



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 04:19 PM UTC

PDB ID : 8G4W / pdb_00008g4w
EMDB ID : EMD-29732
Title : Cryo-EM consensus structure of Escherichia coli que-PEC (paused elongation complex) RNA Polymerase plus preQ1 ligand
Authors : Porta, J.C.; Chauvier, A.; Deb, I.; Ellinger, E.; Frank, A.T.; Meze, K.; Ohi, M.D.; Walter, N.G.
Deposited on : 2023-02-10
Resolution : 3.80 Å (reported)
Based on initial model : 6ASX

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:

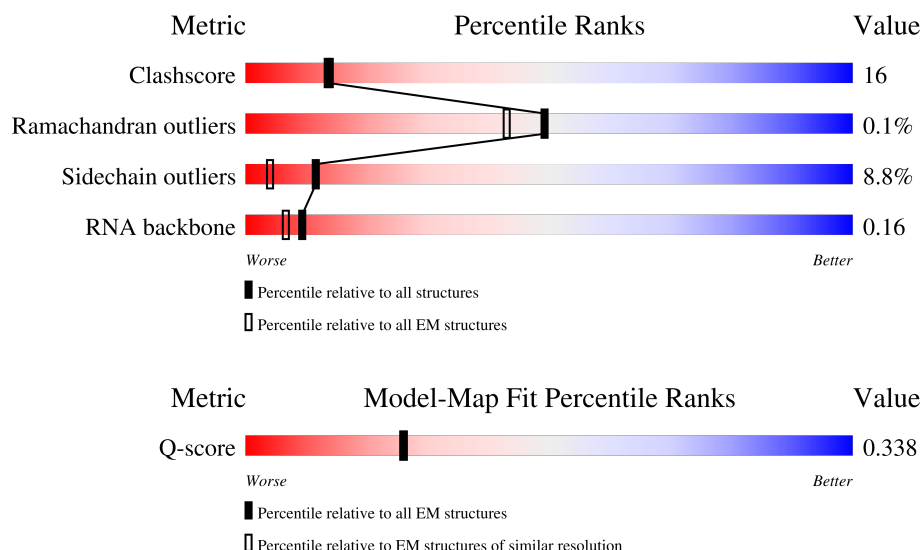
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	39	
2	B	31	

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Mol	Chain	Length	Quality of chain
3	G	235	23%61%33%6%
3	H	235	42%38%40%15%7%
4	K	79	52%57%35%8%
5	R	47	83%40%49%6%
6	I	1340	41%63%33%..
7	J	1358	45%61%36%..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 26842 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 DNA chain called DNA (39-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	19	Total	C	N	O	P	0	0
			388	186	78	107	17		

- Molecule 2 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	31	Total	C	N	O	P	0	0
			631	301	107	192	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	221	Total	C	N	O	S	0	0
			1708	1069	303	330	6		
3	H	219	Total	C	N	O	S	0	0
			1693	1058	298	331	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	235	GLU	-	expression tag	UNP A0A5B9AW69
H	235	GLU	-	expression tag	UNP A0A5B9AW69

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a RNA chain called RNA (47-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	47	Total	C	N	O	P	0	0
			997	449	185	317	46		

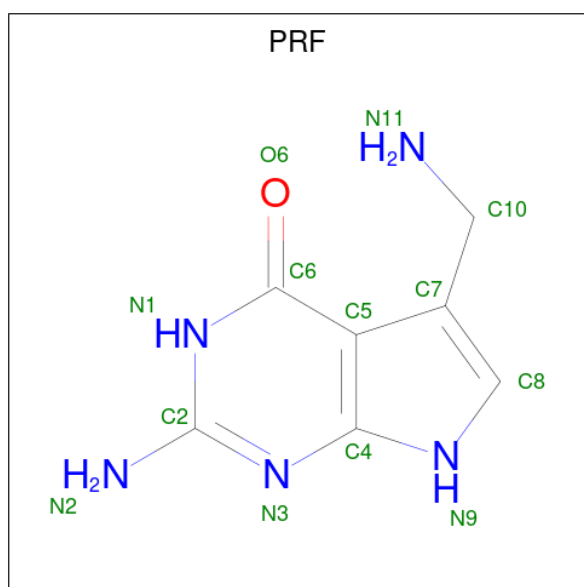
- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	1316	Total	C	N	O	S	0	0
			10381	6514	1810	2014	43		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	1337	Total	C	N	O	S	0	0
			10403	6536	1856	1961	50		

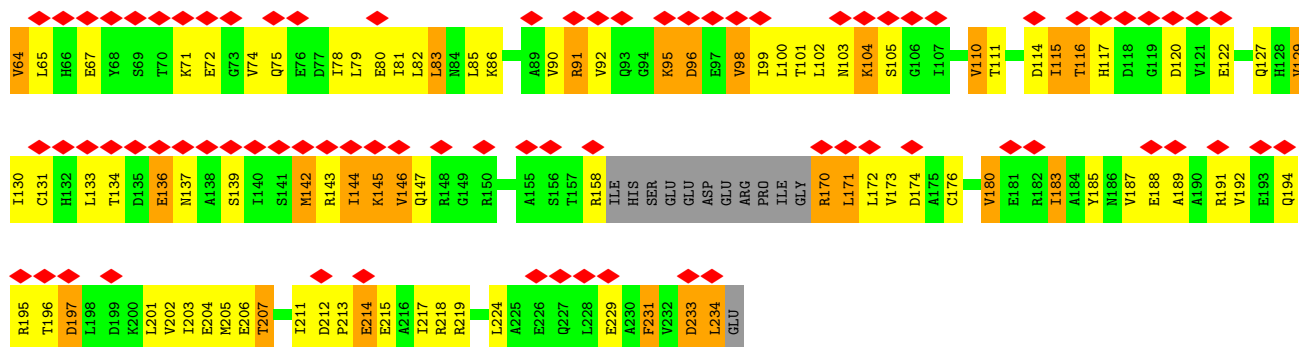
- Molecule 8 is 7-DEAZA-7-AMINOMETHYL-GUANINE (CCD ID: PRF) (formula: $C_7H_9N_5O$) (labeled as "Ligand of Interest" by depositor).



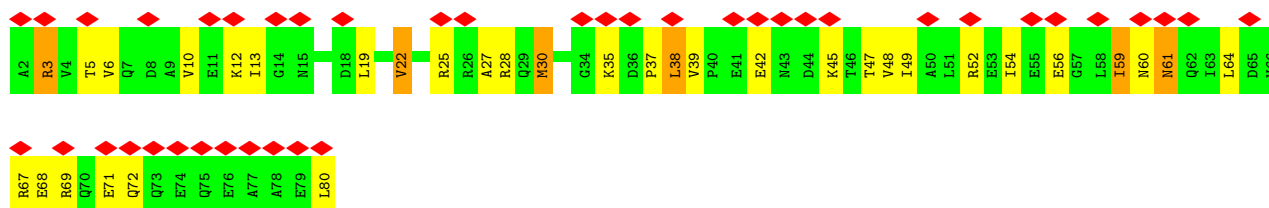
Mol	Chain	Residues	Atoms				AltConf
8	R	1	Total	C	N	O	0
			13	7	5	1	

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

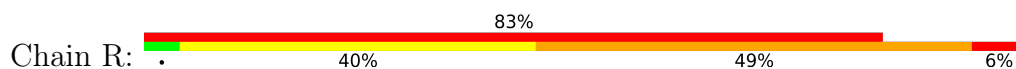
Mol	Chain	Residues	Atoms		AltConf
9	J	1	Total	Mg	0
			1	1	



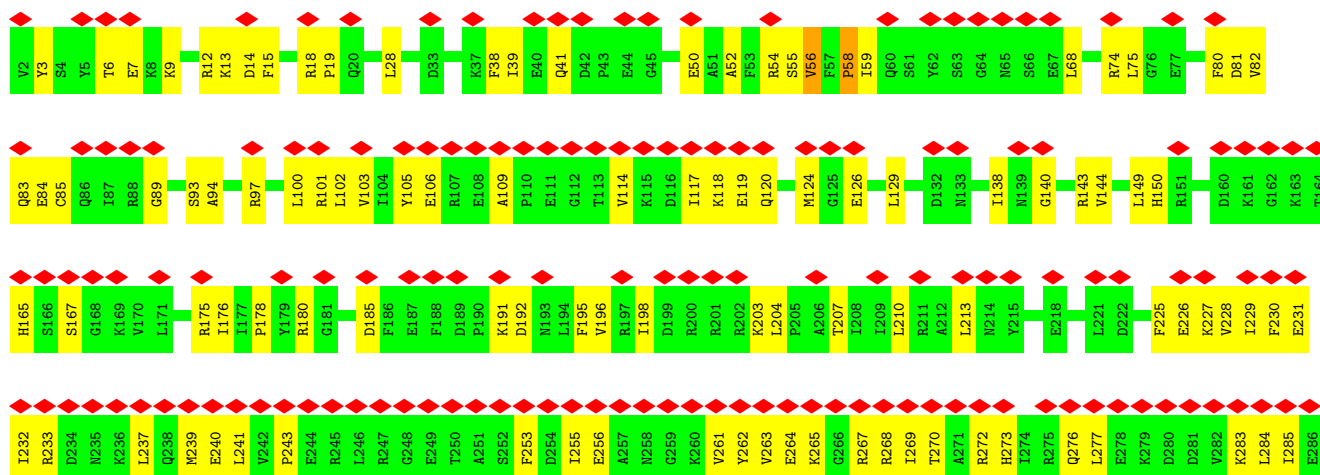
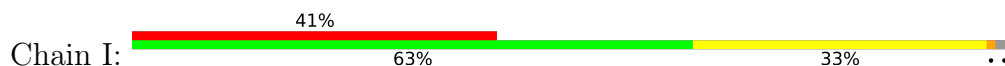
• Molecule 4: DNA-directed RNA polymerase subunit omega



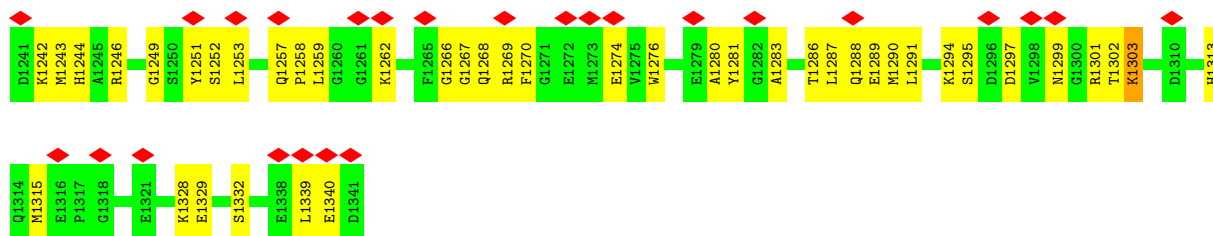
• Molecule 5: RNA (47-MER)



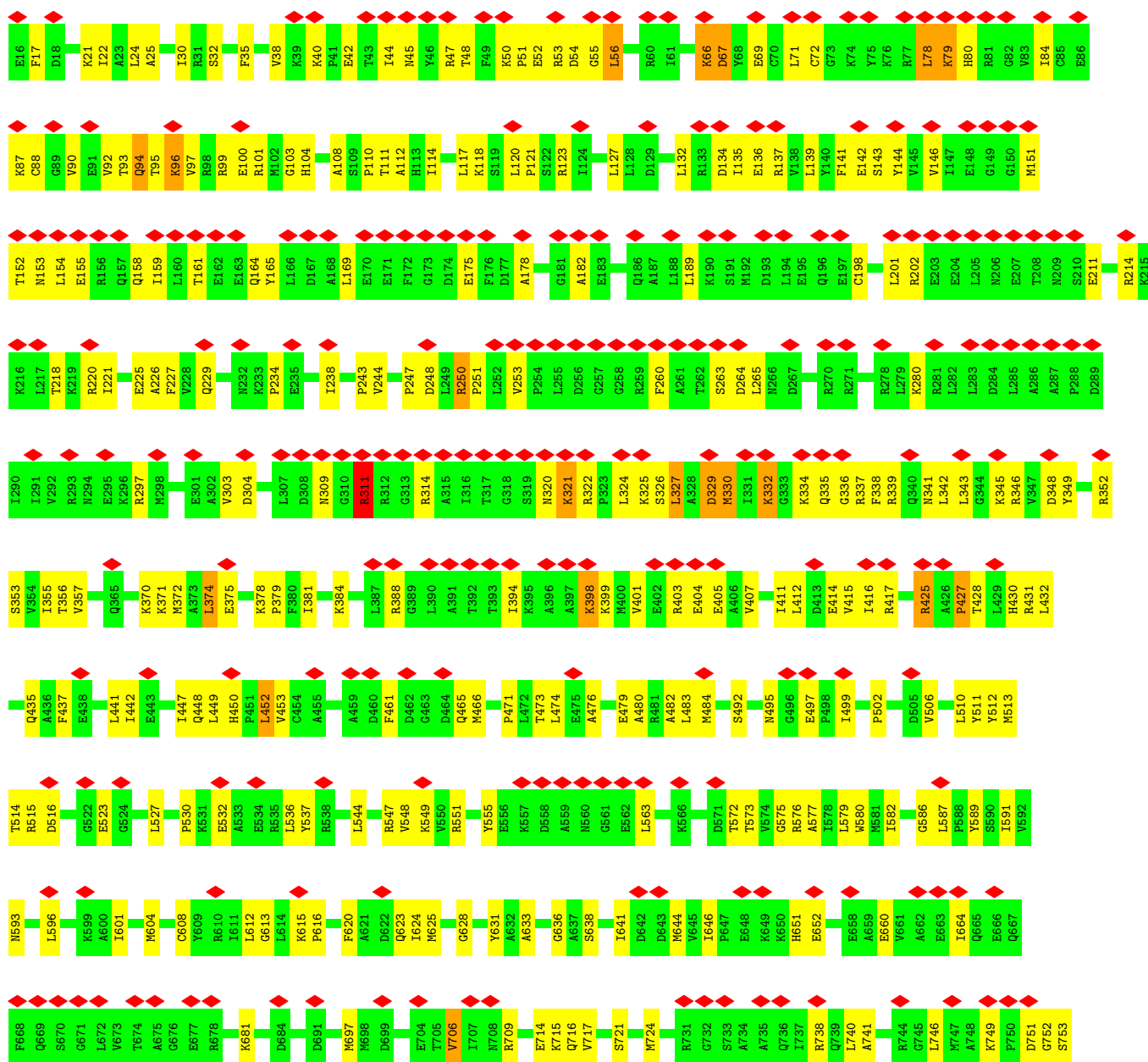
• Molecule 6: DNA-directed RNA polymerase subunit beta

