



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 04:36 PM UTC

PDB ID : 6PSV / pdb_00006psv
EMDB ID : EMD-20465
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TpreR_{Po})
with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.50 Å (reported)

This is a wwPDB EM Validation Summary 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:

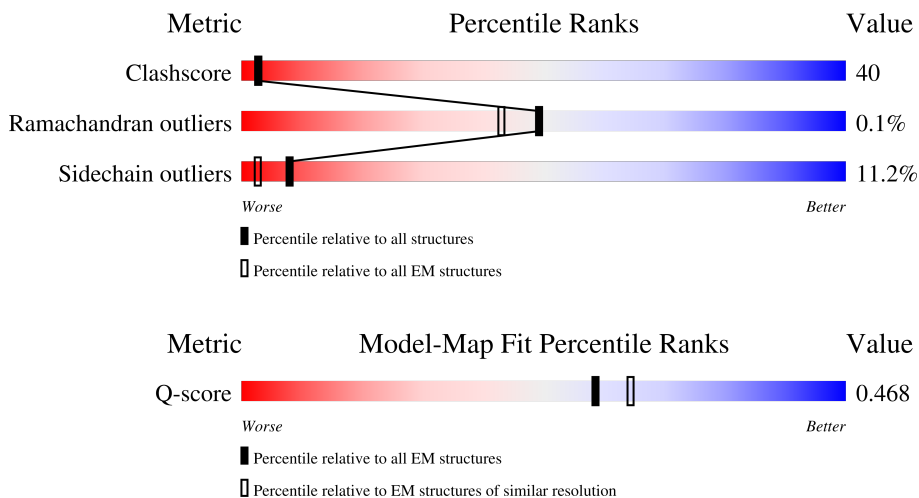
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.50 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.





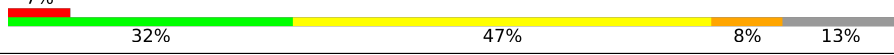
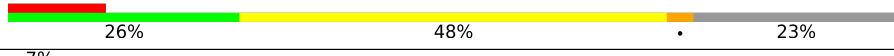
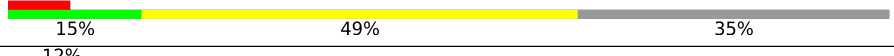
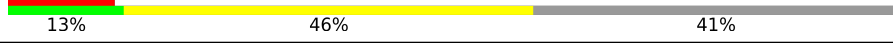
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	N	72	
2	G	329	
2	H	329	
2	M	329	

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Mol	Chain	Length	Quality of chain
3	I	1342	
4	J	1430	
5	K	91	
6	L	616	
7	O	85	
8	P	85	

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 32487 atoms, of which 156 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 Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	72	571	353	105	108	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	228	1761	1099	312	344	6	0	0
2	H	219	1664	1040	291	327	6	0	0
2	M	73	572	362	100	108	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	1340	10564	6628	1838	2055	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	1345	10466	6577	1867	1972	50	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

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

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	474	3846	2409	685	729	23	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	55	1128	539	211	323	55	0	0

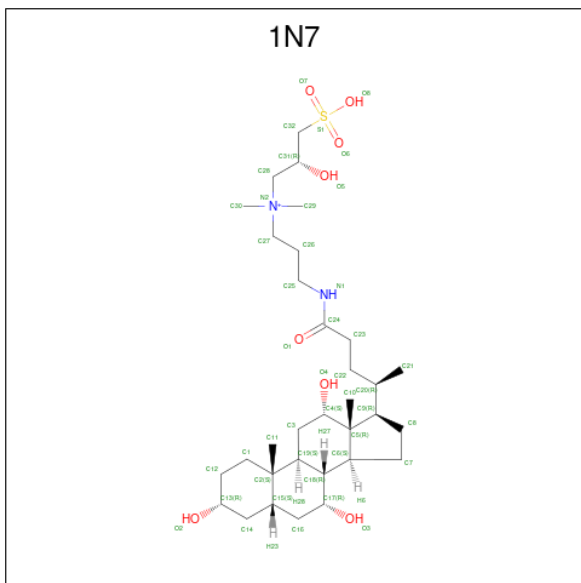
- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	50	1020	491	169	310	50	0	0

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	N	1	1	1	0
9	J	2	2	2	0

- Molecule 10 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



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Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
10	L	1	66	24	39	3	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

3 Residue-property plots [i](#)

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.

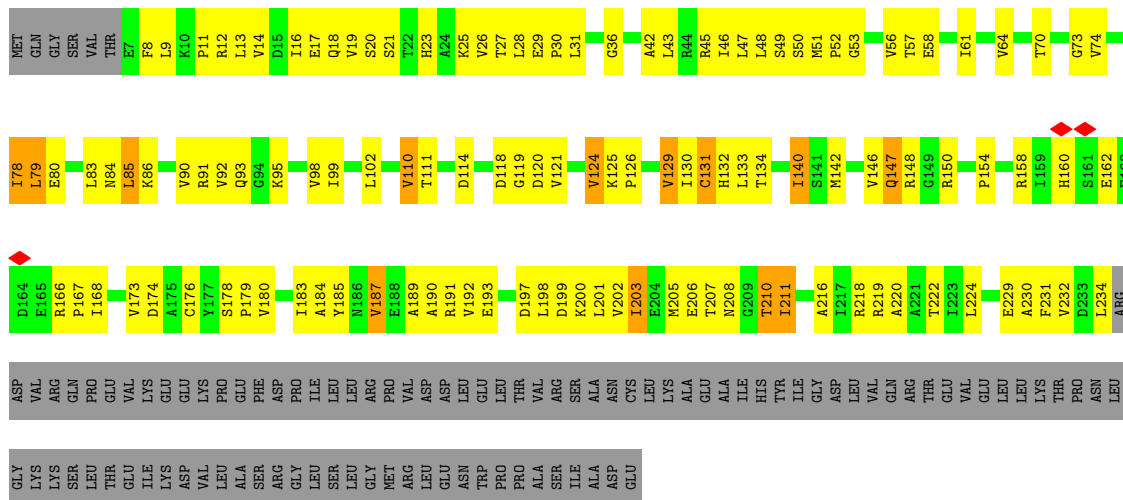
- Molecule 1: Protein TraR

Chain N: 




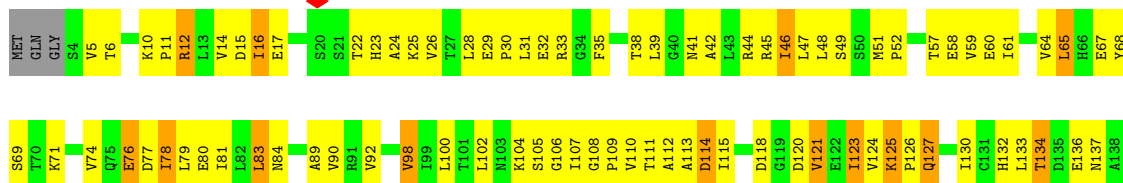
- Molecule 2: DNA-directed RNA polymerase subunit alpha

