ASP:HA	1.96	0.47
2:C:518:ASN:O	2:C:691:PRO:HD3	2.14	0.47
3:D:416:ILE:O	3:D:416:ILE:HG22	2.14	0.47
3:D:664:ILE:HG22	3:D:678:ARG:HB2	1.95	0.47
3:D:1263:LYS:HB2	3:D:1307:LEU:HD13	1.95	0.47
2:C:69:GLN:HB2	2:C:101:ARG:HG3	1.95	0.47
3:D:954:ASN:N	3:D:993:GLU:OE1	2.47	0.47
3:D:1163:VAL:HG12	3:D:1177:ILE:HG13	1.96	0.47
1:A:191:ARG:NH2	1:A:192:VAL:O	2.43	0.47
1:B:41:ASN:HA	1:B:44:ARG:HG2	1.96	0.47
2:C:98:VAL:O	2:C:122:VAL:HG12	2.13	0.47
2:C:221:LEU:HB3	2:C:336:LEU:HD21	1.96	0.47
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.49	0.47
2:C:1214:ASP:O	2:C:1218:GLY:N	2.47	0.47
2:C:119:GLU:HB2	2:C:488:MET:HE3	1.96	0.47
2:C:306:THR:HG23	2:C:308:GLU:H	1.79	0.47
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.96	0.47
2:C:980:VAL:HG22	2:C:986:ALA:HB2	1.96	0.47
3:D:822:MET:HE2	3:D:838:ARG:HB3	1.96	0.47
3:D:1269:ALA:HB2	3:D:1274:PHE:HA	1.96	0.47
1:A:9:LEU:HD11	1:A:194:GLN:OE1	2.14	0.47
1:A:95:LYS:HD3	1:A:96:ASP:N	2.29	0.47
2:C:160:ASP:HB2	2:C:171:LEU:HB2	1.95	0.47
3:D:1321:SER:HB3	3:D:1349:GLU:OE2	2.14	0.47
4:E:65:ASP:OD2	4:E:66:VAL:N	2.47	0.47
2:C:115:LYS:HE2	2:C:485:ASP:HA	1.97	0.47
2:C:555:TYR:CE1	2:C:660:VAL:HG11	2.50	0.47
2:C:987:GLU:HG2	2:C:988:LYS:N	2.29	0.47
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.78	0.47
3:D:265:LEU:HD11	3:D:327:LEU:HD13	1.97	0.47
3:D:863:LEU:HD11	3:D:901:ARG:HD2	1.97	0.47
1:B:47:LEU:HD23	1:B:51:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LEU:HD11	1:B:140:ILE:HG22	1.97	0.47
2:C:105:TYR:HA	2:C:113:THR:HA	1.97	0.47
2:C:232:ILE:HB	2:C:331:LYS:HA	1.96	0.47
2:C:371:ARG:NH2	2:C:374:GLU:OE2	2.48	0.47
2:C:601:ASP:N	2:C:601:ASP:OD1	2.47	0.47
2:C:678:ARG:NH1	2:C:1073:LYS:HE3	2.30	0.47
2:C:821:ARG:NH2	2:C:1082:ILE:HG12	2.30	0.47
3:D:424:ASN:OD1	3:D:467:ALA:HB3	2.15	0.47
3:D:607:THR:HA	3:D:610:ARG:HG2	1.97	0.47
3:D:1081:VAL:HG12	3:D:1087:ASP:HA	1.97	0.47
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.97	0.47
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.96	0.47
1:B:65:LEU:HD23	1:B:169:GLY:H	1.79	0.47
2:C:630:VAL:HG23	2:C:631:GLU:HG3	1.97	0.47
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.33	0.47
3:D:523:GLU:HA	3:D:546:ALA:HB1	1.96	0.47
3:D:1161:GLY:HA2	3:D:1203:ARG:NH2	2.30	0.47
1:B:86:LYS:NZ	1:B:174:ASP:HB2	2.28	0.47
1:A:33:ARG:HD3	1:A:34:GLY:H	1.80	0.47
2:C:471:VAL:O	2:C:475:VAL:HG12	2.14	0.47
2:C:758:ARG:HE	2:C:835:GLU:CD	2.23	0.47
3:D:957:SER:HB3	3:D:1008:GLY:HA2	1.97	0.47
1:A:53:GLY:HA3	1:A:177:TYR:O	2.16	0.46
2:C:562:GLU:OE1	2:C:574:SER:OG	2.23	0.46
3:D:118:LYS:HB3	3:D:311:ARG:HD2	1.97	0.46
3:D:357:VAL:HG22	3:D:461:PHE:CZ	2.50	0.46
3:D:511:TYR:HE1	3:D:724:MET:HG3	1.80	0.46
4:E:70:GLN:HA	4:E:73:GLN:OE1	2.15	0.46
1:B:11:PRO:CB	1:B:28:LEU:HD21	2.39	0.46
2:C:42:ASP:HB2	2:C:50:GLU:HG2	1.97	0.46
1:B:124:VAL:HG11	1:B:210:THR:HA	1.96	0.46
2:C:1101:LEU:HD13	3:D:504:GLN:HG3	1.97	0.46
3:D:1045:THR:HB	3:D:1076:PRO:HG3	1.97	0.46
4:E:51:LEU:O	4:E:55:GLU:HG3	2.16	0.46
4:E:67:ARG:O	4:E:70:GLN:HB3	2.16	0.46
1:A:224:LEU:HD23	1:B:228:LEU:HD11	1.96	0.46
1:B:106:GLY:N	1:B:138:ALA:O	2.40	0.46
1:B:141:SER:O	1:B:142:MET:HE2	2.16	0.46
2:C:1109:ILE:HD11	3:D:763:PHE:C	2.40	0.46
2:C:81:ASP:N	2:C:84:GLU:OE2	2.35	0.46
2:C:799:ASN:O	2:C:800:MET:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:812:PHE:CD2	2:C:813:GLU:HG2	2.50	0.46
2:C:1276:TRP:CE3	3:D:801:VAL:HG21	2.51	0.46
3:D:247:PRO:HA	3:D:250:ARG:NH1	2.29	0.46
3:D:1061:VAL:HG13	3:D:1076:PRO:HG2	1.97	0.46
1:B:37:HIS:HE1	2:C:1217:THR:HA	1.80	0.46
3:D:494:ALA:HB1	3:D:1248:ILE:HD12	1.96	0.46
3:D:615:LYS:HA	3:D:618:VAL:HG12	1.98	0.46
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	1.97	0.46
5:G:45:MET:O	5:G:49:GLN:HG2	2.16	0.46
3:D:24:LEU:H	3:D:232:ASN:ND2	2.14	0.46
3:D:405:GLU:O	3:D:408:VAL:HG22	2.14	0.46
3:D:848:VAL:HG11	3:D:872:LEU:HD11	1.96	0.46
2:C:189:ASP:OD1	2:C:193:ASN:N	2.25	0.46
2:C:225:PHE:CE2	2:C:347:ILE:HB	2.50	0.46
2:C:705:GLU:HB3	2:C:794:LEU:H	1.80	0.46
2:C:1297:ASP:OD2	2:C:1300:GLY:HA3	2.16	0.46
2:C:1313:HIS:HB2	3:D:474:LEU:CD2	2.39	0.46
2:C:359:ARG:HE	2:C:363:LEU:HD11	1.81	0.45
3:D:144:TYR:O	3:D:160:LEU:N	2.35	0.45
3:D:308:ASP:OD2	3:D:311:ARG:HG2	2.15	0.45
3:D:721:SER:O	3:D:725:MET:HB2	2.16	0.45
3:D:1158:GLU:HA	3:D:1223:LEU:HD11	1.97	0.45
3:D:1274:PHE:CD2	5:G:95:SER:HB2	2.51	0.45
5:G:76:LEU:HD12	5:G:115:ALA:HB2	1.97	0.45
2:C:94:ALA:C	2:C:126:GLU:HG3	2.40	0.45
2:C:972:PHE:CD2	2:C:994:ARG:HG2	2.52	0.45
2:C:1281:TYR:CD2	3:D:484:MET:HE1	2.51	0.45
3:D:355:ILE:CG2	3:D:466:MET:HB2	2.46	0.45
1:A:231:PHE:CD2	1:B:43:LEU:HD11	2.51	0.45
2:C:89:GLY:HA2	2:C:140:GLY:HA3	1.99	0.45
2:C:642:SER:HB2	3:D:770:LEU:HD21	1.99	0.45
3:D:333:GLY:HA3	3:D:338:PHE:CE1	2.51	0.45
3:D:1189:MET:HE2	3:D:1189:MET:HA	1.98	0.45
1:A:158:ARG:HD3	1:A:158:ARG:N	2.31	0.45
1:B:156:SER:HA	1:B:159:ILE:HG22	1.98	0.45
2:C:519:ASN:OD1	2:C:520:PRO:HD2	2.17	0.45
3:D:980:THR:HB	3:D:997:VAL:HB	1.97	0.45
3:D:1036:ARG:HB2	3:D:1079:LYS:HB3	1.99	0.45
2:C:1151:LEU:HD13	2:C:1201:LEU:HD11	1.98	0.45
2:C:1246:ARG:HD3	2:C:1267:GLY:N	2.31	0.45
3:D:17:PHE:HD2	3:D:18:ASP:O	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:23:ALA:HB2	4:E:54:ILE:HD13	1.98	0.45
2:C:756:TYR:HA	2:C:764:CYS:SG	2.57	0.45
2:C:772:SER:H	2:C:775:GLU:CD	2.24	0.45
3:D:514:THR:O	3:D:576:ARG:NE	2.46	0.45
4:E:26:ARG:NH1	4:E:35:LYS:HD3	2.32	0.45
1:B:61:ILE:HG22	1:B:63:GLY:H	1.82	0.45
2:C:951:MET:N	2:C:951:MET:HE2	2.31	0.45
3:D:1238:GLN:NE2	3:D:1250:ASP:OD1	2.50	0.45
1:A:9:LEU:C	1:A:10:LYS:HD2	2.42	0.45
1:B:151:GLY:O	3:D:535:ARG:NH2	2.49	0.45
3:D:60:ARG:HA	3:D:91:GLU:HB2	1.99	0.45
3:D:250:ARG:HH11	3:D:266:ASN:ND2	2.14	0.45
3:D:336:GLY:HA3	3:D:1324:SER:OG	2.17	0.45
3:D:495:ASN:HD22	3:D:1247:LYS:HE2	1.82	0.45
4:E:2:ALA:N	4:E:42:GLU:OE1	2.49	0.45
1:B:111:THR:HG22	1:B:129:VAL:HA	1.98	0.45
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.17	0.45
2:C:1276:TRP:CZ3	3:D:798:ARG:HA	2.52	0.45
3:D:1059:LEU:O	3:D:1107:VAL:N	2.44	0.45
2:C:1213:TYR:CE2	2:C:1220:GLN:HB3	2.52	0.45
3:D:308:ASP:OD1	3:D:309:ASN:N	2.50	0.45
3:D:420:PRO:HD3	3:D:481:ARG:HH22	1.82	0.45
3:D:478:LEU:HA	3:D:478:LEU:HD23	1.68	0.45
3:D:1194:ARG:HB3	3:D:1211:SER:HB2	1.98	0.45
1:A:212:ASP:O	1:A:215:GLU:HG2	2.16	0.44
2:C:10:ARG:NH2	2:C:790:ASP:O	2.50	0.44
3:D:247:PRO:HA	3:D:250:ARG:CZ	2.47	0.44
3:D:615:LYS:HB3	3:D:616:PRO:HD3	1.99	0.44
3:D:787:ALA:O	3:D:790:THR:OG1	2.30	0.44
3:D:826:ILE:HG12	3:D:831:VAL:HG22	1.98	0.44
3:D:860:ARG:HH21	3:D:861:ASN:HB3	1.82	0.44
3:D:1289:ASN:O	3:D:1292:LEU:HB3	2.17	0.44
5:G:125:ALA:HA	5:G:128:ASN:ND2	2.32	0.44
8:J:16:A:H2'	8:J:17:G:C8	2.50	0.44
2:C:368:ARG:HD3	2:C:376:PRO:HG3	1.99	0.44
2:C:825:GLU:OE1	2:C:827:ARG:NH1	2.42	0.44
3:D:166:LEU:O	3:D:169:LEU:N	2.51	0.44
1:A:179:PRO:C	1:A:207:THR:HG1	2.23	0.44
1:B:32:GLU:OE1	1:B:32:GLU:N	2.48	0.44
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.97	0.44
