



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 10:01 AM UTC

PDB ID : 6C9Y / pdb_00006c9y
EMDB ID : EMD-7438
Title : Cryo-EM structure of E. coli RNAP sigma70 holoenzyme
Authors : Narayanan, A.; Vago, F.; Li, K.; Qayyum, M.Z.; Yenool, D.; Jiang, W.; Murakami, K.S.
Deposited on : 2018-01-29
Resolution : 4.25 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

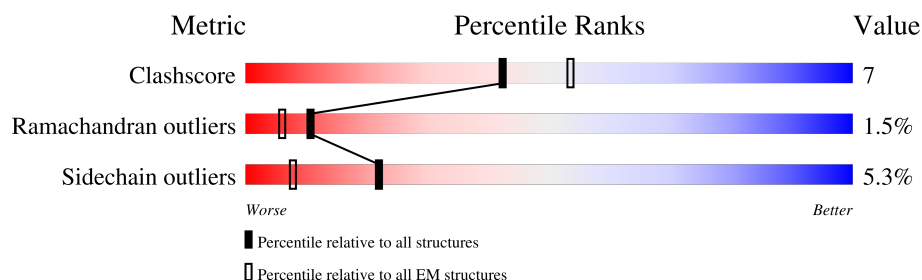
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	329	37% 52% 17% 30%
1	B	329	34% 52% 13% 33%
2	C	1342	65% 80% 18%
3	D	1407	63% 72% 22%
4	E	91	75% 74% 8% 16%
5	F	613	70% 61% 15% 24%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28920 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
			1787	1112	317	352	6		
1	B	221	Total	C	N	O	S	0	0
			1708	1067	302	333	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	1350	Total	C	N	O	S	0	0
			10434	6553	1856	1976	49		

- 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
			605	368	115	121	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	468	Total	C	N	O	S	0	0
			3813	2389	678	723	23		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
6	D	1	Total 1	Mg 1	0

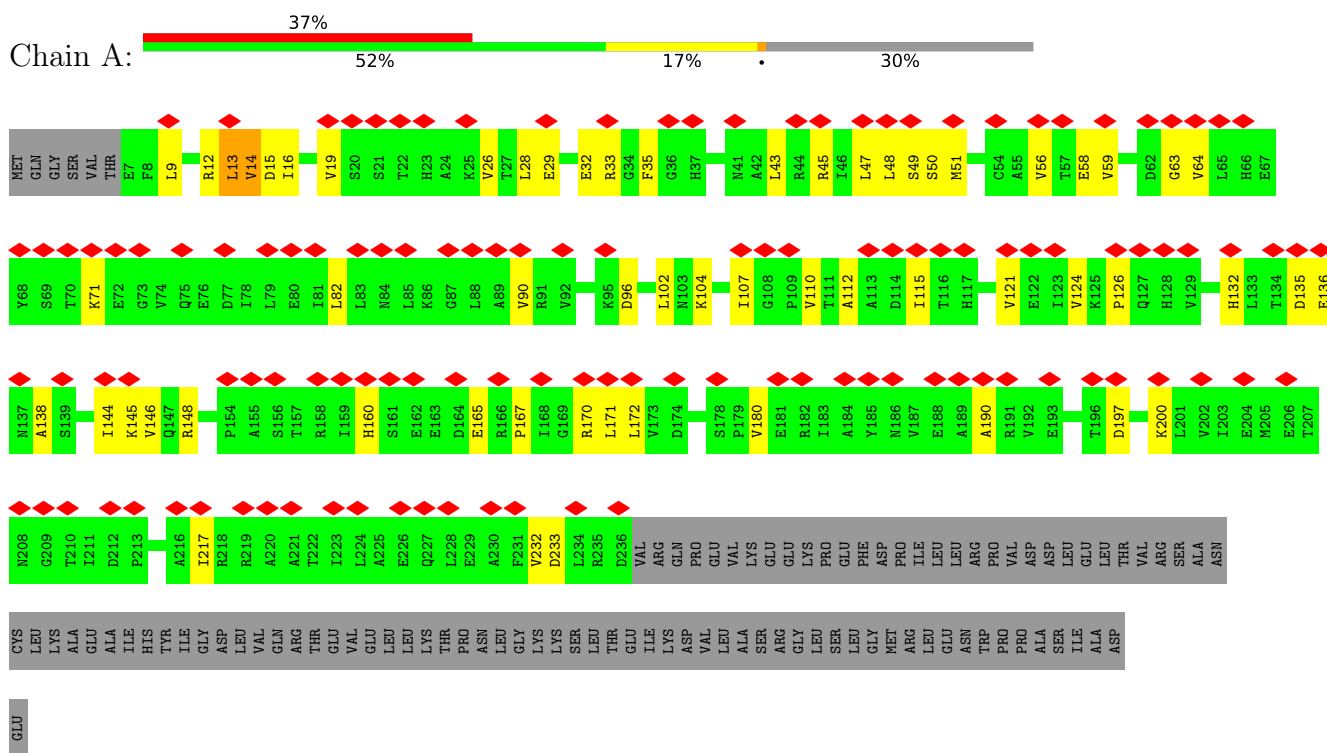
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total 2	Zn 2	0

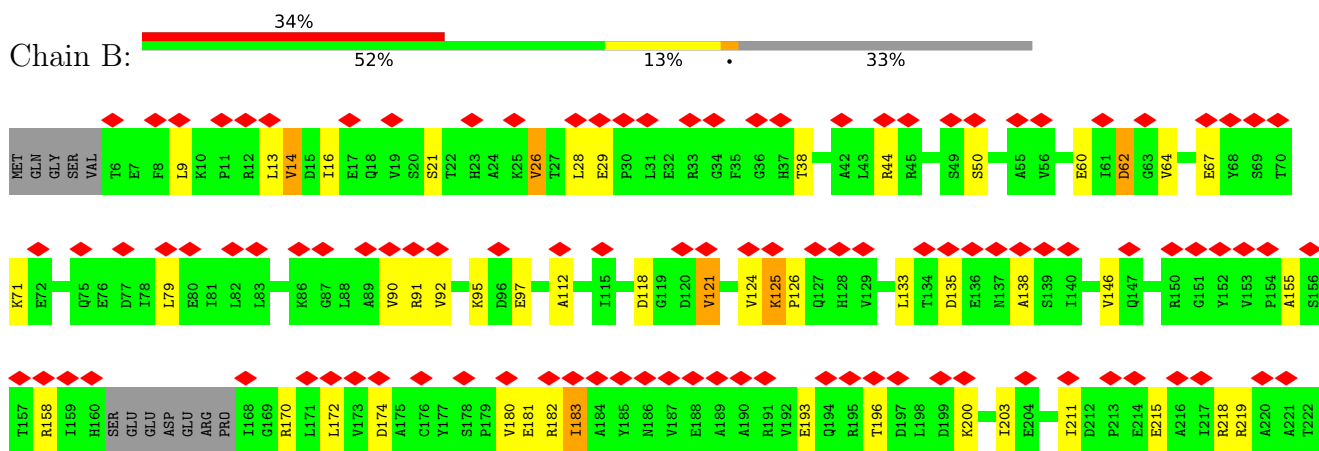
3 Residue-property plots

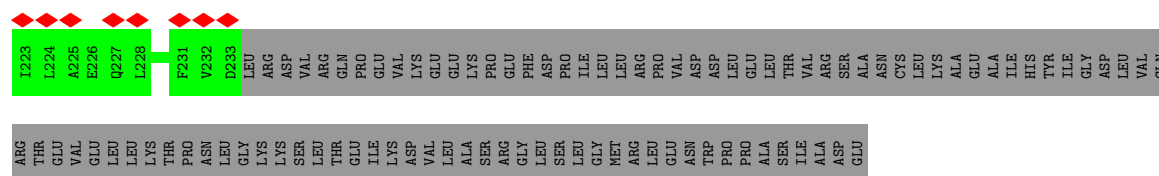
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