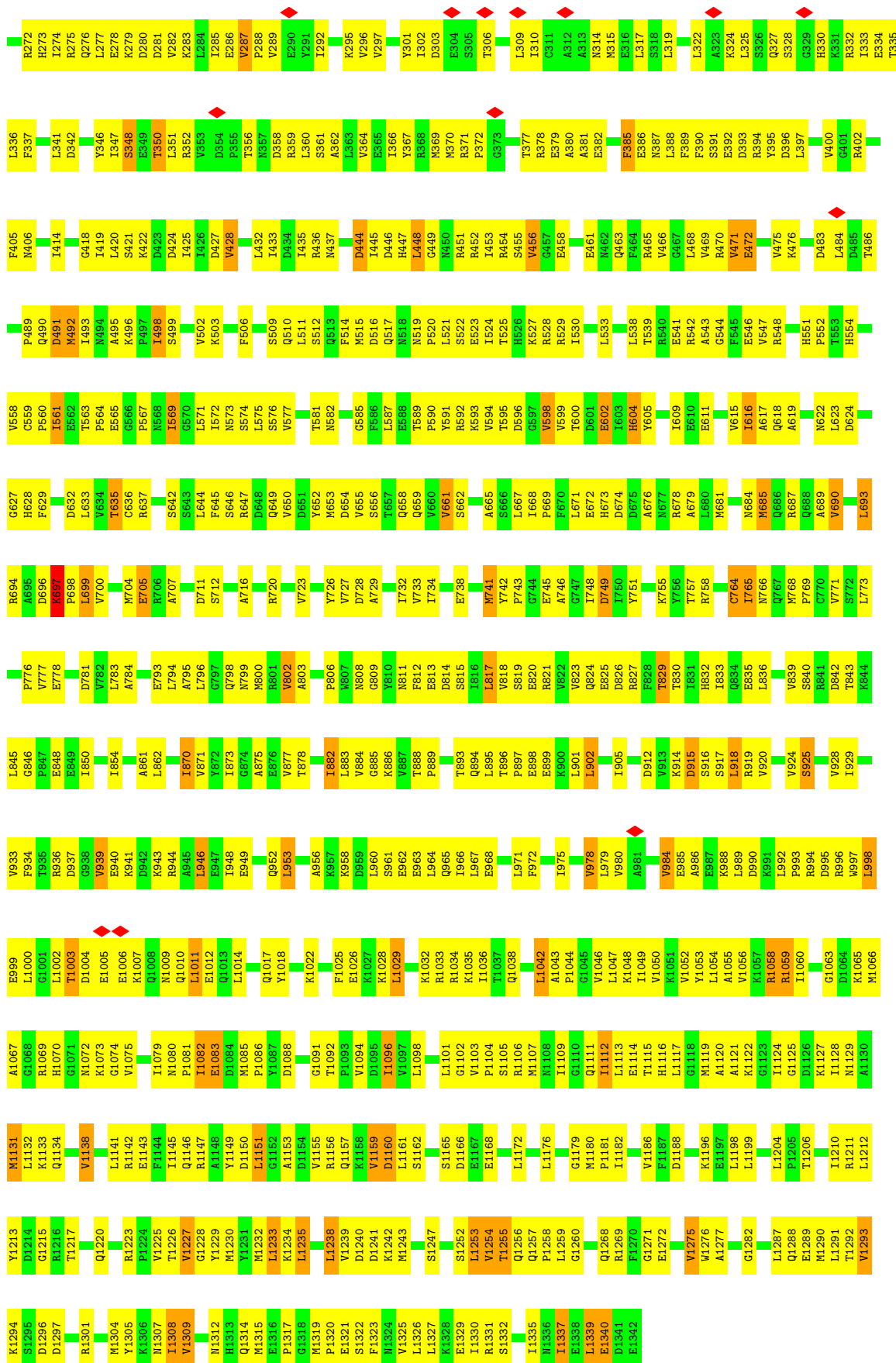
Chain G: 



- Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain H: 





• Molecule 4: DNA-directed RNA polymerase subunit beta'