2:C:98:VAL:HB	2:C:124:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:233:ARG:HG3	2:C:238:GLN:HG3	1.98	0.44
2:C:1281:TYR:C	2:C:1283:ALA:H	2.26	0.44
3:D:342:LEU:HA	3:D:343:LEU:HA	1.60	0.44
1:A:155:ALA:HB3	2:C:1059:ARG:NH1	2.33	0.44
1:B:125:LYS:HG2	1:B:128:HIS:HB2	1.98	0.44
2:C:276:GLN:HA	2:C:279:LYS:HG2	1.98	0.44
2:C:1032:LYS:HA	2:C:1032:LYS:HD3	1.81	0.44
2:C:1131:MET:HE1	2:C:1144:PHE:CD2	2.52	0.44
3:D:1234:VAL:HA	3:D:1253:ILE:HG21	1.98	0.44
3:D:1364:ALA:HB1	4:E:18:ASP:OD2	2.18	0.44
1:A:13:LEU:HG	1:B:231:PHE:CZ	2.52	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
2:C:173:ASN:OD1	2:C:174:ALA:N	2.50	0.44
2:C:204:LEU:HG	2:C:369:MET:HE3	1.98	0.44
2:C:236:LYS:HD2	2:C:289:VAL:H	1.82	0.44
2:C:448:LEU:HD11	2:C:554:HIS:CD2	2.53	0.44
2:C:841:ARG:H	2:C:848:GLU:HB2	1.82	0.44
2:C:1252:SER:OG	2:C:1259:LEU:HB2	2.18	0.44
3:D:145:VAL:HG22	3:D:159:ILE:HG22	2.00	0.44
3:D:1274:PHE:HD1	3:D:1275:LEU:HD23	1.81	0.44
2:C:56:VAL:HG21	2:C:468:LEU:HB3	2.00	0.44
2:C:1243:MET:SD	3:D:372:MET:HG3	2.57	0.44
3:D:160:LEU:HD13	3:D:165:TYR:HA	2.00	0.44
3:D:721:SER:HA	3:D:724:MET:HE2	2.00	0.44
2:C:130:MET:SD	2:C:134:GLY:HA2	2.57	0.44
2:C:184:LEU:HD13	2:C:389:PHE:HZ	1.83	0.44
3:D:141:PHE:HA	3:D:180:MET:SD	2.58	0.44
3:D:705:THR:OG1	3:D:718:SER:HA	2.17	0.44
3:D:1290:ARG:HG2	3:D:1296:GLY:HA2	2.00	0.44
1:A:11:PRO:HB2	1:A:28:LEU:HD23	1.99	0.44
2:C:560:PRO:HG2	2:C:561:ILE:HG23	1.99	0.44
2:C:815:SER:HB3	2:C:1077:SER:OG	2.17	0.44
2:C:836:LEU:HB3	2:C:918:LEU:HD21	2.00	0.44
2:C:1066:MET:SD	2:C:1232:MET:HB3	2.58	0.44
3:D:505:ASP:HB3	3:D:629:PHE:CE1	2.51	0.44
3:D:750:PRO:HD3	3:D:777:HIS:CG	2.53	0.44
2:C:200:ARG:HB3	7:I:14:DA:N3	2.32	0.44
2:C:255:ILE:HB	2:C:263:VAL:HB	1.98	0.44
2:C:883:LEU:HD11	2:C:1054:LEU:HD21	2.00	0.44
3:D:641:ILE:HD11	3:D:764:ARG:HG3	1.99	0.44
3:D:675:ALA:O	3:D:678:ARG:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:749:LYS:HB3	3:D:755:ILE:HG13	2.00	0.44
3:D:1370:MET:HE2	3:D:1370:MET:HA	1.99	0.44
1:B:176:CYS:SG	3:D:535:ARG:NH1	2.90	0.43
2:C:811:ASN:HB3	2:C:1099:ASN:HB2	2.00	0.43
3:D:115:TRP:HB3	3:D:1333:THR:HG21	1.99	0.43
3:D:528:THR:H	3:D:532:GLU:HG3	1.83	0.43
3:D:758:PRO:HG2	3:D:760:THR:HG22	2.00	0.43
3:D:1368:ASP:HA	3:D:1371:ARG:HE	1.83	0.43
5:G:78:ARG:HH11	5:G:79:LYS:HG2	1.83	0.43
2:C:426:ILE:HA	2:C:429:MET:HE3	1.99	0.43
2:C:1107:MET:HB3	3:D:763:PHE:HE2	1.83	0.43
3:D:262:THR:HB	3:D:325:LYS:HG2	2.00	0.43
3:D:1135:THR:H	3:D:1140:ARG:HE	1.66	0.43
4:E:16:ARG:HG3	4:E:17:PHE:CE1	2.52	0.43
1:B:22:THR:HG22	1:B:206:GLU:HB3	1.99	0.43
2:C:521:LEU:HA	2:C:524:ILE:HG22	1.99	0.43
3:D:892:PHE:HD1	3:D:1345:ARG:NH1	2.17	0.43
3:D:957:SER:HB2	3:D:985:ILE:O	2.18	0.43
4:E:70:GLN:HA	4:E:73:GLN:CD	2.43	0.43
7:I:27:DC:H2"	7:I:28:DC:C5	2.53	0.43
2:C:165:HIS:ND1	6:H:6:DT:H5"	2.34	0.43
2:C:1066:MET:HE3	2:C:1066:MET:HB3	1.84	0.43
3:D:123:ARG:HG3	3:D:1337:VAL:HG11	2.00	0.43
3:D:692:ARG:HA	3:D:695:LYS:HE2	2.01	0.43
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.34	0.43
3:D:902:ASP:C	3:D:903:LEU:HD12	2.43	0.43
5:G:85:LEU:HD21	5:G:91:PHE:CE1	2.53	0.43
3:D:743:MET:HE2	3:D:743:MET:HB3	1.87	0.43
2:C:423:ASP:HA	2:C:426:ILE:HG12	1.99	0.43
2:C:463:GLN:HG3	2:C:505:PHE:HB2	2.01	0.43
3:D:740:LEU:O	3:D:762:ASN:HB3	2.19	0.43
3:D:844:THR:OG1	3:D:846:GLU:O	2.30	0.43
3:D:972:LYS:HB3	3:D:974:VAL:HG23	1.99	0.43
1:B:182:ARG:HG2	1:B:204:GLU:OE2	2.19	0.43
1:B:196:THR:HG22	1:B:196:THR:O	2.18	0.43
2:C:339:ASN:N	2:C:345:PRO:HD3	2.33	0.43
2:C:1281:TYR:CE2	3:D:431:ARG:HG2	2.53	0.43
3:D:151:MET:HG2	5:G:37:VAL:HG21	2.00	0.43
3:D:605:LEU:HD23	3:D:605:LEU:HA	1.87	0.43
3:D:1145:PHE:HB3	3:D:1309:ILE:HG13	2.00	0.43
3:D:1171:GLY:HA2	6:H:2:DG:H21	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1276:TRP:HH2	3:D:798:ARG:HA	1.81	0.43
3:D:278:ARG:HG2	3:D:281:ARG:HH21	1.84	0.43
3:D:892:PHE:HA	3:D:1345:ARG:NH1	2.34	0.43
5:G:55:ALA:HA	5:G:58:ARG:HE	1.83	0.43
1:B:101:THR:HA	1:B:143:ARG:HE	1.84	0.43
2:C:607:SER:H	2:C:610:GLU:HB2	1.84	0.43
1:B:64:VAL:HG13	1:B:168:ILE:HB	2.01	0.43
2:C:224:PHE:CD2	2:C:347:ILE:HG21	2.54	0.43
2:C:475:VAL:HG23	2:C:492:MET:HG3	2.00	0.43
2:C:1269:ARG:NH1	6:H:16:DA:OP2	2.52	0.43
3:D:510:LEU:HD11	3:D:624:ILE:HG12	2.01	0.43
3:D:526:VAL:HA	3:D:549:LYS:O	2.19	0.43
3:D:1157:ALA:N	3:D:1208:ASP:O	2.48	0.43
2:C:672:GLU:HB3	2:C:1187:PHE:HD1	1.84	0.42
2:C:1244:HIS:HE1	2:C:1268:GLN:HE22	1.66	0.42
2:C:1259:LEU:HD23	3:D:346:ARG:HD2	2.02	0.42
3:D:1046:ILE:HG22	3:D:1061:VAL:HA	2.00	0.42
3:D:1162:ILE:HD11	3:D:1201:GLY:HA2	2.01	0.42
8:J:15:G:C2	8:J:16:A:C8	3.07	0.42
1:A:27:THR:HA	1:A:201:LEU:O	2.19	0.42
1:A:167:PRO:HB2	1:A:170:ARG:HG3	2.02	0.42
3:D:253:VAL:O	3:D:253:VAL:HG13	2.19	0.42
3:D:799:ARG:HH21	3:D:1146:GLU:HG2	1.83	0.42
3:D:1239:ASP:O	3:D:1243:LEU:HG	2.18	0.42
4:E:21:LEU:O	4:E:25:ARG:HG2	2.19	0.42
6:H:26:DG:H5'	6:H:26:DG:C8	2.55	0.42
1:B:89:ALA:HB3	1:B:125:LYS:HB2	2.01	0.42
1:B:182:ARG:NH2	3:D:531:LYS:HD3	2.34	0.42
2:C:13:LYS:N	2:C:1181:PRO:O	2.53	0.42
2:C:97:ARG:HB3	2:C:121:GLU:HB3	2.01	0.42
2:C:107:ARG:HA	2:C:108:GLU:HA	1.66	0.42
2:C:619:ALA:HB2	2:C:654:ASP:HB2	1.99	0.42
3:D:146:VAL:HG12	3:D:149:GLY:H	1.83	0.42
3:D:722:ILE:HA	3:D:725:MET:HB2	2.01	0.42
3:D:841:GLY:HA3	3:D:902:ASP:OD1	2.19	0.42
3:D:902:ASP:H	3:D:1251:LYS:NZ	2.18	0.42
3:D:1350:ASN:HA	3:D:1353:VAL:HG22	2.01	0.42
5:G:100:LEU:HB2	5:G:105:CYS:SG	2.60	0.42
2:C:192:ASP:HB3	2:C:346:TYR:HD1	1.83	0.42
5:G:93:MET:HE1	5:G:98:GLU:HB2	2.02	0.42
1:A:35:PHE:HE2	1:B:227:GLN:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.87	0.42
2:C:657:THR:HG21	2:C:1188:ASP:HB2	2.01	0.42
2:C:840:SER:OG	2:C:848:GLU:O	2.36	0.42
2:C:1191:LYS:O	2:C:1195:ILE:HG13	2.20	0.42
3:D:424:ASN:N	3:D:466:MET:HE3	2.34	0.42
5:G:73:TRP:CE2	5:G:112:LEU:HB2	2.54	0.42
1:A:10:LYS:NZ	1:B:227:GLN:HE21	2.18	0.42
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	2.01	0.42
1:B:65:LEU:HD23	1:B:168:ILE:HA	2.02	0.42
2:C:37:LYS:NZ	2:C:46:GLN:HB3	2.35	0.42
2:C:732:ILE:HG12	2:C:753:LEU:HD11	2.02	0.42
2:C:802:VAL:CG2	2:C:1098:LEU:HD12	2.50	0.42
2:C:1119:MET:HB2	2:C:1228:GLY:CA	2.50	0.42
2:C:1315:MET:H	4:E:28:ARG:HH22	1.68	0.42
3:D:546:ALA:O	3:D:573:THR:HA	2.20	0.42
2:C:690:VAL:HG12	2:C:1234:LYS:O	2.19	0.42
2:C:802:VAL:HG21	2:C:1098:LEU:HD12	2.01	0.42
2:C:1028:LYS:O	2:C:1032:LYS:HG2	2.19	0.42
2:C:1196:LYS:HB3	2:C:1200:LYS:HZ3	1.83	0.42
2:C:1273:MET:HB3	3:D:428:THR:OG1	2.20	0.42
3:D:1155:ILE:HG23	3:D:1210:ILE:HB	2.02	0.42
3:D:1221:LEU:HD13	3:D:1229:VAL:HG11	2.02	0.42
5:G:92:ILE:HD11	5:G:101:GLU:HG2	2.02	0.42
1:A:91:ARG:NH2	1:A:209:GLY:O	2.50	0.42
1:B:182:ARG:HH12	3:D:531:LYS:HA	1.84	0.42
2:C:44:GLU:HG3	2:C:46:GLN:HG2	2.01	0.42
2:C:425:ILE:HA	2:C:428:VAL:HG12	2.01	0.42
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.55	0.42
3:D:16:GLU:HG2	3:D:16:GLU:O	2.20	0.42
3:D:500:ILE:HG22	3:D:500:ILE:O	2.19	0.42
3:D:702:GLN:HE22	3:D:703:THR:HG22	1.83	0.42
1:A:235:ARG:HH12	1:B:12:ARG:HD3	1.84	0.42
1:B:73:GLY:O	1:B:136:GLU:HB2	2.20	0.42