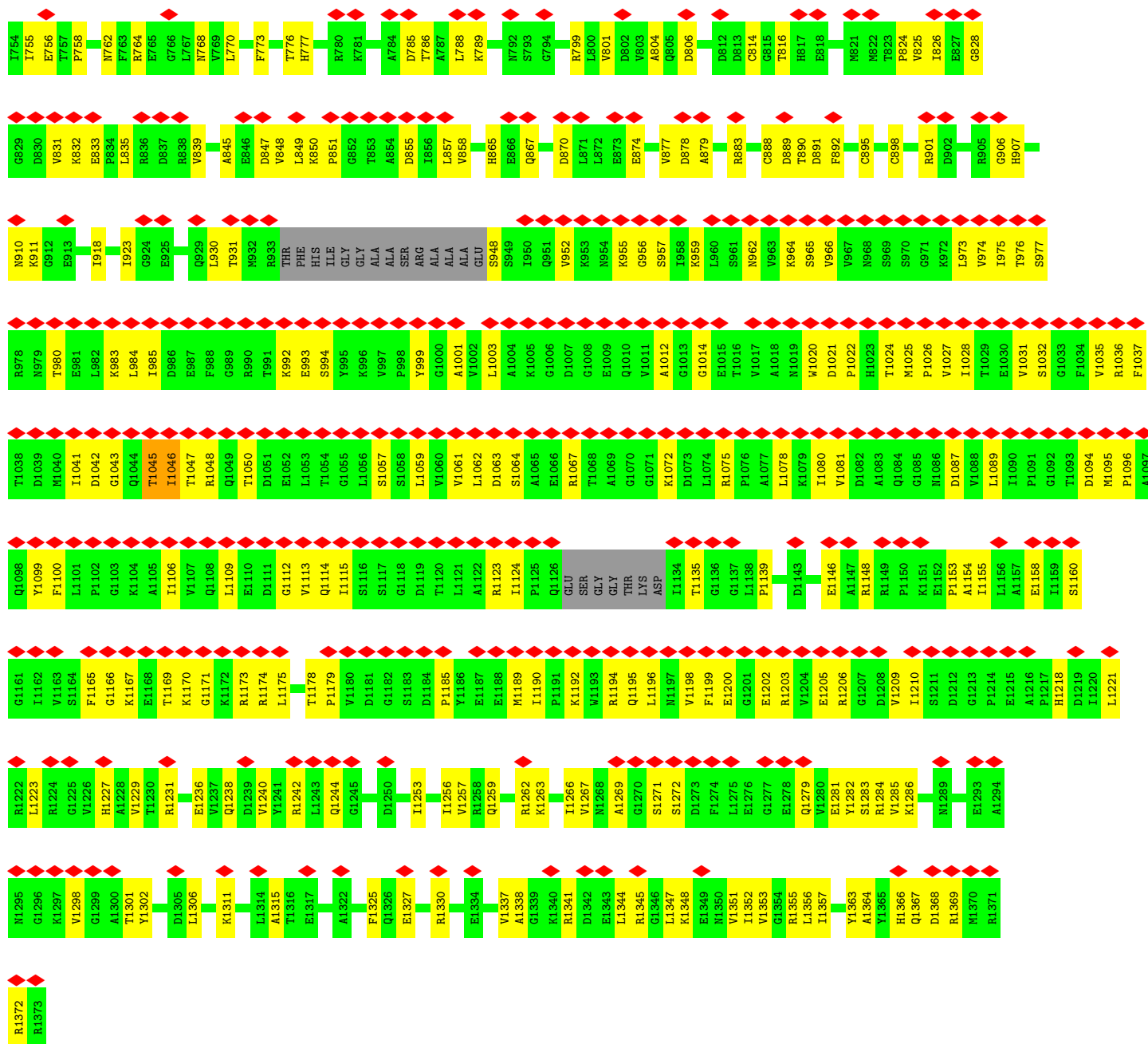


R1156	K1078	L1002	S1077	R1156	K1158	D1166	E1167	E1168	V1169	M1170	R1171	E1174	K1178	P1181	I1182	T1184	P1185	V1186	F1187	D1188	G1189	K1190	K1191	E1192	I1195	K1196	G1202	D1203	L1204	P1205	T1206	Q1209	I1210	R1211	Y1212	Y1213	D1214	G1215	R1216	R1223	P1224	V1225	T1227	V1228	G1228	Y1229	M1230	M1232	L1235	D1240										
I1079	I1079	E1006	I1082	E1083	D1084	M1085	P1086	Y1087	D1088	E1089	M1090	G1091	D1095	I1096	A1015	E1016	Q1017	Y1018	D1019	E1020	L1021	K1022	H1023	E1024	F1025	E1026	K1027	K1028	L1029	E1030	A1031	K1032	R1033	R1034	K1035	I1036	T1037	Q1038	G1039	D1040	D1041	L1042	A1043	E985	P1044	G1045	V1046	L1047	K1048	I1049	V1050	K1051	K1057	R1058	R1069	H1070	G1071	N1072	K1073	
E940	K941	D942	K943	R944	A945	E949	E950	M951	Q952	L953	K954	Q955	A956	K957	K958	D959	L960	S961	E962	E963	L964	Q965	I966	L967	G970	L971	F972	S973	R974	I975	R976	A977	V978	L979	V980	A981	G982	G983	V984	E985	A986	E987	K988	L989	D990	K991	L992	P993	R994	D995	R996	K997	L998	E999	L1000	G1001				
T878	G879	G880	D881	L882	L883	V884	G885	K886	V887	T888	R889	K890	GLY	GLU	THR	GLN	LEU	THR	PRO	GLU	LYS	LEU	LEU	ARG	ALA	ILE	PHE	GLY	GLU	LYS	ALA	SER	ASP	VAL	LYS	D915	S916	S917	L918	R919	V920	P921	N922	G923	V924	S925	G926	I929	P930	V931	Q932	F933	F934	T935	R936	D937	G938			
V939	E940	K941	D942	K943	R944	A945	E949	E950	M951	Q952	L953	K954	Q955	A956	K957	K958	D959	L960	S961	E962	E963	L964	Q965	I966	L967	G970	L971	F972	S973	R974	I975	R976	A977	V978	L979	V980	A981	G982	G983	V984	E985	A986	E987	K988	L989	D990	K991	L992	P993	R994	D995	R996	K997	L998	E999	L1000	G1001			
L1002	T1003	D1004	E1006	E1006	K1007	Q1008	N1009	Q1010	E1011	E1012	Q1013	L1014	A1015	E1016	Q1017	Y1018	D1019	E1020	L1021	K1022	H1023	E1024	F1025	E1026	K1027	K1028	L1029	E1030	A1031	K1032	R1033	R1034	K1035	I1036	T1037	Q1038	G1039	D1040	D1041	L1042	A1043	E985	P1044	G1045	V1046	L1047	K1048	I1049	V1050	K1051	K1057	R1058	R1069	H1070	G1071	N1072	K1073			
R1156	K1158	D1166	E1167	E1168	V1169	M1170	R1171	E1174	K1178	P1181	I1182	T1184	P1185	V1186	F1187	D1188	G1189	K1190	K1191	E1192	I1195	K1196	G1202	D1203	L1204	P1205	T1206	Q1209	I1210	R1211	Y1212	Y1213	D1214	G1215	R1216	R1223	P1224	V1225	T1227	V1228	G1228	Y1229	M1230	M1232	L1235	D1240														
S1077	K1078	L1002	I1079	E1083	D1084	M1085	P1086	Y1087	D1088	E1089	M1090	G1091	D1095	I1096	A1015	E1016	Q1017	Y1018	D1019	E1020	L1021	K1022	H1023	E1024	F1025	E1026	K1027	K1028	L1029	E1030	A1031	K1032	R1033	R1034	K1035	I1036	T1037	Q1038	G1039	D1040	D1041	L1042	A1043	E985	P1044	G1045	V1046	L1047	K1048	I1049	V1050	K1051	K1057	R1058	R1069	H1070	G1071	N1072	K1073	
R352	V353	D354	P355	P356	N357	D358	R359	L363	V364	E365	I366	Y367	R368	M369	M370	R371	P372	G373	E374	P375	A313	T377	R378	E379	A381	E382	S383	E386	N387	L388	F389	F390	S391	E392	D393	R394	Y395	D396	L397	R402	R407	L410	R411	E412	E413	I414	E415	G416	I419	K422	D423									
D424	I425	V428	M429	K430	K431	I435	R436	M437	G438	K439	G440	E441	V442	D443	D444	I445	D446	H447	L448	R451	R452	I453	R454	E458	M459	A460	E461	M462	Q463	F464	R465	L468	V469	E472	R473	A474	V475	K476	E477	S480	L481	G482	D483	L484	D485	T486	L487	M488	P489	Q490	D491	M492								
I493	M494	A495	K496	A500	A501	V502	K503	E504	F505	F506	G507	S508	S509	Q510	L511	S512	Q513	D516	Q517	N518	N519	P520	L521	K527	R528	R529	G536	G537	L538	T539	R540	E541	R542	A543	G544	F545	E546	V547	R548	D549	V550	H551	P552	T553	H554	T555	G556	R557	V558	C559	P560	I561	E562	T563	P564					
E565	N568	L571	L572	L587	P590	Y591	R592	K593	V594	T595	D596	G597	V598	V599	T600	D601	E602	L606	L609	E610	G611	G612	N613	Y614	V615	I616	L693	A617	Q618	A619	N620	S621	N622	L623	D624	E625	E626	G627	D632	C636	K639	G640	S643	L644	F645	S646	R647	D648	Q649	V650										
D651	Y652	M653	D654	V655	V660	V661	S662	A665	S666	L667	I668	L671	E672	H673	D674	D675	R678	A679	L680	M681	N684	G685	Q686	R687	Q688	A689	V690	P691	T692	L693	R694	A695	D696	K697	P698	L699	V700	G701	T702	G703	M704	E705	R706	A707	V708	D711	V714	T715	F718	K719	R720									
V727	D728	L732	V733	L734	K735	V736	N737	E738	D739	E740	N741	V742	P743	G744	E745	A746	G747	I748	D749	N752	L753	T754	K755	S759	N760	Q761	I765	N766	G767	R768	P769	S772	L773	G774	E775	G776	V777	E778	R779	G780	D781	L782	V783	A784	D785	G786	P787	D790	E793	L794	A795									
L796	G797	Q798	R801	V802	M805	P806	M807	N808	E813	D814	E820	R821	V822	E825	D826	R827	T830	L836	A837	C838	R841	D842	T843	K844	L845	G846	P847	E848	E849	T850	T851	A852	D853	L854	P855	N856	V857	G858	E859	A860	K864	L865	D866	E867	S868	G869	L870	E876	V877											



• Molecule 7: DNA-directed RNA polymerase subunit beta'





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	51824	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 ($e^-/\text{\AA}^2$)	62.00	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.135	Depositor
Minimum map value	-0.541	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.4	Depositor
Map size ($\text{\AA}$)	300.0, 300.0, 300.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.22	0/436	0.39	0/670
2	B	0.19	0/704	0.38	0/1084
3	G	0.16	0/1728	0.32	0/2341
3	H	0.95	0/1712	1.31	1/2320 (0.0%)
4	K	0.86	0/629	1.28	0/847
5	R	1.80	21/1116 (1.9%)	1.51	19/1736 (1.1%)
6	I	0.37	0/10547	0.59	6/14232 (0.0%)
7	J	0.42	0/10560	0.64	3/14257 (0.0%)
All	All	0.57	21/27432 (0.1%)	0.74	29/37487 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	R	0	13

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	24	U	O3'-P	-7.26	1.50	1.61
5	R	27	A	P-O5'	-7.13	1.49	1.59
5	R	3	A	C5'-C4'	6.94	1.61	1.51
5	R	14	C	C5'-C4'	6.79	1.61	1.51
5	R	20	C	C3'-C2'	6.69	1.62	1.52
5	R	19	C	O5'-C5'	6.67	1.52	1.42
5	R	10	C	C1'-N1	6.46	1.58	1.48
5	R	18	A	C5'-C4'	6.43	1.60	1.51
5	R	3	A	C4'-O4'	-6.35	1.36	1.45
5	R	13	G	C2'-C1'	-6.29	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	33	C	P-O5'	-6.05	1.50	1.59
5	R	4	G	C5'-C4'	6.01	1.60	1.51
5	R	15	U	C5'-C4'	5.94	1.60	1.51
5	R	29	A	C2'-C1'	-5.92	1.44	1.53
5	R	8	U	C4'-O4'	5.84	1.54	1.45
5	R	6	G	C5'-C4'	5.80	1.59	1.51
5	R	17	C	C2'-C1'	5.64	1.61	1.53
5	R	21	C	C5'-C4'	5.50	1.59	1.51
5	R	20	C	O3'-P	-5.44	1.52	1.61
5	R	24	U	C3'-C2'	5.29	1.60	1.52
5	R	12	A	C2'-O2'	-5.26	1.34	1.42

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	3	A	P-O5'-C5'	9.04	134.47	120.90
5	R	17	C	P-O5'-C5'	7.03	131.45	120.90
5	R	32	A	P-O5'-C5'	6.25	130.28	120.90
5	R	19	C	C5'-C4'-O4'	6.17	119.05	109.80
5	R	11	U	C1'-O4'-C4'	-6.07	103.83	109.90
5	R	21	C	O4'-C1'-N1	5.96	117.44	108.50
5	R	27	A	C2'-C3'-O3'	5.82	118.22	109.50
5	R	20	C	C4'-C3'-C2'	-5.79	96.81	102.60
3	H	116	THR	CB-CA-C	5.78	121.92	110.42
5	R	3	A	O3'-P-O5'	5.72	112.58	104.00
7	J	80	HIS	N-CA-C	-5.70	106.12	114.39
5	R	22	U	P-O5'-C5'	5.65	129.38	120.90
6	I	997	TRP	N-CA-C	-5.51	106.56	113.28
6	I	58	PRO	N-CA-C	-5.46	101.22	112.47
5	R	1	G	C2'-C3'-O3'	5.43	117.65	109.50
5	R	23	C	C4'-C3'-C2'	-5.38	97.22	102.60
5	R	32	A	P-O3'-C3'	5.34	128.21	120.20
5	R	19	C	P-O5'-C5'	-5.30	112.95	120.90
7	J	311	ARG	N-CA-C	-5.28	105.61	111.36
5	R	25	A	C4'-C3'-O3'	5.24	117.27	109.40
7	J	335	GLN	N-CA-C	-5.23	105.58	111.28
6	I	993	PRO	N-CA-C	-5.15	103.10	111.03
5	R	19	C	C5'-C4'-C3'	-5.11	108.33	116.00
6	I	926	GLY	CA-C-O	-5.07	118.67	122.37
5	R	6	G	O4'-C4'-C3'	-5.06	98.94	104.00
5	R	26	U	O5'-C5'-C4'	-5.05	104.13	111.70
6	I	56	VAL	CA-C-N	-5.00	117.25	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	56	VAL	C-N-CA	-5.00	117.25	123.21
5	R	21	C	P-O3'-C3'	5.00	127.70	120.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	R	1	G	Sidechain
5	R	10	C	Sidechain
5	R	12	A	Sidechain
5	R	13	G	Sidechain
5	R	19	C	Sidechain
5	R	21	C	Sidechain
5	R	23	C	Sidechain
5	R	24	U	Sidechain
5	R	30	A	Sidechain
5	R	31	A	Sidechain
5	R	4	G	Sidechain
5	R	7	G	Sidechain
5	R	9	U	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	388	0	216	11	0
2	B	631	0	352	13	0
3	G	1708	0	1752	53	0
3	H	1693	0	1727	66	0
4	K	627	0	634	11	0
5	R	997	0	511	10	0
6	I	10381	0	10391	341	0
7	J	10403	0	10636	385	0
8	R	13	0	9	0	0
9	J	1	0	0	0	0
All	All	26842	0	26228	820	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 16.