VAL	L139	E204	V272	K345	E418	L491	S668	M644	E713	G782	L849	G916
LYS	E142	L205	I273	R346	V421	I499	L569	V645	E714	L783	K850	A919
ASP	E144	M206	M274	V547	L422	I500	K570	I646	K715	L786	P851	A920
LEU	V145	E207	R275	Y348	L423	V501	T572	K649	V177	K789	T853	E925
LEU	V146	T208	M276	Y349	M424	P502	T573	K650	S718	T790	D855	P926
PHE	K74	N209	N277	R278	R425	S503	T574	H653	F719	S793	L857	E930
LEU	K75	S210	L279	S853	A426	Q504	R576	E652	M720	G794	L858	L930
LEU	K76	K213	L282	V354	P427	D505	M581	I653	S721	G794	V858	N932
ALA	R77	G150	L283	I355	H430	V506	I654	I654	I722	V859	P859	N933
ALA	R78	R215	L286	T356	H431	V507	I655	S655	V723	R860	R860	R933
GLN	R79	K216	L288	T357	R431	L508	V653	E656	M724	R798	N861	T934
THR	K80	T152	A286	V357	L432	G509	V654	E666	M725	R799	T862	
LYS	H80	M153	A287	L363	G433	L510	L587	E660	R731	L800	L863	
LYS	H81	L154	A288	L364	I434	Y511	P588	V661	G732	L801	L864	
THR	H82	L155	P288	Q365	L435	Y512	P589	I662	G733	V801	L865	
GLU	H83	E155	D289	Q366	E438	H513	S590	E663	A735	G802	H866	
E16	V83	R220	I290	P369	P439	T514	I591	E664	Q736	V803	E866	
F17	V90	K222	I291	P370	V440	R515	V592	Q665	I737	D804	Q867	
F17	E91	Q158	V292	K370	L441	D516	V592	E666	R738	Q805	Q868	
L20	V92	I159	R293	K371	L442	C517	A595	Q669	A741	D806	C869	
K21	K96	T160	R294	M372	L443	V518	L596	Q670	G742	L807	D870	
I22	V97	L161	R295	A373	K445	G522	I601	Q671	G743	V808	L871	
S26	R98	E162	R296	L374	A446	E523	G671	G671	M743	V809	L872	
P27	R99	F227	R297	L375	L447	E524	L672	L672	R744	M744	L873	
D28	R99	Q164	M298	F377	Q448	G524	V673	V673	G745	G745	E811	
M29	R101	Y165	R299	K376	L449	M525	M604	A674	L746	L746	D812	
I30	M102	L166	R300	P379	L450	M526	M605	A675	M747	A675	D813	
R31	G103	D167	L306	F380	L451	V526	L606	A676	M748	G676	G814	
S34	H104	A168	L307	I381	L452	M527	M606	L676	M749	G676	G815	
F35	I105	H104	D308	I382	L453	T528	N606	L677	K749	E677	G816	
G36	E106	I105	R309	K384	Y457	G529	C608	C608	P750	R678	T816	
E37	L107	E171	M309	L385	M458	P530	Y609	Y609	D751	V679	V883	
V38	T111	F172	G310	E386	D460	A533	R610	M680	G752	M680	S884	
E42	A112	G173	R311	L387	F461	A534	I611	I611	I612	G681	V885	
T43	H113	L242	R312	L388	D461	R535	G612	G612	E534	V682	V886	
I44	H114	L243	R313	L389	F462	R536	G613	G613	I754	I754	V887	
M45	H115	V244	R314	L390	Q465	L536	L614	L614	E755	E755	C888	
Y46	H116	L245	R315	L391	M466	L537	K615	K615	T757	T757	D889	
R47	L117	P246	R316	L392	A467	A542	P616	P616	F758	F758	T890	
T48	L118	P247	R317	L393	V468	M543	T617	T617	M689	M689	G893	
P51	L119	R250	R318	L394	H469	H544	V618	V618	T760	T760	V894	
E52	L120	R251	R319	L395	V470	A545	I619	I619	A761	A761	G894	
R53	L121	V253	R320	L396	P471	R547	F620	F620	V693	V693	H897	
D54	L122	L255	R321	L397	L472	V548	G621	G621	M697	M697	G900	
G55	R123	L256	R322	L398	L473	K549	D622	D622	M698	M698	E933	
L56	G125	R259	R323	L399	L474	V550	Q623	Q623	D699	D699	P834	
F57	L126	F260	R324	L400	E475	R551	I624	I624	N700	N700	L835	
G58	L127	A261	R325	L401	A476	I552	G624	G624	L701	L701	D902	
A59	L128	M192	R326	L402	E479	T553	T627	T627	Q702	Q702	L903	
R60	L129	L194	R327	L403	A480	E554	G628	G628	T703	T703	A904	
I61	M130	L194	R328	L404	R481	T555	F629	F629	E704	E704	R905	
F62	P131	S263	R329	L405	A482	E556	A633	A633	T705	T705	L940	
G63	L132	D264	R330	L406	L483	K557	R634	R634	V706	V706	G941	
P64	R133	R265	R331	L407	L484	D558	G635	G635	I707	I707	B942	
V65	D134	D267	R332	L408	I411	A559	S635	S635	T708	T708	V943	
K66	I135	L268	R333	L409	M485	N560	V639	V639	R709	R709	T944	
D67	V138	R270	R334	L410	S486	G561	G640	G640	A779	A779	A945	
		R271	R335	L411	T487	E562	G641	G641	D710	D710	E946	
			R336	L412	I490	T567	I641	I641	G711	G711	D947	
			R337	L413			G642	G642	K781	K781	V948	
			R338	L414			G643	G643				
			R339	L415			G644	G644				
			R340	L416			G645	G645				
			R341	L417			G646	G646				
			R342	L418			G647	G647				
			R343	L419			G648	G648				
			R344	L420			G649	G649				
			R345	L421			G650	G650				
			R346	L422			G651	G651				
			R347	L423			G652	G652				
			R348	L424			G653	G653				
			R349	L425			G654	G654				
			R350	L426			G655	G655				
			R351	L427			G656	G656				
			R352	L428			G657	G657				
			R353	L429			G658	G658				
			R354	L430			G659	G659				
			R355	L431			G660	G660				
			R356	L432			G661	G661				
			R357	L433			G662	G662				
			R358	L434			G663	G663				
			R359	L435			G664	G664				
			R360	L436			G665	G665				
			R361	L437			G666	G666				
			R362	L438			G667	G667				
			R363	L439			G668	G668				
			R364	L440			G669	G669				
			R365	L441			G670	G670				
			R366	L442			G671	G671				
			R367	L443			G672	G672				
			R368	L444			G673	G673				
			R369	L445			G674	G674				
			R370	L446			G675	G675				
			R371	L447			G676	G676				
			R372	L448			G677	G677				
			R373	L449			G678	G678				
			R374	L450			G679	G679				
			R375	L451			G680	G680				
			R376	L452			G681	G681				
			R377	L453			G682	G682				
			R378	L454			G683	G683				
			R379	L455			G684	G684				
			R380	L456			G685	G685				
			R381	L457			G686	G686				
			R382	L458			G687	G687				
			R383	L459			G688	G688				
			R384	L460			G689	G689				
			R385	L461			G690	G690				
			R386	L462			G691	G691				
			R387	L463			G692	G692				
			R388	L464			G693	G693				
			R389	L465			G694	G694				
			R390	L466			G695	G695				
			R391	L467			G696	G696				
			R392	L468			G697	G697				
			R393	L469			G698	G698				
			R394	L470			G699	G699				
			R395	L471			G700	G700				
			R396	L472			G701	G701				
			R397	L473			G702	G702				
			R398	L474			G703	G703				
			R399	L475			G704	G704				
			R400	L476			G705	G705				
			R401	L477			G706	G706				
			R402	L478			G707	G707				
			R403	L479			G708	G708				
			R404	L480			G709	G709				
			R405	L481			G710	G710				
			R406	L482			G711	G711				
			R407	L483			G712	G712				
			R408	L484			G713	G713				
			R409	L485			G714	G714				
			R410	L486			G715	G715				
			R411	L487			G716	G716				
			R412	L488	</							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81732	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 ($e^-/\text{\AA}^2$)	80	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	0.226	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1N7, MG

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	N	0.42	0/581	0.56	0/785
2	G	0.48	0/1783	0.63	0/2417
2	H	0.44	0/1683	0.66	2/2285 (0.1%)
2	M	0.23	0/579	0.51	0/784
3	I	0.49	0/10733	0.63	6/14482 (0.0%)
4	J	0.46	0/10625	0.61	0/14345
5	K	0.36	0/629	0.56	0/847
6	L	0.28	0/3898	0.54	0/5242
7	O	0.25	0/1266	0.44	0/1948
8	P	0.25	0/1138	0.44	0/1752
All	All	0.43	0/32915	0.60	8/44887 (0.0%)

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	H	0	1
3	I	0	1
4	J	0	1
6	L	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	516	ASP	N-CA-C	-6.69	99.93	109.96
3	I	1096	ILE	CA-C-N	-5.87	117.39	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1096	ILE	C-N-CA	-5.87	117.39	122.96
2	H	194	GLN	CA-C-N	5.47	131.55	121.70
2	H	194	GLN	C-N-CA	5.47	131.55	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	12	ARG	Peptide
3	I	81	ASP	Peptide
4	J	177	ASP	Peptide
6	L	110	LEU	Peptide
6	L	500	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	571	0	558	45	0
2	G	1761	0	1787	126	0
2	H	1664	0	1672	145	0
2	M	572	0	602	67	0
3	I	10564	0	10571	865	0
4	J	10466	0	10689	926	0
5	K	627	0	634	62	0
6	L	3846	0	3896	432	0
7	O	1128	0	621	78	0
8	P	1020	0	573	63	0
9	J	2	0	0	0	0
9	N	1	0	0	0	0
10	I	27	39	38	6	0
10	J	27	39	37	3	0
10	L	27	39	37	3	0
10	N	27	39	38	4	0
11	J	1	0	0	0	0
All	All	32331	156	31753	2594	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 40.