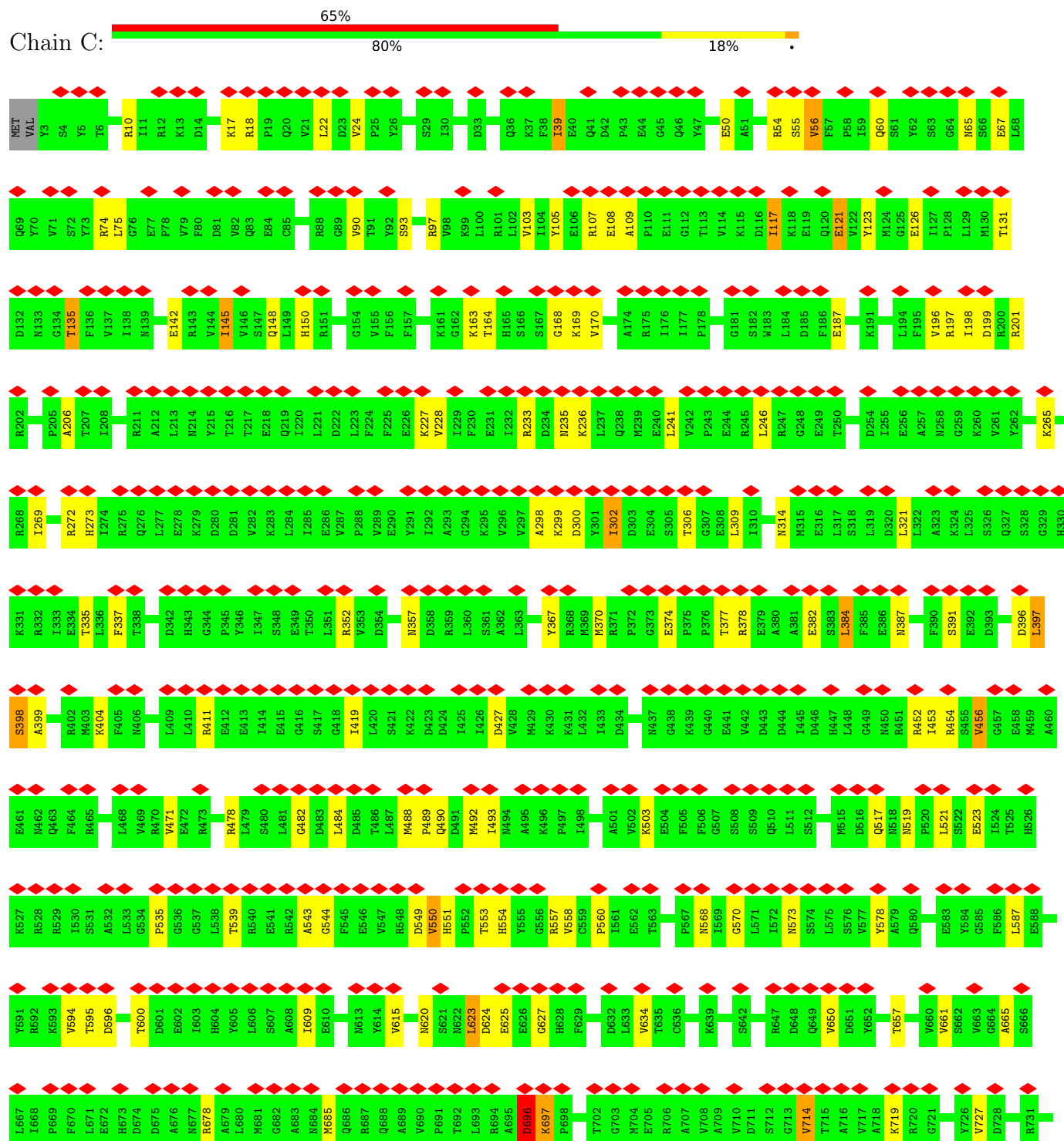


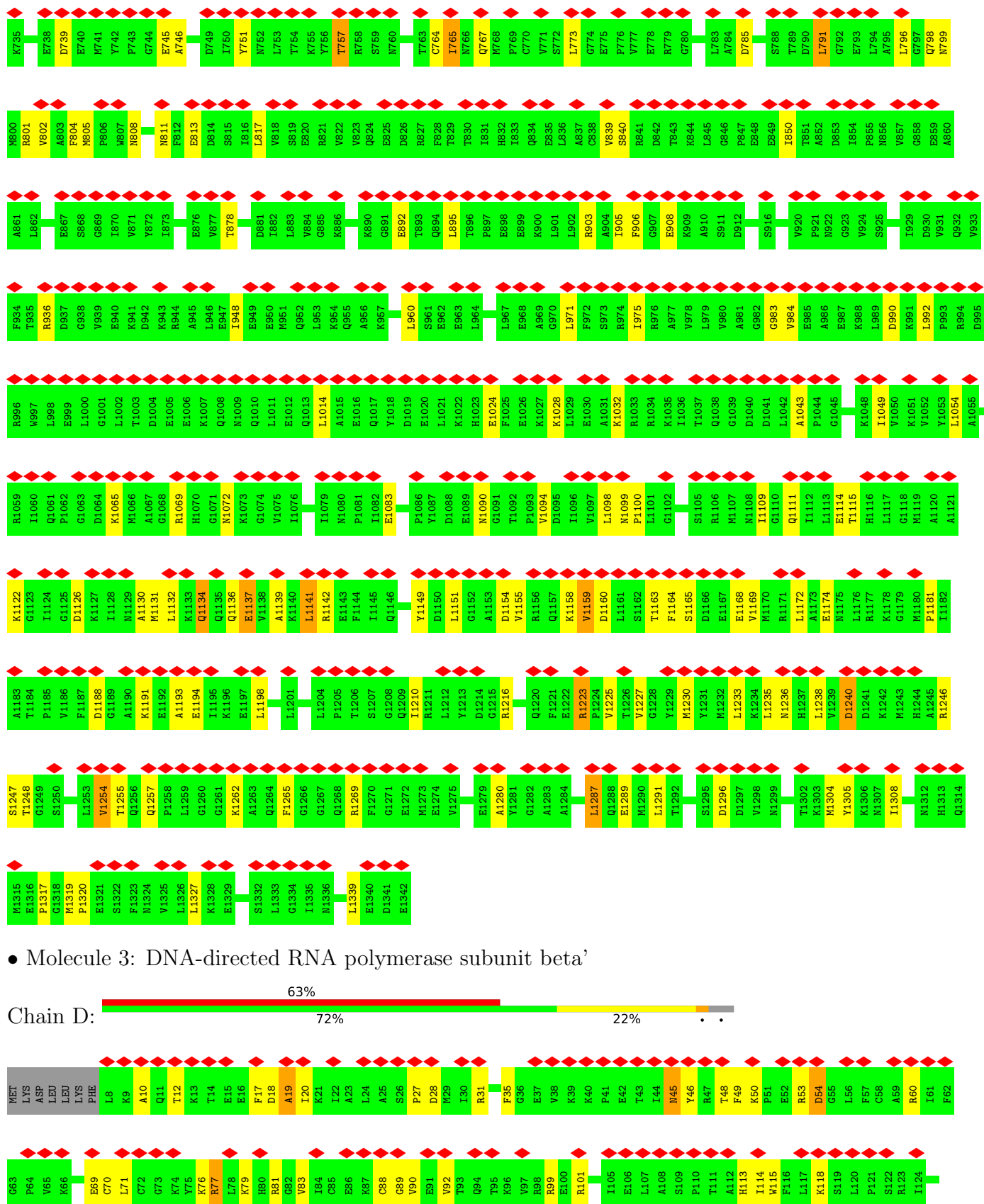
• Molecule 1: DNA-directed RNA polymerase subunit alpha



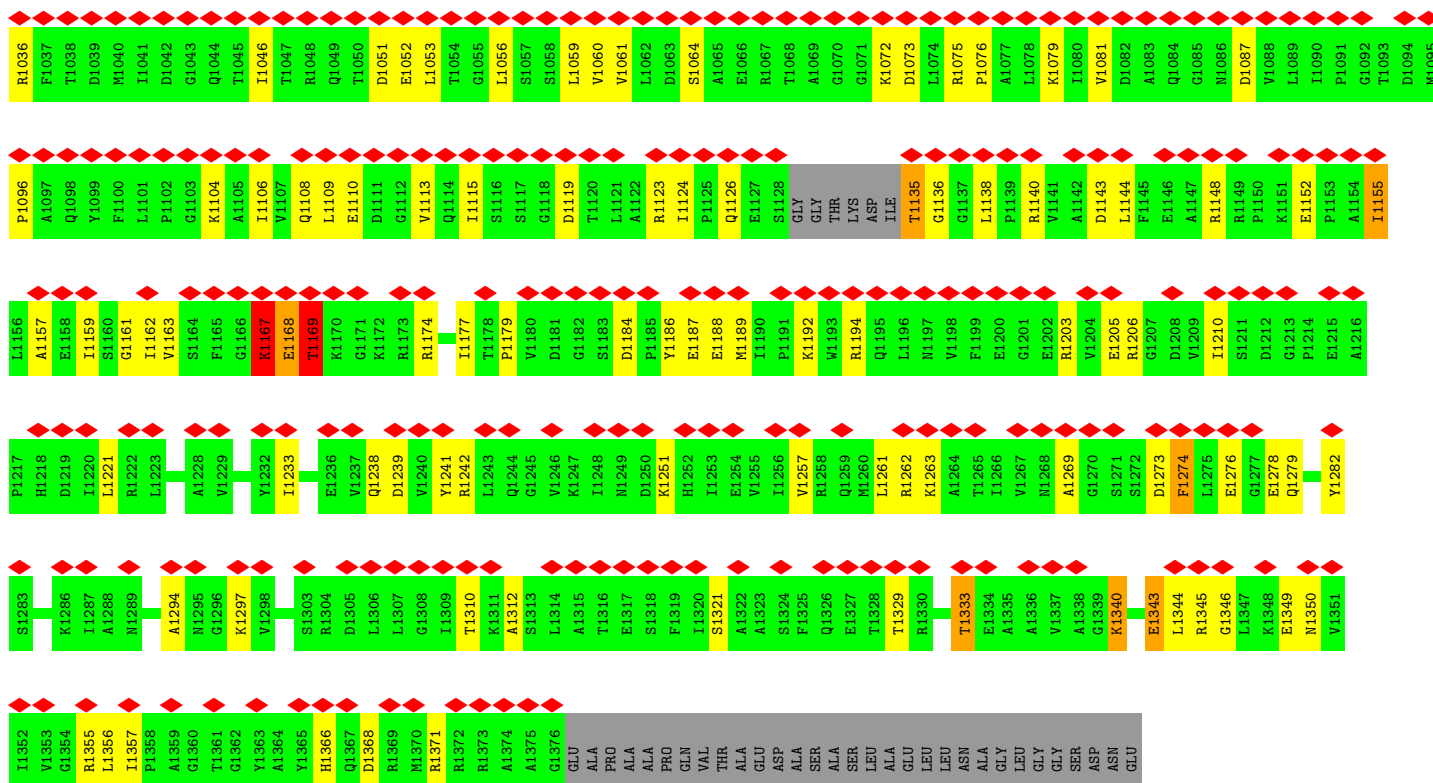


• Molecule 2: DNA-directed RNA polymerase subunit beta

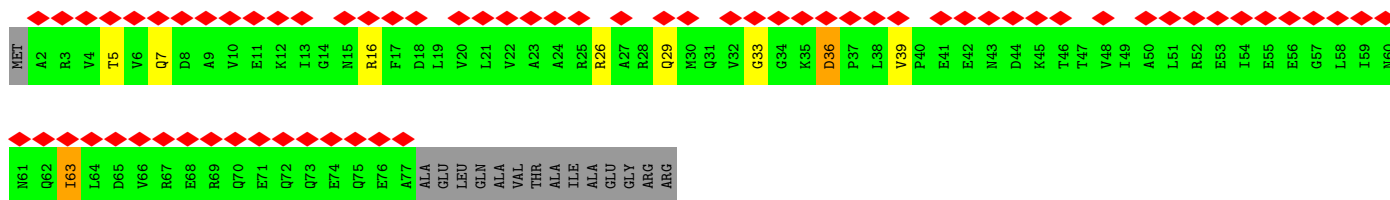
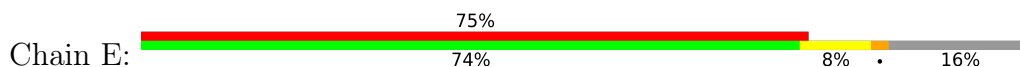




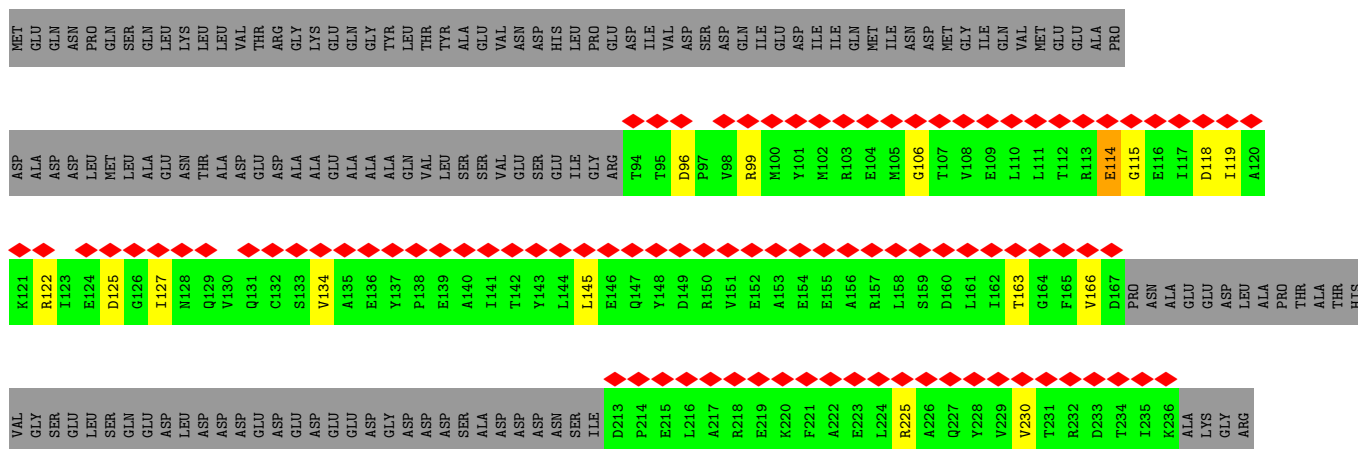
V974	A914	L849	L783	P647	H581	G512	L449	L385	G319	L189	L128
V975	I915	K850	A784	H651	I582	H513	H450	E386	S319	K190	D129
V976	G916	P851	D785	E652	V583	T614	P451	L387	N320	S191	M130
S977	G917	G852	T786	E653	P584	R515	L452	R388	K321	M192	P131
S978	I918	T853	A787	T654	G586	D516	L453	G389	R322	D193	L132
S979	A919	L854	L788	W723	L587	G517	C454	L390	R323	R259	R133
T980	A920	V855	K789	W724	P588	V518	A455	A391	L324	E195	D134
E981	Q921	P859	T790	W725	Y589	N519	A456	T392	K325	A261	I135
E982	S922	R860	A791	A657	Y590	A520	Y457	T393	K326	E196	E136
K983	I923	E861	A792	E659	S590	K521	N458	I394	T262	C198	R137
L984	G924	L863	W793	E660	V592	L527	D460	K398	D329	E199	V138
E985	E925	L864	G794	W661	N593	T528	F461	K399	M330	Q200	L139
F986	F926	H865	A795	A662	Q594	G529	D462	M400	I331	E200	Y140
G989	Q927	E866	L796	E663	A595	P530	D463	M401	K332	R202	F141
R990	T928	Q867	T797	E664	L596	K531	G463	E401	G333	E203	E142
T991	W868	R869	R798	Q665	G597	E532	D464	A402	K334	E204	S143
Q929	C869	E866	R799	Q666	K598	A533	Q465	R403	Q335	R270	Y144
K992	D870	L800	W801	Q667	K599	E534	A466	E404	G336	V146	V145
E993	L871	L872	D802	F668	A600	R535	V468	E404	R337	T208	I147
S994	L873	E873	W803	Q669	I601	L536	H469	V408	F338	N209	I147
Y995	F927	E874	R804	S670	S602	Y537	V470	W409	N341	S210	E148
K996	L796	E875	Q805	S671	K604	R538	P471	D410	L342	E211	G149
T997	T797	E876	D806	L672	L605	S539	L472	I411	L343	T212	G150
P998	W877	R878	T810	W673	L606	G540	T473	L412	R280	K213	M151
Y999	L746	A879	D813	T674	A542	L541	L474	D413	G344	R214	T152
G1000	W747	E880	E814	T675	S543	H545	E475	V415	K345	K215	M153
A1001	A748	G676	W815	G676	L544	H546	A476	I416	R346	K216	L154
V1002	K749	E877	E816	E877	H547	A548	Q477	R417	V347	L217	E155
L1003	P750	R678	E817	W679	K548	R548	L478	E418	D248	T218	R156
A1004	D751	W680	E818	H680	L614	S549	E479	R419	L285	K219	K218
K1005	G752	W681	E819	W681	K615	E554	M484	S350	A286	R220	Q157
G1006	S753	T685	E820	W682	P616	Y555	R425	G351	A287	R221	Q158
D1007	T754	W686	E821	W683	T617	E556	A426	R352	P288	K222	I159
S948	W755	A689	E822	W684	W618	E557	S486	S353	D289	L223	L160
Q1008	E756	W690	E823	W685	L619	D558	L483	V354	I290	L224	E162
E1009	T757	W691	E824	W686	F620	E561	M485	I355	I291	E225	E163
I950	W758	W692	E825	W687	A621	E562	S486	T356	V292	A226	Q164
Q951	T759	W693	E826	W688	D622	E567	N489	V357	R293	F227	Y165
V952	W760	W694	E827	W689	Q623	D568	L422	L361	N294	V228	L166
K953	T761	W695	E828	W690	E624	E569	L423	R362	R297	Q229	D167
G893	W762	W696	E829	W691	H625	N560	H430	L363	M298	S230	L169
V894	F763	W697	E830	W692	W626	G561	R431	G366	E301	M237	E171
C895	W764	W698	E831	W693	T627	E562	L432	G367	A302	I238	F172
A896	E765	W699	E832	W694	G628	E563	H431	L363	G304	L239	G173
H897	W766	W699	E833	W695	F629	E564	L433	G367	A305	T240	D174
C898	W767	W699	E834	W696	E632	E565	H432	G367	L306	V241	E175
G900	W768	W699	E835	W697	A633	E566	L433	G367	L307	L242	F176
P901	W769	W699	E836	W698	E634	E567	H433	G367	D308	P243	D177
L903	W770	W699	E837	W699	E635	E568	L434	G367	N309	V244	A178
A904	W771	W699	E838	W699	E636	E569	H434	G367	L245	L245	K179
G906	W772	W699	E839	W699	E637	E570	L435	G367	R311	P246	M180
R907	W773	W699	E840	W699	E638	E571	H435	G367	G312	D247	E183
I908	W774	W699	E841	W699	E639	E572	L436	G367	R313	L249	A184
N909	W775	W699	E842	W699	E640	E573	H436	G367	A315	R251	Q186
S970	W776	W699	E843	W699	E641	E574	L437	G367	I316	L252	
Q971	W777	W699	E844	W699	E642	E575	H437	G367	T317		
K972	W778	W699	E845	W699	E643	E576	L438	G367			
L973	W779	W699	E846	W699	E644	E577	H438	G367			
F1034	W780	W699	E847	W699	E645	E578	L439	G367			
V1035	W781	W699	E848	W699	E646	E579	H439	G367			