All (820) 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:H:16:ILE:CG2	3:H:26:VAL:HG13	1.63	1.25
7:J:1048:ARG:HG2	7:J:1059:LEU:CD2	1.68	1.21
7:J:1048:ARG:CG	7:J:1059:LEU:CD2	2.19	1.19
7:J:118:LYS:CE	7:J:136:GLU:OE2	1.90	1.19
6:I:1294:LYS:HG2	7:J:348:ASP:OD1	1.44	1.15
7:J:118:LYS:HE2	7:J:136:GLU:OE2	0.99	1.15
7:J:1048:ARG:CG	7:J:1059:LEU:HD23	1.79	1.09
7:J:1048:ARG:HG2	7:J:1059:LEU:HD23	1.28	1.09
7:J:375:GLU:HA	7:J:378:LYS:HE3	1.12	1.08
3:H:16:ILE:HG23	3:H:26:VAL:CG1	1.82	1.08
7:J:1048:ARG:CG	7:J:1059:LEU:HD21	1.84	1.06
3:H:41:ASN:ND2	3:H:45:ARG:NH1	2.09	1.00
7:J:114:ILE:HD11	7:J:118:LYS:HD2	1.43	0.99
7:J:348:ASP:OD2	7:J:349:TYR:CE2	2.17	0.97
7:J:1048:ARG:HG3	7:J:1059:LEU:CD2	1.90	0.97
6:I:1257:GLN:CG	6:I:1258:PRO:HD3	1.95	0.96
7:J:375:GLU:CA	7:J:378:LYS:HE3	1.94	0.96
3:H:16:ILE:HG23	3:H:26:VAL:HG13	0.98	0.96
3:H:41:ASN:HD21	3:H:45:ARG:NH1	1.63	0.95
7:J:375:GLU:HA	7:J:378:LYS:CE	1.94	0.95
7:J:251:PRO:HB2	7:J:253:VAL:HG22	1.48	0.94
3:H:22:THR:CG2	3:H:207:THR:O	2.18	0.92
3:H:22:THR:HG23	3:H:207:THR:O	1.70	0.90
6:I:850:ILE:HG21	6:I:1048:LYS:NZ	1.86	0.90
6:I:1294:LYS:CG	7:J:348:ASP:OD1	2.22	0.87
3:H:26:VAL:HG21	3:H:217:ILE:HD13	1.57	0.87
7:J:1048:ARG:HG3	7:J:1059:LEU:HD21	1.50	0.87
6:I:1257:GLN:HG3	6:I:1258:PRO:HD3	1.57	0.85
7:J:263:SER:O	7:J:264:ASP:OD1	1.95	0.84
3:H:41:ASN:ND2	3:H:45:ARG:CZ	2.40	0.84
7:J:506:VAL:HG23	7:J:628:GLY:HA3	1.61	0.82
6:I:1257:GLN:HG2	6:I:1258:PRO:HD3	1.63	0.80
4:K:25:ARG:NH1	4:K:61:ASN:HD21	1.81	0.79
3:G:232:VAL:HA	3:H:218:ARG:HD2	1.63	0.79
5:R:45:C:H2'	5:R:46:G:H8	1.48	0.78
6:I:253:PHE:HA	6:I:265:LYS:HD2	1.65	0.78
3:G:91:ARG:NH2	3:G:209:GLY:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:348:ASP:CG	7:J:349:TYR:CD2	2.63	0.77
7:J:44:ILE:HG22	7:J:51:PRO:HA	1.66	0.77
6:I:1257:GLN:NE2	7:J:348:ASP:HB3	2.00	0.77
7:J:348:ASP:CG	7:J:349:TYR:CE2	2.65	0.74
7:J:814:CYS:SG	7:J:890:THR:OG1	2.44	0.74
6:I:598:VAL:HG23	6:I:627:GLY:HA3	1.69	0.74
7:J:697:MET:HE1	7:J:738:ARG:HA	1.69	0.74
7:J:1368:ASP:O	7:J:1372:ARG:HG3	1.87	0.73
7:J:349:TYR:HE1	7:J:379:PRO:HG2	1.54	0.73
6:I:1072:ASN:ND2	6:I:1111:GLN:OE1	2.21	0.73
7:J:591:ILE:HD12	7:J:604:MET:HG3	1.71	0.73
6:I:560:PRO:HB2	7:J:776:THR:HG21	1.70	0.73
5:R:45:C:H2'	5:R:46:G:C8	2.24	0.73
6:I:195:PHE:HD2	6:I:203:LYS:HE2	1.55	0.72
7:J:582:ILE:HD12	7:J:623:GLN:HB3	1.72	0.72
6:I:1212:LEU:HD22	6:I:1225:VAL:HG11	1.72	0.71
2:B:23:DG:OP1	6:I:143:ARG:NH2	2.23	0.70
3:H:16:ILE:HG22	3:H:26:VAL:HG13	1.69	0.70
6:I:1030:GLU:CG	6:I:1034:ARG:HE	2.05	0.70
7:J:1067:ARG:HE	7:J:1072:LYS:HA	1.56	0.70
6:I:317:LEU:HD11	6:I:335:THR:HG21	1.74	0.70
6:I:1253:LEU:HD22	7:J:251:PRO:HG3	1.74	0.70
7:J:118:LYS:HE2	7:J:136:GLU:CD	2.10	0.69
7:J:1158:GLU:HA	7:J:1223:LEU:HD11	1.74	0.69
7:J:99:ARG:HB3	7:J:248:ASP:HB2	1.75	0.69
3:G:61:ILE:HB	3:G:64:VAL:HG12	1.74	0.69
6:I:557:ARG:NH1	6:I:611:GLU:OE1	2.23	0.69
7:J:1035:VAL:HG12	7:J:1078:LEU:HD21	1.74	0.69
3:G:60:GLU:OE1	3:G:143:ARG:NH2	2.25	0.69
3:H:41:ASN:ND2	3:H:45:ARG:HH12	1.89	0.69
6:I:551:HIS:HD2	6:I:552:PRO:HD2	1.56	0.69
3:H:86:LYS:HG2	3:H:176:CYS:HB2	1.74	0.69
6:I:102:LEU:HD23	6:I:118:LYS:HD3	1.76	0.68
7:J:848:VAL:HB	7:J:858:VAL:HB	1.76	0.68
3:H:212:ASP:HB2	3:H:215:GLU:HG2	1.75	0.67
6:I:1119:MET:HE2	6:I:1228:GLY:HA2	1.76	0.67
7:J:889:ASP:O	7:J:1286:LYS:NZ	2.27	0.67
7:J:1178:THR:HB	7:J:1185:PRO:HB3	1.77	0.67
2:B:26:DA:H8	2:B:27:DG:H2'	1.58	0.67
7:J:1032:SER:OG	7:J:1114:GLN:NE2	2.27	0.67
7:J:1281:GLU:HB2	7:J:1284:ARG:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:348:ASP:OD2	7:J:349:TYR:HE2	1.74	0.67
6:I:302:ILE:HA	6:I:309:LEU:HA	1.77	0.67
7:J:247:PRO:HG3	7:J:250:ARG:HH21	1.58	0.67
7:J:514:THR:HG21	7:J:596:LEU:HD12	1.77	0.67
6:I:727:VAL:HG11	6:I:772:SER:HA	1.77	0.67
6:I:1257:GLN:HG3	6:I:1258:PRO:CD	2.23	0.67
6:I:1313:HIS:HB2	7:J:474:LEU:HD12	1.77	0.67
7:J:1109:LEU:HD22	7:J:1115:ILE:HG12	1.77	0.66
3:H:26:VAL:HG21	3:H:217:ILE:CD1	2.25	0.66
7:J:1135:THR:HG21	7:J:1139:PRO:HB2	1.78	0.66
1:A:31:DA:H2'	1:A:32:DT:H71	1.77	0.66
6:I:836:LEU:HB3	6:I:918:LEU:HD21	1.78	0.66
6:I:808:ASN:H	7:J:633:ALA:HB2	1.60	0.66
3:H:41:ASN:HD22	3:H:45:ARG:NH2	1.92	0.65
6:I:180:ARG:NH2	6:I:396:ASP:OD2	2.29	0.65
3:G:185:TYR:HB2	3:G:201:LEU:HD11	1.79	0.65
6:I:55:SER:OG	6:I:465:ARG:NH1	2.29	0.65
6:I:454:ARG:HG2	6:I:458:GLU:HB3	1.78	0.65
3:G:45:ARG:NH2	6:I:1084:ASP:OD1	2.30	0.65
6:I:681:MET:SD	6:I:1073:LYS:NZ	2.68	0.65
3:G:102:LEU:HD12	3:G:115:ILE:HG12	1.78	0.65
6:I:552:PRO:HA	7:J:773:PHE:HE2	1.62	0.65
6:I:933:VAL:HG13	6:I:1050:VAL:HG22	1.79	0.65
7:J:955:LYS:HG2	7:J:1012:ALA:HA	1.79	0.65
6:I:798:GLN:OE1	6:I:827:ARG:NH1	2.30	0.64
7:J:799:ARG:HG2	7:J:1325:PHE:HE1	1.63	0.64
7:J:1238:GLN:HB3	7:J:1242:ARG:HE	1.63	0.64
7:J:144:TYR:HB3	7:J:178:ALA:HB1	1.79	0.64
6:I:448:LEU:H	6:I:553:THR:HG21	1.62	0.64
6:I:989:LEU:HD22	6:I:997:TRP:HD1	1.63	0.64
7:J:127:LEU:O	7:J:220:ARG:NH2	2.30	0.64
6:I:801:ARG:HB3	6:I:1095:ASP:H	1.62	0.64
7:J:515:ARG:HH22	7:J:717:VAL:HG22	1.61	0.64
7:J:948:SER:N	7:J:1020:TRP:O	2.31	0.64
7:J:824:PRO:HD3	7:J:835:LEU:HB2	1.80	0.63
3:G:145:LYS:NZ	3:G:147:GLN:OE1	2.30	0.63
3:G:12:ARG:H	3:G:30:PRO:HD2	1.64	0.63
7:J:749:LYS:HZ2	7:J:753:SER:HB3	1.63	0.63
7:J:1089:LEU:HA	7:J:1096:PRO:HA	1.80	0.63
6:I:41:GLN:NE2	6:I:50:GLU:OE1	2.31	0.62
7:J:225:GLU:O	7:J:229:GLN:NE2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1081:VAL:HG12	7:J:1087:ASP:HA	1.80	0.62
6:I:551:HIS:CD2	6:I:552:PRO:HD2	2.34	0.62
7:J:1356:LEU:O	7:J:1366:HIS:NE2	2.28	0.62
6:I:1281:TYR:HB3	7:J:484:MET:HE1	1.82	0.62
7:J:247:PRO:HA	7:J:250:ARG:HE	1.65	0.62
7:J:975:ILE:HG21	7:J:980:THR:HG21	1.81	0.61
6:I:1257:GLN:HE22	7:J:348:ASP:CG	2.07	0.61
3:G:104:LYS:HG2	3:G:110:VAL:HG12	1.82	0.61
3:H:16:ILE:CG2	3:H:26:VAL:CG1	2.56	0.61
6:I:9:LYS:HG2	6:I:1171:ARG:HD3	1.82	0.61
6:I:850:ILE:HG21	6:I:1048:LYS:HZ1	1.64	0.61
3:H:41:ASN:HD22	3:H:45:ARG:CZ	2.11	0.61
3:G:91:ARG:NH1	3:G:210:THR:O	2.34	0.61
6:I:283:LYS:HG3	6:I:284:LEU:HD12	1.82	0.61
6:I:106:GLU:HB2	6:I:109:ALA:HB3	1.81	0.61
6:I:402:ARG:HD3	6:I:416:GLY:H	1.66	0.61
7:J:374:LEU:O	7:J:378:LYS:HG3	2.01	0.61
6:I:646:SER:HB3	6:I:649:GLN:HG3	1.82	0.60
7:J:151:MET:HB2	7:J:175:GLU:HG2	1.83	0.60
3:G:58:GLU:OE1	3:G:170:ARG:NH2	2.29	0.60
3:G:167:PRO:HD2	3:G:170:ARG:HD3	1.82	0.60
5:R:42:A:O3'	6:I:510:GLN:NE2	2.34	0.60
6:I:559:CYS:HB2	6:I:662:SER:HB3	1.83	0.60
7:J:370:LYS:HA	7:J:441:LEU:HD22	1.83	0.60
7:J:1075:ARG:HH21	7:J:1200:GLU:HB3	1.66	0.60
6:I:1257:GLN:NE2	7:J:348:ASP:CB	2.65	0.60
7:J:114:ILE:HD11	7:J:118:LYS:CD	2.27	0.60
7:J:120:LEU:HD12	7:J:1330:ARG:HD3	1.82	0.60
6:I:312:ALA:H	6:I:315:MET:HE2	1.67	0.60
7:J:21:LYS:NZ	7:J:22:ILE:O	2.35	0.60
7:J:892:PHE:HB3	7:J:1345:ARG:HH12	1.65	0.60
6:I:1223:ARG:HH22	7:J:721:SER:N	1.99	0.59
7:J:339:ARG:HA	7:J:343:LEU:HD12	1.83	0.59
7:J:983:LYS:HA	7:J:994:SER:HA	1.84	0.59
6:I:228:VAL:HG13	6:I:337:PHE:HB2	1.82	0.59
6:I:240:GLU:HA	6:I:284:LEU:HA	1.83	0.59
6:I:1294:LYS:CB	7:J:348:ASP:OD1	2.49	0.59
7:J:586:GLY:HA3	7:J:612:LEU:HD21	1.84	0.59
7:J:664:ILE:HD12	7:J:681:LYS:HE2	1.84	0.59
6:I:850:ILE:HG21	6:I:1048:LYS:HZ3	1.67	0.59
6:I:50:GLU:OE2	6:I:54:ARG:NH2	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1251:TYR:HB3	6:I:1257:GLN:HA	1.84	0.59
7:J:789:LYS:HE2	7:J:931:THR:HA	1.85	0.59
7:J:901:ARG:HD3	7:J:906:GLY:HA2	1.83	0.59
6:I:19:PRO:HA	6:I:1156:ARG:HD3	1.85	0.59
6:I:93:SER:HB2	6:I:126:GLU:HG2	1.85	0.59
6:I:521:LEU:HD22	6:I:667:LEU:HD12	1.84	0.59
6:I:660:VAL:HG13	6:I:661:VAL:HG13	1.84	0.59
7:J:911:LYS:HE2	7:J:1363:TYR:HE2	1.67	0.59
6:I:681:MET:O	6:I:685:MET:HG2	2.03	0.58
3:G:29:GLU:HB3	3:G:30:PRO:HD3	1.85	0.58
3:G:97:GLU:HB2	3:G:145:LYS:HE2	1.85	0.58
4:K:37:PRO:HB3	4:K:49:ILE:HG21	1.86	0.58
7:J:1024:THR:HG23	7:J:1026:PRO:HD3	1.86	0.58
3:G:102:LEU:HB3	3:G:142:MET:HG2	1.85	0.58
7:J:384:LYS:O	7:J:388:ARG:HG2	2.02	0.58
7:J:544:LEU:HD11	7:J:631:TYR:HD1	1.68	0.58
7:J:1100:PHE:HB2	7:J:1200:GLU:HB2	1.85	0.58
7:J:1199:PHE:HB3	7:J:1202:GLU:HB2	1.86	0.58
6:I:694:ARG:O	6:I:798:GLN:NE2	2.36	0.58
7:J:329:ASP:HA	7:J:332:LYS:HE2	1.85	0.58
6:I:348:SER:O	6:I:352:ARG:HG2	2.04	0.57
6:I:1005:GLU:H	6:I:1008:GLN:HB2	1.68	0.57
6:I:1340:GLU:HG2	7:J:1341:ARG:HH22	1.69	0.57
7:J:814:CYS:SG	7:J:895:CYS:HB2	2.44	0.57
6:I:12:ARG:HG3	6:I:1181:PRO:HB2	1.85	0.57
3:H:41:ASN:HD22	3:H:45:ARG:NH1	2.01	0.57
5:R:41:C:H2'	5:R:42:A:C8	2.40	0.57
6:I:692:THR:HA	6:I:830:THR:HG22	1.87	0.57
7:J:537:TYR:CZ	7:J:544:LEU:HG	2.40	0.57
5:R:41:C:H2'	5:R:42:A:H8	1.69	0.57
6:I:105:TYR:HA	6:I:114:VAL:HA	1.87	0.57
6:I:870:ILE:HG21	6:I:931:VAL:HG11	1.86	0.57
6:I:975:ILE:HG23	6:I:979:LEU:HD22	1.86	0.57
7:J:660:GLU:O	7:J:664:ILE:HG12	2.04	0.57
6:I:233:ARG:H	6:I:237:LEU:HA	1.70	0.57
6:I:621:SER:HB2	6:I:653:MET:HE3	1.87	0.57
7:J:572:THR:HG21	7:J:589:TYR:HE2	1.69	0.57
7:J:576:ARG:NH1	7:J:593:ASN:O	2.38	0.57
7:J:108:ALA:HB2	7:J:280:LYS:HG3	1.86	0.57
7:J:527:LEU:HD22	7:J:548:VAL:HG21	1.86	0.57
7:J:646:ILE:HD11	7:J:764:ARG:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1263:LYS:HD2	7:J:1279:GLN:HG2	1.85	0.57
6:I:594:VAL:HG22	6:I:599:VAL:HA	1.86	0.57
7:J:1062:LEU:O	7:J:1067:ARG:NH1	2.35	0.57
6:I:850:ILE:HG21	6:I:1048:LYS:CE	2.34	0.57
6:I:979:LEU:HG	6:I:989:LEU:HD13	1.85	0.57
7:J:825:VAL:HG12	7:J:833:GLU:HB2	1.86	0.57
3:H:23:HIS:HE1	3:H:204:GLU:HB3	1.70	0.56
6:I:1246:ARG:HH21	6:I:1249:GLY:N	2.03	0.56
6:I:1313:HIS:HB3	7:J:473:THR:HA	1.86	0.56
7:J:146:VAL:HG12	7:J:178:ALA:HB2	1.85	0.56
6:I:339:ASN:O	6:I:343:HIS:N	2.37	0.56
6:I:444:ASP:HB3	6:I:447:HIS:HB2	1.86	0.56
6:I:268:ARG:NH1	6:I:269:ILE:O	2.37	0.56
7:J:134:ASP:OD1	7:J:137:ARG:NH2	2.39	0.56
7:J:375:GLU:HG2	7:J:378:LYS:HE3	1.87	0.56
7:J:502:PRO:HB3	7:J:506:VAL:CG1	2.34	0.56
7:J:1171:GLY:O	7:J:1192:LYS:NZ	2.35	0.56
5:R:44:A:OP2	6:I:540:ARG:NH2	2.39	0.56
7:J:973:LEU:HB2	7:J:1003:LEU:HB3	1.87	0.56
6:I:94:ALA:HB2	6:I:129:LEU:HD11	1.87	0.56
7:J:1198:VAL:HG23	7:J:1210:ILE:HA	1.86	0.56
7:J:826:ILE:HG21	7:J:993:GLU:HA	1.88	0.56
7:J:826:ILE:HG22	7:J:828:GLY:H	1.70	0.56
3:G:231:PHE:HE2	3:H:39:LEU:HD23	1.71	0.56
7:J:201:LEU:HD11	7:J:220:ARG:HH11	1.71	0.56
7:J:449:LEU:HB2	7:J:466:MET:HE1	1.87	0.56
7:J:506:VAL:HG21	7:J:625:MET:HA	1.88	0.56
6:I:207:THR:HA	6:I:210:LEU:HD12	1.88	0.56
6:I:265:LYS:O	6:I:267:ARG:NH1	2.39	0.56
3:H:144:ILE:HG22	3:H:146:VAL:HG22	1.88	0.55
7:J:161:THR:O	7:J:165:TYR:N	2.32	0.55
6:I:176:ILE:HD11	6:I:428:VAL:HG11	1.89	0.55
6:I:319:LEU:HD23	6:I:322:LEU:HD12	1.89	0.55
3:G:54:CYS:SG	3:G:92:VAL:HG22	2.46	0.55
6:I:453:ILE:HD12	6:I:587:LEU:HD21	1.89	0.55
6:I:613:ASN:OD1	6:I:614:TYR:N	2.39	0.55
2:B:29:DA:H2''	2:B:30:DC:H5'	1.88	0.55
6:I:1287:LEU:HD23	7:J:1357:ILE:HD13	1.89	0.55
7:J:965:SER:HB2	7:J:975:ILE:HG12	1.89	0.55
3:G:23:HIS:HB3	3:G:206:GLU:HA	1.87	0.55
6:I:303:ASP:HB3	6:I:310:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1289:GLU:HG2	6:I:1294:LYS:HD2	1.89	0.55
7:J:895:CYS:HB3	7:J:898:CYS:HB2	1.88	0.55
3:G:71:LYS:NZ	3:G:139:SER:O	2.37	0.55
6:I:226:GLU:HG2	6:I:337:PHE:HB3	1.88	0.55
6:I:231:GLU:OE2	6:I:332:ARG:NH1	2.39	0.55
6:I:1253:LEU:HD22	7:J:251:PRO:CG	2.37	0.55
3:G:180:VAL:HG12	3:G:207:THR:HG22	1.88	0.54
6:I:255:ILE:N	6:I:263:VAL:O	2.37	0.54
6:I:1291:LEU:HD11	7:J:1351:VAL:HG13	1.89	0.54
7:J:751:ASP:OD1	7:J:752:GLY:N	2.39	0.54
7:J:1046:ILE:HG22	7:J:1062:LEU:H	1.72	0.54
7:J:1062:LEU:HB2	7:J:1067:ARG:HB3	1.89	0.54
7:J:1153:PRO:O	7:J:1194:ARG:NH1	2.40	0.54
6:I:230:PHE:HB2	6:I:333:ILE:HB	1.89	0.54
6:I:1030:GLU:HG2	6:I:1034:ARG:HE	1.73	0.54
7:J:374:LEU:O	7:J:378:LYS:CG	2.55	0.54
6:I:198:ILE:HG12	6:I:369:MET:HE1	1.90	0.54
6:I:520:PRO:HG3	6:I:714:VAL:HG11	1.88	0.54
7:J:572:THR:HG21	7:J:589:TYR:CE2	2.42	0.54
7:J:1042:ASP:O	7:J:1047:THR:HG22	2.07	0.54
3:H:105:SER:HB2	3:H:139:SER:HA	1.89	0.54
3:H:189:ALA:HB1	3:H:197:ASP:HB2	1.88	0.54
7:J:338:PHE:HA	7:J:342:LEU:HD12	1.89	0.54
7:J:381:ILE:HD11	7:J:412:LEU:HD13	1.89	0.54
7:J:112:ALA:HA	7:J:238:ILE:HA	1.90	0.54
7:J:483:LEU:HB2	7:J:484:MET:HE2	1.89	0.54
7:J:826:ILE:HG13	7:J:831:VAL:HA	1.88	0.54
3:G:192:VAL:HG21	3:G:198:LEU:HD12	1.90	0.54
7:J:480:ALA:HA	7:J:484:MET:HB2	1.90	0.54
6:I:138:ILE:HD12	6:I:143:ARG:HD2	1.89	0.54
7:J:348:ASP:OD1	7:J:349:TYR:CD2	2.61	0.54
4:K:27:ALA:HB1	7:J:474:LEU:HD23	1.90	0.54
6:I:256:GLU:HB3	6:I:261:VAL:HG22	1.90	0.54
6:I:617:ALA:HB2	6:I:650:VAL:HG21	1.90	0.54