The worst 5 of 2594 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)
10:L:701:1N7:C19	10:L:701:1N7:C3	1.84	1.55
10:N:102:1N7:C19	10:N:102:1N7:C3	1.82	1.55
10:I:1401:1N7:C3	10:I:1401:1N7:C19	1.83	1.53
10:J:1504:1N7:C19	10:J:1504:1N7:C3	1.84	1.51
4:J:697:MET:HE2	4:J:741:ALA:HB3	1.36	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	70/72 (97%)	66 (94%)	4 (6%)	0	100	100
2	G	226/329 (69%)	192 (85%)	34 (15%)	0	100	100
2	H	215/329 (65%)	185 (86%)	30 (14%)	0	100	100
2	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
3	I	1338/1342 (100%)	1164 (87%)	170 (13%)	4 (0%)	36	67
4	J	1339/1430 (94%)	1202 (90%)	137 (10%)	0	100	100
5	K	77/91 (85%)	66 (86%)	10 (13%)	1 (1%)	9	39
6	L	468/616 (76%)	433 (92%)	35 (8%)	0	100	100
All	All	3804/4538 (84%)	3376 (89%)	423 (11%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	82	VAL

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Mol	Chain	Res	Type
5	K	61	ASN
3	I	81	ASP
3	I	1059	ARG
3	I	697	LYS

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	N	61/61 (100%)	52 (85%)	9 (15%)	3 17
2	G	194/286 (68%)	172 (89%)	22 (11%)	5 25
2	H	181/286 (63%)	157 (87%)	24 (13%)	4 20
2	M	65/286 (23%)	62 (95%)	3 (5%)	24 50
3	I	1154/1157 (100%)	1015 (88%)	139 (12%)	5 23
4	J	1128/1189 (95%)	991 (88%)	137 (12%)	5 22
5	K	67/75 (89%)	61 (91%)	6 (9%)	9 32
6	L	418/543 (77%)	391 (94%)	27 (6%)	15 42
All	All	3268/3883 (84%)	2901 (89%)	367 (11%)	8 25

5 of 367 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	499	ILE
4	J	930	LEU
4	J	553	THR
4	J	746	LEU
4	J	1089	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	1146	GLN

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Mol	Chain	Res	Type
4	J	488	ASN
6	L	437	GLN
3	I	1244	HIS
4	J	266	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
10	1N7	J	1504	-	30,30,46	5.20	19 (63%)	47,48,72	2.17	12 (25%)
10	1N7	L	701	-	30,30,46	5.24	15 (50%)	47,48,72	2.34	18 (38%)
10	1N7	I	1401	-	30,30,46	5.11	15 (50%)	47,48,72	2.58	21 (44%)
10	1N7	N	102	-	30,30,46	5.00	15 (50%)	47,48,72	2.42	17 (36%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	1N7	J	1504	-	-	3/7/72/92	0/4/4/4
10	1N7	L	701	-	-	4/7/72/92	0/4/4/4
10	1N7	I	1401	-	-	2/7/72/92	0/4/4/4
10	1N7	N	102	-	-	2/7/72/92	0/4/4/4

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	701	1N7	C3-C19	18.84	1.84	1.53
10	J	1504	1N7	C3-C19	18.79	1.84	1.53
10	I	1401	1N7	C3-C19	18.34	1.83	1.53
10	N	102	1N7	C3-C19	17.76	1.82	1.53
10	L	701	1N7	C3-C4	12.47	1.73	1.53

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1504	1N7	C7-C6-C18	-7.80	107.66	118.36
10	I	1401	1N7	C7-C6-C18	-5.81	110.39	118.36
10	I	1401	1N7	C9-C5-C4	-5.81	112.44	117.67
10	N	102	1N7	C9-C5-C4	-5.51	112.71	117.67
10	L	701	1N7	C9-C5-C4	-5.46	112.75	117.67

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

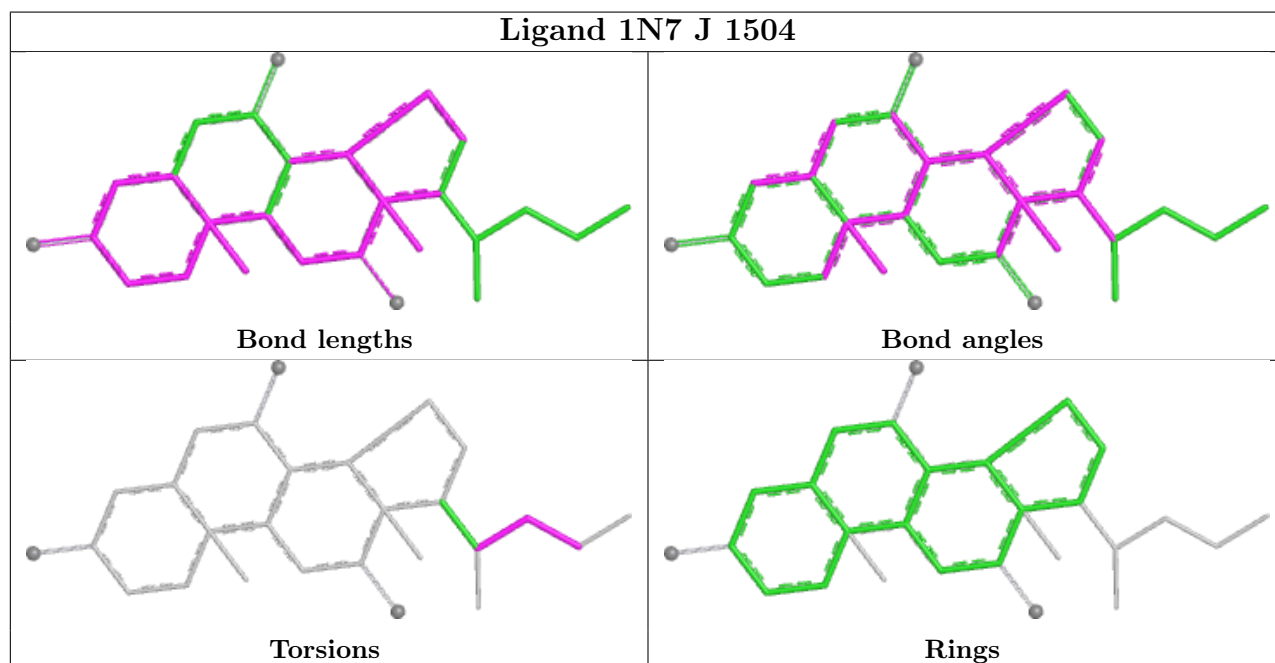
Mol	Chain	Res	Type	Atoms
10	N	102	1N7	C21-C20-C22-C23
10	J	1504	1N7	C9-C20-C22-C23
10	L	701	1N7	C22-C20-C9-C5
10	J	1504	1N7	C21-C20-C22-C23
10	L	701	1N7	C21-C20-C9-C5