2:C:582:ASN:ND2	2:C:583:GLU:OE2	2.53	0.42
2:C:1246:ARG:HB3	2:C:1264:GLN:NE2	2.35	0.42
3:D:416:ILE:CG2	3:D:439:PRO:HG2	2.48	0.42
3:D:683:ILE:HD12	3:D:754:ILE:HD13	2.02	0.42
3:D:901:ARG:HB2	3:D:907:HIS:O	2.19	0.42
3:D:1135:THR:N	3:D:1140:ARG:HH21	2.17	0.42
1:B:131:CYS:O	1:B:132:HIS:ND1	2.53	0.41
2:C:13:LYS:HB3	2:C:1182:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:VAL:O	2:C:22:LEU:HB3	2.20	0.41
2:C:557:ARG:HH21	2:C:607:SER:C	2.28	0.41
2:C:655:VAL:N	2:C:659:GLN:OE1	2.53	0.41
2:C:874:GLY:N	2:C:928:VAL:O	2.53	0.41
2:C:1086:PRO:CB	2:C:1212:LEU:HD13	2.50	0.41
3:D:123:ARG:HH21	3:D:1334:GLU:HG2	1.85	0.41
3:D:152:THR:HA	5:G:37:VAL:HG11	2.01	0.41
3:D:343:LEU:HA	3:D:344:GLY:HA2	1.77	0.41
3:D:352:ARG:NH1	6:H:16:DA:O3'	2.52	0.41
2:C:820:GLU:HG2	2:C:824:GLN:NE2	2.28	0.41
3:D:101:ARG:O	3:D:246:PRO:HG3	2.20	0.41
3:D:948:SER:HA	3:D:1022:PRO:HA	2.02	0.41
3:D:1280:VAL:HG21	3:D:1304:ARG:CZ	2.49	0.41
1:B:112:ALA:HB1	1:B:123:ILE:HG21	2.02	0.41
1:B:215:GLU:HA	1:B:218:ARG:HG2	2.02	0.41
2:C:642:SER:HB2	3:D:770:LEU:CD2	2.50	0.41
3:D:355:ILE:HD11	3:D:460:ASP:O	2.20	0.41
3:D:1179:PRO:HD2	3:D:1184:ASP:HA	2.03	0.41
3:D:1232:TYR:O	3:D:1236:GLU:HG2	2.20	0.41
5:G:43:ASN:C	5:G:43:ASN:HD22	2.28	0.41
2:C:1270:PHE:CE1	2:C:1274:GLU:HB3	2.56	0.41
3:D:77:ARG:HD3	3:D:77:ARG:HA	1.83	0.41
3:D:424:ASN:C	3:D:466:MET:HE3	2.46	0.41
3:D:1364:ALA:HB1	4:E:18:ASP:CG	2.45	0.41
1:A:230:ALA:HB2	1:B:12:ARG:NH2	2.36	0.41
1:B:53:GLY:O	1:B:148:ARG:HA	2.21	0.41
2:C:364:VAL:HG13	2:C:376:PRO:HG3	2.02	0.41
2:C:374:GLU:O	2:C:375:PRO:C	2.63	0.41
2:C:565:GLU:OE1	2:C:681:MET:HG3	2.20	0.41
3:D:264:ASP:HB2	3:D:325:LYS:O	2.21	0.41
3:D:796:LEU:O	3:D:800:LEU:HD23	2.21	0.41
3:D:819:GLY:H	3:D:881:LYS:HE2	1.85	0.41
3:D:951:GLN:HB3	3:D:1014:GLY:HA2	2.02	0.41
3:D:1316:THR:HG22	3:D:1318:SER:H	1.86	0.41
2:C:176:ILE:HB	2:C:184:LEU:HB3	2.03	0.41
2:C:1105:SER:HB2	3:D:731:ARG:HB3	2.03	0.41
3:D:15:GLU:O	3:D:17:PHE:HD1	2.04	0.41
3:D:388:ARG:HH21	3:D:414:GLU:CD	2.26	0.41
3:D:430:HIS:ND1	3:D:925:GLU:OE1	2.53	0.41
3:D:495:ASN:ND2	3:D:1247:LYS:HE2	2.36	0.41
3:D:536:LEU:O	3:D:539:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:73:TRP:HZ2	5:G:108:ALA:HB1	1.85	0.41
1:A:35:PHE:CE2	1:B:227:GLN:HG3	2.56	0.41
1:B:74:VAL:HG12	1:B:76:GLU:H	1.85	0.41
2:C:232:ILE:HD11	2:C:325:LEU:HD11	2.01	0.41
2:C:722:GLY:HA2	2:C:737:ASN:CG	2.46	0.41
2:C:818:VAL:HA	2:C:1096:ILE:HD13	2.02	0.41
2:C:1087:TYR:CZ	2:C:1213:TYR:HB2	2.56	0.41
3:D:985:ILE:HD13	3:D:991:THR:HB	2.01	0.41
1:A:219:ARG:O	1:A:223:ILE:HG13	2.21	0.41
1:B:183:ILE:HD12	1:B:183:ILE:HA	1.96	0.41
2:C:459:MET:HE2	2:C:505:PHE:CE1	2.56	0.41
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.86	0.41
2:C:1281:TYR:CZ	3:D:431:ARG:HG2	2.56	0.41
2:C:1284:ALA:H	3:D:479:GLU:CD	2.29	0.41
3:D:841:GLY:HA3	3:D:902:ASP:CG	2.46	0.41
3:D:849:LEU:HD13	3:D:854:ALA:HA	2.01	0.41
4:E:10:VAL:HG22	4:E:16:ARG:HB2	2.03	0.41
4:E:46:THR:HG22	4:E:49:ILE:HD11	2.03	0.41
1:A:112:ALA:HB2	1:A:128:HIS:HB3	2.03	0.41
1:B:37:HIS:ND1	2:C:1216:ARG:HG3	2.36	0.41
1:B:107:ILE:HA	1:B:133:LEU:O	2.21	0.41
2:C:40:GLU:O	2:C:73:TYR:OH	2.38	0.41
2:C:138:ILE:HG22	2:C:139:ASN:OD1	2.21	0.41
2:C:364:VAL:HG13	2:C:376:PRO:CG	2.51	0.41
2:C:458:GLU:O	2:C:461:GLU:HG2	2.21	0.41
2:C:1280:ALA:HB3	3:D:431:ARG:HG3	2.03	0.41
2:C:1327:LEU:HD22	2:C:1328:LYS:NZ	2.36	0.41
3:D:44:ILE:HD11	3:D:252:LEU:HD11	2.02	0.41
3:D:98:ARG:O	3:D:98:ARG:NH1	2.42	0.41
3:D:113:HIS:HB3	3:D:116:PHE:CD1	2.56	0.41
3:D:204:GLU:HG2	5:G:108:ALA:HB1	2.03	0.41
3:D:497:GLU:HG2	3:D:498:PRO:HD2	2.03	0.41
3:D:552:ILE:CD1	3:D:570:LYS:HG3	2.51	0.41
3:D:696:ALA:O	3:D:700:ASN:ND2	2.40	0.41
3:D:720:ASN:ND2	3:D:722:ILE:HG22	2.36	0.41
3:D:1061:VAL:HG21	3:D:1101:LEU:HD13	2.03	0.41
3:D:1270:GLY:HA2	3:D:1298:VAL:N	2.36	0.41
3:D:1309:ILE:HD13	3:D:1309:ILE:HA	1.90	0.41
5:G:44:ALA:O	5:G:48:ILE:HG12	2.21	0.41
1:B:51:MET:O	1:B:150:ARG:HA	2.20	0.41
2:C:95:PRO:HA	2:C:126:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:ASP:OD1	2:C:313:ALA:N	2.43	0.41
2:C:706:ARG:HA	2:C:792:GLY:O	2.21	0.41
2:C:847:PRO:HB2	2:C:1047:LEU:HD11	2.03	0.41
2:C:1117:LEU:HD13	2:C:1195:ILE:HG23	2.02	0.41
2:C:1161:LEU:HD11	2:C:1165:SER:HA	2.02	0.41
2:C:1196:LYS:HG2	2:C:1206:THR:O	2.21	0.41
3:D:755:ILE:HG22	3:D:757:THR:H	1.86	0.41
4:E:54:ILE:HG22	4:E:59:ILE:HB	2.03	0.41
1:A:70:THR:HG21	2:C:755:LYS:NZ	2.36	0.40
1:A:231:PHE:CE1	1:B:28:LEU:HD13	2.30	0.40
1:B:85:LEU:HD12	1:B:86:LYS:HD3	2.02	0.40
2:C:693:LEU:N	2:C:829:THR:O	2.54	0.40
2:C:1030:GLU:O	2:C:1034:ARG:HG2	2.21	0.40
3:D:161:THR:HG23	3:D:163:GLU:HG3	2.03	0.40
3:D:220:ARG:CZ	5:G:27:GLN:HG3	2.51	0.40
3:D:578:ILE:O	3:D:581:MET:HB2	2.21	0.40
1:A:14:VAL:HG12	1:A:27:THR:O	2.22	0.40
2:C:185:ASP:O	2:C:196:VAL:HA	2.21	0.40
2:C:676:ALA:HA	3:D:772:TYR:OH	2.21	0.40
2:C:698:PRO:HG3	2:C:1231:TYR:CZ	2.56	0.40
2:C:1216:ARG:HG2	2:C:1216:ARG:HH11	1.86	0.40
2:C:1281:TYR:OH	3:D:432:LEU:HA	2.22	0.40
1:A:65:LEU:O	1:A:169:GLY:HA2	2.21	0.40
1:B:71:LYS:HD2	1:B:72:GLU:H	1.86	0.40
2:C:765:ILE:O	2:C:765:ILE:HG13	2.21	0.40
3:D:185:ILE:HG22	3:D:238:ILE:HD11	2.04	0.40
3:D:218:THR:HA	3:D:221:ILE:HG22	2.03	0.40
3:D:1297:LYS:HA	3:D:1298:VAL:HA	1.64	0.40
3:D:1322:ALA:HB3	3:D:1331:VAL:HG11	2.04	0.40
2:C:461:GLU:HG3	2:C:465:ARG:HH21	1.87	0.40
2:C:962:GLU:HA	2:C:962:GLU:OE1	2.21	0.40
2:C:1042:LEU:HD21	2:C:1046:VAL:HG12	2.03	0.40
2:C:1103:VAL:HG21	2:C:1112:ILE:HD11	2.03	0.40
4:E:63:ILE:HD12	4:E:63:ILE:H	1.87	0.40
2:C:7:GLU:HG2	2:C:11:ILE:HD13	2.04	0.40
2:C:403:MET:O	2:C:407:ARG:HG2	2.22	0.40
2:C:1107:MET:HB3	3:D:763:PHE:CE2	2.56	0.40
2:C:1156:ARG:O	2:C:1156:ARG:HG2	2.22	0.40
3:D:394:ILE:O	3:D:398:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/231 (99%)	211 (92%)	16 (7%)	1 (0%)	30	60
1	B	226/231 (98%)	219 (97%)	7 (3%)	0	100	100
2	C	1338/1340 (100%)	1280 (96%)	57 (4%)	1 (0%)	48	75
3	D	1348/1363 (99%)	1290 (96%)	53 (4%)	5 (0%)	30	60
4	E	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
5	G	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	16	45
All	All	3341/3370 (99%)	3191 (96%)	142 (4%)	8 (0%)	44	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	79	LYS
3	D	1097	ALA
3	D	594	GLN
2	C	1158	LYS
3	D	1152	GLU
1	A	195	ARG
5	G	54	SER
3	D	497	GLU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/199 (100%)	198 (100%)	0	100	100
1	B	196/199 (98%)	196 (100%)	0	100	100
2	C	1155/1155 (100%)	1155 (100%)	0	100	100
3	D	1129/1136 (99%)	1129 (100%)	0	100	100
4	E	65/65 (100%)	65 (100%)	0	100	100
5	G	112/112 (100%)	112 (100%)	0	100	100
All	All	2855/2866 (100%)	2855 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	B	93	GLN
1	B	147	GLN
1	B	227	GLN
2	C	31	GLN
2	C	69	GLN
2	C	276	GLN
2	C	339	ASN
2	C	628	HIS
2	C	686	GLN
2	C	824	GLN
2	C	932	GLN
2	C	1010	GLN
2	C	1017	GLN
2	C	1038	GLN
2	C	1175	ASN
2	C	1244	HIS
3	D	477	GLN
3	D	669	GLN
3	D	762	ASN
3	D	910	ASN
3	D	1098	GLN
3	D	1244	GLN
3	D	1350	ASN
3	D	1367	GLN