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96067	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.032	Depositor
Map size ($\text{\AA}$)	315.84, 315.84, 315.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.316, 1.316, 1.316	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, ZN

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	0.40	0/1809	1.15	11/2451 (0.4%)
1	B	0.36	0/1728	1.00	3/2341 (0.1%)
2	C	0.37	0/10739	0.92	23/14489 (0.2%)
3	D	0.36	0/10591	0.95	17/14307 (0.1%)
4	E	0.34	0/607	0.91	0/817
5	F	0.34	0/3864	1.02	9/5194 (0.2%)
All	All	0.36	0/29338	0.96	63/39599 (0.2%)

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
2	C	0	4
3	D	0	2
5	F	0	3
All	All	0	9

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LEU	CA-C-N	8.92	130.84	119.78
1	A	28	LEU	C-N-CA	8.92	130.84	119.78
3	D	1343	GLU	CA-C-N	8.79	138.34	121.54
3	D	1343	GLU	C-N-CA	8.79	138.34	121.54
1	A	160	HIS	N-CA-C	-7.70	105.85	114.62
2	C	1160	ASP	CA-C-N	7.16	134.58	121.70
2	C	1160	ASP	C-N-CA	7.16	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	168	GLY	N-CA-C	-7.12	96.31	113.18
2	C	233	ARG	CA-C-N	6.78	134.49	121.54
2	C	233	ARG	C-N-CA	6.78	134.49	121.54
1	B	91	ARG	CG-CD-NE	-6.58	97.52	112.00
2	C	397	LEU	CA-C-N	6.53	134.01	121.54
2	C	397	LEU	C-N-CA	6.53	134.01	121.54
5	F	601	PRO	CA-C-N	6.47	133.91	121.54
5	F	601	PRO	C-N-CA	6.47	133.91	121.54
1	A	132	HIS	CA-C-N	-6.32	114.08	122.99
1	A	132	HIS	C-N-CA	-6.32	114.08	122.99
1	A	29	GLU	N-CA-C	6.32	120.81	112.35
2	C	398	SER	N-CA-C	-6.27	97.45	110.80
1	A	50	SER	CA-C-N	-6.23	114.21	122.56
1	A	50	SER	C-N-CA	-6.23	114.21	122.56
3	D	45	ASN	CA-C-N	6.19	133.36	121.54
3	D	45	ASN	C-N-CA	6.19	133.36	121.54
2	C	624	ASP	CA-C-N	6.05	133.11	121.54
2	C	624	ASP	C-N-CA	6.05	133.11	121.54
2	C	399	ALA	N-CA-C	-6.03	104.07	112.45
2	C	396	ASP	CA-C-N	-6.00	111.11	121.66
2	C	396	ASP	C-N-CA	-6.00	111.11	121.66
1	B	135	ASP	CA-C-N	5.91	132.82	121.54
1	B	135	ASP	C-N-CA	5.91	132.82	121.54
3	D	1168	GLU	CA-C-N	5.86	132.74	121.54
3	D	1168	GLU	C-N-CA	5.86	132.74	121.54
1	A	19	VAL	N-CA-C	-5.83	107.07	113.43
3	D	77	ARG	CA-CB-CG	5.72	125.55	114.10
5	F	166	VAL	CA-C-N	5.69	131.95	121.70
5	F	166	VAL	C-N-CA	5.69	131.95	121.70
2	C	595	THR	N-CA-C	-5.60	100.16	109.46
2	C	1158	LYS	CA-CB-CG	5.44	124.97	114.10
3	D	859	PRO	CA-C-N	5.42	131.90	121.54
3	D	859	PRO	C-N-CA	5.42	131.90	121.54
5	F	585	GLU	CA-C-N	5.40	127.83	120.54
5	F	585	GLU	C-N-CA	5.40	127.83	120.54
3	D	46	TYR	CA-CB-CG	5.40	123.61	113.90
3	D	826	ILE	N-CA-C	5.30	120.37	109.34
3	D	515	ARG	N-CA-C	-5.26	101.30	109.24
1	A	14	VAL	CA-C-N	5.22	131.51	121.54
1	A	14	VAL	C-N-CA	5.22	131.51	121.54
2	C	1136	GLN	CA-C-N	5.21	131.49	121.54
2	C	1136	GLN	C-N-CA	5.21	131.49	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	565	ILE	CA-C-N	5.18	131.44	121.54
5	F	565	ILE	C-N-CA	5.18	131.44	121.54
2	C	696	ASP	CA-C-N	5.16	134.39	121.80
2	C	696	ASP	C-N-CA	5.16	134.39	121.80
3	D	425	ARG	CA-C-N	5.15	134.38	121.80
3	D	425	ARG	C-N-CA	5.15	134.38	121.80
5	F	490	PRO	N-CA-C	5.09	122.96	112.47
3	D	230	SER	N-CA-C	5.09	121.64	110.80
2	C	1262	LYS	CA-C-N	5.06	131.21	121.54
2	C	1262	LYS	C-N-CA	5.06	131.21	121.54
3	D	1167	LYS	CA-C-N	5.04	128.36	120.75
3	D	1167	LYS	C-N-CA	5.04	128.36	120.75
2	C	745	GLU	CA-C-N	5.03	131.15	121.54
2	C	745	GLU	C-N-CA	5.03	131.15	121.54

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	397	LEU	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
5	F	569	THR	Peptide
5	F	582	VAL	Peptide
5	F	600	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1787	0	1810	33	0
1	B	1708	0	1741	28	0
2	C	10570	0	10582	125	0
3	D	10434	0	10599	181	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	605	0	612	6	0
5	F	3813	0	3880	52	0
6	D	1	0	0	0	0
7	D	2	0	0	0	0
All	All	28920	0	29224	392	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 7.