6:I:727:VAL:HG23	6:I:732:ILE:HG12	1.90	0.54
6:I:975:ILE:HA	6:I:1011:LEU:HD22	1.89	0.54
7:J:511:TYR:OH	7:J:515:ARG:NH1	2.41	0.54
3:G:11:PRO:HG2	3:H:231:PHE:HZ	1.74	0.53
6:I:6:THR:HA	6:I:9:LYS:HE2	1.90	0.53
3:H:98:VAL:HA	3:H:146:VAL:HG23	1.89	0.53
7:J:226:ALA:HB1	7:J:1338:ALA:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1072:ASN:HD21	6:I:1230:MET:HE1	1.72	0.53
7:J:646:ILE:HD12	7:J:762:ASN:ND2	2.24	0.53
6:I:243:PRO:HB3	6:I:277:LEU:HB3	1.90	0.53
6:I:518:ASN:HB2	6:I:761:GLN:HG3	1.91	0.53
6:I:1030:GLU:OE2	6:I:1034:ARG:HD2	2.08	0.53
7:J:1099:TYR:HB3	7:J:1199:PHE:HZ	1.74	0.53
6:I:239:MET:HE1	6:I:241:LEU:HD13	1.90	0.53
7:J:956:GLY:HA3	7:J:984:LEU:HD21	1.90	0.53
3:G:184:ALA:HB2	6:I:1091:GLY:HA3	1.90	0.53
6:I:1141:LEU:HD23	6:I:1170:MET:HE1	1.89	0.53
7:J:338:PHE:CZ	7:J:1352:ILE:HG12	2.44	0.53
3:G:13:LEU:HB3	3:G:16:ILE:HD11	1.91	0.53
6:I:12:ARG:NH2	6:I:793:GLU:OE1	2.31	0.53
6:I:807:TRP:CZ2	6:I:1216:ARG:HD2	2.44	0.53
7:J:870:ASP:O	7:J:874:GLU:HG2	2.09	0.53
7:J:1253:ILE:O	7:J:1257:VAL:HG23	2.08	0.53
6:I:89:GLY:HA2	6:I:140:GLY:HA3	1.91	0.53
6:I:519:ASN:ND2	6:I:796:LEU:HD22	2.24	0.53
6:I:821:ARG:HB2	6:I:1082:ILE:HD12	1.90	0.53
7:J:851:PRO:HD3	7:J:877:VAL:HG22	1.91	0.53
7:J:962:ASN:OD1	7:J:964:LYS:NZ	2.42	0.53
6:I:934:PHE:O	6:I:1048:LYS:HG3	2.10	0.52
6:I:83:GLN:NE2	6:I:84:GLU:HG3	2.25	0.52
6:I:101:ARG:HG3	6:I:119:GLU:HB2	1.92	0.52
6:I:102:LEU:O	6:I:118:LYS:N	2.41	0.52
6:I:1030:GLU:O	6:I:1034:ARG:HG3	2.09	0.52
6:I:1339:LEU:HD23	7:J:17:PHE:CD1	2.44	0.52
7:J:114:ILE:HA	7:J:117:LEU:HB3	1.91	0.52
6:I:81:ASP:OD2	6:I:82:VAL:N	2.38	0.52
6:I:301:TYR:O	6:I:310:ILE:N	2.41	0.52
7:J:114:ILE:HD13	7:J:304:ASP:OD2	2.09	0.52
3:G:107:ILE:HD11	6:I:773:LEU:HD22	1.91	0.52
7:J:1025:MET:HB2	7:J:1124:ILE:HB	1.91	0.52
7:J:17:PHE:O	7:J:1369:ARG:NH2	2.43	0.52
3:G:109:PRO:HA	3:G:132:HIS:HA	1.92	0.52
6:I:838:CYS:SG	6:I:884:VAL:HG11	2.50	0.52
6:I:997:TRP:HE1	6:I:1002:LEU:HB2	1.75	0.52
2:B:19:DT:H2'	2:B:20:DG:C8	2.45	0.52
7:J:375:GLU:HG2	7:J:378:LYS:CE	2.40	0.52
7:J:513:MET:SD	7:J:579:LEU:HB2	2.50	0.52
3:G:222:THR:HG21	3:H:233:ASP:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:192:ASP:HB3	6:I:346:TYR:HD1	1.75	0.52
6:I:1242:LYS:HD2	7:J:465:GLN:HE22	1.74	0.51
7:J:337:ARG:HG2	7:J:341:ASN:HD21	1.76	0.51
7:J:1050:THR:HA	7:J:1057:SER:HA	1.92	0.51
3:G:31:LEU:HD13	3:G:36:GLY:HA2	1.91	0.51
5:R:37:G:H22	6:I:1259:LEU:HD11	1.75	0.51
6:I:561:ILE:HD13	6:I:661:VAL:HG12	1.92	0.51
7:J:375:GLU:HA	7:J:378:LYS:HG3	1.93	0.51
7:J:930:LEU:HG	7:J:1244:GLN:HG3	1.92	0.51
1:A:28:DG:H5''	7:J:1148:ARG:NH1	2.25	0.51
3:H:111:THR:HA	3:H:129:VAL:HA	1.92	0.51
7:J:123:ARG:HG2	7:J:1337:VAL:HG21	1.92	0.51
6:I:700:VAL:HG13	6:I:1069:ARG:HH22	1.75	0.51
7:J:964:LYS:HG2	7:J:977:SER:HB2	1.93	0.51
6:I:232:ILE:HA	6:I:237:LEU:HG	1.93	0.51
6:I:714:VAL:HB	6:I:787:PRO:HD2	1.93	0.51
6:I:359:ARG:HG2	6:I:363:LEU:HD13	1.93	0.51
6:I:1096:ILE:HD13	6:I:1232:MET:HE2	1.93	0.51
7:J:651:HIS:CE1	7:J:652:GLU:HG3	2.46	0.51
3:H:21:SER:O	3:H:213:PRO:CD	2.59	0.51
6:I:822:VAL:HG13	6:I:827:ARG:HB2	1.93	0.51
7:J:799:ARG:HG2	7:J:1325:PHE:CE1	2.43	0.51
7:J:1263:LYS:NZ	7:J:1315:ALA:O	2.38	0.51
3:H:41:ASN:ND2	3:H:45:ARG:NH2	2.57	0.50
6:I:705:GLU:HB3	6:I:794:LEU:H	1.76	0.50
7:J:865:HIS:ND1	7:J:867:GLN:OE1	2.43	0.50
7:J:865:HIS:HA	7:J:901:ARG:HH21	1.76	0.50
6:I:1138:VAL:HG23	6:I:1170:MET:HE3	1.92	0.50
6:I:1246:ARG:HH21	6:I:1249:GLY:H	1.60	0.50
6:I:1258:PRO:HG2	7:J:346:ARG:C	2.37	0.50
6:I:1140:LYS:O	6:I:1143:GLU:HG3	2.10	0.50
6:I:1315:MET:HB2	7:J:473:THR:HG21	1.93	0.50
3:H:56:VAL:HB	3:H:147:GLN:HB3	1.93	0.50
6:I:13:LYS:HD3	6:I:1149:TYR:HA	1.92	0.50
7:J:132:LEU:O	7:J:135:ILE:N	2.45	0.50
7:J:816:THR:O	7:J:883:ARG:NH1	2.44	0.50
6:I:262:TYR:HB3	6:I:276:GLN:HE22	1.76	0.50
6:I:448:LEU:HD21	6:I:587:LEU:HD12	1.94	0.50
7:J:375:GLU:CB	7:J:378:LYS:HE3	2.41	0.50
7:J:1045:THR:HG21	7:J:1067:ARG:HB2	1.93	0.50
3:H:11:PRO:HB3	3:H:31:LEU:HG	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:149:LEU:HD11	6:I:451:ARG:HB3	1.94	0.50
6:I:838:CYS:SG	6:I:1050:VAL:HB	2.52	0.50
7:J:1036:ARG:HH12	7:J:1112:GLY:HA2	1.75	0.50
7:J:1048:ARG:HE	7:J:1059:LEU:HD21	1.77	0.50
6:I:68:LEU:HD11	6:I:100:LEU:HB3	1.94	0.50
6:I:144:VAL:HG11	6:I:527:LYS:HA	1.94	0.50
4:K:25:ARG:HH12	4:K:61:ASN:HD21	1.60	0.49
7:J:1206:ARG:NH1	7:J:1223:LEU:O	2.45	0.49
7:J:1267:VAL:N	7:J:1301:THR:O	2.45	0.49
7:J:1271:SER:OG	7:J:1298:VAL:O	2.22	0.49
3:G:59:VAL:HG22	3:G:144:ILE:HG22	1.94	0.49
3:G:100:LEU:HD21	3:G:121:VAL:HG11	1.93	0.49
6:I:805:MET:HE3	7:J:636:GLY:HA2	1.95	0.49
6:I:1257:GLN:HB3	6:I:1301:ARG:CZ	2.42	0.49
7:J:135:ILE:O	7:J:139:LEU:HD23	2.12	0.49
7:J:189:LEU:HB3	7:J:234:PRO:HB2	1.93	0.49
7:J:1174:ARG:HG3	7:J:1189:MET:HE1	1.93	0.49
6:I:866:ASP:OD1	6:I:869:GLY:N	2.45	0.49
7:J:35:PHE:HB3	7:J:101:ARG:HH21	1.77	0.49
7:J:334:LYS:HE3	7:J:339:ARG:HH12	1.77	0.49
7:J:1021:ASP:HB3	7:J:1024:THR:HG22	1.93	0.49
6:I:678:ARG:HD3	6:I:1106:ARG:HB3	1.95	0.49
6:I:1297:ASP:H	6:I:1301:ARG:HD3	1.78	0.49
7:J:948:SER:N	7:J:1022:PRO:HD3	2.27	0.49
7:J:1166:GLY:N	7:J:1174:ARG:O	2.45	0.49
3:G:81:ILE:HG12	3:G:131:CYS:HB3	1.93	0.49
6:I:178:PRO:HB3	6:I:395:TYR:CZ	2.47	0.49
7:J:353:SER:HB3	7:J:447:ILE:HG13	1.95	0.49
7:J:587:LEU:HD21	7:J:608:CYS:HA	1.94	0.49
7:J:1031:VAL:HG23	7:J:1080:ILE:HG21	1.94	0.49
6:I:13:LYS:HB3	6:I:1182:ILE:HD13	1.93	0.49
6:I:315:MET:HE3	6:I:321:LEU:HD11	1.94	0.49
6:I:618:GLN:HE22	7:J:770:LEU:HB2	1.78	0.49
6:I:600:THR:HG22	6:I:602:GLU:HG2	1.95	0.49
3:G:61:ILE:HD13	3:G:142:MET:HB3	1.95	0.49
6:I:519:ASN:HD21	6:I:796:LEU:HD22	1.78	0.49
6:I:1294:LYS:HB3	7:J:348:ASP:OD1	2.11	0.49
6:I:1332:SER:HA	7:J:243:PRO:HB2	1.94	0.49
7:J:227:PHE:CE1	7:J:1337:VAL:HG13	2.47	0.49
7:J:620:PHE:CZ	7:J:624:ILE:HD11	2.48	0.49
6:I:661:VAL:HB	6:I:665:ALA:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:1119:MET:HG3	6:I:1204:LEU:HD13	1.95	0.48
7:J:94:GLN:HB3	7:J:96:LYS:HG2	1.95	0.48
7:J:907:HIS:NE2	7:J:910:ASN:OD1	2.46	0.48
7:J:1042:ASP:OD1	7:J:1043:GLY:N	2.46	0.48
6:I:746:ALA:H	6:I:974:ARG:HH22	1.62	0.48
6:I:1290:MET:HE3	6:I:1294:LYS:HZ2	1.78	0.48
6:I:411:ARG:NH2	6:I:424:ASP:OD1	2.45	0.48
3:G:18:GLN:NE2	3:G:20:SER:O	2.32	0.48
6:I:165:HIS:CG	6:I:167:SER:HG	2.32	0.48
6:I:232:ILE:O	6:I:331:LYS:NZ	2.47	0.48
6:I:1211:ARG:NH1	6:I:1213:TYR:OH	2.46	0.48
7:J:247:PRO:HG3	7:J:250:ARG:NH2	2.28	0.48
7:J:321:LYS:HA	7:J:321:LYS:HD2	1.47	0.48
7:J:555:TYR:HB3	7:J:563:LEU:HD22	1.95	0.48
6:I:297:VAL:HA	6:I:335:THR:HG22	1.95	0.48
6:I:1257:GLN:NE2	7:J:348:ASP:CG	2.71	0.48
7:J:161:THR:HB	7:J:164:GLN:HB2	1.95	0.48
7:J:355:ILE:HD11	7:J:466:MET:HG3	1.96	0.48
6:I:732:ILE:HD11	6:I:769:PRO:HB3	1.94	0.48
6:I:56:VAL:HG11	6:I:468:LEU:HB3	1.96	0.48
7:J:375:GLU:CG	7:J:378:LYS:HE3	2.43	0.48
6:I:954:LYS:O	6:I:958:LYS:HG3	2.13	0.48
6:I:1027:LYS:HA	6:I:1027:LYS:HD3	1.61	0.48
3:H:47:LEU:HD13	3:H:180:VAL:HG11	1.96	0.47
7:J:388:ARG:HG3	7:J:411:ILE:HD11	1.95	0.47
5:R:40:C:H2'	5:R:41:C:C6	2.50	0.47
6:I:3:TYR:HB3	6:I:7:GLU:HB3	1.96	0.47
7:J:1155:ILE:HB	7:J:1210:ILE:HB	1.96	0.47
7:J:1344:LEU:O	7:J:1345:ARG:HG2	2.14	0.47
3:G:11:PRO:HG2	3:H:231:PHE:CZ	2.49	0.47
7:J:352:ARG:HH21	7:J:465:GLN:HB2	1.79	0.47
7:J:878:ASP:OD1	7:J:879:ALA:N	2.47	0.47
6:I:1077:SER:HA	7:J:356:THR:HG23	1.96	0.47
6:I:1166:ASP:OD1	6:I:1167:GLU:N	2.46	0.47
7:J:338:PHE:CE2	7:J:1352:ILE:HG12	2.48	0.47
7:J:348:ASP:OD1	7:J:349:TYR:HD2	1.97	0.47
7:J:1203:ARG:NH2	7:J:1205:GLU:OE2	2.48	0.47
7:J:398:LYS:HE2	7:J:398:LYS:HB2	1.77	0.47
3:H:130:ILE:HG21	3:H:142:MET:HA	1.97	0.47
7:J:132:LEU:HD12	7:J:135:ILE:HB	1.97	0.47
7:J:198:CYS:SG	7:J:202:ARG:NH1	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:432:LEU:HD13	7:J:499:ILE:HG12	1.97	0.47
2:B:18:DG:OP2	7:J:346:ARG:NH2	2.48	0.47
3:H:41:ASN:HD22	3:H:45:ARG:HH22	1.60	0.47
3:H:59:VAL:HB	3:H:143:ARG:HD2	1.96	0.47
6:I:52:ALA:HA	6:I:465:ARG:HH12	1.80	0.47
6:I:124:MET:HE2	6:I:124:MET:HB3	1.80	0.47
6:I:213:LEU:HB3	6:I:422:LYS:HD3	1.97	0.47
6:I:753:LEU:HB3	6:I:767:GLN:HB3	1.97	0.47
6:I:802:VAL:HG21	6:I:1230:MET:HB3	1.96	0.47
7:J:111:THR:HG21	7:J:303:VAL:HB	1.95	0.47
4:K:6:VAL:HG11	7:J:482:ALA:HA	1.96	0.47
6:I:28:LEU:HD22	6:I:527:LYS:HD2	1.96	0.47
7:J:510:LEU:HD11	7:J:624:ILE:HG23	1.96	0.47
7:J:865:HIS:CE1	7:J:867:GLN:HB2	2.50	0.47
3:G:11:PRO:HB3	3:G:31:LEU:HG	1.97	0.47
7:J:152:THR:HG23	7:J:175:GLU:HG3	1.96	0.47
7:J:502:PRO:HB3	7:J:506:VAL:HG13	1.96	0.47
7:J:1048:ARG:HG2	7:J:1059:LEU:CG	2.42	0.47
7:J:1327:GLU:OE1	7:J:1330:ARG:NH2	2.48	0.47
1:A:33:DT:H2''	1:A:34:DC:H2'	1.96	0.47
6:I:1047:LEU:H	6:I:1047:LEU:HG	1.55	0.47
6:I:1268:GLN:HG3	7:J:352:ARG:HG3	1.96	0.47
7:J:847:ASP:OD1	7:J:847:ASP:O	2.33	0.47
7:J:1175:LEU:HD22	7:J:1190:ILE:HD11	1.97	0.47
3:G:219:ARG:O	3:G:222:THR:OG1	2.27	0.46
7:J:218:THR:HA	7:J:221:ILE:HG22	1.97	0.46
7:J:137:ARG:HH21	7:J:159:ILE:HG12	1.79	0.46
7:J:741:ALA:O	7:J:762:ASN:ND2	2.30	0.46
7:J:1063:ASP:O	7:J:1067:ARG:HG2	2.16	0.46
7:J:1173:ARG:HH21	7:J:1190:ILE:HG21	1.80	0.46
6:I:690:VAL:HG13	6:I:830:THR:HG21	1.97	0.46
7:J:537:TYR:CE1	7:J:544:LEU:HG	2.51	0.46
7:J:806:ASP:OD1	7:J:1259:GLN:NE2	2.48	0.46
7:J:1259:GLN:HA	7:J:1262:ARG:HG3	1.97	0.46
3:H:54:CYS:HB2	3:H:92:VAL:HA	1.96	0.46
6:I:1280:ALA:HB1	7:J:918:ILE:HG12	1.97	0.46
7:J:104:HIS:HA	7:J:243:PRO:HA	1.97	0.46
6:I:473:ARG:O	6:I:477:GLU:HG2	2.16	0.46
6:I:545:PHE:CZ	7:J:788:LEU:HD22	2.51	0.46
7:J:356:THR:HB	7:J:448:GLN:HG2	1.97	0.46
1:A:33:DT:H2''	1:A:34:DC:H5'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:115:ILE:HG21	3:H:144:ILE:HG12	1.97	0.46
6:I:270:THR:OG1	6:I:273:HIS:ND1	2.35	0.46
6:I:423:ASP:OD1	6:I:424:ASP:N	2.49	0.46
7:J:66:LYS:HA	7:J:66:LYS:HD3	1.55	0.46
7:J:601:ILE:HD11	7:J:624:ILE:HG21	1.98	0.46
3:H:102:LEU:HD23	3:H:102:LEU:HA	1.80	0.46
6:I:459:MET:SD	6:I:511:LEU:HD13	2.56	0.46
7:J:850:LYS:HB3	7:J:855:ASP:HB2	1.98	0.46
7:J:891:ASP:HB3	7:J:1283:SER:HB2	1.97	0.46
6:I:1070:HIS:ND1	6:I:1114:GLU:OE1	2.47	0.46
6:I:1303:LYS:HD2	6:I:1303:LYS:HA	1.51	0.46
3:G:89:ALA:HB1	3:G:124:VAL:HB	1.99	0.46
3:H:185:TYR:HB2	3:H:201:LEU:HD11	1.98	0.46
6:I:356:THR:HG21	6:I:365:GLU:HG3	1.98	0.46
6:I:596:ASP:OD1	6:I:597:GLY:N	2.44	0.46
7:J:1198:VAL:HG12	7:J:1199:PHE:O	2.16	0.46
3:G:64:VAL:HG21	3:G:78:ILE:HG13	1.97	0.45
6:I:6:THR:HG23	6:I:781:ASP:OD2	2.17	0.45
6:I:472:GLU:HA	6:I:475:VAL:HG12	1.97	0.45
6:I:636:CYS:HB2	6:I:645:PHE:HD2	1.80	0.45
6:I:935:THR:HG21	6:I:941:LYS:HD2	1.98	0.45
7:J:265:LEU:HD11	7:J:327:LEU:HG	1.97	0.45
7:J:437:PHE:CZ	7:J:453:VAL:HG11	2.52	0.45
3:G:106:GLY:HA2	3:G:136:GLU:HA	1.97	0.45
6:I:425:ILE:O	6:I:429:MET:HG3	2.16	0.45
6:I:615:VAL:HG13	6:I:650:VAL:HA	1.98	0.45
6:I:1225:VAL:HG13	6:I:1227:VAL:HG23	1.98	0.45
2:B:6:DA:H2"	2:B:7:DA:C8	2.51	0.45
6:I:989:LEU:HD22	6:I:997:TRP:CD1	2.46	0.45
6:I:688:GLN:HB2	6:I:1235:LEU:HD22	1.98	0.45
6:I:772:SER:OG	6:I:773:LEU:N	2.49	0.45
6:I:1002:LEU:HB3	6:I:1008:GLN:HE21	1.81	0.45
6:I:1137:GLU:HG3	6:I:1139:ALA:H	1.80	0.45
7:J:330:MET:O	7:J:336:GLY:HA2	2.16	0.45
7:J:1155:ILE:HG22	7:J:1210:ILE:HD12	1.99	0.45
6:I:590:PRO:HG2	6:I:655:VAL:HG11	1.97	0.45
7:J:549:LYS:HE3	7:J:549:LYS:HB3	1.70	0.45
7:J:52:GLU:HB3	7:J:55:GLY:HA3	1.97	0.45
3:G:56:VAL:HG12	3:G:146:VAL:HG22	1.97	0.45
7:J:141:PHE:HB2	7:J:297:ARG:NE	2.32	0.45
7:J:253:VAL:HG12	7:J:260:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:DC:H2''	1:A:13:DC:C6	2.51	0.45
3:H:170:ARG:HB2	3:H:171:LEU:H	1.51	0.45
6:I:15:PHE:CD2	6:I:1190:ALA:HB2	2.52	0.45
6:I:519:ASN:ND2	6:I:689:ALA:HB3	2.32	0.45
6:I:554:HIS:HD2	6:I:558:VAL:HB	1.82	0.45
6:I:1132:LEU:HD23	6:I:1132:LEU:HA	1.83	0.45
6:I:1276:TRP:CD2	7:J:801:VAL:HG11	2.52	0.45
7:J:103:GLY:C	7:J:244:VAL:HG12	2.41	0.45
3:G:182:ARG:HB3	3:G:206:GLU:HB3	1.99	0.45
5:R:40:C:H2'	5:R:41:C:H6	1.82	0.45
6:I:685:MET:HE3	6:I:1073:LYS:HD3	1.99	0.45
6:I:1257:GLN:HG2	6:I:1295:SER:HA	1.98	0.45
7:J:137:ARG:HG2	7:J:142:GLU:OE1	2.17	0.45
7:J:1106:ILE:O	7:J:1123:ARG:NH2	2.50	0.45
3:H:105:SER:HA	3:H:110:VAL:HG11	1.98	0.44
6:I:820:GLU:HG2	6:I:1079:ILE:HG22	2.00	0.44
7:J:341:ASN:O	7:J:345:LYS:HG3	2.17	0.44
7:J:644:MET:HE3	7:J:740:LEU:HB3	1.99	0.44
2:B:17:DC:C2	2:B:18:DG:C8	3.05	0.44
3:G:54:CYS:HB2	3:G:90:VAL:O	2.16	0.44
5:R:46:G:H2'	5:R:47:A:C8	2.52	0.44
6:I:1030:GLU:HG2	6:I:1034:ARG:NE	2.31	0.44
6:I:1122:LYS:HG2	6:I:1229:TYR:CE2	2.52	0.44