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Mol	Chain	Res	Type
4	E	29	GLN
4	E	43	ASN
5	G	29	GLN
5	G	50	ASN
5	G	71	ASN
5	G	128	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	J	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	J	12	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

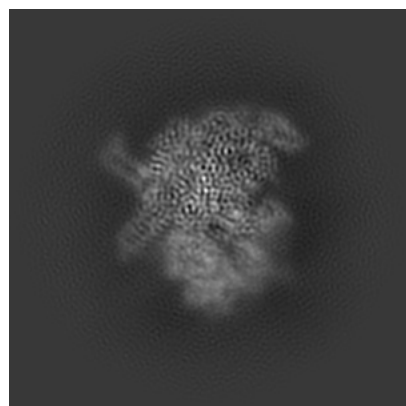
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36899. These allow visual inspection of the internal detail of the map and identification of artifacts.

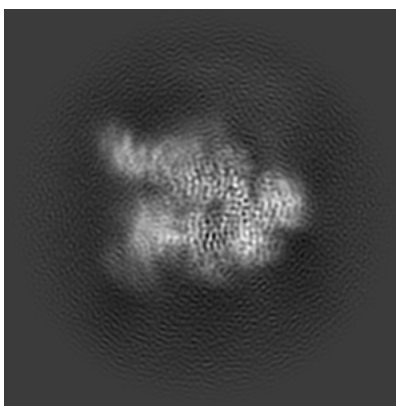
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