All (392) 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:D:1140:ARG:HH12	3:D:1144:LEU:HG	1.32	0.94
1:A:233:ASP:HA	1:B:218:ARG:HH12	1.40	0.87
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.06	0.87
2:C:299:LYS:NZ	2:C:300:ASP:O	2.11	0.81
1:A:33:ARG:NH2	1:A:197:ASP:OD2	2.13	0.79
3:D:518:VAL:HA	3:D:547:ARG:HH12	1.45	0.79
3:D:1263:LYS:NZ	3:D:1279:GLN:OE1	2.16	0.79
1:A:232:VAL:O	1:B:218:ARG:NH1	2.16	0.77
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.15	0.76
2:C:17:LYS:NZ	2:C:1194:GLU:OE2	2.15	0.76
2:C:50:GLU:OE2	2:C:54:ARG:NE	2.20	0.74
2:C:1223:ARG:HH12	3:D:724:MET:HE1	1.53	0.73
3:D:1278:GLU:OE2	3:D:1279:GLN:NE2	2.21	0.73
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.22	0.72
3:D:77:ARG:HG3	3:D:79:LYS:HG2	1.72	0.71
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.25	0.70
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.74	0.69
5:F:493:LYS:NZ	5:F:496:LYS:NZ	2.41	0.69
5:F:493:LYS:HZ2	5:F:496:LYS:NZ	1.91	0.69
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.26	0.68
1:B:211:ILE:HG12	1:B:219:ARG:HH22	1.59	0.68
1:A:49:SER:HB3	2:C:1083:GLU:OE2	1.95	0.67
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.77	0.66
5:F:490:PRO:HB2	5:F:493:LYS:HG3	1.76	0.66
2:C:378:ARG:NE	2:C:382:GLU:OE2	2.27	0.65
2:C:719:LYS:HZ3	2:C:751:TYR:HE1	1.44	0.65
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.78	0.65
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.77	0.65
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:479:THR:HG22	5:F:482:GLU:HG3	1.80	0.64
5:F:587:ILE:HD12	5:F:590:ILE:HD12	1.79	0.64
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.80	0.64
2:C:551:HIS:H	2:C:554:HIS:HD2	1.45	0.64
1:A:63:GLY:O	1:A:71:LYS:NZ	2.29	0.63
1:B:180:VAL:O	3:D:535:ARG:NH2	2.30	0.63
3:D:214:ARG:HA	3:D:217:LEU:HB3	1.80	0.63
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.79	0.62
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.31	0.62
3:D:31:ARG:HE	3:D:241:VAL:HG21	1.64	0.62
2:C:517:GLN:HG3	2:C:523:GLU:OE2	1.99	0.62
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.81	0.62
3:D:1073:ASP:HA	3:D:1168:GLU:HG2	1.80	0.62
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.81	0.62
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.82	0.61
2:C:272:ARG:HD3	2:C:273:HIS:HD2	1.65	0.61
2:C:1072:ASN:ND2	2:C:1111:GLN:OE1	2.34	0.61
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.33	0.61
5:F:493:LYS:NZ	5:F:496:LYS:HZ1	1.98	0.61
3:D:518:VAL:HA	3:D:547:ARG:NH1	2.15	0.61
3:D:741:ALA:O	3:D:762:ASN:ND2	2.32	0.61
2:C:374:GLU:OE1	5:F:99:ARG:NH1	2.34	0.60
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.81	0.60
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.83	0.60
4:E:36:ASP:N	4:E:36:ASP:OD1	2.32	0.60
2:C:187:GLU:OE2	2:C:197:ARG:NH2	2.34	0.60
3:D:1140:ARG:NH1	3:D:1144:LEU:HG	2.12	0.60
2:C:1223:ARG:NH1	3:D:724:MET:HE1	2.16	0.60
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.83	0.59
3:D:709:ARG:NH1	3:D:710:ASP:HB3	2.16	0.59
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.35	0.59
2:C:960:LEU:HD21	2:C:1032:LYS:NZ	2.18	0.59
3:D:708:ASN:OD1	3:D:708:ASN:N	2.35	0.59
3:D:532:GLU:HB2	3:D:535:ARG:NH1	2.18	0.59
3:D:1238:GLN:HG3	3:D:1242:ARG:HE	1.66	0.59
3:D:832:LYS:NZ	3:D:1242:ARG:NH1	2.51	0.59
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.84	0.59
3:D:128:LEU:HA	3:D:192:MET:HE1	1.84	0.59
3:D:1140:ARG:NH1	3:D:1140:ARG:O	2.36	0.59
3:D:832:LYS:HZ2	3:D:832:LYS:HB3	1.67	0.59
2:C:93:SER:OG	2:C:126:GLU:OE1	2.13	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:479:THR:HG23	5:F:481:GLU:H	1.68	0.58
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.37	0.58
3:D:45:ASN:ND2	3:D:48:THR:OG1	2.36	0.58
1:A:64:VAL:HG13	1:A:71:LYS:HE2	1.85	0.58
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.11	0.58
3:D:17:PHE:O	3:D:1355:ARG:NH2	2.36	0.58
3:D:435:GLN:HE21	3:D:486:SER:HA	1.69	0.58
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.68	0.58
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.37	0.57
5:F:115:GLY:HA2	5:F:118:ASP:HB2	1.86	0.57
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.85	0.57
5:F:371:LYS:HA	5:F:374:ARG:NH1	2.18	0.57
3:D:905:ARG:HH21	3:D:907:HIS:HB2	1.69	0.57
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.85	0.57
2:C:719:LYS:NZ	2:C:751:TYR:HE1	2.01	0.57
2:C:714:VAL:O	2:C:767:GLN:NE2	2.37	0.57
3:D:957:SER:HB3	3:D:985:ILE:HB	1.87	0.57
5:F:508:GLU:OE1	5:F:518:HIS:ND1	2.38	0.57
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.87	0.56
3:D:646:ILE:HD11	3:D:764:ARG:HD3	1.86	0.56
2:C:387:ASN:HA	2:C:391:SER:HB2	1.88	0.56
3:D:54:ASP:N	3:D:54:ASP:OD1	2.39	0.56
3:D:473:THR:HG23	3:D:476:ALA:H	1.70	0.56
3:D:538:ARG:NH1	3:D:634:ARG:NH1	2.54	0.56
2:C:551:HIS:H	2:C:554:HIS:CD2	2.23	0.56
3:D:437:PHE:HZ	3:D:453:VAL:HG11	1.71	0.56
1:A:233:ASP:HA	1:B:218:ARG:NH1	2.16	0.56
5:F:312:SER:OG	5:F:313:ASP:N	2.39	0.56
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.88	0.55
2:C:18:ARG:HE	2:C:620:ASN:HA	1.72	0.55
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.55
3:D:60:ARG:HA	3:D:90:VAL:HG22	1.90	0.55
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.71	0.55
3:D:615:LYS:NZ	4:E:7:GLN:HB3	2.23	0.54
2:C:227:LYS:NZ	2:C:298:ALA:HB1	2.21	0.54
2:C:1304:MET:HE3	2:C:1308:ILE:HD11	1.88	0.54
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.89	0.54
3:D:1321:SER:HB2	3:D:1349:GLU:OE2	2.08	0.54
3:D:832:LYS:HZ1	3:D:1242:ARG:NH1	2.06	0.54
5:F:274:ARG:NH2	5:F:369:GLU:OE1	2.40	0.54
1:A:104:LYS:HD3	1:A:110:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:LYS:NZ	1:B:97:GLU:O	2.40	0.54
3:D:1061:VAL:O	3:D:1104:LYS:N	2.40	0.54
5:F:285:ARG:HD2	5:F:288:MET:HE2	1.89	0.54
2:C:1142:ARG:HG2	2:C:1169:VAL:HG11	1.90	0.53
3:D:1262:ARG:NH2	3:D:1312:ALA:O	2.42	0.53
3:D:388:ARG:NH2	3:D:414:GLU:OE1	2.42	0.53
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.91	0.53
2:C:1289:GLU:OE2	3:D:472:LEU:HB2	2.08	0.53
2:C:1269:ARG:HG3	3:D:346:ARG:NH1	2.24	0.53
3:D:1087:ASP:HB3	3:D:1096:PRO:HB3	1.91	0.53
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.91	0.53
3:D:1060:VAL:HG22	3:D:1106:ILE:HG12	1.90	0.53
3:D:970:SER:HB2	3:D:972:LYS:HZ3	1.73	0.53
3:D:1036:ARG:HD2	3:D:1079:LYS:HD3	1.90	0.53
5:F:612:ASP:OD1	5:F:612:ASP:N	2.39	0.53
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.24	0.52
3:D:1143:ASP:HA	3:D:1148:ARG:NH1	2.23	0.52
2:C:903:ARG:NH2	5:F:612:ASP:OD1	2.43	0.52
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.41	0.52
2:C:489:PRO:HA	2:C:492:MET:HE3	1.92	0.52
3:D:694:SER:OG	3:D:738:ARG:NE	2.43	0.52
3:D:722:ILE:HA	3:D:725:MET:HE3	1.90	0.52
3:D:1046:ILE:HD12	3:D:1059:LEU:HD22	1.92	0.52
5:F:262:VAL:HG11	5:F:264:LYS:HZ2	1.74	0.52
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.91	0.52
3:D:930:LEU:HD11	3:D:1241:TYR:HE1	1.75	0.52
5:F:376:LYS:NZ	5:F:417:ASP:HA	2.24	0.52
2:C:367:TYR:HD1	2:C:384:LEU:HD22	1.75	0.52
1:B:182:ARG:NH1	3:D:534:GLU:OE1	2.43	0.51
3:D:1340:LYS:HB2	3:D:1340:LYS:NZ	2.25	0.51
1:B:62:ASP:OD1	1:B:62:ASP:N	2.34	0.51
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.75	0.51
3:D:370:LYS:HA	3:D:441:LEU:HD12	1.91	0.51
3:D:576:ARG:NH1	3:D:593:ASN:O	2.43	0.51
3:D:709:ARG:O	3:D:711:GLY:N	2.43	0.51
3:D:1109:LEU:HD22	3:D:1113:VAL:HG11	1.93	0.51
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.43	0.51
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.76	0.51
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.92	0.51
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.51
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1100:PRO:HB3	3:D:639:VAL:HG12	1.92	0.51
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.76	0.51
2:C:148:GLN:NE2	2:C:535:PRO:O	2.38	0.50
3:D:69:GLU:HG3	3:D:76:LYS:HG2	1.93	0.50
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.92	0.50
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.93	0.50
2:C:905:ILE:HG23	5:F:595:LEU:HD13	1.93	0.50
5:F:274:ARG:NH1	5:F:365:MET:HE3	2.26	0.50
1:B:215:GLU:CD	1:B:219:ARG:HH12	2.19	0.50
2:C:227:LYS:HZ3	2:C:298:ALA:HB1	1.76	0.50
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.93	0.50
3:D:843:VAL:HG13	3:D:883:ARG:HD3	1.94	0.50
1:B:125:LYS:NZ	1:B:125:LYS:HB3	2.26	0.50
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.19	0.50
3:D:1002:VAL:N	3:D:1019:ASN:O	2.42	0.50
1:A:58:GLU:HG2	1:A:145:LYS:HE3	1.94	0.49
3:D:1051:ASP:HB2	3:D:1056:LEU:HB2	1.93	0.49
3:D:1034:PHE:N	3:D:1081:VAL:O	2.44	0.49
1:A:59:VAL:HG13	1:A:144:ILE:HG12	1.94	0.49
2:C:1240:ASP:N	2:C:1240:ASP:OD1	2.45	0.49
1:A:167:PRO:HB2	1:A:170:ARG:HG2	1.95	0.49
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.94	0.49
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.94	0.49
3:D:48:THR:O	3:D:50:LYS:N	2.43	0.49
2:C:1269:ARG:HB3	3:D:343:LEU:HD22	1.95	0.49
5:F:554:ARG:HH21	5:F:587:ILE:HD13	1.76	0.49
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.94	0.49
3:D:1329:THR:O	3:D:1333:THR:OG1	2.27	0.48
2:C:272:ARG:HD3	2:C:273:HIS:CD2	2.47	0.48
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.95	0.48
3:D:1059:LEU:HG	3:D:1110:GLU:OE2	2.14	0.48
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.96	0.48
1:B:14:VAL:HB	1:B:28:LEU:HD13	1.95	0.48
3:D:1186:TYR:OH	3:D:1188:GLU:OE1	2.23	0.48
3:D:549:LYS:NZ	3:D:569:LEU:O	2.46	0.48
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.95	0.48
3:D:352:ARG:NH1	3:D:465:GLN:OE1	2.47	0.48
1:A:102:LEU:HD23	1:A:115:ILE:HG12	1.95	0.47
3:D:1159:ILE:HD12	3:D:1206:ARG:HD2	1.96	0.47
1:A:16:ILE:HG12	1:A:26:VAL:HG12	1.96	0.47
3:D:1064:SER:O	3:D:1072:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:122:ARG:HA	5:F:125:ASP:HB2	1.97	0.47