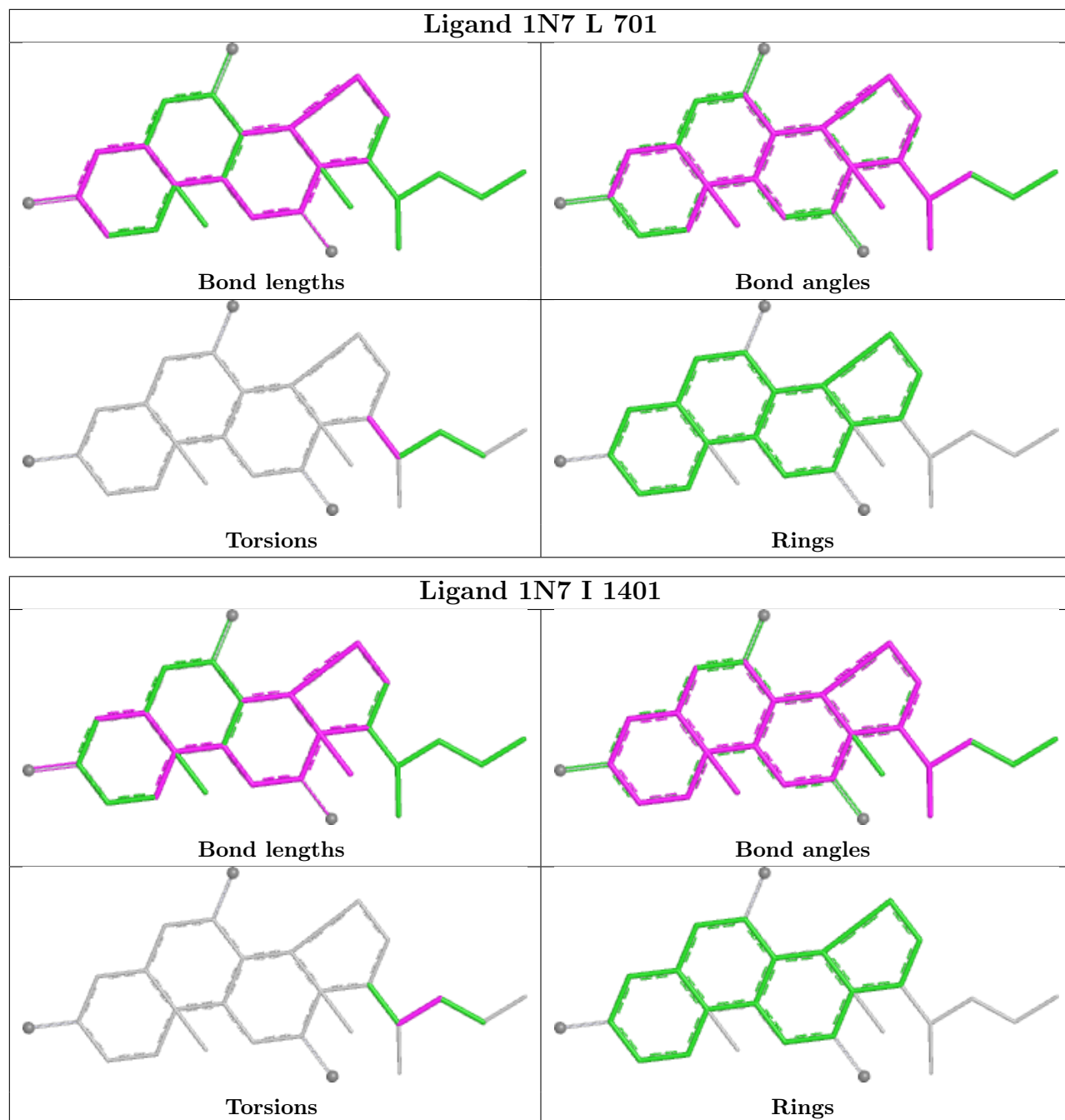
There are no ring outliers.

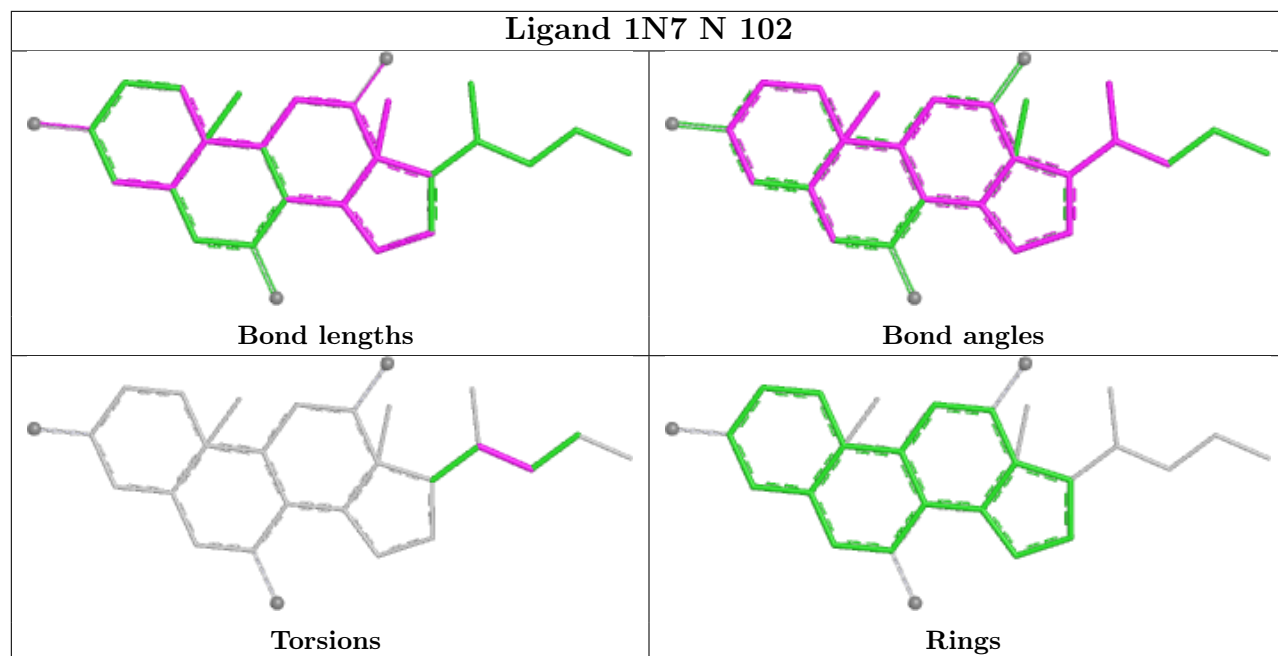
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	1504	1N7	3	0
10	L	701	1N7	3	0
10	I	1401	1N7	6	0
10	N	102	1N7	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

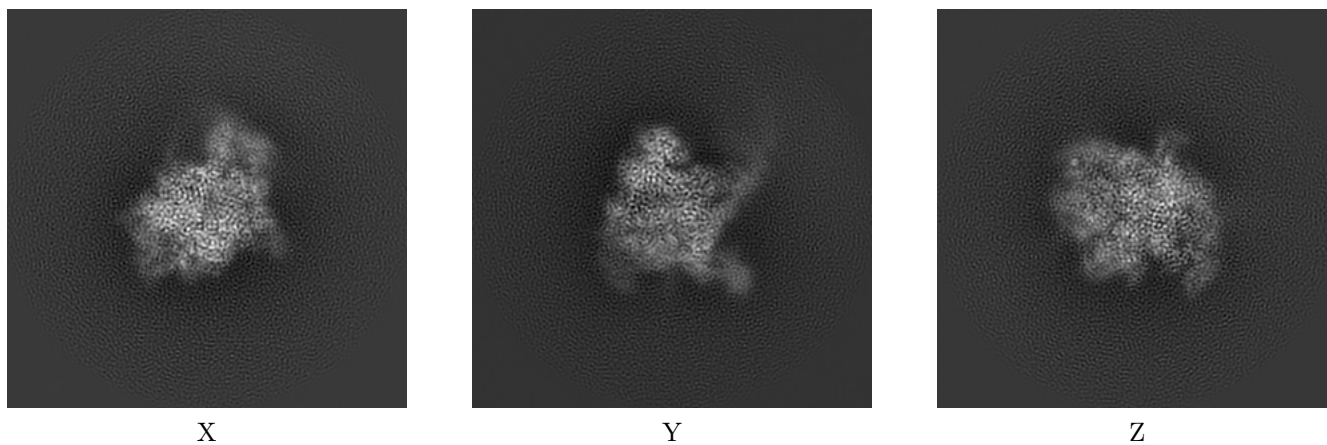
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20465. 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](#)