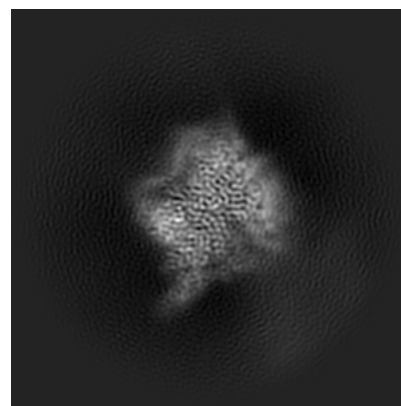
6.1.1 Primary map



X

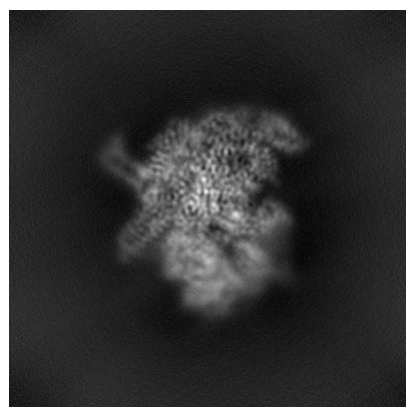


Y

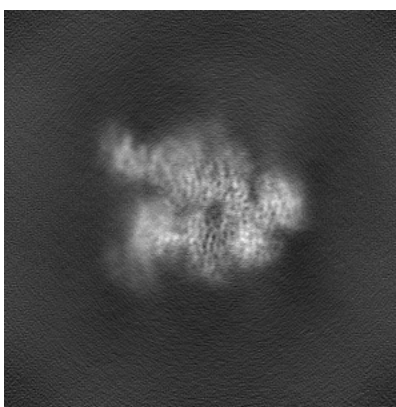


Z

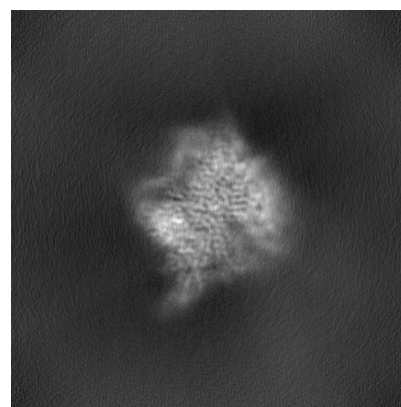
6.1.2 Raw map



X



Y

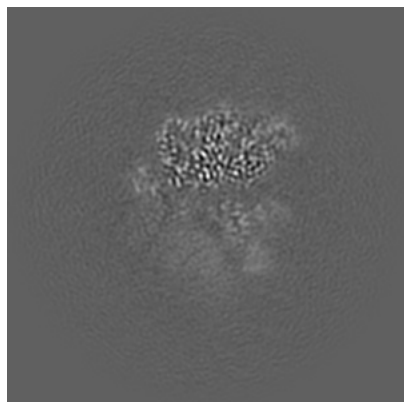


Z

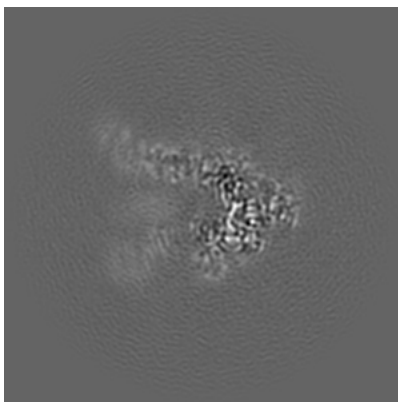
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

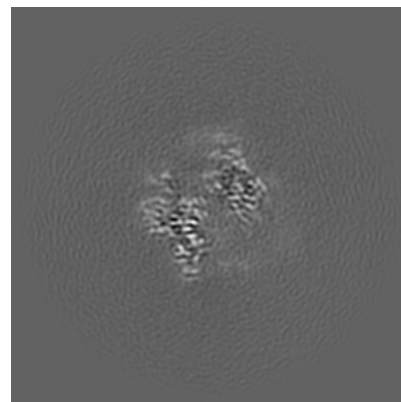
6.2.1 Primary map



X Index: 168

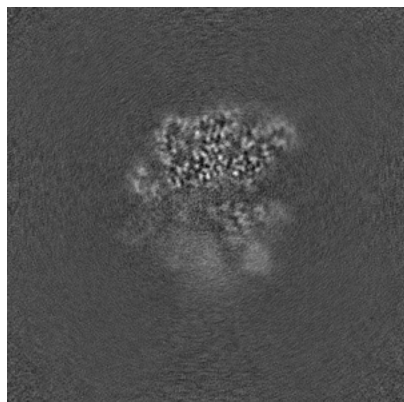


Y Index: 168

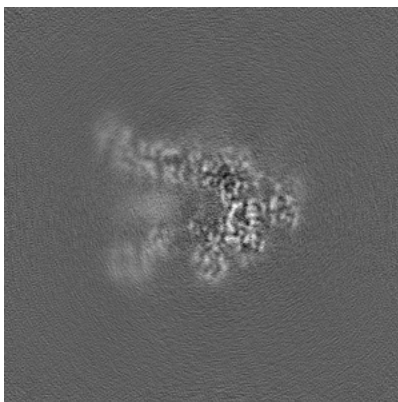


Z Index: 168

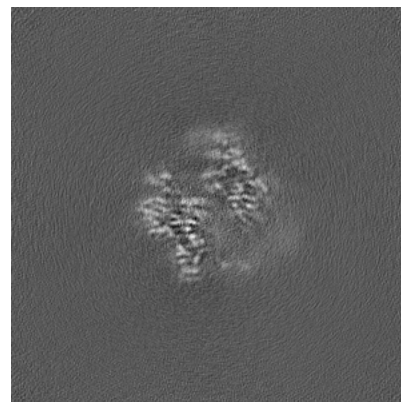
6.2.2 Raw map



X Index: 168



Y Index: 168

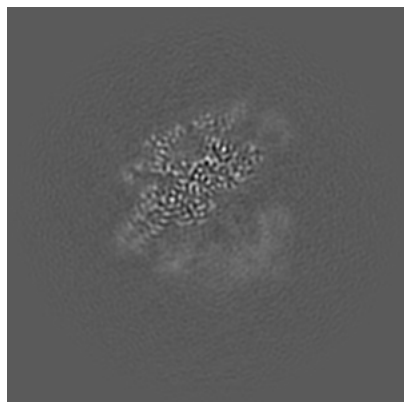


Z Index: 168

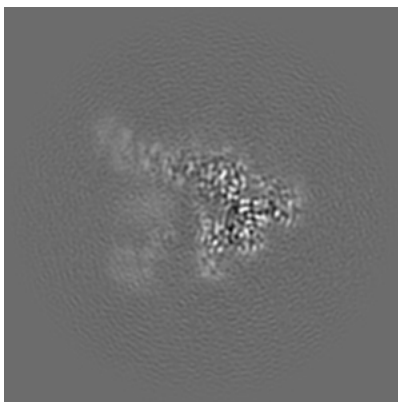
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