1:B:16:ILE:HB	1:B:26:VAL:HG13	1.96	0.47
2:C:201:ARG:HG3	2:C:201:ARG:HH11	1.79	0.47
2:C:201:ARG:HH12	2:C:370:MET:HA	1.78	0.47
1:B:133:LEU:HD23	1:B:138:ALA:HB1	1.97	0.47
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.96	0.47
3:D:322:ARG:NH1	3:D:322:ARG:HB2	2.29	0.47
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.97	0.47
5:F:145:LEU:O	5:F:225:ARG:NH2	2.47	0.47
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.96	0.47
2:C:314:ASN:O	2:C:352:ARG:NH1	2.43	0.47
5:F:493:LYS:HZ3	5:F:496:LYS:HZ1	1.63	0.47
3:D:35:PHE:CD2	3:D:101:ARG:HD3	2.50	0.46
2:C:107:ARG:HA	2:C:108:GLU:HA	1.56	0.46
3:D:495:ASN:O	3:D:497:GLU:N	2.48	0.46
2:C:785:ASP:OD2	2:C:791:LEU:N	2.48	0.46
2:C:906:PHE:HE2	5:F:607:LEU:HB3	1.81	0.46
1:B:158:ARG:NH1	1:B:172:LEU:HD13	2.30	0.46
3:D:1036:ARG:HH21	3:D:1081:VAL:HG21	1.80	0.46
2:C:145:ILE:HG21	2:C:456:VAL:HG13	1.98	0.46
5:F:493:LYS:NZ	5:F:496:LYS:HZ2	2.12	0.46
2:C:488:MET:O	2:C:490:GLN:N	2.46	0.46
3:D:370:LYS:HD3	3:D:443:GLU:OE2	2.16	0.46
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.51	0.46
3:D:819:GLY:N	3:D:881:LYS:HZ3	2.13	0.46
3:D:1203:ARG:NH1	3:D:1205:GLU:OE2	2.45	0.46
3:D:342:LEU:HA	3:D:343:LEU:HA	1.76	0.46
3:D:1356:LEU:HD23	3:D:1356:LEU:HA	1.76	0.46
4:E:26:ARG:NH1	4:E:29:GLN:OE1	2.48	0.46
5:F:262:VAL:HG11	5:F:264:LYS:NZ	2.31	0.45
1:B:60:GLU:HB3	1:B:170:ARG:HG2	1.99	0.45
1:B:155:ALA:N	1:B:174:ASP:OD1	2.50	0.45
2:C:1149:TYR:HB3	2:C:1159:VAL:HG21	1.99	0.45
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.98	0.45
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.77	0.45
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.87	0.45
3:D:962:ASN:O	3:D:980:THR:OG1	2.34	0.45
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.51	0.45
5:F:280:VAL:HG22	5:F:347:ILE:HG21	1.99	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.58	0.45
3:D:609:TYR:HE1	3:D:614:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:947:GLU:O	3:D:1020:TRP:NE1	2.49	0.45
3:D:977:SER:OG	3:D:980:THR:OG1	2.34	0.45
2:C:990:ASP:OD1	2:C:990:ASP:N	2.49	0.45
2:C:1132:LEU:HD11	2:C:1174:GLU:OE2	2.17	0.45
3:D:615:LYS:HZ2	4:E:7:GLN:HB3	1.82	0.45
1:A:43:LEU:HD13	1:A:217:ILE:HD11	1.99	0.45
1:A:45:ARG:HG2	1:B:38:THR:HB	1.98	0.45
2:C:568:ASN:OD1	2:C:568:ASN:N	2.50	0.45
3:D:953:LYS:HB2	3:D:993:GLU:OE2	2.16	0.45
1:B:215:GLU:OE2	1:B:219:ARG:NH1	2.50	0.45
2:C:549:ASP:OD1	2:C:550:VAL:N	2.49	0.45
3:D:638:SER:OG	3:D:639:VAL:N	2.47	0.45
5:F:558:VAL:HA	5:F:576:VAL:HG11	1.98	0.45
1:A:9:LEU:HB2	1:A:32:GLU:HG2	1.98	0.44
2:C:1024:GLU:HG2	2:C:1028:LYS:HD3	1.98	0.44
3:D:930:LEU:HD12	3:D:1138:LEU:HD13	1.98	0.44
1:A:47:LEU:HD23	1:A:51:MET:HE3	1.99	0.44
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.99	0.44
3:D:1023:HIS:ND1	3:D:1126:GLN:O	2.32	0.44
1:A:14:VAL:HG22	1:A:15:ASP:H	1.82	0.44
2:C:1247:SER:OG	2:C:1248:THR:N	2.50	0.44
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.48	0.44
5:F:525:ASP:OD2	5:F:528:LEU:HG	2.16	0.44
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.35	0.44
2:C:560:PRO:O	3:D:780:ARG:NH2	2.45	0.44
2:C:623:LEU:HD12	2:C:627:GLY:HA2	1.99	0.44
3:D:416:ILE:HD13	3:D:416:ILE:HA	1.80	0.44
3:D:1075:ARG:HD2	3:D:1076:PRO:HD2	2.00	0.44
5:F:395:THR:OG1	5:F:396:ASN:N	2.51	0.44
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.99	0.44
5:F:470:MET:HB2	5:F:478:PRO:HG3	2.00	0.44
5:F:592:ALA:O	5:F:595:LEU:HB2	2.17	0.44
2:C:1130:ALA:O	2:C:1134:GLN:NE2	2.51	0.44
2:C:1319:MET:HA	2:C:1320:PRO:HD3	1.92	0.44
2:C:678:ARG:HA	2:C:678:ARG:HD3	1.79	0.44
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.51	0.44
2:C:975:ILE:HD11	2:C:1014:LEU:HB3	2.00	0.44
3:D:19:ALA:HA	3:D:1343:GLU:HA	2.00	0.44
3:D:88:CYS:O	3:D:90:VAL:N	2.51	0.44
3:D:275:ARG:NH1	3:D:298:MET:HB3	2.33	0.44
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	2.00	0.44
2:C:503:LYS:HD3	2:C:503:LYS:HA	1.84	0.43
2:C:1164:PHE:HB2	2:C:1168:GLU:HG3	2.01	0.43
3:D:70:CYS:SG	3:D:71:LEU:N	2.90	0.43
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.98	0.43
2:C:228:VAL:O	2:C:335:THR:OG1	2.28	0.43
3:D:1269:ALA:HB2	3:D:1274:PHE:HD1	1.84	0.43
3:D:18:ASP:N	3:D:18:ASP:OD1	2.47	0.43
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.84	0.43
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.84	0.43
3:D:848:VAL:HG12	3:D:858:VAL:HG22	2.00	0.43
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.51	0.43
1:B:181:GLU:HA	3:D:535:ARG:HH22	1.83	0.43
2:C:357:ASN:OD1	2:C:357:ASN:N	2.49	0.43
3:D:372:MET:HE2	3:D:372:MET:HB3	1.84	0.43
3:D:959:LYS:NZ	3:D:985:ILE:HG13	2.34	0.43
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.86	0.43
2:C:1083:GLU:H	2:C:1083:GLU:HG3	1.55	0.43
2:C:1339:LEU:HA	3:D:20:ILE:HG12	2.00	0.43
3:D:516:ASP:HB3	3:D:573:THR:HG21	2.00	0.43
3:D:667:GLN:HG2	3:D:672:LEU:HD22	2.00	0.43
5:F:114:GLU:H	5:F:114:GLU:HG3	1.57	0.43
1:B:67:GLU:OE1	1:B:67:GLU:N	2.49	0.43
2:C:404:LYS:HD2	2:C:404:LYS:HA	1.81	0.43
2:C:908:GLU:OE2	5:F:611:LEU:HB3	2.18	0.43
3:D:581:MET:HE2	3:D:581:MET:HB3	1.91	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HG22	2.01	0.43
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.43
1:A:12:ARG:NH1	1:A:13:LEU:O	2.51	0.43
3:D:27:PRO:O	3:D:31:ARG:HG3	2.19	0.43
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.16	0.43
3:D:1344:LEU:O	3:D:1346:GLY:N	2.44	0.43
3:D:118:LYS:HB3	3:D:118:LYS:HE2	1.92	0.43
1:A:71:LYS:HD3	1:A:71:LYS:HA	1.90	0.42
2:C:1065:LYS:HD3	2:C:1235:LEU:HD12	2.01	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.54	0.42
1:B:196:THR:HG23	3:D:443:GLU:HG3	2.01	0.42
2:C:802:VAL:HG11	2:C:1230:MET:HB3	2.00	0.42
2:C:971:LEU:HG	2:C:1014:LEU:HD23	2.00	0.42
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	2.01	0.42
2:C:24:VAL:HG22	2:C:578:TYR:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:222:LYS:HA	3:D:222:LYS:HD2	1.85	0.42
3:D:511:TYR:HE2	3:D:724:MET:HG2	1.85	0.42
1:A:82:LEU:HD23	1:A:82:LEU:HA	1.88	0.42
3:D:429:LEU:HD13	3:D:429:LEU:HA	1.92	0.42
5:F:134:VAL:HG22	5:F:273:MET:HE1	2.00	0.42
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.44	0.42
3:D:1021:ASP:HB3	3:D:1024:THR:HB	2.00	0.42
3:D:1157:ALA:HB3	3:D:1206:ARG:HA	2.02	0.42
5:F:106:GLY:O	5:F:385:ARG:NH2	2.53	0.42
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.70	0.42
2:C:39:ILE:HD11	2:C:75:LEU:HG	2.01	0.42
3:D:510:LEU:HD22	3:D:601:ILE:HD11	2.00	0.42
3:D:819:GLY:H	3:D:881:LYS:HZ3	1.68	0.42
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.40	0.42
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.80	0.42
2:C:570:GLY:O	2:C:573:ASN:ND2	2.45	0.42
3:D:1203:ARG:NH1	3:D:1205:GLU:HG2	2.35	0.42
5:F:387:VAL:HG21	5:F:412:LEU:HD22	2.01	0.42
5:F:476:ARG:HB3	5:F:477:GLU:H	1.62	0.42
1:A:9:LEU:HD23	1:A:9:LEU:HA	1.89	0.41
1:B:112:ALA:HB3	1:B:126:PRO:HA	2.02	0.41
2:C:1137:GLU:HG3	2:C:1139:ALA:H	1.84	0.41
1:A:165:GLU:OE2	1:A:172:LEU:HD11	2.20	0.41
3:D:863:LEU:HD11	3:D:901:ARG:HB3	2.02	0.41
3:D:1152:GLU:OE2	3:D:1194:ARG:HG2	2.21	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:A:90:VAL:HG21	1:A:146:VAL:HG21	2.02	0.41
2:C:1305:TYR:HE2	5:F:535:ALA:HB2	1.85	0.41
5:F:495:ARG:HD3	5:F:495:ARG:H	1.86	0.41
1:B:71:LYS:HA	1:B:71:LYS:HD3	1.84	0.41
2:C:117:ILE:H	2:C:117:ILE:HG12	1.64	0.41
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.03	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.88	0.41
2:C:549:ASP:OD2	3:D:750:PRO:HB3	2.20	0.41
2:C:594:VAL:HG11	2:C:650:VAL:HG23	2.03	0.41
3:D:538:ARG:HA	3:D:538:ARG:HD2	1.93	0.41
2:C:55:SER:OG	2:C:56:VAL:N	2.51	0.41
2:C:135:THR:HG21	2:C:142:GLU:OE2	2.20	0.41
2:C:805:MET:HE3	2:C:805:MET:HB2	1.92	0.41
3:D:1115:ILE:HB	3:D:1119:ASP:HB2	2.02	0.41
5:F:274:ARG:HH12	5:F:365:MET:HE3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:309:ASN:HB3	5:F:310:GLU:H	1.67	0.41
3:D:1025:MET:HB3	3:D:1124:ILE:HB	2.03	0.41
3:D:1174:ARG:NH2	3:D:1187:GLU:OE2	2.54	0.41
3:D:148:GLU:H	3:D:156:ARG:HG3	1.84	0.41
3:D:753:SER:O	3:D:753:SER:OG	2.38	0.41
3:D:1167:LYS:HE3	3:D:1167:LYS:HB3	1.85	0.41
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.36	0.41
2:C:799:ASN:OD1	2:C:799:ASN:N	2.54	0.41
3:D:139:LEU:HD23	3:D:139:LEU:HA	1.84	0.41
1:B:26:VAL:O	1:B:203:ILE:N	2.47	0.41
1:B:118:ASP:HB2	1:B:121:VAL:HB	2.03	0.41
2:C:685:MET:HE3	2:C:685:MET:HB2	1.82	0.41
3:D:813:ASP:HB2	3:D:897:HIS:CE1	2.56	0.41
1:A:96:ASP:OD1	1:A:148:ARG:NH1	2.54	0.40
2:C:17:LYS:N	2:C:1188:ASP:OD2	2.54	0.40
3:D:161:THR:HG22	3:D:164:GLN:HB2	2.03	0.40
3:D:242:LEU:HA	3:D:243:PRO:HD3	1.90	0.40
3:D:278:ARG:HD3	5:F:407:GLU:OE2	2.20	0.40
3:D:587:LEU:HD23	3:D:591:ILE:HG21	2.02	0.40
3:D:1052:GLU:HG2	3:D:1053:LEU:H	1.86	0.40
4:E:63:ILE:HD13	4:E:63:ILE:HA	1.92	0.40
2:C:804:PHE:HE2	2:C:1115:THR:HG21	1.85	0.40
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	2.02	0.40
5:F:589:GLN:O	5:F:593:LYS:N	2.49	0.40
1:A:171:LEU:HD13	1:A:171:LEU:HA	1.91	0.40
2:C:123:TYR:OH	2:C:126:GLU:HG3	2.21	0.40
3:D:371:LYS:HA	3:D:371:LYS:HD2	1.95	0.40
3:D:1036:ARG:HB3	3:D:1079:LYS:HB3	2.03	0.40
2:C:228:VAL:HG23	2:C:337:PHE:HB2	2.03	0.40
2:C:1255:THR:O	2:C:1257:GLN:N	2.55	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.40
5:F:505:ILE:HD12	5:F:505:ILE:HA	1.95	0.40
2:C:727:VAL:HG23	2:C:773:LEU:HD23	2.03	0.40
2:C:1236:ASN:HA	2:C:1238:LEU:HD12	2.04	0.40
3:D:1282:TYR:HD1	3:D:1282:TYR:HA	1.77	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	228/329 (69%)	204 (90%)	24 (10%)	0	100	100
1	B	217/329 (66%)	196 (90%)	18 (8%)	3 (1%)	9	39
2	C	1338/1342 (100%)	1209 (90%)	109 (8%)	20 (2%)	8	38
3	D	1344/1407 (96%)	1212 (90%)	105 (8%)	27 (2%)	6	31
4	E	74/91 (81%)	70 (95%)	3 (4%)	1 (1%)	9	39
5	F	462/613 (75%)	430 (93%)	27 (6%)	5 (1%)	11	45
All	All	3663/4111 (89%)	3321 (91%)	286 (8%)	56 (2%)	11	38