7:J:532:GLU:O	7:J:536:LEU:HD23	2.18	0.44
7:J:999:TYR:HE2	7:J:1027:VAL:HG22	1.82	0.44
7:J:1146:GLU:OE2	7:J:1148:ARG:NH2	2.50	0.44
7:J:1160:SER:O	7:J:1179:PRO:HB3	2.17	0.44
7:J:1167:LYS:HE3	7:J:1170:LYS:HB3	1.98	0.44
1:A:36:DG:H1'	1:A:37:DA:C8	2.52	0.44
2:B:17:DC:H5'	6:I:1269:ARG:HD3	1.98	0.44
6:I:348:SER:HA	6:I:351:LEU:HD12	1.99	0.44
6:I:697:LYS:HD2	6:I:1181:PRO:HG3	2.00	0.44
6:I:801:ARG:HD2	6:I:1229:TYR:HE1	1.82	0.44
6:I:1113:LEU:HD13	7:J:641:ILE:HG13	1.99	0.44
7:J:375:GLU:HA	7:J:378:LYS:CD	2.45	0.44
7:J:992:LYS:HA	7:J:992:LYS:HD3	1.82	0.44
7:J:1046:ILE:HB	7:J:1061:VAL:HA	1.99	0.44
1:A:31:DA:H4'	7:J:120:LEU:O	2.17	0.44
6:I:560:PRO:HG2	6:I:561:ILE:HD12	2.00	0.44
6:I:801:ARG:HA	6:I:1229:TYR:CD1	2.52	0.44
6:I:979:LEU:HD12	6:I:979:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:984:LEU:N	7:J:993:GLU:O	2.44	0.44
6:I:297:VAL:HB	6:I:317:LEU:HD21	1.98	0.44
7:J:437:PHE:HZ	7:J:453:VAL:HG11	1.83	0.44
7:J:596:LEU:HD23	7:J:596:LEU:HA	1.83	0.44
7:J:835:LEU:O	7:J:839:VAL:HG12	2.16	0.44
7:J:1227:HIS:O	7:J:1231:ARG:HG3	2.16	0.44
6:I:14:ASP:HB3	6:I:1157:GLN:HG3	2.00	0.44
6:I:80:PHE:HB2	6:I:85:CYS:SG	2.58	0.44
6:I:175:ARG:NH1	6:I:185:ASP:OD2	2.50	0.44
6:I:431:LYS:O	6:I:435:ILE:HG12	2.17	0.44
6:I:618:GLN:HG3	6:I:620:ASN:H	1.82	0.44
6:I:988:LYS:HA	6:I:988:LYS:HD3	1.45	0.44
7:J:1094:ASP:OD1	7:J:1095:MET:N	2.50	0.44
6:I:297:VAL:HG12	6:I:315:MET:O	2.17	0.44
7:J:311:ARG:HA	7:J:311:ARG:HD2	1.45	0.44
3:H:136:GLU:H	3:H:136:GLU:HG3	1.43	0.44
4:K:38:LEU:H	4:K:38:LEU:HG	1.58	0.44
7:J:78:LEU:HD12	7:J:79:LYS:H	1.82	0.44
4:K:3:ARG:HH22	7:J:615:LYS:HD2	1.82	0.44
6:I:120:GLN:HE21	6:I:489:PRO:HD2	1.83	0.44
6:I:1117:LEU:HD12	6:I:1195:ILE:HG12	2.00	0.44
7:J:746:LEU:HD23	7:J:758:PRO:HB3	2.00	0.44
7:J:1158:GLU:OE1	7:J:1223:LEU:HD21	2.18	0.44
1:A:27:DA:H4'	1:A:28:DG:OP1	2.18	0.43
1:A:35:DA:H2''	1:A:36:DG:N7	2.32	0.43
2:B:19:DT:H5''	6:I:1262:LYS:HB2	2.00	0.43
3:H:85:LEU:HB3	3:H:145:LYS:HE2	2.00	0.43
6:I:196:VAL:N	6:I:204:LEU:O	2.44	0.43
6:I:951:MET:O	6:I:955:GLN:HG3	2.17	0.43
6:I:996:ARG:HD2	6:I:996:ARG:HA	1.32	0.43
6:I:1286:THR:O	6:I:1290:MET:HG3	2.18	0.43
7:J:357:VAL:HG22	7:J:461:PHE:CE2	2.52	0.43
7:J:845:ALA:HA	7:J:883:ARG:HG3	1.99	0.43
7:J:957:SER:N	7:J:985:ILE:O	2.50	0.43
7:J:1221:LEU:HD13	7:J:1229:VAL:HG11	1.99	0.43
3:G:112:ALA:HB3	3:G:126:PRO:HA	2.00	0.43
6:I:587:LEU:HD23	6:I:587:LEU:HA	1.83	0.43
7:J:24:LEU:HD12	7:J:25:ALA:H	1.83	0.43
7:J:1169:THR:HG22	7:J:1173:ARG:HB2	2.01	0.43
6:I:103:VAL:HG12	6:I:117:ILE:HG22	2.00	0.43
7:J:530:PRO:HB3	7:J:577:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:749:LYS:HB3	7:J:755:ILE:HD11	2.00	0.43
6:I:303:ASP:OD2	6:I:305:SER:OG	2.35	0.43
6:I:617:ALA:N	6:I:652:TYR:O	2.36	0.43
7:J:1347:LEU:HD12	7:J:1357:ILE:HB	2.01	0.43
3:G:45:ARG:HH12	3:H:37:HIS:HB3	1.84	0.43
3:G:118:ASP:HB2	3:G:121:VAL:HG12	2.00	0.43
3:H:234:LEU:HD13	3:H:234:LEU:HA	1.84	0.43
6:I:39:ILE:HB	6:I:75:LEU:HD11	2.00	0.43
6:I:239:MET:SD	6:I:241:LEU:HB2	2.59	0.43
6:I:264:GLU:HB2	6:I:267:ARG:HG3	2.00	0.43
6:I:500:ALA:O	6:I:504:GLU:HG3	2.19	0.43
6:I:807:TRP:CH2	6:I:1216:ARG:HD2	2.53	0.43
7:J:110:PRO:O	7:J:182:ALA:HB3	2.18	0.43
7:J:1075:ARG:NH1	7:J:1165:PHE:H	2.16	0.43
1:A:29:DA:H2''	1:A:30:DG:C8	2.53	0.43
3:H:47:LEU:H	3:H:47:LEU:HG	1.74	0.43
7:J:375:GLU:HA	7:J:378:LYS:CG	2.49	0.43
7:J:471:PRO:HB3	7:J:476:ALA:HB1	2.01	0.43
7:J:523:GLU:OE1	7:J:547:ARG:N	2.52	0.43
7:J:1227:HIS:HB3	7:J:1231:ARG:NH1	2.33	0.43
7:J:1238:GLN:O	7:J:1242:ARG:N	2.40	0.43
7:J:1348:LYS:O	7:J:1352:ILE:HD12	2.18	0.43
2:B:23:DG:H2'	2:B:24:DT:C6	2.53	0.43
3:G:68:TYR:OH	6:I:1057:LYS:HE3	2.18	0.43
6:I:350:THR:O	6:I:354:ASP:N	2.49	0.43
6:I:772:SER:H	6:I:775:GLU:CD	2.26	0.43
6:I:1114:GLU:CD	6:I:1230:MET:HG3	2.44	0.43
6:I:1270:PHE:CE1	6:I:1274:GLU:HB3	2.53	0.43
7:J:127:LEU:HD22	7:J:227:PHE:HE2	1.84	0.43
7:J:959:LYS:HD2	7:J:959:LYS:HA	1.84	0.43
3:H:96:ASP:O	3:H:147:GLN:HA	2.19	0.43
7:J:740:LEU:O	7:J:762:ASN:HB2	2.19	0.43
6:I:101:ARG:HA	6:I:119:GLU:HA	2.01	0.43
6:I:273:HIS:O	6:I:276:GLN:HG3	2.18	0.43
6:I:715:THR:OG1	6:I:784:ALA:O	2.30	0.43
6:I:1042:LEU:HD23	6:I:1042:LEU:HA	1.85	0.43
7:J:1353:VAL:HG11	7:J:1355:ARG:HE	1.84	0.43
3:H:58:GLU:HG3	3:H:173:VAL:H	1.84	0.43
6:I:777:VAL:HG13	6:I:781:ASP:HB3	2.00	0.43
6:I:1252:SER:OG	6:I:1253:LEU:N	2.52	0.43
7:J:66:LYS:HB3	7:J:69:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:155:GLU:OE2	7:J:158:GLN:HB2	2.17	0.43
7:J:414:GLU:HG2	7:J:417:ARG:HH21	1.84	0.43
7:J:441:LEU:HD23	7:J:441:LEU:HA	1.81	0.43
7:J:832:LYS:HG2	7:J:1242:ARG:HD2	2.00	0.43
4:K:22:VAL:HG23	4:K:64:LEU:HD12	2.01	0.42
6:I:850:ILE:HD12	6:I:850:ILE:HA	1.86	0.42
6:I:1225:VAL:HG23	7:J:638:SER:HB2	2.01	0.42
7:J:375:GLU:HG2	7:J:378:LYS:NZ	2.34	0.42
7:J:547:ARG:HA	7:J:573:THR:HA	2.01	0.42
6:I:150:HIS:CG	6:I:454:ARG:HH21	2.37	0.42
7:J:450:HIS:O	7:J:453:VAL:HG12	2.19	0.42
3:H:183:ILE:HD13	3:H:183:ILE:C	2.44	0.42
6:I:765:ILE:HD13	6:I:787:PRO:HG3	2.01	0.42
7:J:1218:HIS:ND1	7:J:1306:LEU:HB3	2.34	0.42
6:I:74:ARG:NH2	6:I:97:ARG:HG3	2.34	0.42
6:I:233:ARG:HH21	6:I:331:LYS:HD3	1.85	0.42
6:I:957:LYS:HG3	6:I:1029:LEU:HD11	2.01	0.42
7:J:785:ASP:OD2	7:J:789:LYS:HE3	2.19	0.42
2:B:27:DG:H2"	2:B:28:DG:OP1	2.19	0.42
3:G:95:LYS:NZ	3:G:120:ASP:OD2	2.30	0.42
3:H:82:LEU:HD13	3:H:173:VAL:HG22	2.02	0.42
3:H:95:LYS:H	3:H:95:LYS:HG3	1.62	0.42
3:H:104:LYS:HB2	3:H:104:LYS:HE2	1.95	0.42
6:I:102:LEU:HB3	6:I:118:LYS:HB2	2.01	0.42
6:I:513:GLN:OE1	6:I:529:ARG:NH2	2.53	0.42
6:I:643:SER:OG	7:J:756:GLU:OE2	2.38	0.42
7:J:30:ILE:HG12	7:J:243:PRO:HG3	2.02	0.42
7:J:67:ASP:HB2	7:J:95:THR:H	1.84	0.42
6:I:295:LYS:HB2	6:I:317:LEU:HD12	2.00	0.42
6:I:591:TYR:CD2	6:I:606:LEU:HD12	2.54	0.42
6:I:618:GLN:HG2	7:J:768:ASN:HD21	1.84	0.42
6:I:978:VAL:HB	6:I:1011:LEU:HD11	2.01	0.42
7:J:582:ILE:HG23	7:J:623:GLN:HB3	2.01	0.42
7:J:706:VAL:HG22	7:J:715:LYS:HD3	2.01	0.42
4:K:30:MET:HE2	4:K:30:MET:HB2	1.68	0.42
6:I:225:PHE:HZ	6:I:345:PRO:HA	1.84	0.42
6:I:1101:LEU:O	6:I:1104:PRO:HD2	2.19	0.42
7:J:1064:SER:OG	7:J:1067:ARG:NH2	2.52	0.42
7:J:1109:LEU:HD23	7:J:1113:VAL:HG12	2.01	0.42
3:H:81:ILE:HG12	3:H:131:CYS:HB2	2.02	0.42
6:I:229:ILE:HD13	6:I:334:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:165:TYR:CZ	7:J:169:LEU:HD11	2.54	0.42
7:J:502:PRO:HB3	7:J:506:VAL:HG11	2.00	0.42
7:J:888:CYS:HB3	7:J:898:CYS:SG	2.60	0.42
7:J:976:THR:HG23	7:J:999:TYR:HE1	1.85	0.42
6:I:225:PHE:CZ	6:I:345:PRO:HA	2.54	0.42
7:J:544:LEU:O	7:J:575:GLY:N	2.49	0.42
6:I:6:THR:HG21	6:I:782:VAL:HG22	2.02	0.42
6:I:165:HIS:ND1	6:I:167:SER:OG	2.52	0.42
6:I:465:ARG:O	6:I:469:VAL:HG13	2.20	0.42
6:I:1028:LYS:HB3	6:I:1028:LYS:HE2	1.39	0.42
6:I:1127:LYS:HD2	6:I:1202:GLY:HA2	2.02	0.42
6:I:1192:GLU:OE1	7:J:764:ARG:NH1	2.52	0.42
7:J:425:ARG:HD3	7:J:427:PRO:HD2	2.01	0.42
7:J:530:PRO:HG2	7:J:580:TRP:HD1	1.85	0.42
7:J:931:THR:H	7:J:1244:GLN:NE2	2.18	0.42
7:J:1364:ALA:O	7:J:1367:GLN:HG3	2.19	0.42
4:K:3:ARG:HD2	4:K:3:ARG:HA	1.28	0.41
6:I:138:ILE:HD13	6:I:506:PHE:HB3	2.01	0.41
6:I:668:ILE:HB	6:I:671:LEU:HD12	2.01	0.41
6:I:686:GLN:HE21	6:I:1069:ARG:HG2	1.85	0.41
6:I:870:ILE:HD12	6:I:1050:VAL:HG11	2.01	0.41
7:J:495:ASN:OD1	7:J:497:GLU:HB2	2.20	0.41
6:I:545:PHE:CE2	7:J:788:LEU:HD22	2.56	0.41
6:I:1196:LYS:HD3	6:I:1206:THR:O	2.20	0.41
7:J:72:CYS:H	7:J:88:CYS:HB3	1.85	0.41
7:J:375:GLU:CA	7:J:378:LYS:HG3	2.50	0.41
7:J:923:ILE:HD12	7:J:1256:ILE:HG13	2.02	0.41
7:J:974:VAL:HA	7:J:1001:ALA:O	2.21	0.41
3:G:53:GLY:HA3	3:G:177:TYR:O	2.20	0.41
3:G:133:LEU:HA	3:G:133:LEU:HD23	1.79	0.41
3:H:55:ALA:HA	3:H:145:LYS:HB3	2.02	0.41
3:H:91:ARG:HE	3:H:91:ARG:HB2	1.54	0.41
6:I:447:HIS:HA	6:I:551:HIS:ND1	2.34	0.41
6:I:1022:LYS:HD2	6:I:1022:LYS:HA	1.58	0.41
7:J:143:SER:HB2	7:J:159:ILE:HD11	2.03	0.41
7:J:857:LEU:HG	7:J:858:VAL:HG23	2.01	0.41
7:J:1236:GLU:O	7:J:1240:VAL:HG23	2.20	0.41
3:G:110:VAL:HG23	3:G:130:ILE:HB	2.03	0.41
3:H:214:GLU:HA	3:H:217:ILE:HD12	2.03	0.41
6:I:97:ARG:HA	6:I:97:ARG:HD3	1.75	0.41
6:I:1243:MET:HE1	7:J:371:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:1154:ALA:HB1	7:J:1209:VAL:HG23	2.03	0.41
3:H:47:LEU:CD1	3:H:183:ILE:HG21	2.51	0.41
6:I:38:PHE:HD1	6:I:461:GLU:HG3	1.85	0.41
6:I:881:ASP:O	6:I:920:VAL:HG23	2.20	0.41
6:I:1244:HIS:NE2	6:I:1266:GLY:O	2.53	0.41
6:I:1288:GLN:CD	6:I:1315:MET:HE1	2.45	0.41
6:I:1328:LYS:NZ	7:J:100:GLU:O	2.51	0.41
7:J:786:THR:HA	7:J:789:LYS:HD2	2.02	0.41
7:J:804:ALA:HA	7:J:1259:GLN:HG3	2.02	0.41
7:J:824:PRO:HD3	7:J:835:LEU:HD13	2.03	0.41
7:J:966:VAL:HB	7:J:1028:ILE:HD12	2.02	0.41
2:B:19:DT:OP1	6:I:1262:LYS:N	2.54	0.41
3:G:48:LEU:HG	3:G:183:ILE:HD12	2.02	0.41
3:H:21:SER:O	3:H:213:PRO:HD3	2.21	0.41
3:H:23:HIS:CE1	3:H:204:GLU:HB3	2.54	0.41
1:A:26:DA:H4'	1:A:27:DA:OP1	2.20	0.41
3:H:43:LEU:O	3:H:47:LEU:HG	2.21	0.41
3:H:61:ILE:HG12	3:H:64:VAL:HG23	2.03	0.41
6:I:521:LEU:HD23	6:I:686:GLN:HB3	2.03	0.41
6:I:759:SER:OG	6:I:765:ILE:HG12	2.20	0.41
6:I:960:LEU:HD13	6:I:1029:LEU:HA	2.02	0.41
6:I:1185:PRO:HD2	6:I:1189:GLY:HA2	2.03	0.41
6:I:1267:GLY:O	7:J:346:ARG:NH1	2.54	0.41
6:I:1283:ALA:HB1	6:I:1286:THR:OG1	2.20	0.41
7:J:449:LEU:HD13	7:J:466:MET:HE1	2.02	0.41
7:J:492:SER:HB3	7:J:499:ILE:HD13	2.02	0.41
7:J:516:ASP:OD1	7:J:516:ASP:N	2.54	0.41
7:J:613:GLY:C	7:J:616:PRO:HD2	2.45	0.41
7:J:1037:PHE:CZ	7:J:1059:LEU:HD13	2.55	0.41
7:J:1048:ARG:CA	7:J:1059:LEU:HD23	2.51	0.41
7:J:1266:ILE:HA	7:J:1302:TYR:HA	2.02	0.41
7:J:1282:TYR:HA	7:J:1285:VAL:HG12	2.03	0.41
6:I:272:ARG:HH21	6:I:276:GLN:N	2.18	0.41
6:I:704:MET:O	6:I:708:VAL:HG23	2.21	0.41
6:I:718:ALA:N	6:I:781:ASP:O	2.53	0.41
6:I:870:ILE:HB	6:I:944:ARG:HG2	2.03	0.41
7:J:38:VAL:HG11	7:J:56:LEU:HA	2.02	0.41
7:J:480:ALA:HA	7:J:484:MET:HG2	2.02	0.41
7:J:499:ILE:HD12	7:J:499:ILE:HA	1.96	0.41
7:J:512:TYR:HD1	7:J:724:MET:HE1	1.86	0.41
7:J:580:TRP:CE3	7:J:589:TYR:HD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:849:LEU:HD23	7:J:849:LEU:H	1.86	0.41
7:J:952:VAL:HG13	7:J:1014:GLY:H	1.86	0.41
3:G:88:LEU:HG	3:G:90:VAL:HG23	2.01	0.41
3:H:46:ILE:HG13	3:H:224:LEU:HD13	2.02	0.41
3:H:83:LEU:HB3	7:J:551:ARG:HH21	1.86	0.41
6:I:18:ARG:NE	6:I:620:ASN:HA	2.36	0.41
6:I:68:LEU:HD13	6:I:102:LEU:HB2	2.03	0.41
6:I:550:VAL:HG13	7:J:777:HIS:ND1	2.35	0.41
7:J:127:LEU:HD23	7:J:189:LEU:HD22	2.03	0.41
7:J:211:GLU:HA	7:J:214:ARG:HB2	2.03	0.41
7:J:544:LEU:HD11	7:J:631:TYR:CD1	2.52	0.41
7:J:1099:TYR:HB3	7:J:1199:PHE:CZ	2.55	0.41
6:I:324:LYS:O	6:I:327:GLN:NE2	2.54	0.41
6:I:538:LEU:HD22	6:I:547:VAL:HG11	2.01	0.41
6:I:699:LEU:HD12	6:I:699:LEU:HA	1.81	0.41
6:I:1329:GLU:OE2	7:J:330:MET:HB2	2.21	0.41
7:J:1306:LEU:HD12	7:J:1306:LEU:HA	1.89	0.41
6:I:191:LYS:HE2	6:I:191:LYS:HB2	1.96	0.40
6:I:241:LEU:HB3	6:I:285:ILE:HD12	2.03	0.40
6:I:667:LEU:HD23	6:I:667:LEU:HA	1.85	0.40
6:I:1339:LEU:HD23	7:J:17:PHE:CG	2.57	0.40
7:J:120:LEU:HB2	7:J:121:PRO:HD3	2.03	0.40
7:J:450:HIS:CE1	7:J:452:LEU:HB2	2.56	0.40
7:J:1311:LYS:HA	7:J:1311:LYS:HD3	1.91	0.40
3:H:83:LEU:HD12	3:H:83:LEU:HA	1.75	0.40
6:I:178:PRO:HA	6:I:397:LEU:HD23	2.02	0.40
6:I:551:HIS:H	6:I:554:HIS:CE1	2.40	0.40
6:I:560:PRO:HB2	7:J:776:THR:CG2	2.46	0.40
6:I:702:THR:HA	6:I:1184:THR:O	2.22	0.40
6:I:976:ARG:HH12	6:I:989:LEU:HB2	1.86	0.40
6:I:1283:ALA:HA	7:J:479:GLU:CD	2.46	0.40
7:J:1269:ALA:O	7:J:1272:SER:OG	2.37	0.40
2:B:4:DT:H2''	2:B:5:DG:O4'	2.21	0.40
4:K:59:ILE:HD13	4:K:59:ILE:HA	1.74	0.40
6:I:473:ARG:O	6:I:476:LYS:HG2	2.22	0.40
6:I:1086:PRO:HB2	6:I:1212:LEU:HD21	2.04	0.40
7:J:153:ASN:OD1	7:J:154:LEU:N	2.55	0.40
7:J:355:ILE:HG22	7:J:461:PHE:HE1	1.87	0.40
7:J:563:LEU:HA	7:J:563:LEU:HD23	1.84	0.40
7:J:641:ILE:HD13	7:J:641:ILE:HA	1.89	0.40
7:J:1195:GLN:NE2	7:J:1196:LEU:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:227:LYS:HD2	6:I:334:GLU:HB3	2.04	0.40
6:I:1290:MET:HE3	6:I:1294:LYS:NZ	2.36	0.40
7:J:384:LYS:HG3	7:J:415:VAL:HG12	2.03	0.40
7:J:770:LEU:HA	7:J:770:LEU:HD23	1.88	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	
3	G	217/235 (92%)	212 (98%)	5 (2%)	0	100	100
3	H	215/235 (92%)	204 (95%)	9 (4%)	2 (1%)	14	45
4	K	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
6	I	1312/1340 (98%)	1271 (97%)	40 (3%)	1 (0%)	48	79
7	J	1331/1358 (98%)	1293 (97%)	37 (3%)	1 (0%)	48	79
All	All	3152/3247 (97%)	3055 (97%)	93 (3%)	4 (0%)	49	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	30	PRO
3	H	90	VAL
6	I	58	PRO
7	J	427	PRO