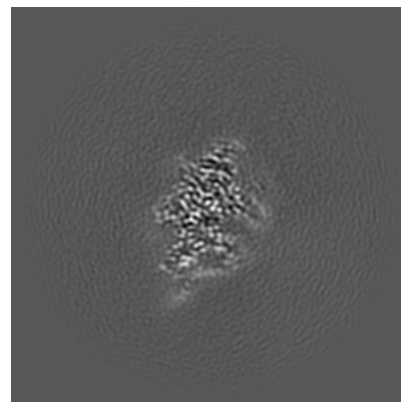
6.3.1 Primary map



X Index: 155

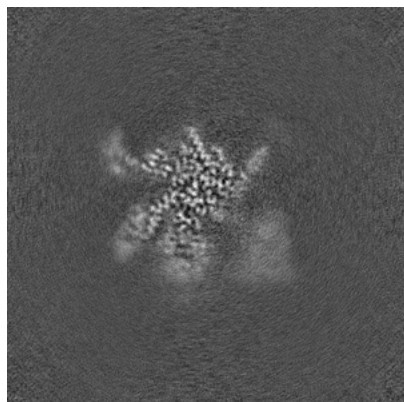


Y Index: 171

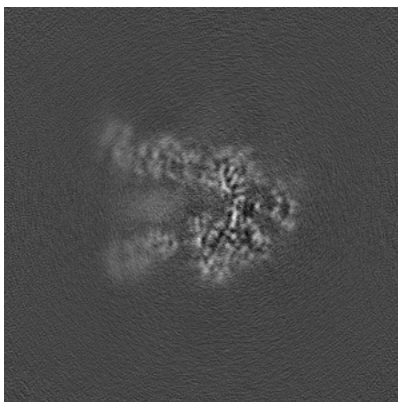


Z Index: 199

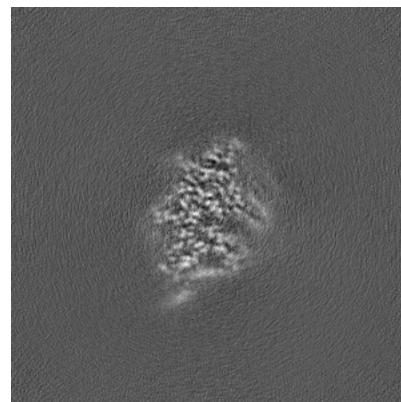
6.3.2 Raw map



X Index: 142



Y Index: 164

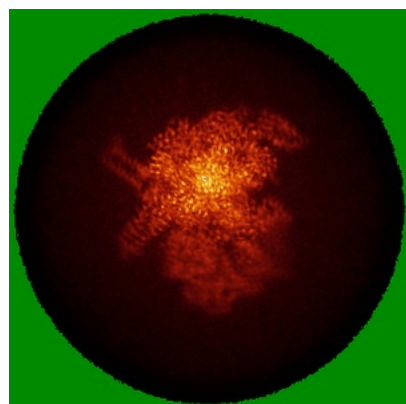


Z Index: 199

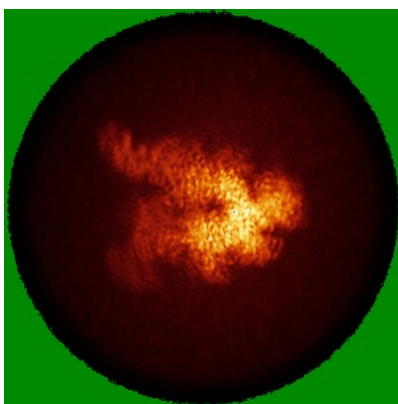
The images above show the largest variance slices of the map in three orthogonal directions.

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

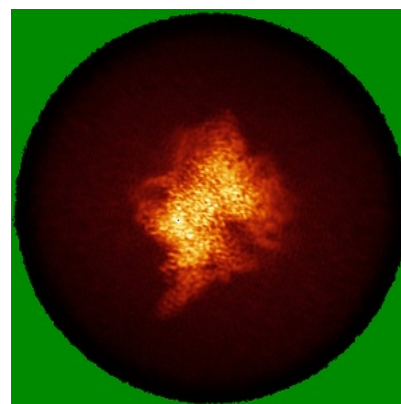
6.4.1 Primary map



X

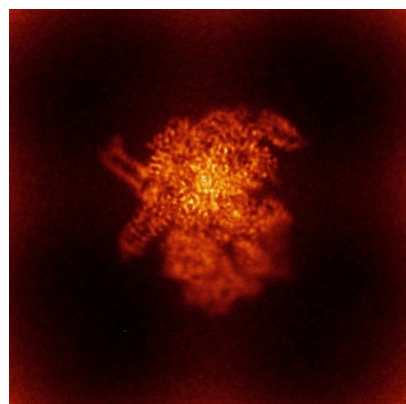


Y

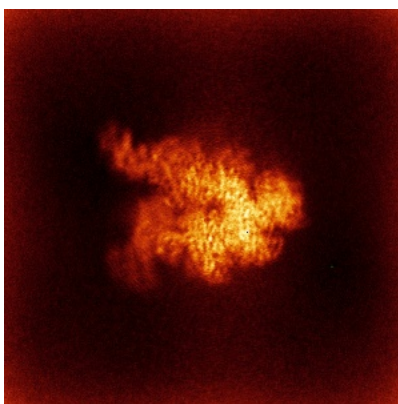


Z

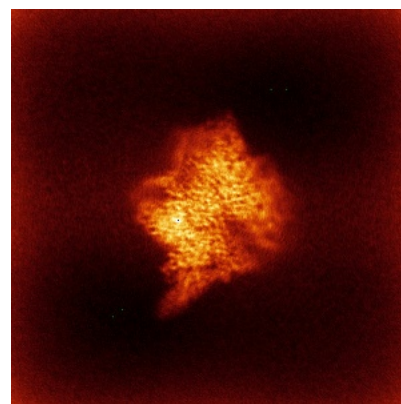
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

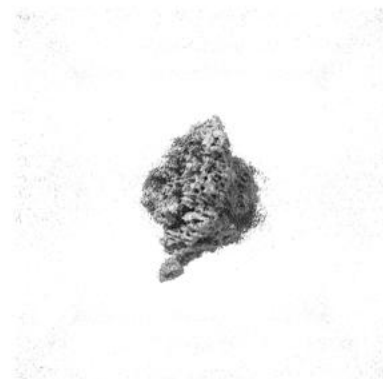
6.5.2 Raw map



X



Y



Z

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.

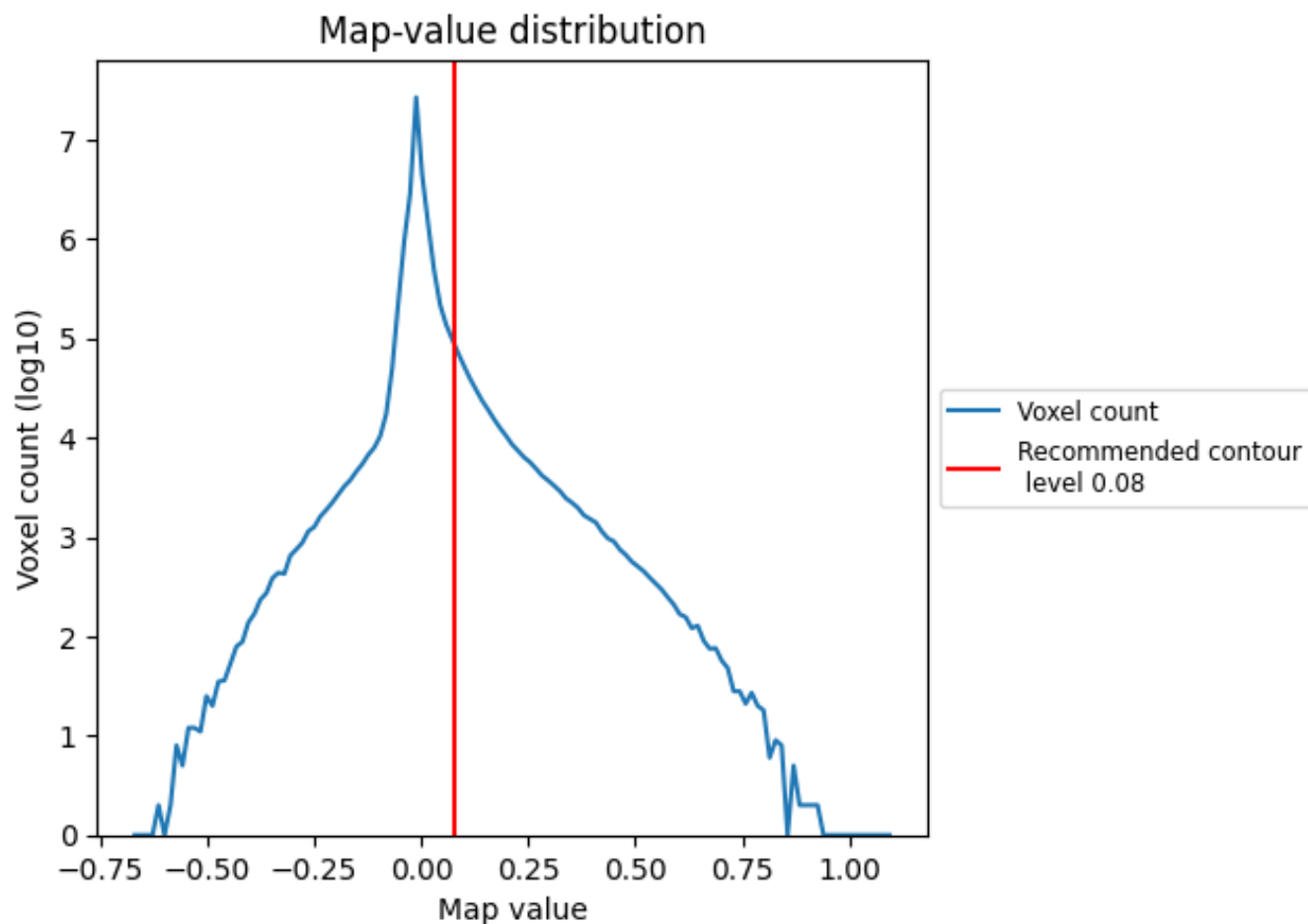
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