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
1	B	193	GLU
2	C	398	SER
2	C	484	LEU
2	C	697	LYS
3	D	10	ALA
3	D	49	PHE
3	D	426	ALA
3	D	496	GLY
3	D	710	ASP
3	D	712	GLN
3	D	745	GLY
3	D	805	GLN
3	D	826	ILE
3	D	831	VAL
3	D	860	ARG
3	D	1169	THR
3	D	1294	ALA
4	E	33	GLY
5	F	490	PRO

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Mol	Chain	Res	Type
5	F	566	ASP
2	C	121	GLU
2	C	596	ASP
2	C	746	ALA
2	C	1137	GLU
2	C	1154	ASP
2	C	1165	SER
3	D	89	GLY
3	D	1167	LYS
5	F	569	THR
1	B	13	LEU
2	C	696	ASP
2	C	892	GLU
2	C	1317	PRO
3	D	19	ALA
2	C	163	LYS
2	C	199	ASP
2	C	235	ASN
2	C	813	GLU
3	D	173	GLY
3	D	314	ARG
3	D	417	ARG
3	D	585	LYS
2	C	625	GLU
3	D	230	SER
3	D	1274	PHE
3	D	1345	ARG
2	C	169	LYS
2	C	983	GLY
2	C	1223	ARG
3	D	152	THR
3	D	1297	LYS
3	D	357	VAL
5	F	96	ASP
5	F	361	ILE
3	D	828	GLY

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	
1	A	198/286 (69%)	194 (98%)	4 (2%)	48	66
1	B	189/286 (66%)	177 (94%)	12 (6%)	16	38
2	C	1155/1157 (100%)	1087 (94%)	68 (6%)	18	41
3	D	1115/1168 (96%)	1053 (94%)	62 (6%)	19	42
4	E	65/75 (87%)	61 (94%)	4 (6%)	16	39
5	F	417/540 (77%)	400 (96%)	17 (4%)	27	49
All	All	3139/3512 (89%)	2972 (95%)	167 (5%)	22	43

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	56	VAL
1	A	121	VAL
1	A	124	VAL
1	B	9	LEU
1	B	14	VAL
1	B	26	VAL
1	B	50	SER
1	B	62	ASP
1	B	64	VAL
1	B	79	LEU
1	B	92	VAL
1	B	121	VAL
1	B	124	VAL
1	B	125	LYS
1	B	183	ILE
2	C	22	LEU
2	C	39	ILE
2	C	56	VAL
2	C	90	VAL
2	C	103	VAL
2	C	117	ILE
2	C	131	THR
2	C	135	THR
2	C	145	ILE
2	C	164	THR
2	C	170	VAL

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Mol	Chain	Res	Type
2	C	265	LYS
2	C	302	ILE
2	C	306	THR
2	C	321	LEU
2	C	377	THR
2	C	384	LEU
2	C	419	ILE
2	C	452	ARG
2	C	453	ILE
2	C	456	VAL
2	C	471	VAL
2	C	493	ILE
2	C	521	LEU
2	C	539	THR
2	C	550	VAL
2	C	553	THR
2	C	558	VAL
2	C	600	THR
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	634	VAL
2	C	657	THR
2	C	714	VAL
2	C	757	THR
2	C	764	CYS
2	C	765	ILE
2	C	791	LEU
2	C	817	LEU
2	C	878	THR
2	C	895	LEU
2	C	948	ILE
2	C	984	VAL
2	C	992	LEU
2	C	1054	LEU
2	C	1090	ASN
2	C	1098	LEU
2	C	1109	ILE
2	C	1134	GLN
2	C	1141	LEU
2	C	1151	LEU
2	C	1155	VAL

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Mol	Chain	Res	Type
2	C	1159	VAL
2	C	1163	THR
2	C	1172	LEU
2	C	1198	LEU
2	C	1210	ILE
2	C	1225	VAL
2	C	1227	VAL
2	C	1233	LEU
2	C	1240	ASP
2	C	1254	VAL
2	C	1265	PHE
2	C	1287	LEU
2	C	1291	LEU
2	C	1296	ASP
2	C	1327	LEU
3	D	12	THR
3	D	54	ASP
3	D	81	ARG
3	D	83	VAL
3	D	92	VAL
3	D	175	GLU
3	D	252	LEU
3	D	255	LEU
3	D	269	TYR
3	D	290	ILE
3	D	292	VAL
3	D	306	LEU
3	D	324	LEU
3	D	343	LEU
3	D	363	LEU
3	D	374	LEU
3	D	386	GLU
3	D	392	THR
3	D	394	ILE
3	D	416	ILE
3	D	423	LEU
3	D	425	ARG
3	D	429	LEU
3	D	442	ILE
3	D	505	ASP
3	D	507	VAL
3	D	510	LEU

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Mol	Chain	Res	Type
3	D	514	THR
3	D	532	GLU
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	573	THR
3	D	639	VAL
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	754	ILE
3	D	770	LEU
3	D	790	THR
3	D	801	VAL
3	D	810	THR
3	D	844	THR
3	D	853	THR
3	D	858	VAL
3	D	903	LEU
3	D	1135	THR
3	D	1155	ILE
3	D	1162	ILE
3	D	1169	THR
3	D	1221	LEU
3	D	1233	ILE
3	D	1251	LYS
3	D	1257	VAL
3	D	1261	LEU
3	D	1310	THR
3	D	1333	THR
3	D	1340	LYS
3	D	1366	HIS
4	E	5	THR
4	E	36	ASP
4	E	39	VAL
4	E	63	ILE
5	F	114	GLU
5	F	127	ILE
5	F	163	THR

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Mol	Chain	Res	Type
5	F	230	VAL
5	F	261	LEU
5	F	305	LEU
5	F	341	LEU
5	F	399	LEU
5	F	450	ILE
5	F	479	THR
5	F	491	GLU
5	F	494	ILE
5	F	526	THR
5	F	527	THR
5	F	530	LEU
5	F	558	VAL
5	F	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	147	GLN
1	B	37	HIS
1	B	84	ASN
1	B	117	HIS
2	C	31	GLN
2	C	235	ASN
2	C	276	GLN
2	C	513	GLN
2	C	517	GLN
2	C	526	HIS
2	C	554	HIS
2	C	752	ASN
2	C	760	ASN
2	C	922	ASN
2	C	1023	HIS
2	C	1090	ASN
2	C	1134	GLN
2	C	1299	ASN
2	C	1324	ASN
3	D	45	ASN
3	D	113	HIS
3	D	209	ASN
3	D	294	ASN

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Mol	Chain	Res	Type
3	D	320	ASN
3	D	430	HIS
3	D	435	GLN
3	D	450	HIS
3	D	865	HIS
3	D	907	HIS
3	D	1010	GLN
3	D	1019	ASN
3	D	1086	ASN
3	D	1289	ASN
3	D	1366	HIS
4	E	31	GLN
5	F	294	GLN
5	F	338	HIS
5	F	446	GLN
5	F	455	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

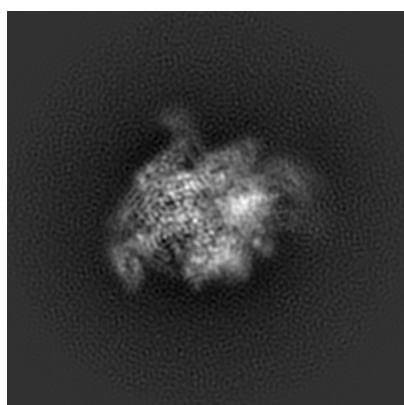
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7438. These allow visual inspection of the internal detail of the map and identification of artifacts.

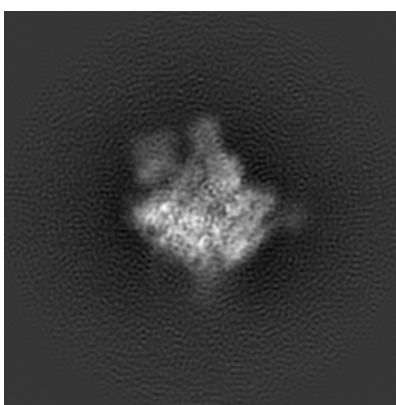
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

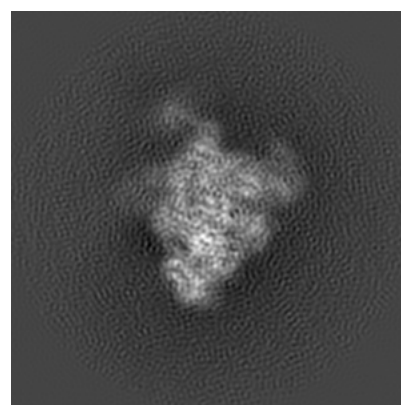
6.1.1 Primary map



X



Y

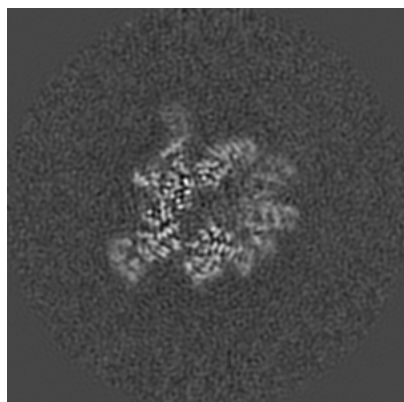


Z

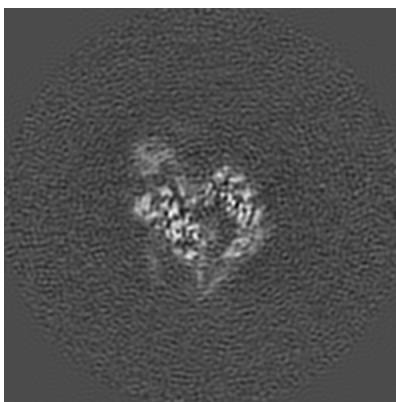
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

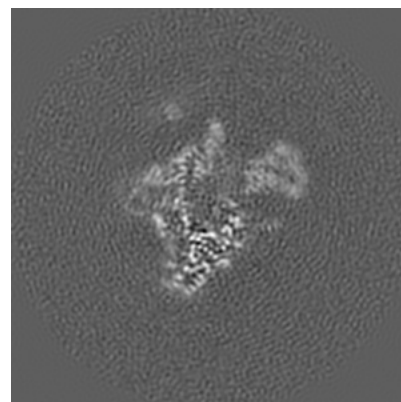
6.2.1 Primary map



X Index: 120



Y Index: 120

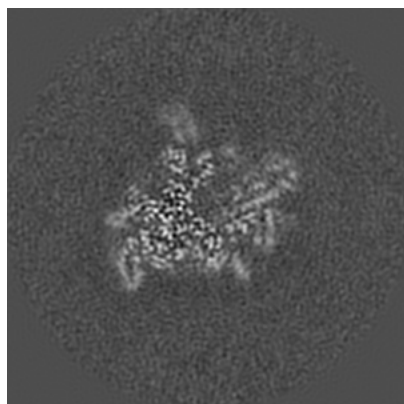


Z Index: 120

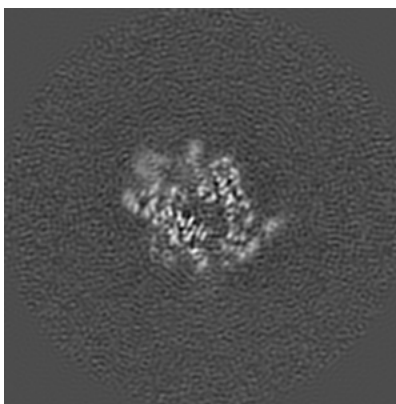
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

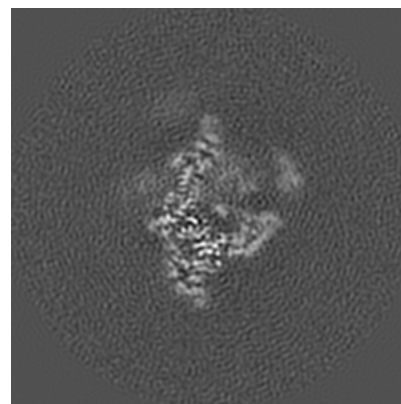
6.3.1 Primary map



X Index: 114



Y Index: 114

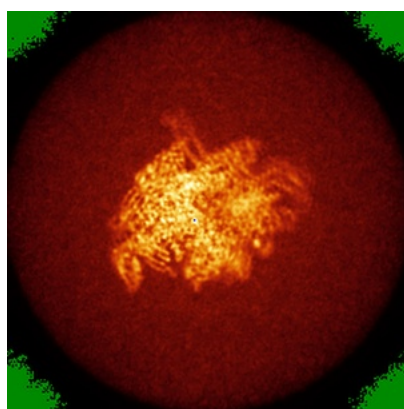


Z Index: 114

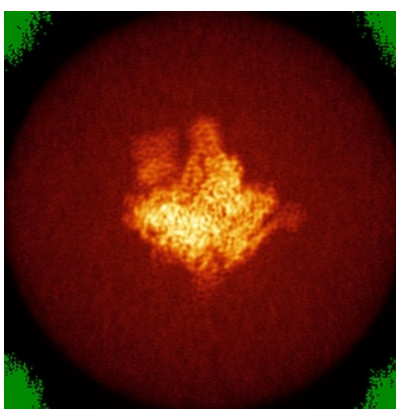
The images above show the largest variance slices of the map in three orthogonal directions.