5.3.2 Protein sidechains [i](#)

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	
3	G	189/202 (94%)	189 (100%)	0	100	100
3	H	188/202 (93%)	96 (51%)	92 (49%)	0	0
4	K	67/67 (100%)	39 (58%)	28 (42%)	0	0
6	I	1135/1155 (98%)	1080 (95%)	55 (5%)	23	47
7	J	1122/1134 (99%)	1060 (94%)	62 (6%)	19	45
All	All	2701/2760 (98%)	2464 (91%)	237 (9%)	11	33

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	5	VAL
3	H	6	THR
3	H	9	LEU
3	H	10	LYS
3	H	13	LEU
3	H	14	VAL
3	H	16	ILE
3	H	18	GLN
3	H	19	VAL
3	H	20	SER
3	H	22	THR
3	H	26	VAL
3	H	27	THR
3	H	28	LEU
3	H	29	GLU
3	H	31	LEU
3	H	33	ARG
3	H	37	HIS
3	H	43	LEU
3	H	45	ARG
3	H	47	LEU
3	H	48	LEU
3	H	50	SER
3	H	51	MET
3	H	54	CYS
3	H	59	VAL
3	H	60	GLU
3	H	62	ASP

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Mol	Chain	Res	Type
3	H	64	VAL
3	H	65	LEU
3	H	67	GLU
3	H	71	LYS
3	H	72	GLU
3	H	74	VAL
3	H	75	GLN
3	H	78	ILE
3	H	79	LEU
3	H	80	GLU
3	H	83	LEU
3	H	91	ARG
3	H	95	LYS
3	H	96	ASP
3	H	98	VAL
3	H	99	ILE
3	H	100	LEU
3	H	101	THR
3	H	103	ASN
3	H	104	LYS
3	H	110	VAL
3	H	114	ASP
3	H	115	ILE
3	H	116	THR
3	H	117	HIS
3	H	120	ASP
3	H	122	GLU
3	H	127	GLN
3	H	129	VAL
3	H	133	LEU
3	H	134	THR
3	H	136	GLU
3	H	137	ASN
3	H	142	MET
3	H	144	ILE
3	H	145	LYS
3	H	146	VAL
3	H	158	ARG
3	H	170	ARG
3	H	171	LEU
3	H	172	LEU
3	H	174	ASP

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Mol	Chain	Res	Type
3	H	180	VAL
3	H	183	ILE
3	H	187	VAL
3	H	188	GLU
3	H	191	ARG
3	H	192	VAL
3	H	194	GLN
3	H	195	ARG
3	H	196	THR
3	H	197	ASP
3	H	202	VAL
3	H	203	ILE
3	H	205	MET
3	H	206	GLU
3	H	207	THR
3	H	211	ILE
3	H	214	GLU
3	H	219	ARG
3	H	229	GLU
3	H	231	PHE
3	H	233	ASP
3	H	234	LEU
4	K	3	ARG
4	K	5	THR
4	K	10	VAL
4	K	12	LYS
4	K	13	ILE
4	K	19	LEU
4	K	22	VAL
4	K	28	ARG
4	K	30	MET
4	K	35	LYS
4	K	38	LEU
4	K	39	VAL
4	K	42	GLU
4	K	45	LYS
4	K	47	THR
4	K	48	VAL
4	K	52	ARG
4	K	54	ILE
4	K	56	GLU
4	K	59	ILE

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Mol	Chain	Res	Type
4	K	60	ASN
4	K	61	ASN
4	K	67	ARG
4	K	68	GLU
4	K	69	ARG
4	K	71	GLU
4	K	72	GLN
4	K	80	LEU
6	I	59	ILE
6	I	563	THR
6	I	568	ASN
6	I	572	ILE
6	I	734	ILE
6	I	735	LYS
6	I	739	ASP
6	I	740	GLU
6	I	748	ILE
6	I	843	THR
6	I	850	ILE
6	I	929	ILE
6	I	933	VAL
6	I	935	THR
6	I	941	LYS
6	I	950	GLU
6	I	953	LEU
6	I	960	LEU
6	I	964	LEU
6	I	966	ILE
6	I	967	LEU
6	I	974	ARG
6	I	975	ILE
6	I	978	VAL
6	I	979	LEU
6	I	980	VAL
6	I	987	GLU
6	I	988	LYS
6	I	991	LYS
6	I	992	LEU
6	I	994	ARG
6	I	995	ASP
6	I	996	ARG
6	I	997	TRP

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Mol	Chain	Res	Type
6	I	998	LEU
6	I	1000	LEU
6	I	1005	GLU
6	I	1007	LYS
6	I	1009	ASN
6	I	1013	GLN
6	I	1019	ASP
6	I	1021	LEU
6	I	1022	LYS
6	I	1026	GLU
6	I	1027	LYS
6	I	1028	LYS
6	I	1030	GLU
6	I	1032	LYS
6	I	1035	LYS
6	I	1046	VAL
6	I	1047	LEU
6	I	1049	ILE
6	I	1299	ASN
6	I	1302	THR
6	I	1303	LYS
7	J	32	SER
7	J	40	LYS
7	J	42	GLU
7	J	45	ASN
7	J	47	ARG
7	J	48	THR
7	J	50	LYS
7	J	53	ARG
7	J	54	ASP
7	J	56	LEU
7	J	66	LYS
7	J	67	ASP
7	J	71	LEU
7	J	78	LEU
7	J	79	LYS
7	J	84	ILE
7	J	87	LYS
7	J	90	VAL
7	J	92	VAL
7	J	93	THR
7	J	94	GLN

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Mol	Chain	Res	Type
7	J	96	LYS
7	J	97	VAL
7	J	250	ARG
7	J	309	ASN
7	J	311	ARG
7	J	314	ARG
7	J	320	ASN
7	J	321	LYS
7	J	322	ARG
7	J	324	LEU
7	J	325	LYS
7	J	326	SER
7	J	327	LEU
7	J	329	ASP
7	J	330	MET
7	J	332	LYS
7	J	372	MET
7	J	374	LEU
7	J	394	ILE
7	J	398	LYS
7	J	399	LYS
7	J	401	VAL
7	J	403	ARG
7	J	404	GLU
7	J	405	GLU
7	J	407	VAL
7	J	416	ILE
7	J	425	ARG
7	J	428	THR
7	J	430	HIS
7	J	431	ARG
7	J	435	GLN
7	J	442	ILE
7	J	452	LEU
7	J	706	VAL
7	J	709	ARG
7	J	714	GLU
7	J	716	GLN
7	J	1041	ILE
7	J	1045	THR
7	J	1046	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39)

such sidechains are listed below:

Mol	Chain	Res	Type
3	G	84	ASN
3	G	128	HIS
3	G	227	GLN
3	H	23	HIS
3	H	41	ASN
3	H	84	ASN
4	K	61	ASN
4	K	70	GLN
4	K	73	GLN
6	I	31	GLN
6	I	41	GLN
6	I	120	GLN
6	I	357	ASN
6	I	462	ASN
6	I	517	GLN
6	I	618	GLN
6	I	620	ASN
6	I	686	GLN
6	I	932	GLN
6	I	1008	GLN
6	I	1009	ASN
6	I	1175	ASN
6	I	1268	GLN
6	I	1288	GLN
6	I	1313	HIS
7	J	80	HIS
7	J	206	ASN
7	J	229	GLN
7	J	419	HIS
7	J	424	ASN
7	J	448	GLN
7	J	458	ASN
7	J	465	GLN
7	J	489	ASN
7	J	979	ASN
7	J	1086	ASN
7	J	1114	GLN
7	J	1195	GLN
7	J	1238	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	R	47/47 (100%)	27 (57%)	2 (4%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	R	2	C
5	R	3	A
5	R	8	U
5	R	9	U
5	R	10	C
5	R	13	G
5	R	14	C
5	R	15	U
5	R	16	A
5	R	17	C
5	R	18	A
5	R	25	A
5	R	26	U
5	R	27	A
5	R	28	A
5	R	30	A
5	R	31	A
5	R	32	A
5	R	33	C
5	R	34	U
5	R	35	A
5	R	36	A
5	R	37	G
5	R	38	G
5	R	39	A
5	R	42	A
5	R	47	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	R	1	G
5	R	15	U

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
8	PRF	R	101	-	14,14,14	0.66	0	14,20,20	1.54	1 (7%)

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
8	PRF	R	101	-	-	0/0/2/2	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	101	PRF	C7-C5-C4	-5.20	106.71	112.68

There are no chirality outliers.

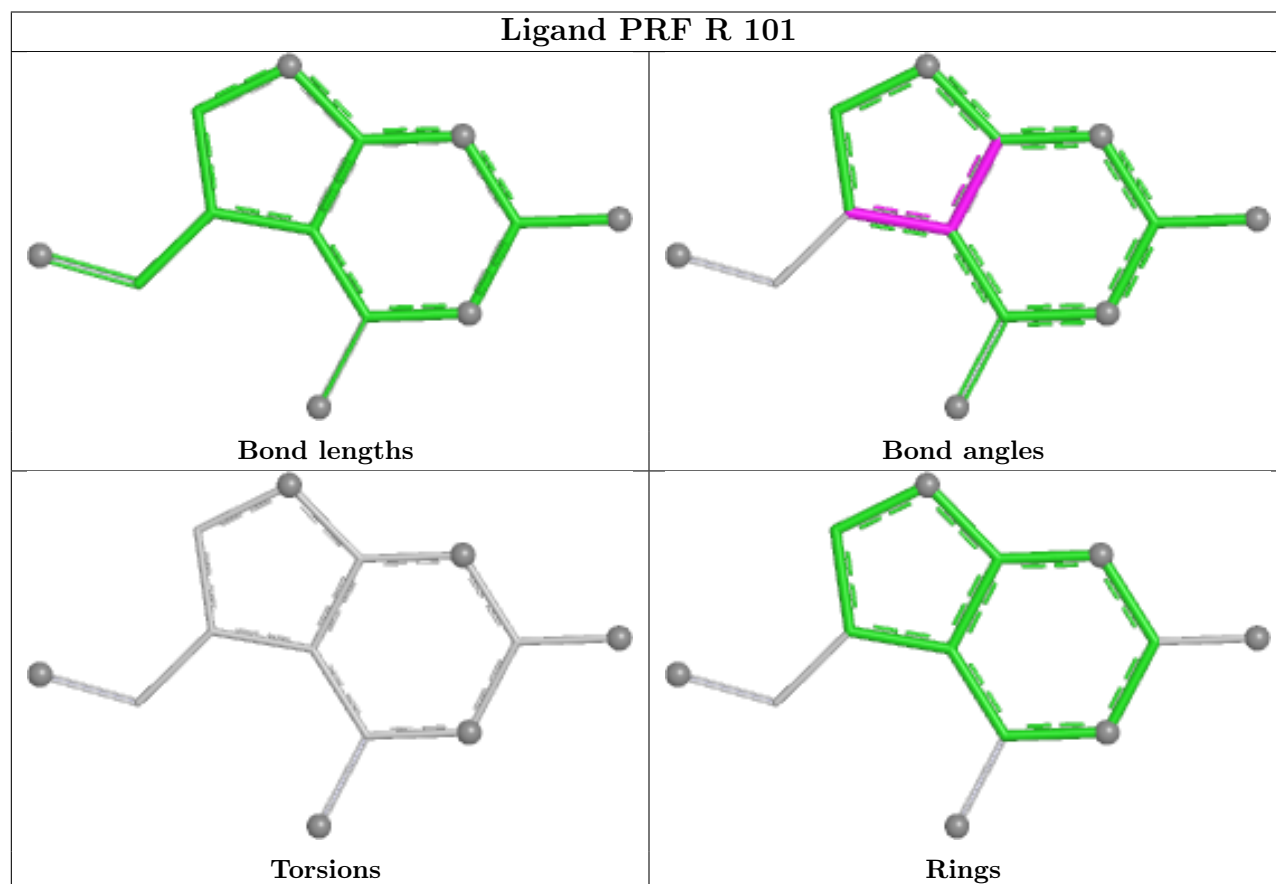
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

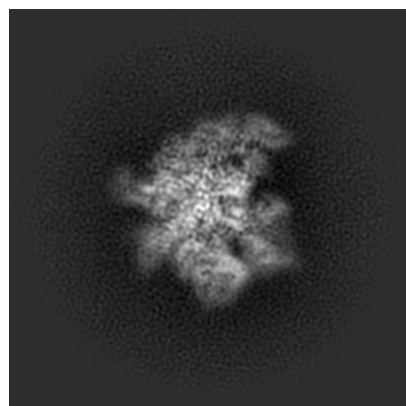
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29732. These allow visual inspection of the internal detail of the map and identification of artifacts.