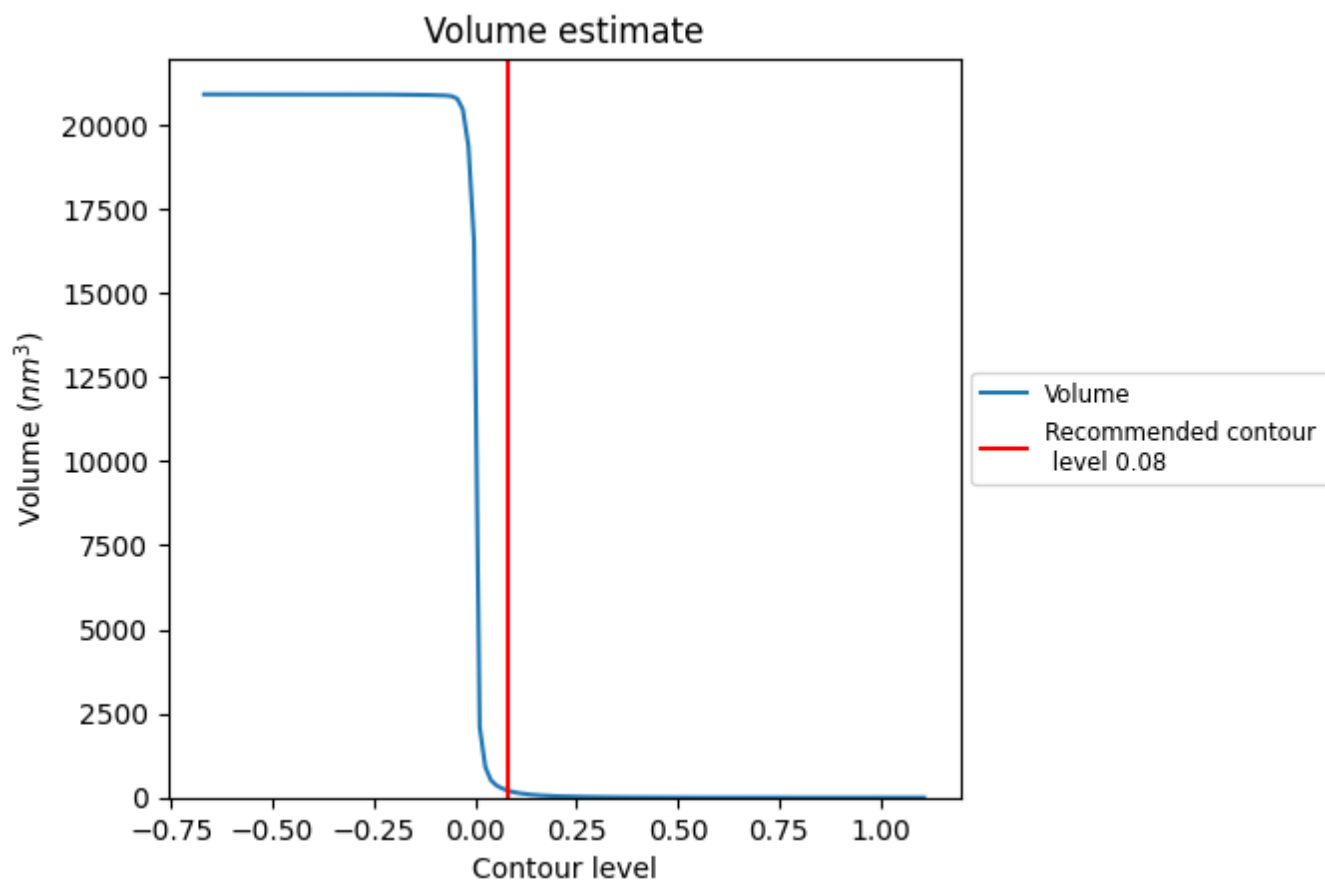
This section contains the results of statistical analysis of the map.

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.

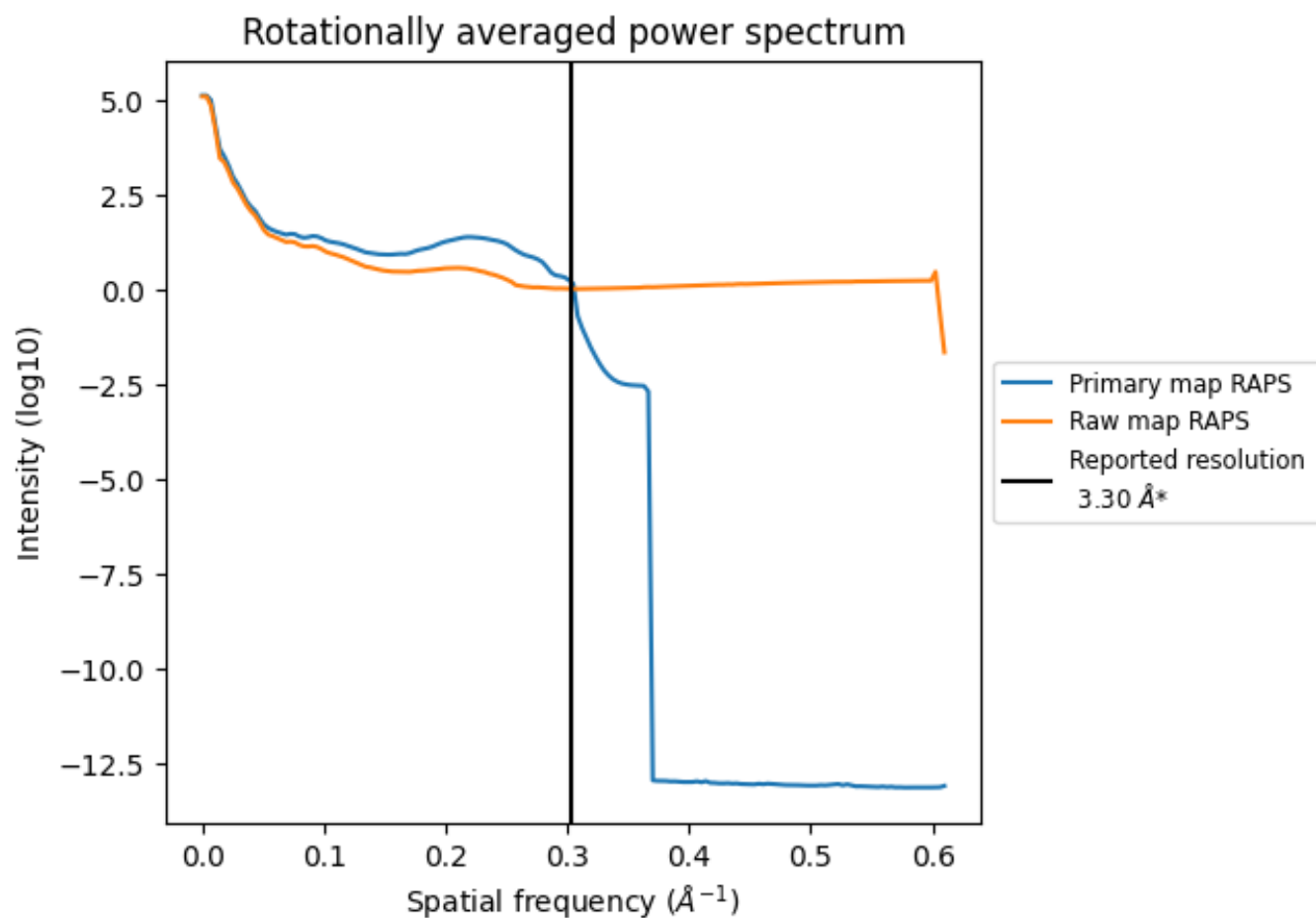
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 191 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 ⓘ