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

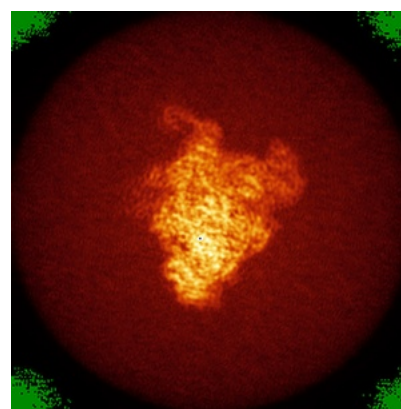
6.4.1 Primary map



X



Y

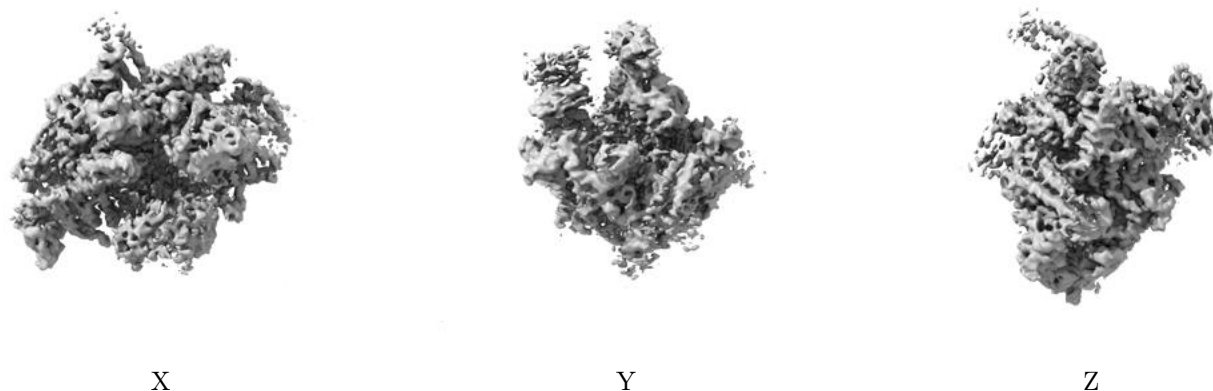


Z

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 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

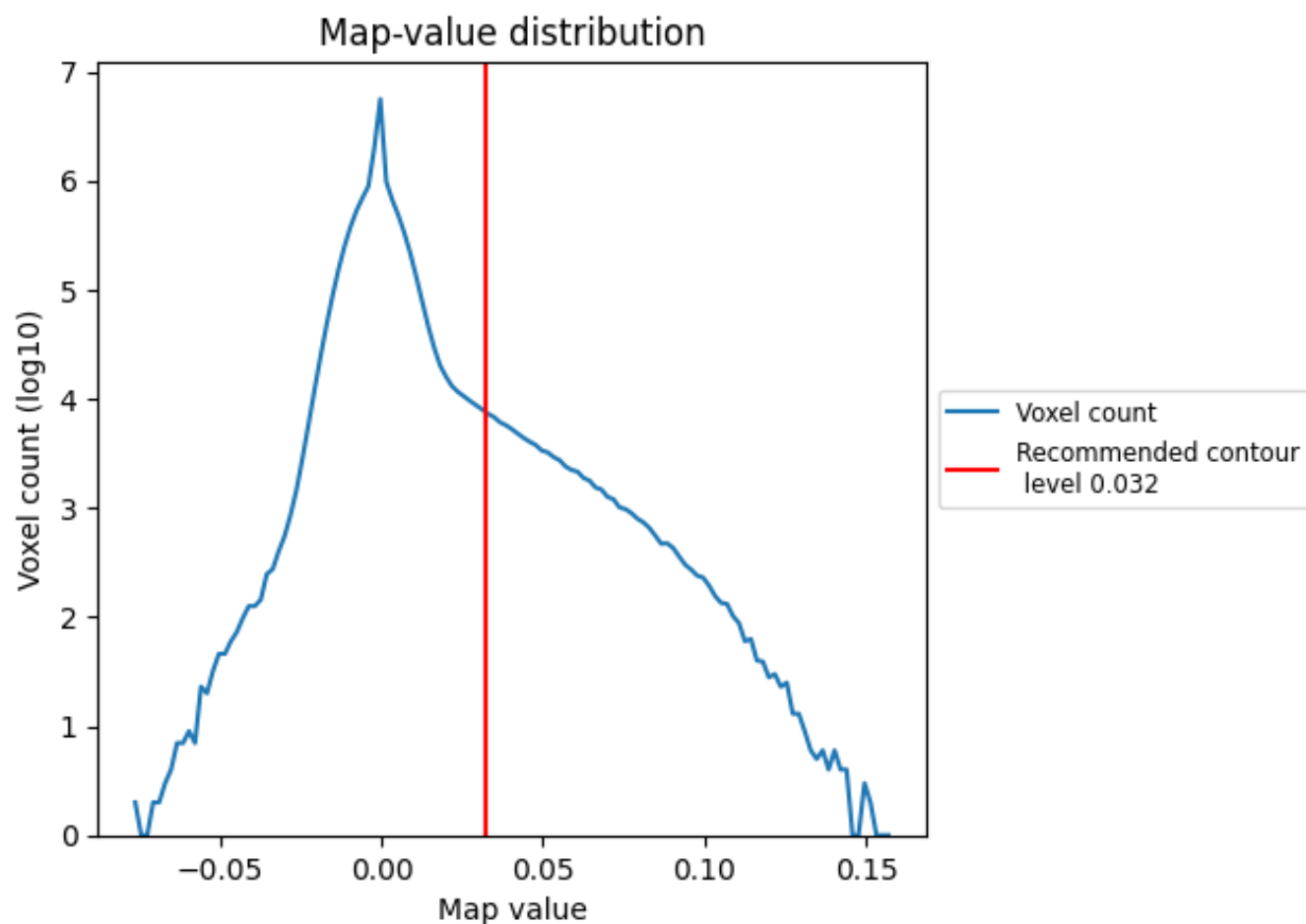
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

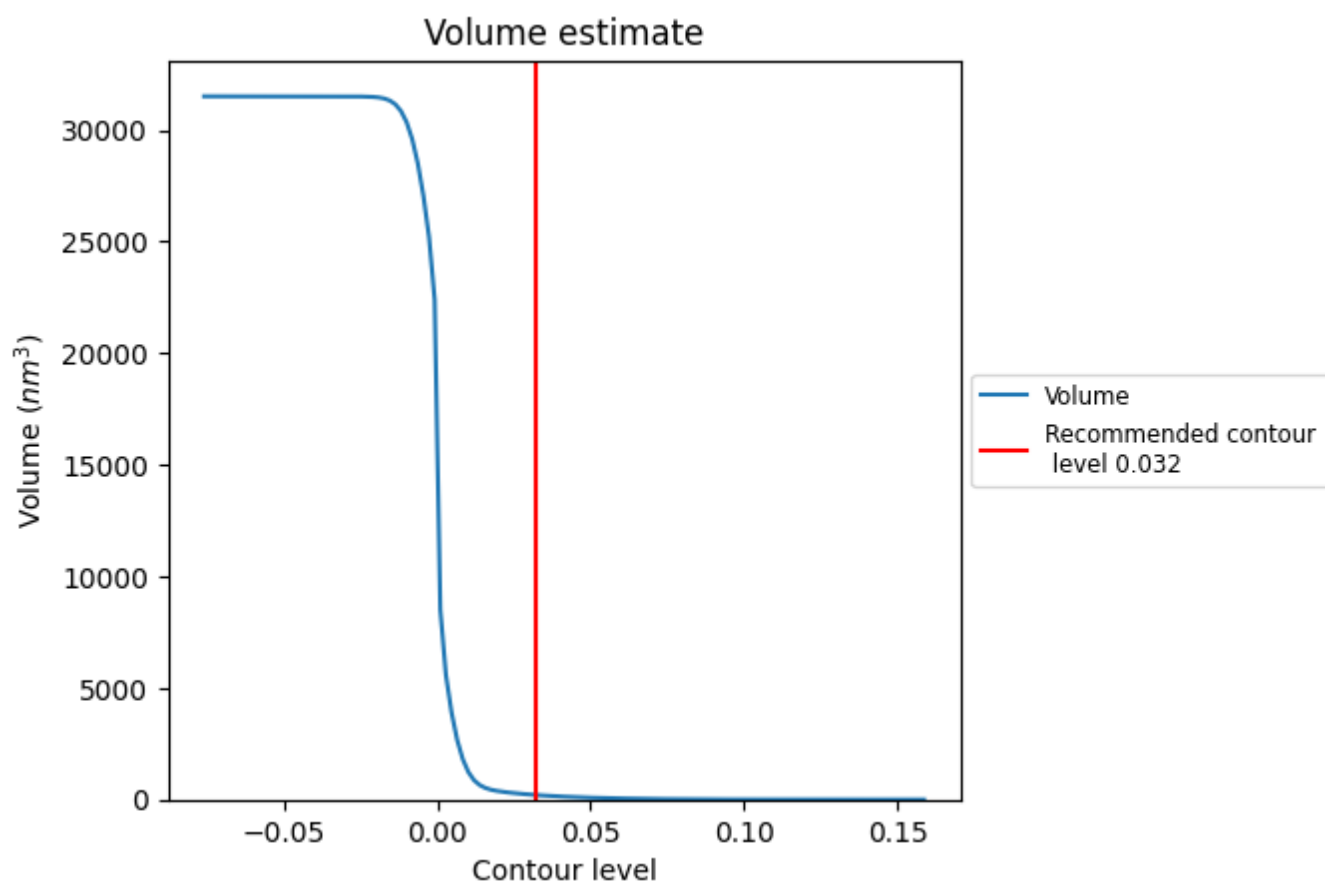
This section contains the results of statistical analysis of the map.

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.