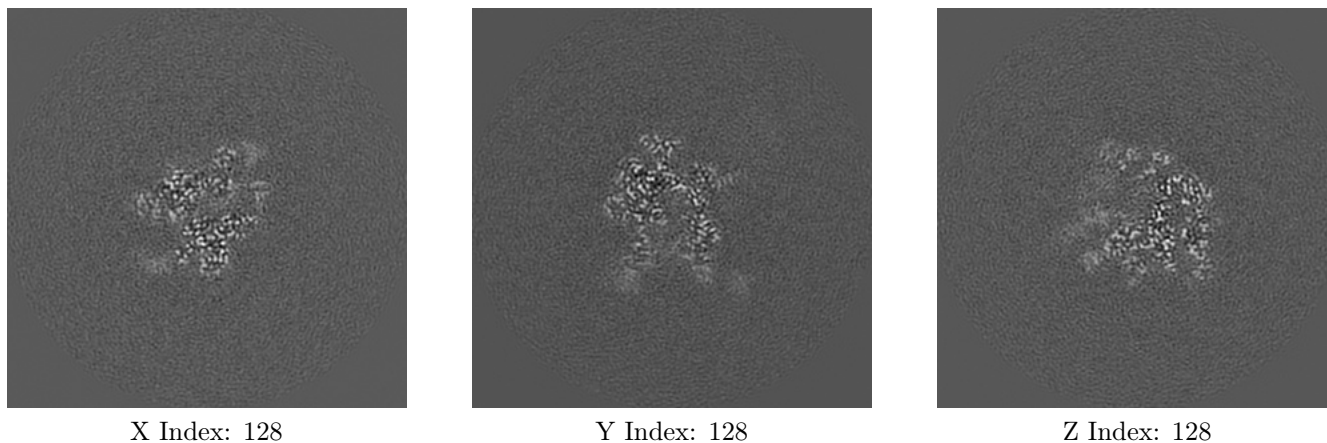
6.1.1 Primary map



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

6.2 Central slices [i](#)

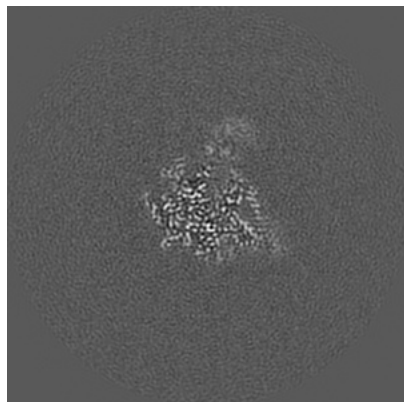
6.2.1 Primary map



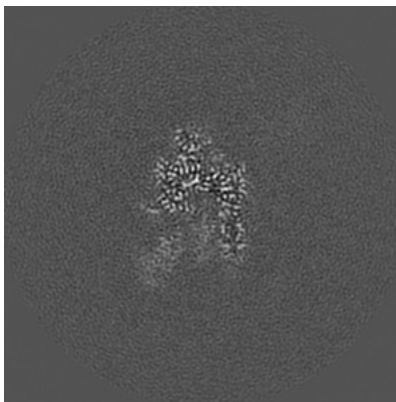
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

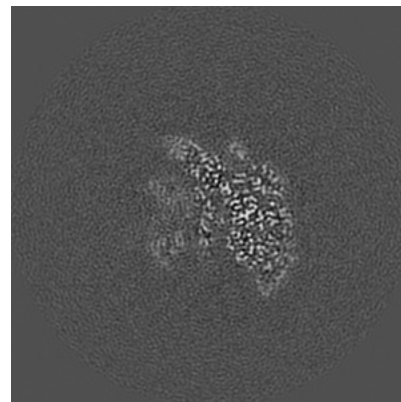
6.3.1 Primary map



X Index: 146



Y Index: 123

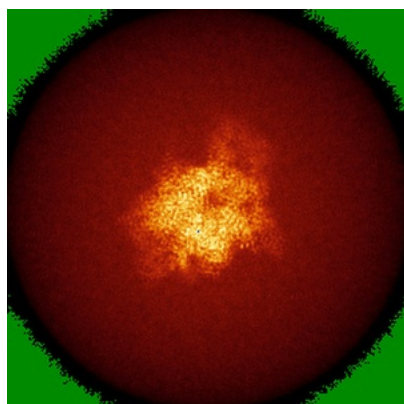


Z Index: 120

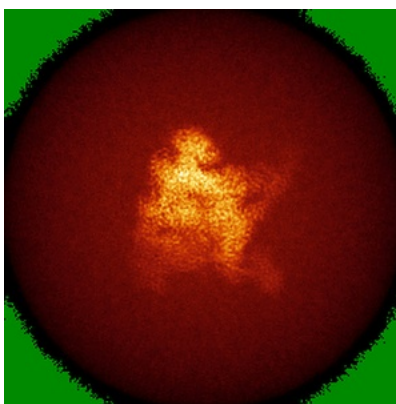
The images above show the largest variance slices of the map in three orthogonal directions.

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

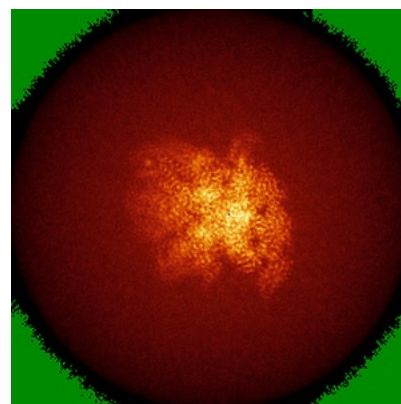
6.4.1 Primary map



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

This section was not generated.