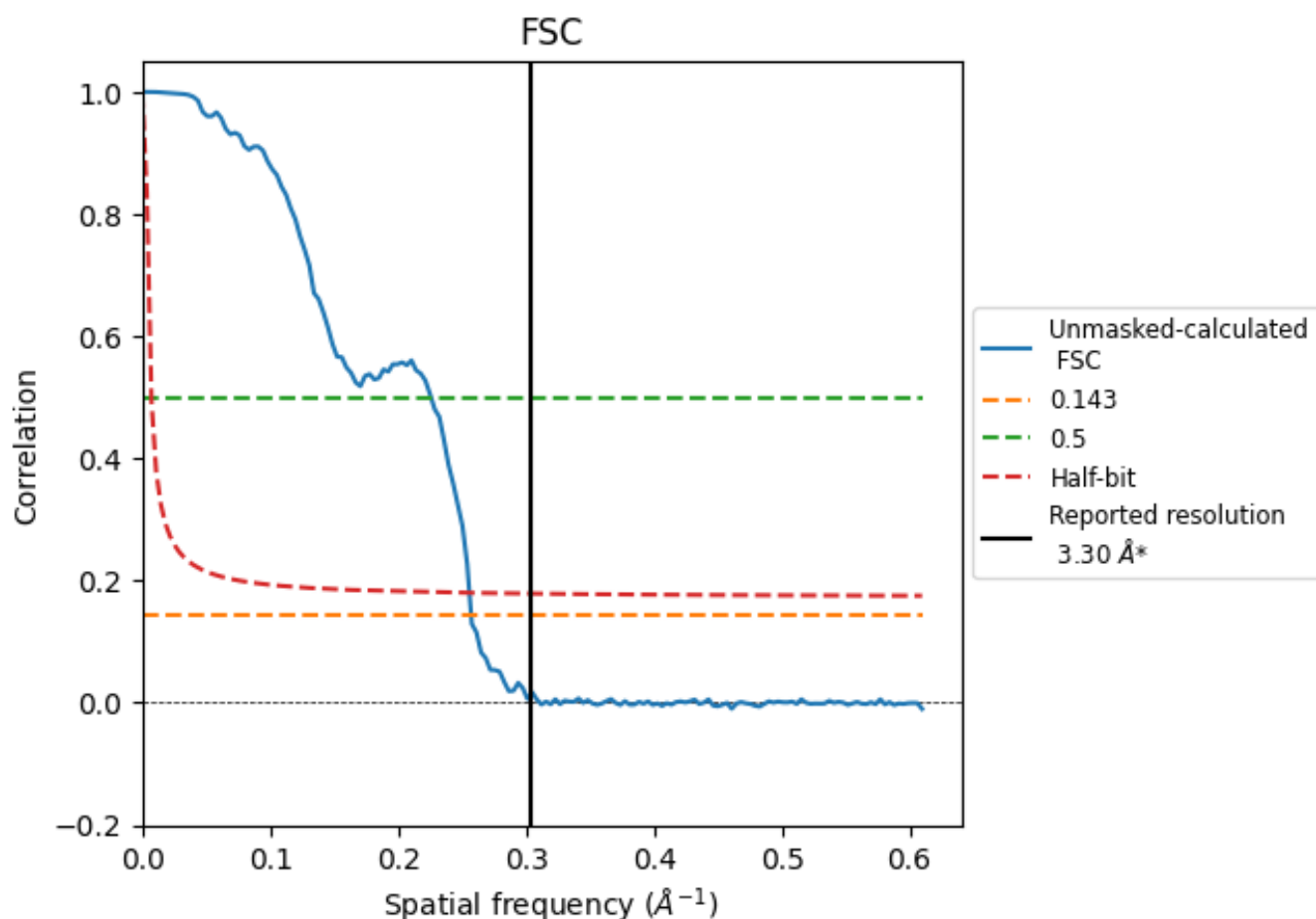


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

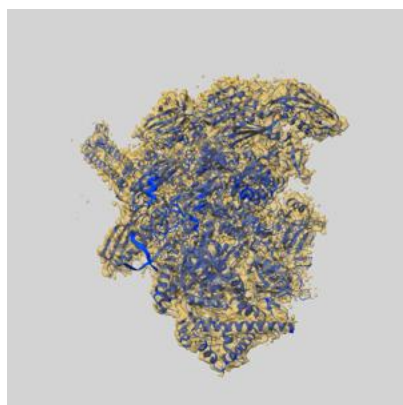
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.89	4.43	3.91

*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 3.89 differs from the reported value 3.3 by more than 10 %

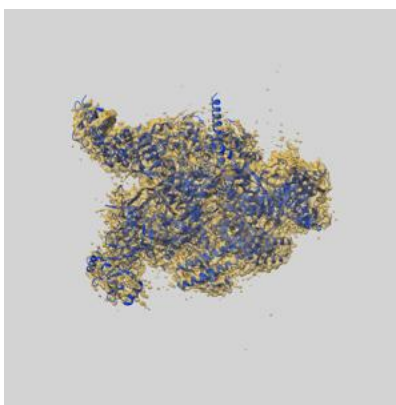
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36899 and PDB model 8K5A. Per-residue inclusion information can be found in section 3 on page 6.

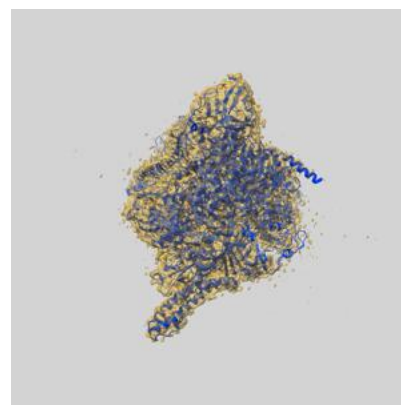
9.1 Map-model overlay [i](#)



X



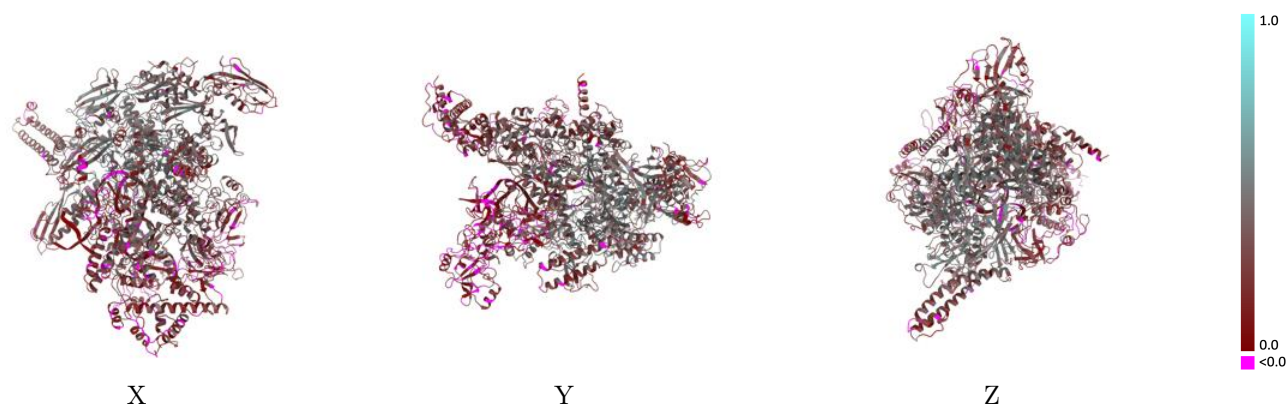
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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](#)

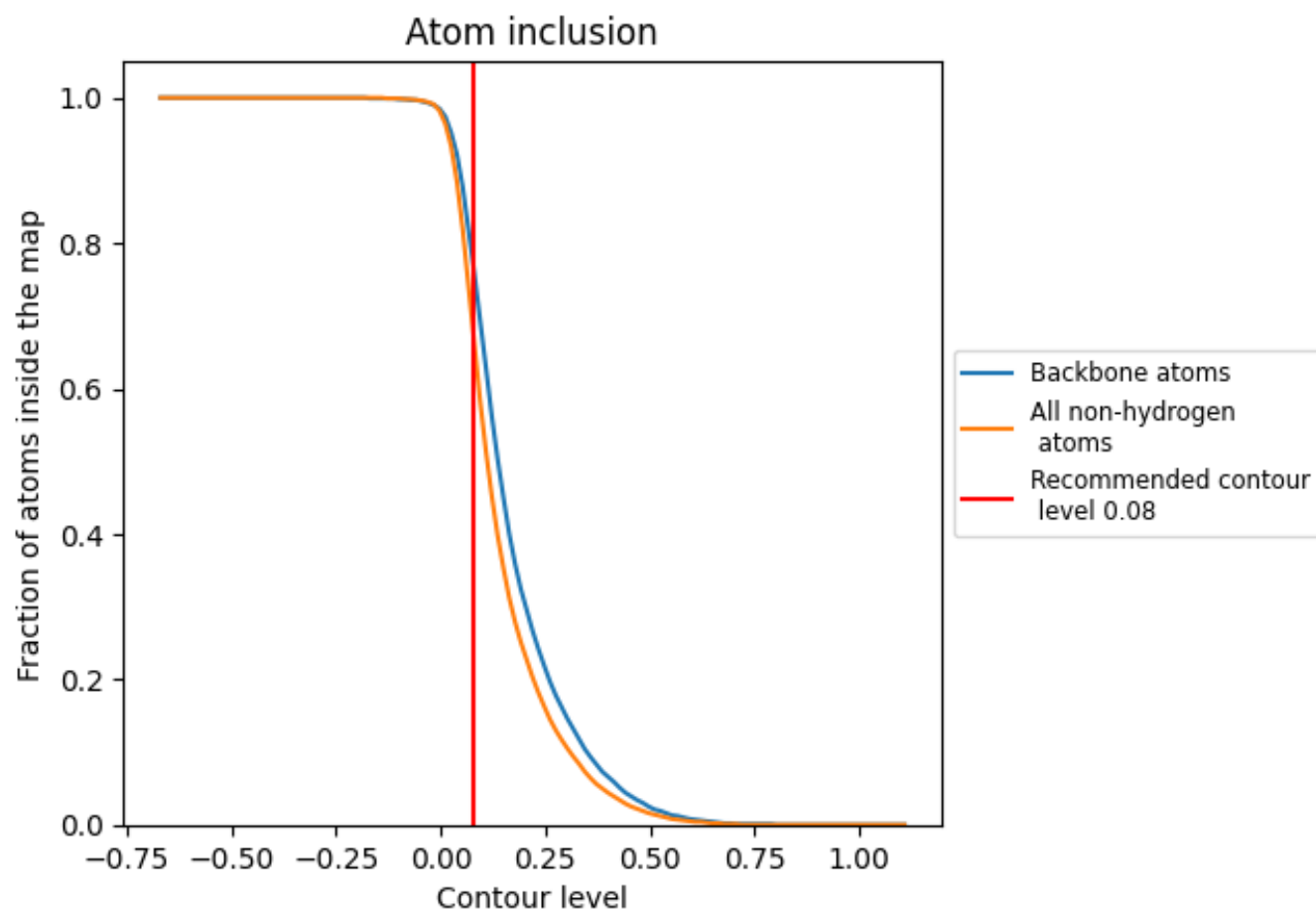


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 66% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6640	0.2950
A	0.7990	0.4000
B	0.7110	0.3000
C	0.7350	0.3380
D	0.6510	0.2740
E	0.3340	0.2260
G	0.5900	0.1650
H	0.1490	0.0990
I	0.1430	0.0550
J	0.1510	0.0510

1.0

0.0

<0.0