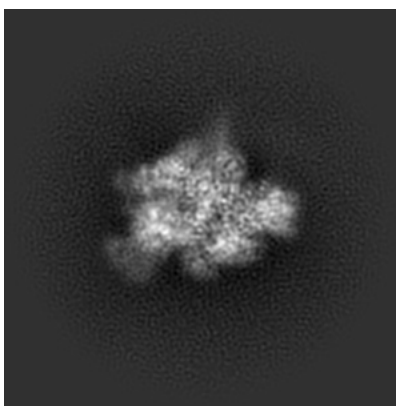
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

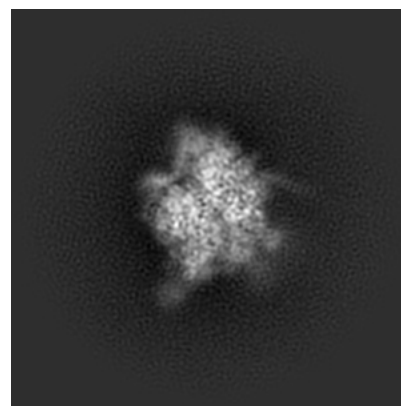
6.1.1 Primary map



X

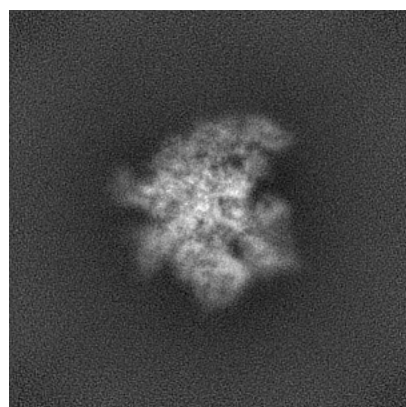


Y

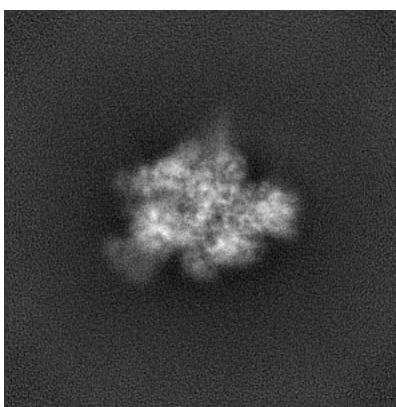


Z

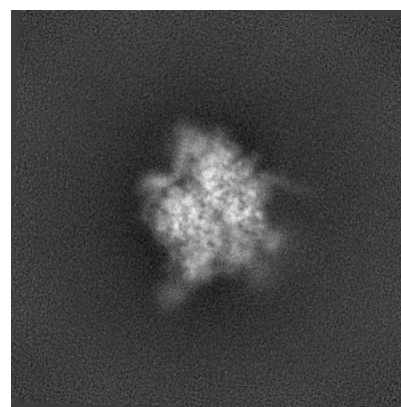
6.1.2 Raw map



X



Y

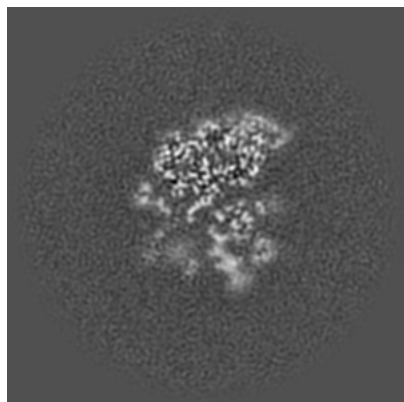


Z

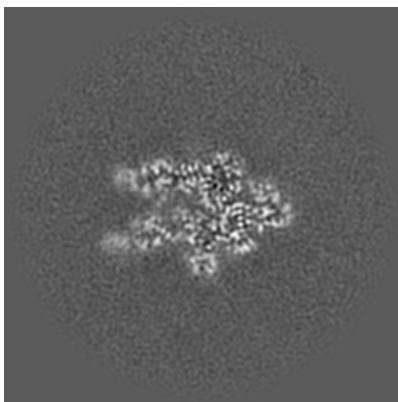
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

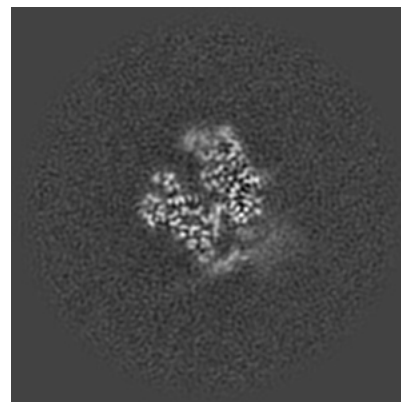
6.2.1 Primary map



X Index: 150

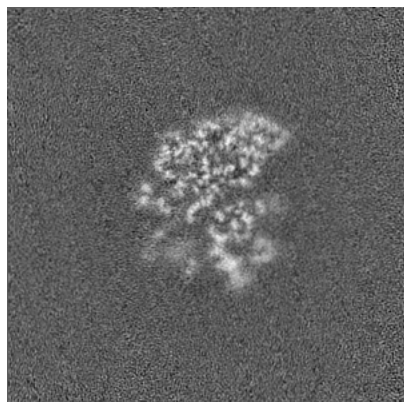


Y Index: 150

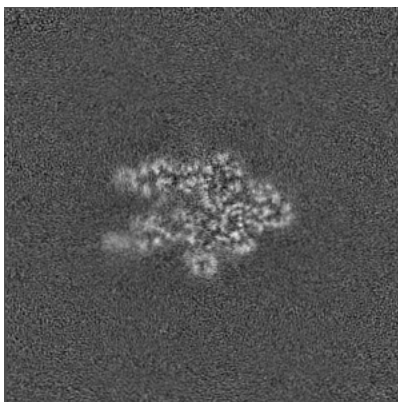


Z Index: 150

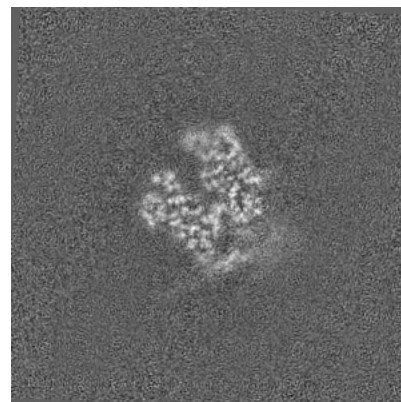
6.2.2 Raw map



X Index: 150



Y Index: 150

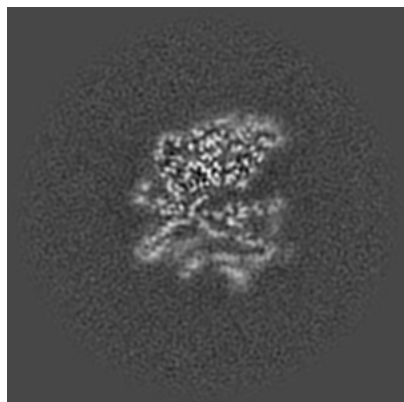


Z Index: 150

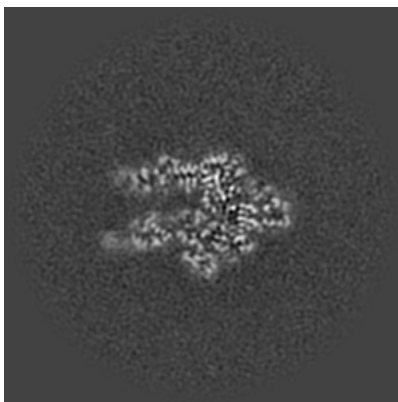
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

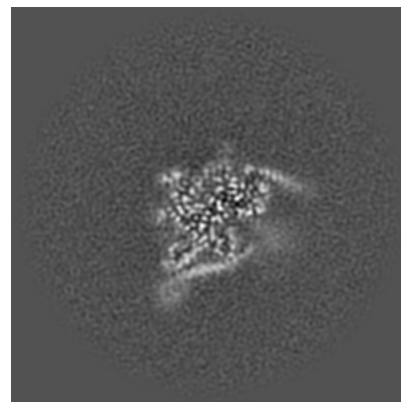
6.3.1 Primary map



X Index: 146

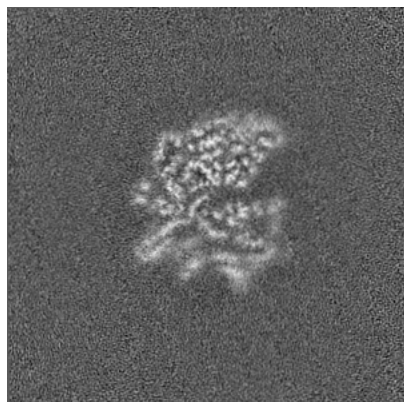


Y Index: 148

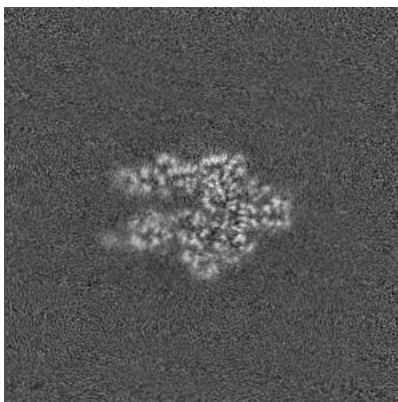


Z Index: 165

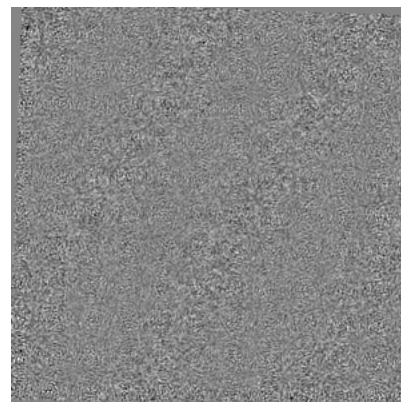
6.3.2 Raw map



X Index: 146



Y Index: 147

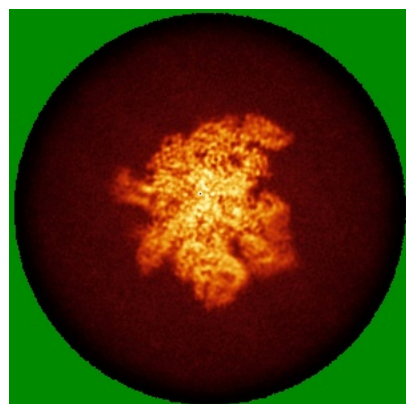


Z Index: 297

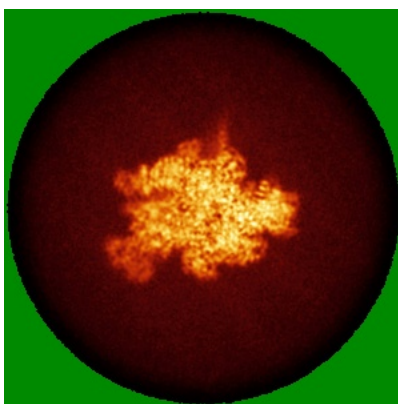
The images above show the largest variance slices of the map in three orthogonal directions.

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

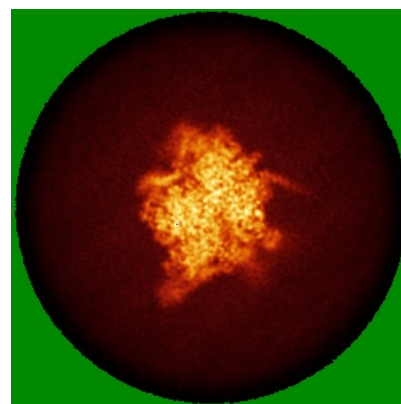
6.4.1 Primary map



X

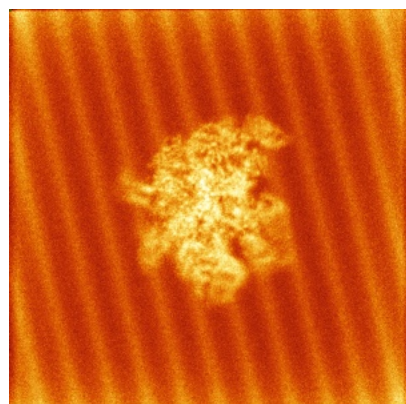


Y

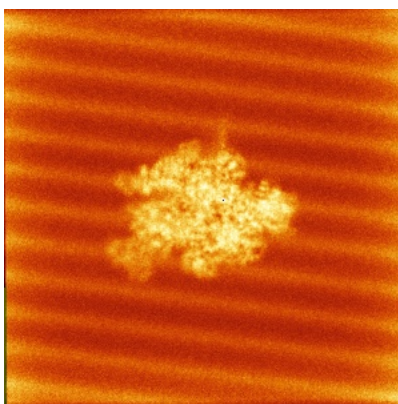


Z

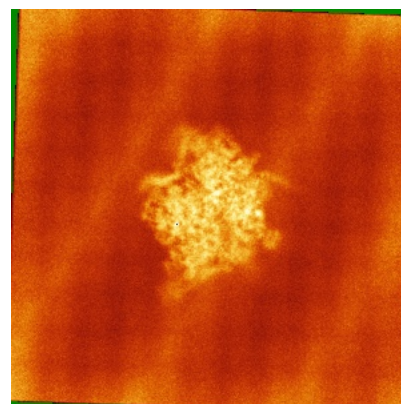
6.4.2 Raw map



X



Y

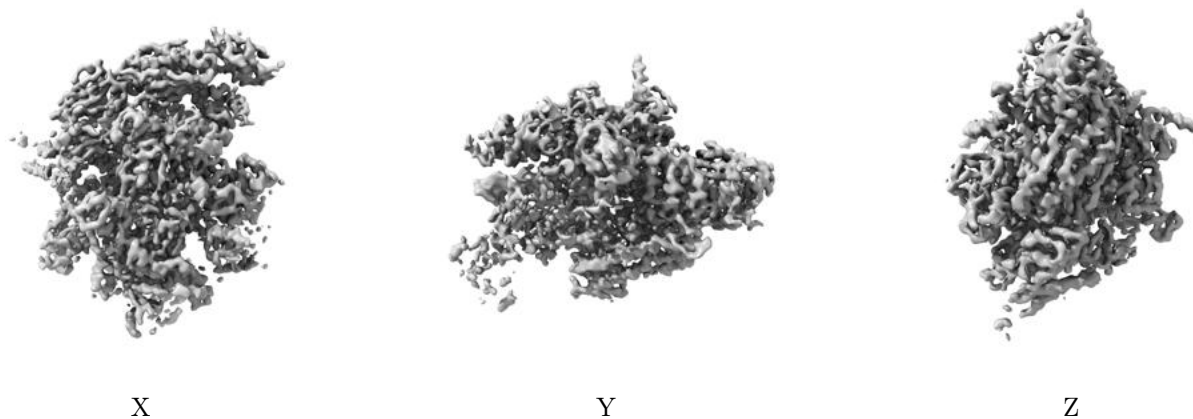


Z

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.

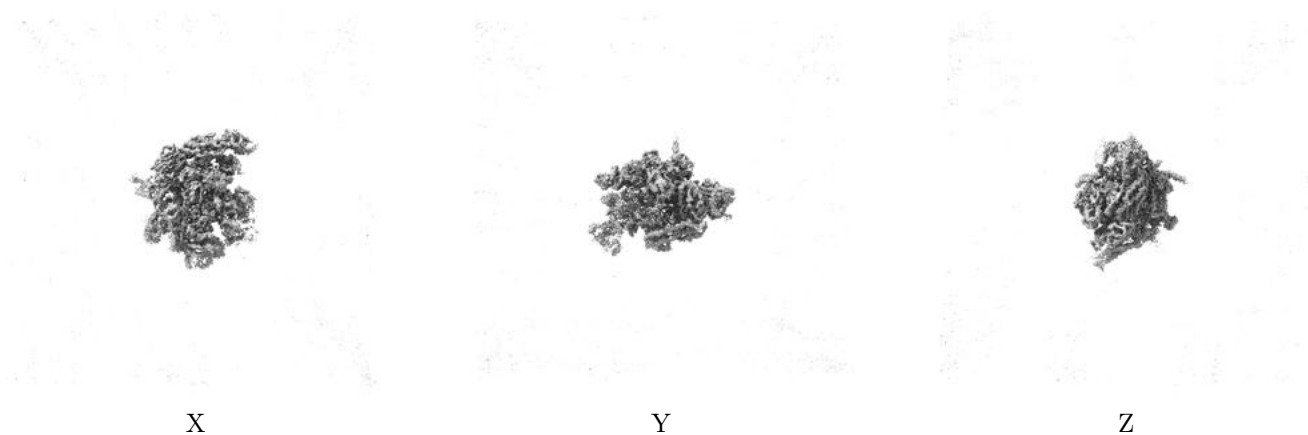
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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.

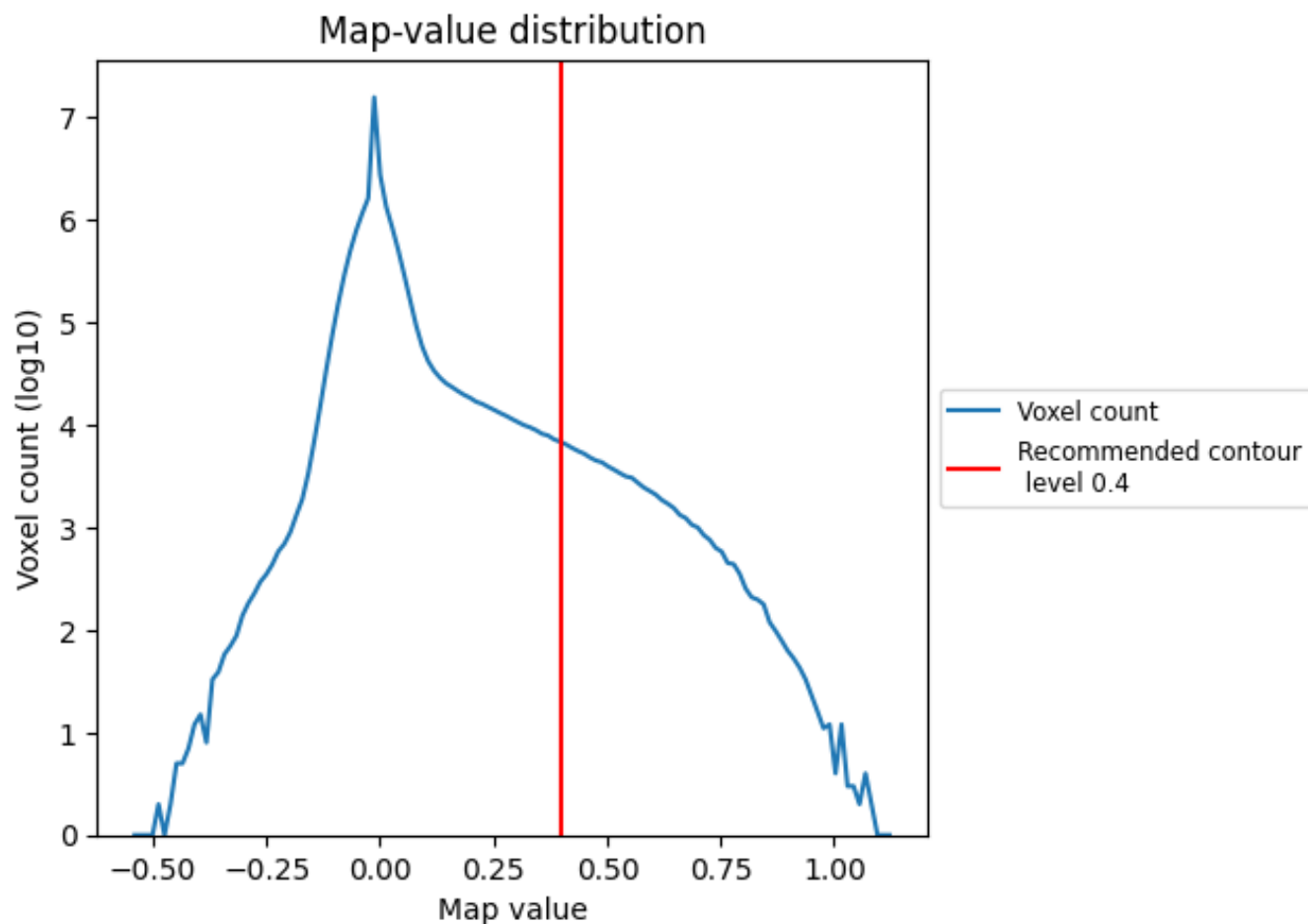
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

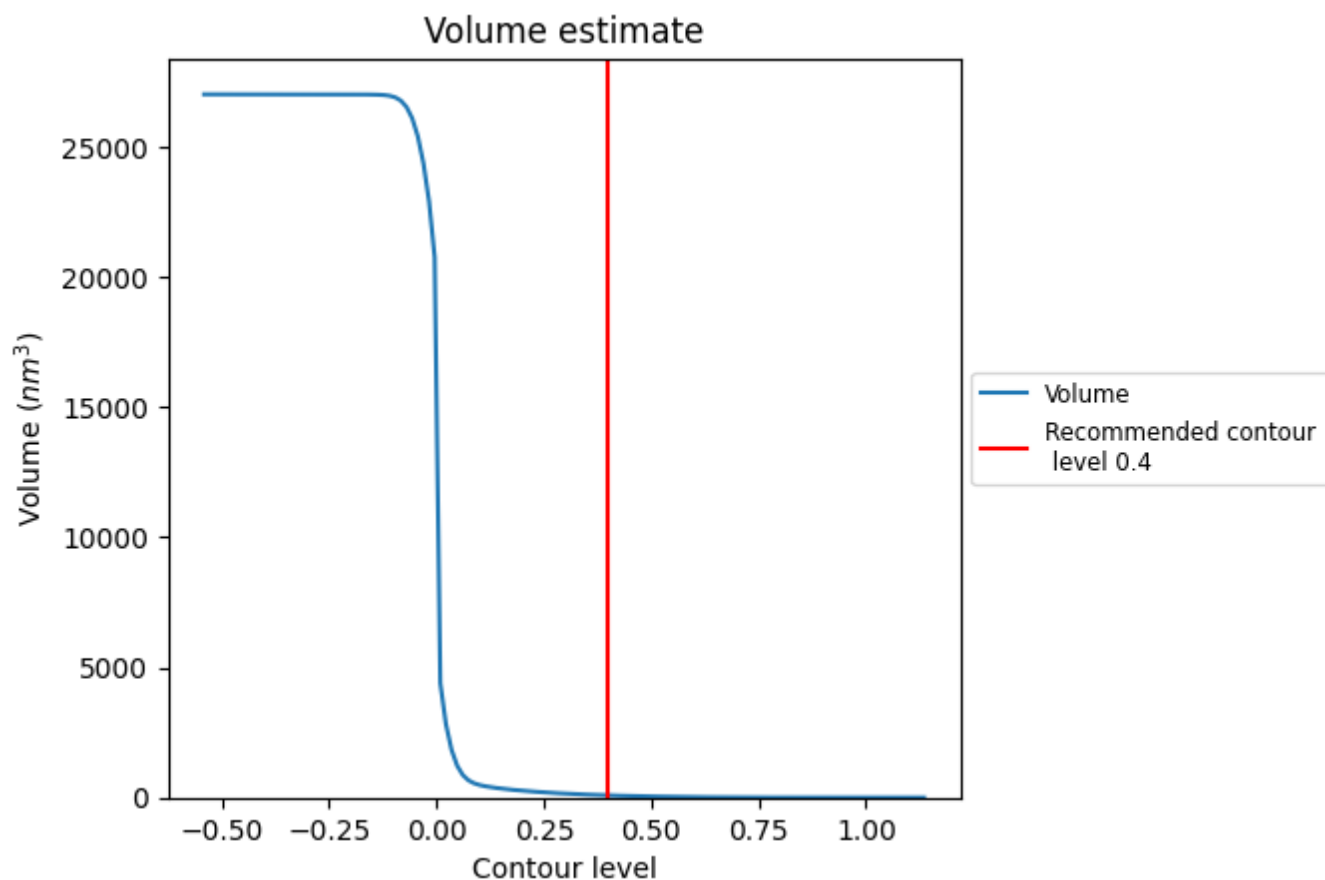
This section contains the results of statistical analysis of the map.