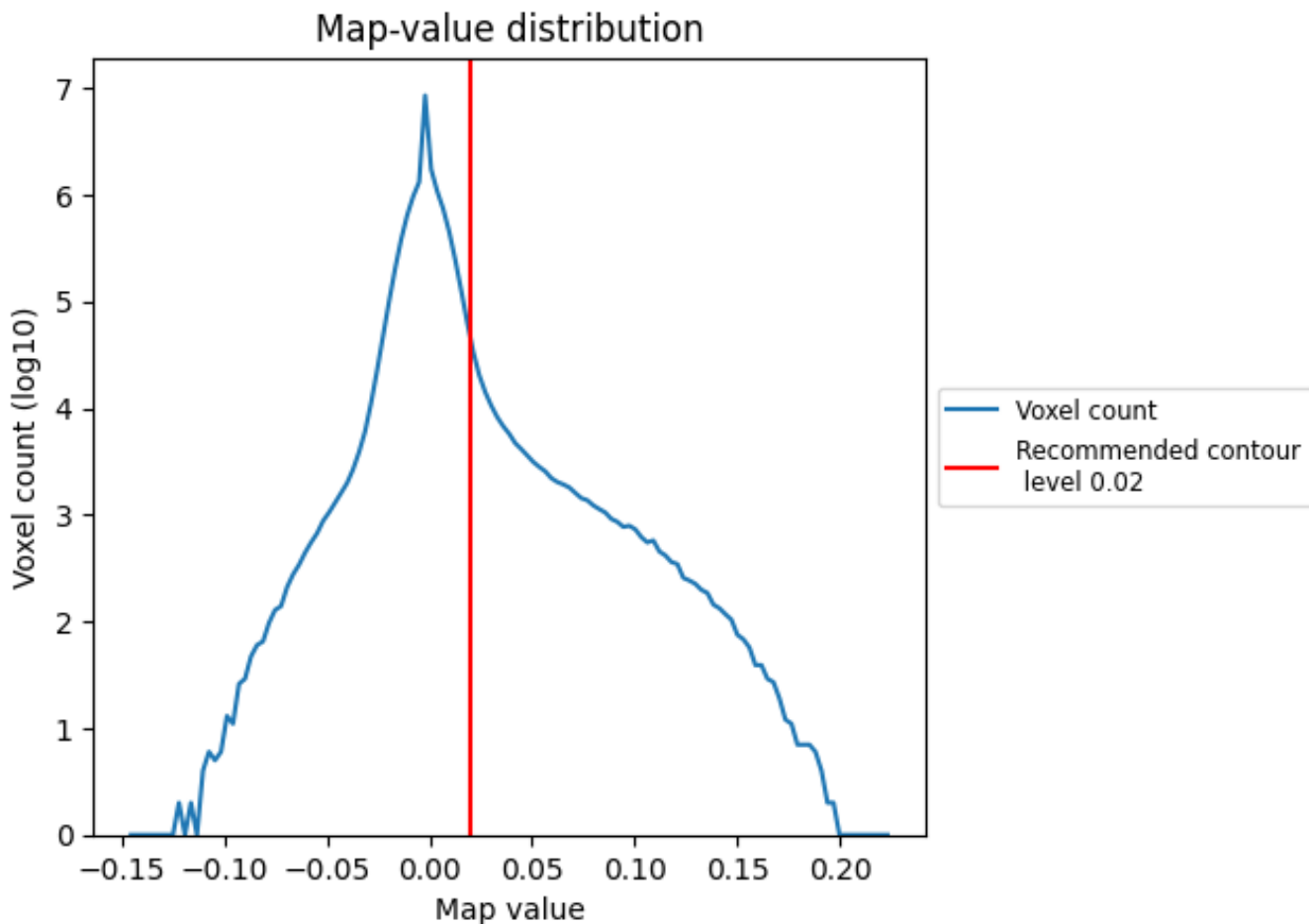
6.6 Mask visualisation

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

7 Map analysis [i](#)

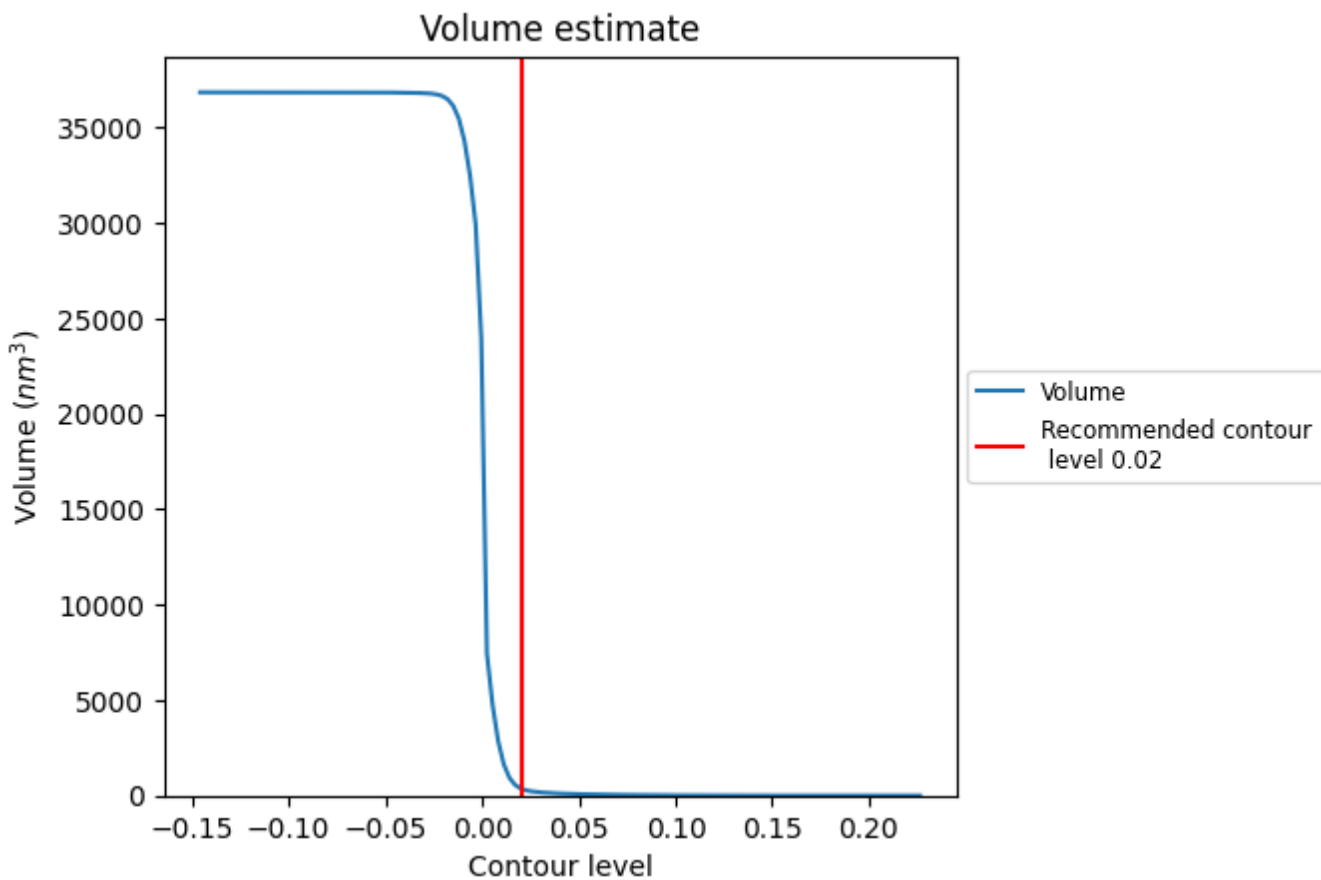
This section contains the results of statistical analysis of the map.

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.