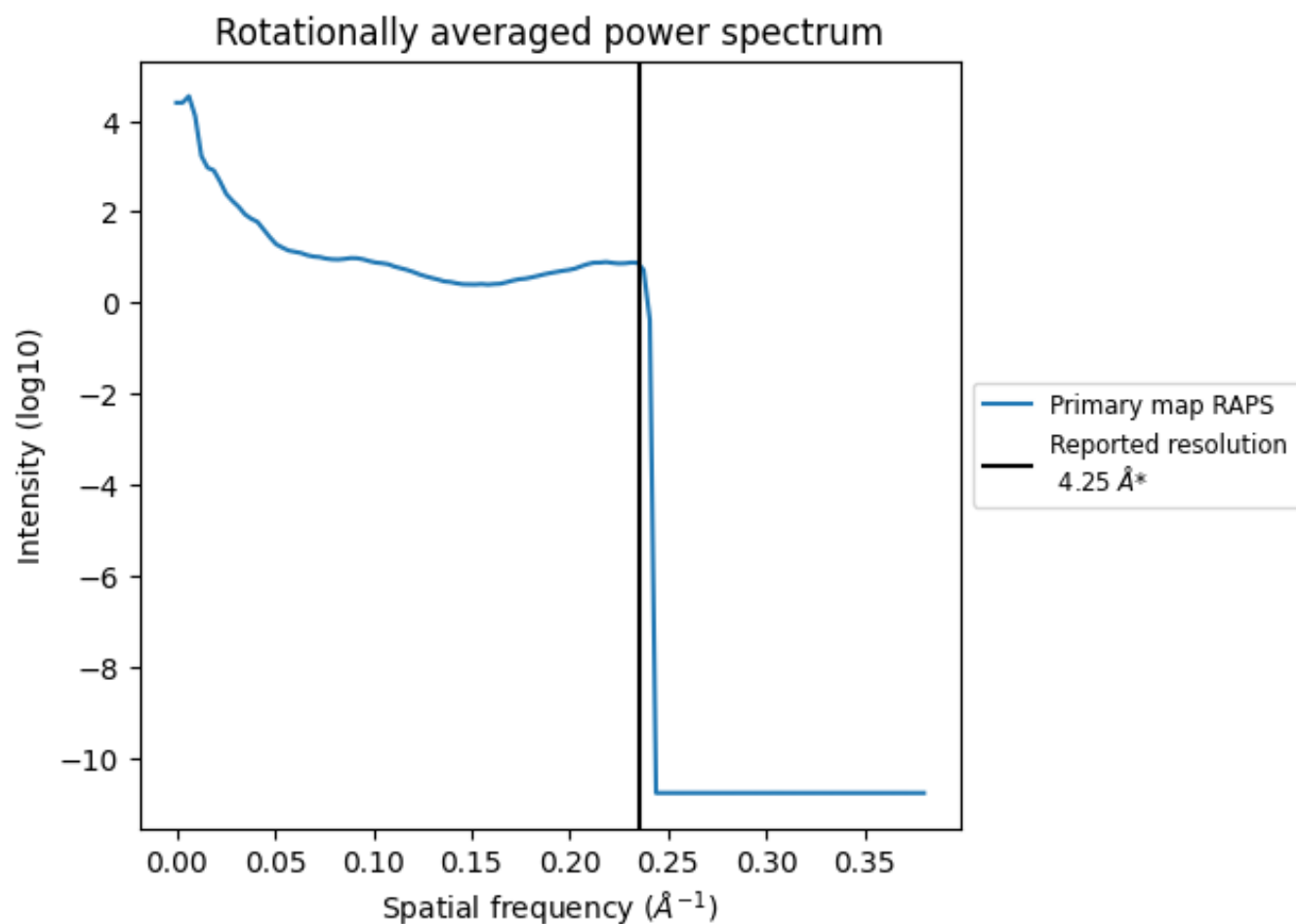
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 206 nm³; this corresponds to an approximate mass of 186 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 0.235 $\text{\AA}^{-1}$

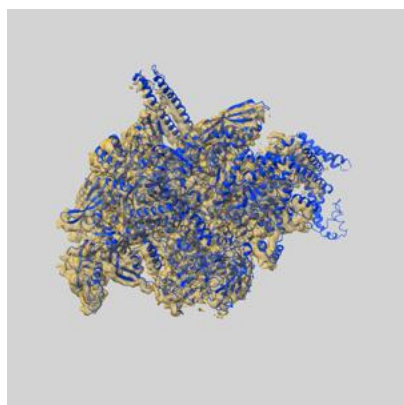
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

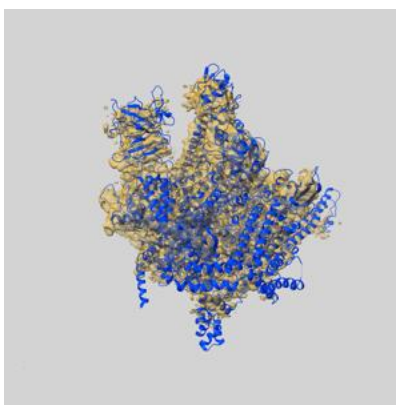
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-7438 and PDB model 6C9Y. Per-residue inclusion information can be found in section [3](#) on page [5](#).

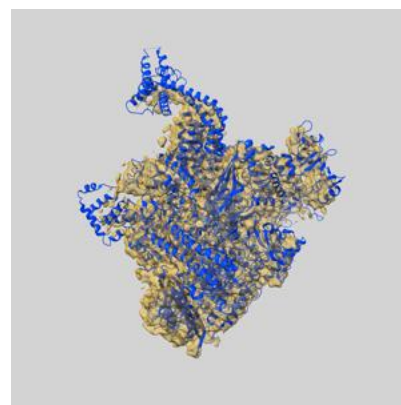
9.1 Map-model overlay [i](#)



X



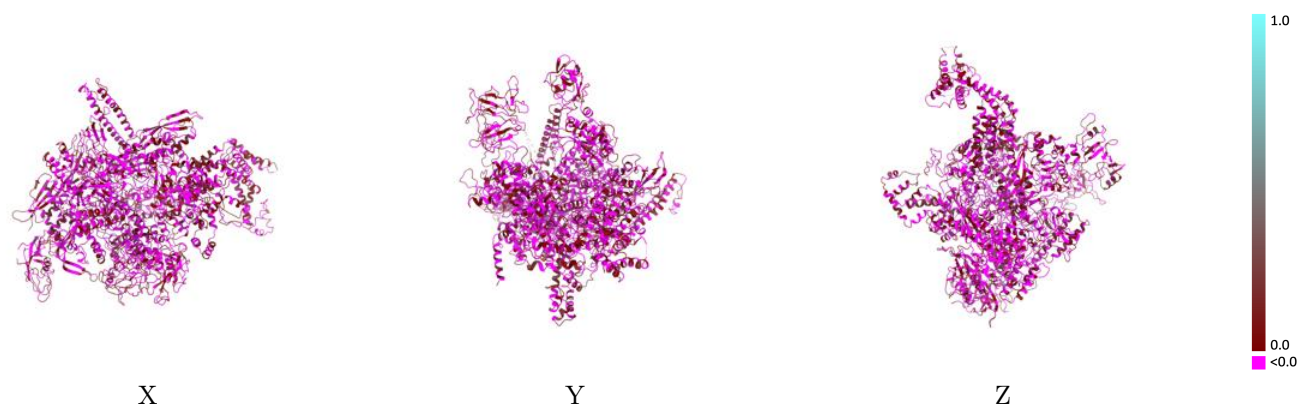
Y



Z

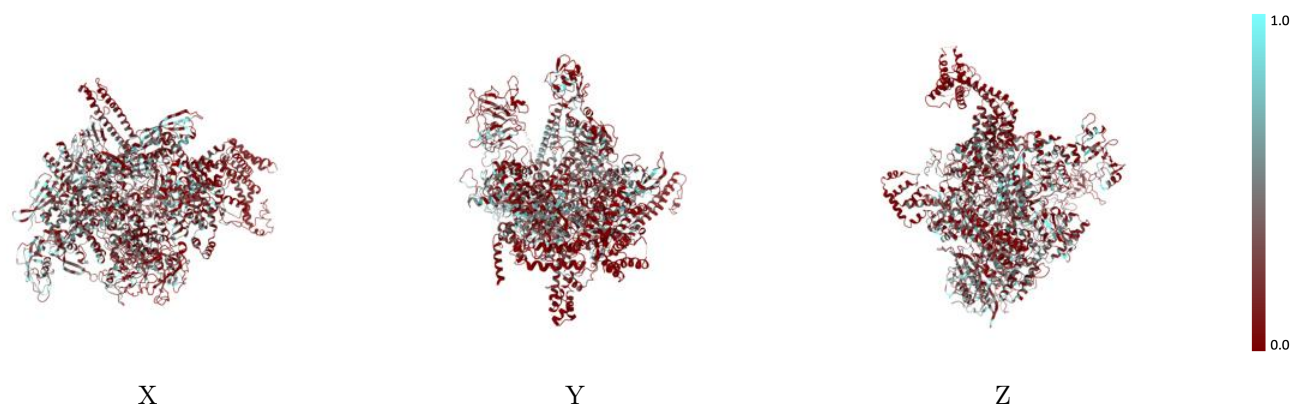
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



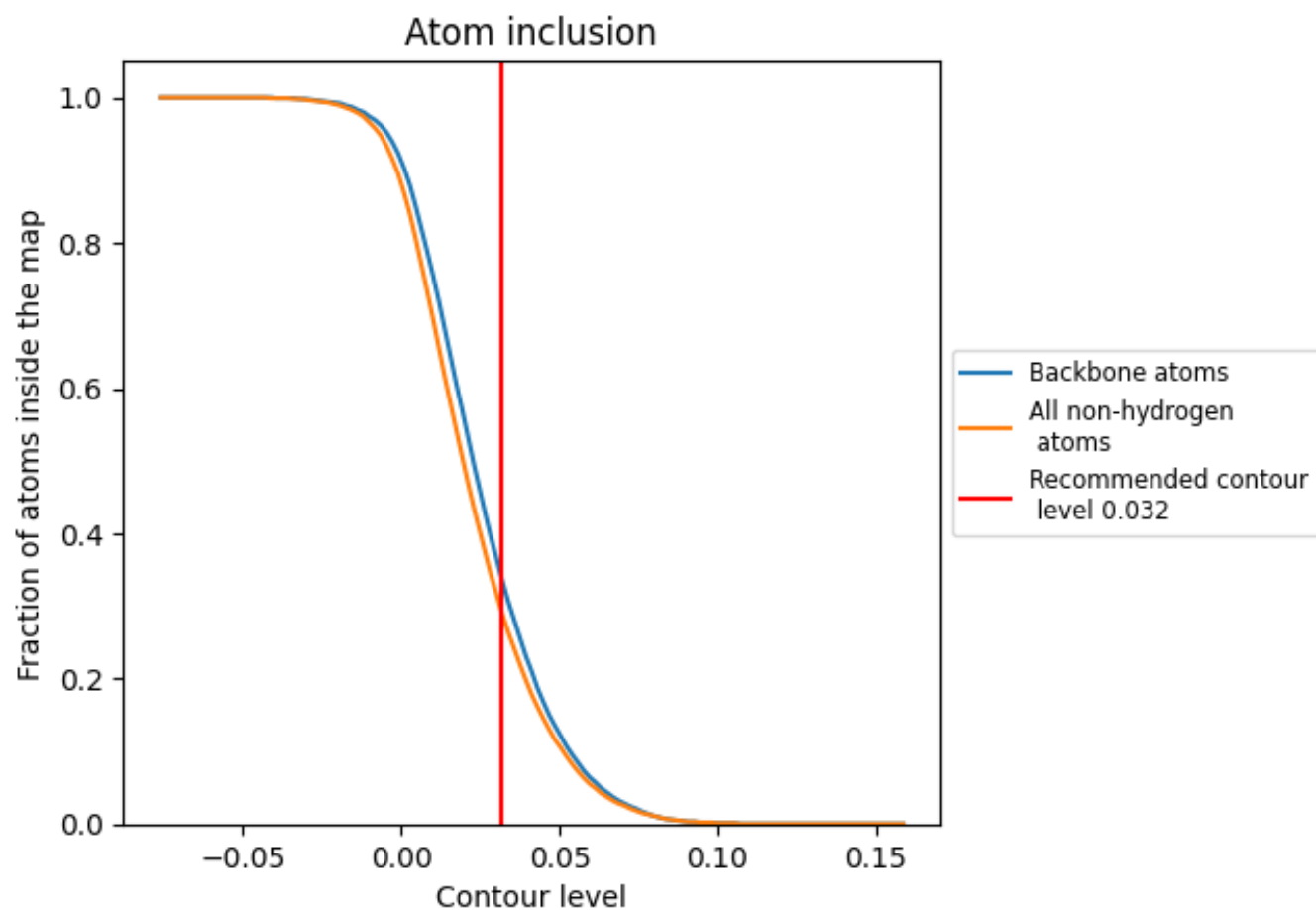
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 29% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2900	-0.0170
A	0.4000	-0.0020
B	0.4190	-0.0130
C	0.3110	-0.0300
D	0.3100	-0.0120
E	0.1140	-0.0490
F	0.0920	0.0030

1.0
0.0
-0.0