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.

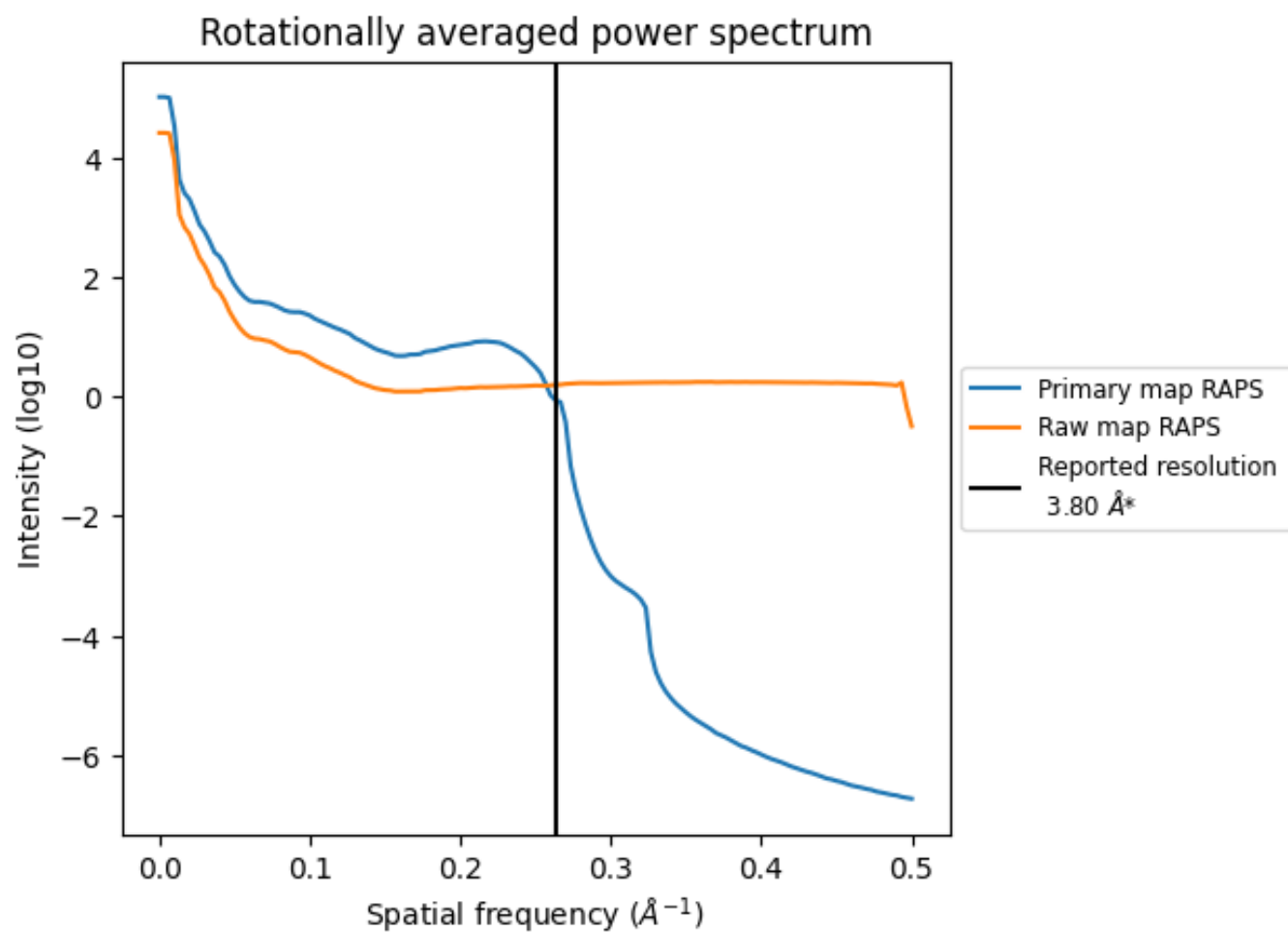
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 84 nm³; this corresponds to an approximate mass of 76 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 ⓘ

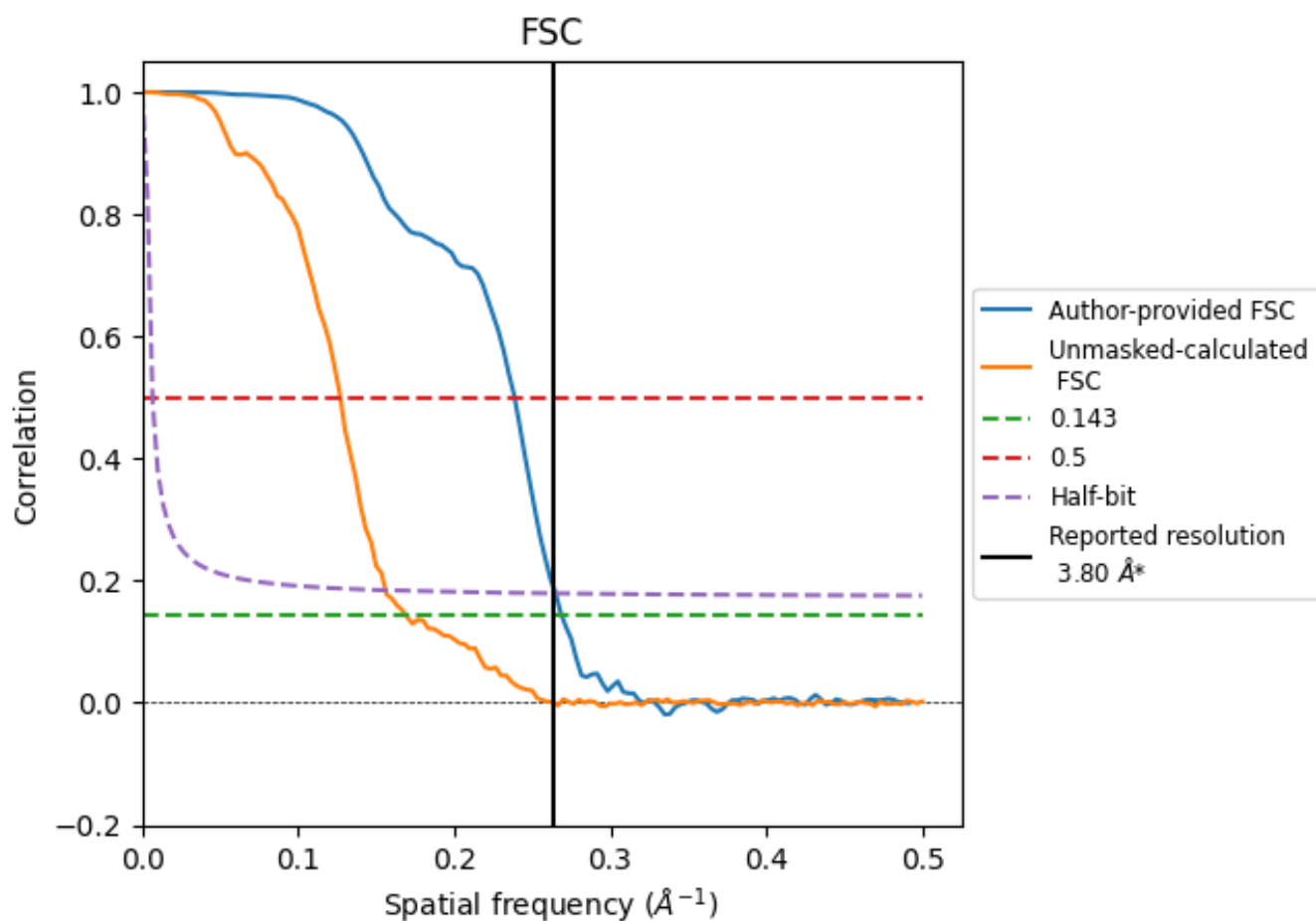


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

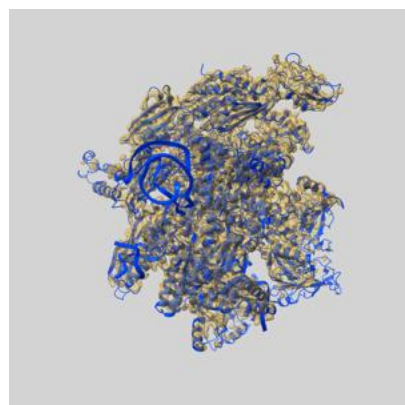
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.72	4.19	3.77
Unmasked-calculated*	5.91	7.87	6.41

*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 5.91 differs from the reported value 3.8 by more than 10 %

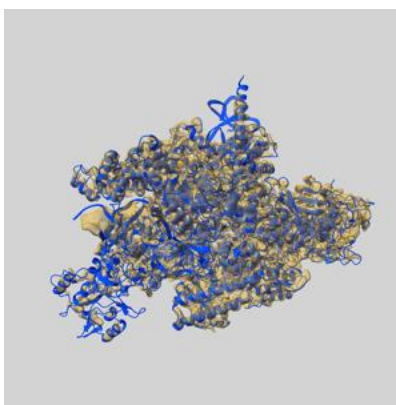
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29732 and PDB model 8G4W. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

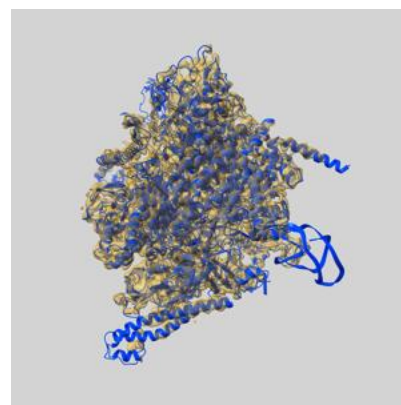
9.1 Map-model overlay [i](#)



X



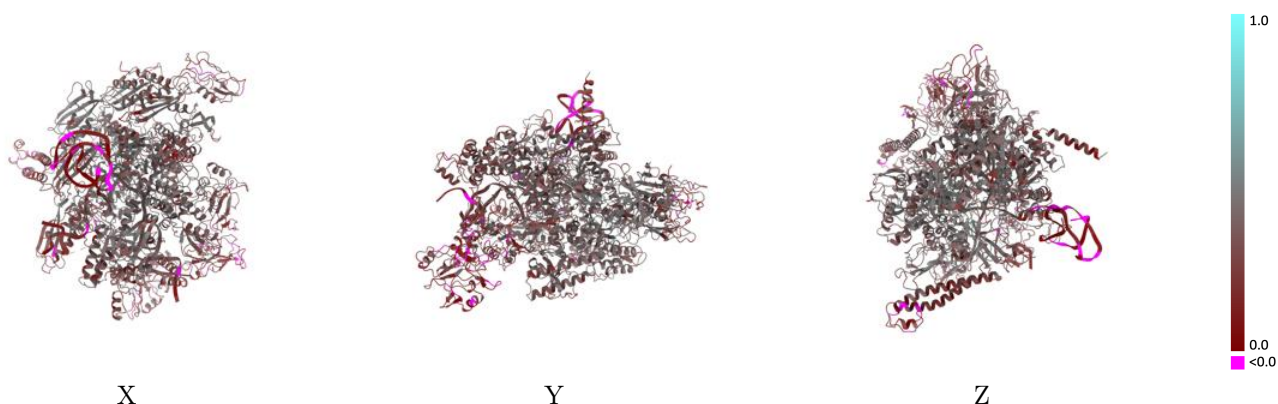
Y



Z

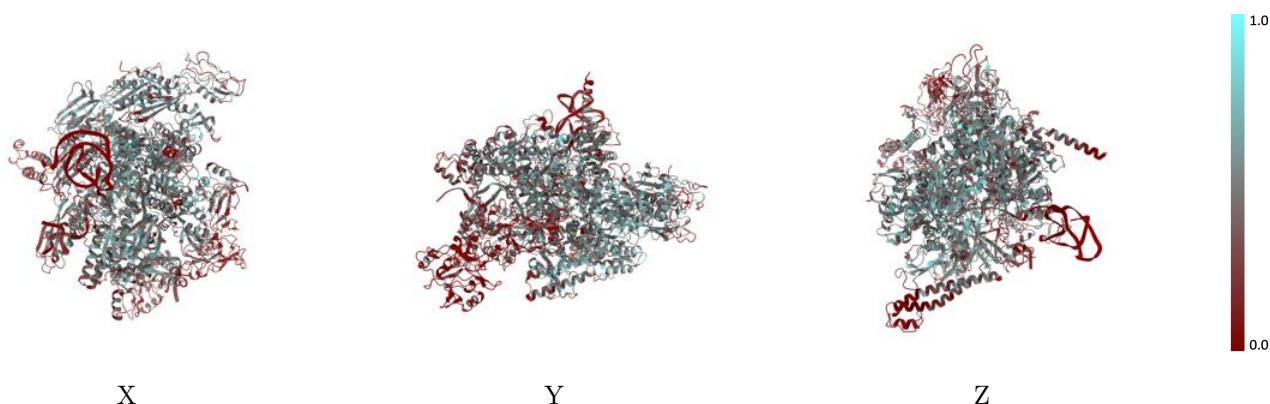
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



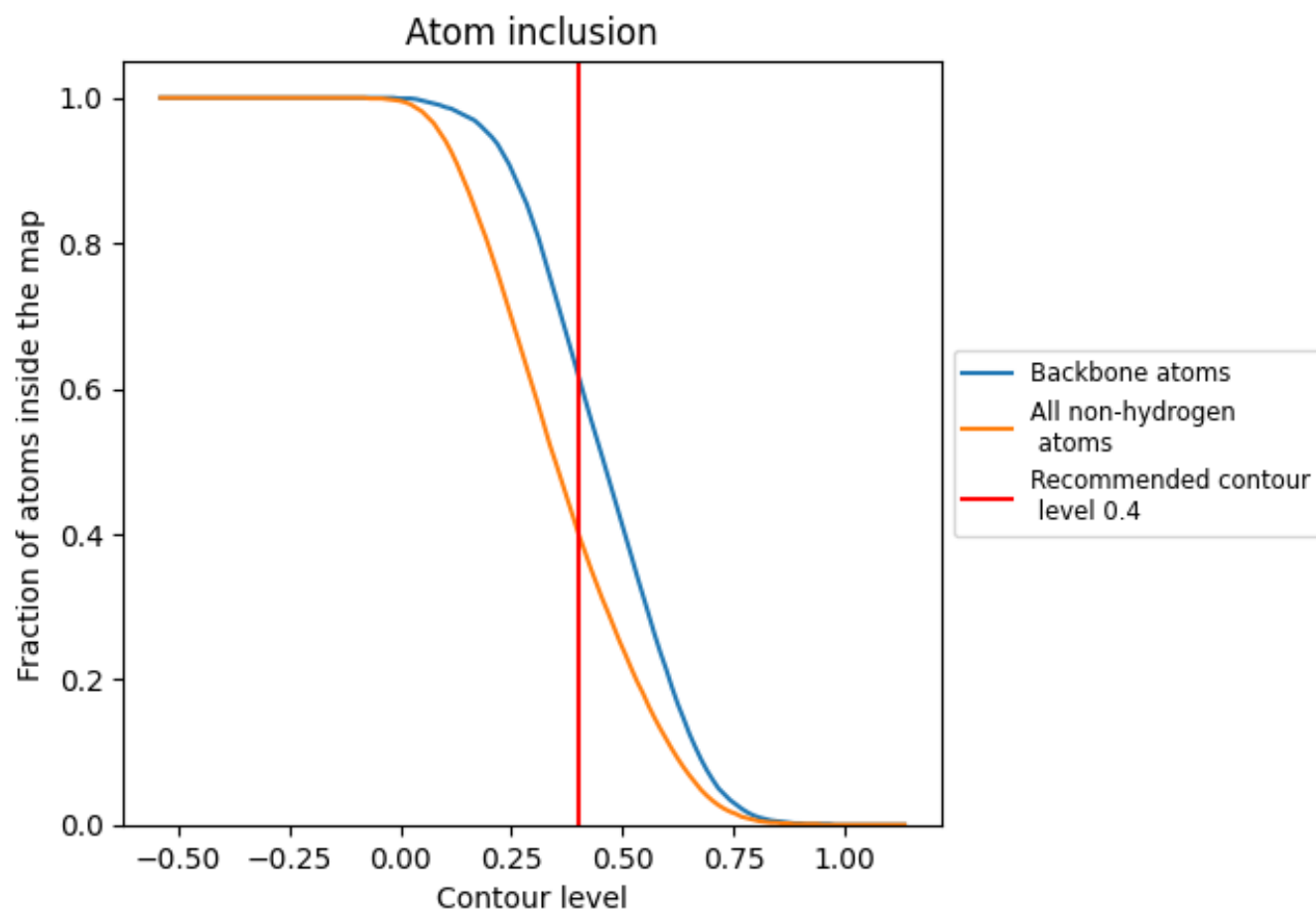
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 40% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4020	0.3380
A	0.4200	0.2700
B	0.4470	0.2870
G	0.5080	0.4040
H	0.3990	0.3080
I	0.4160	0.3580
J	0.3970	0.3410
K	0.3630	0.3290
R	0.1210	0.1030

1.0

0.0

<0.0