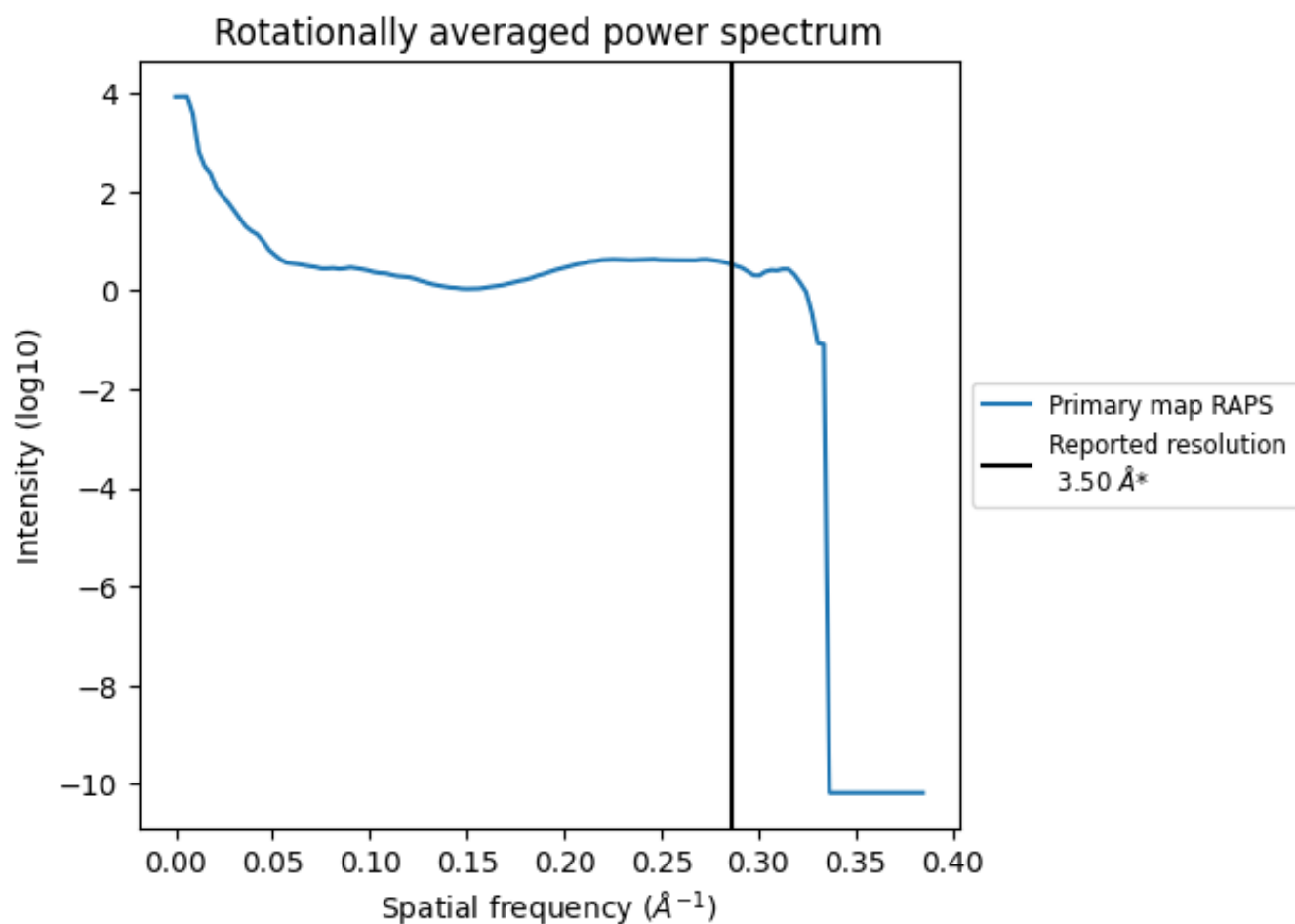
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 368 nm^3 ; this corresponds to an approximate mass of 332 kDa.

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

7.3 Rotationally averaged power spectrum i

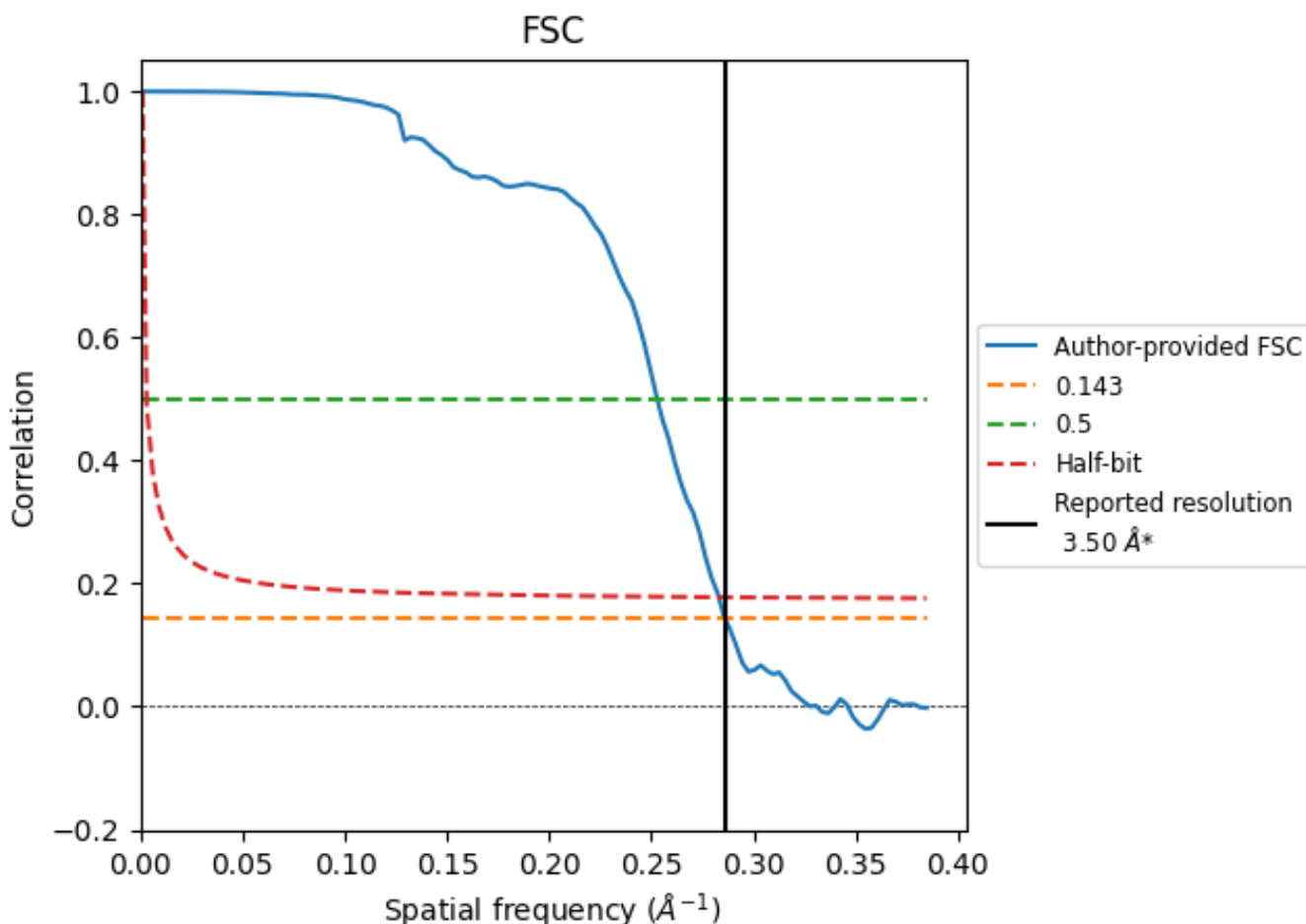


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

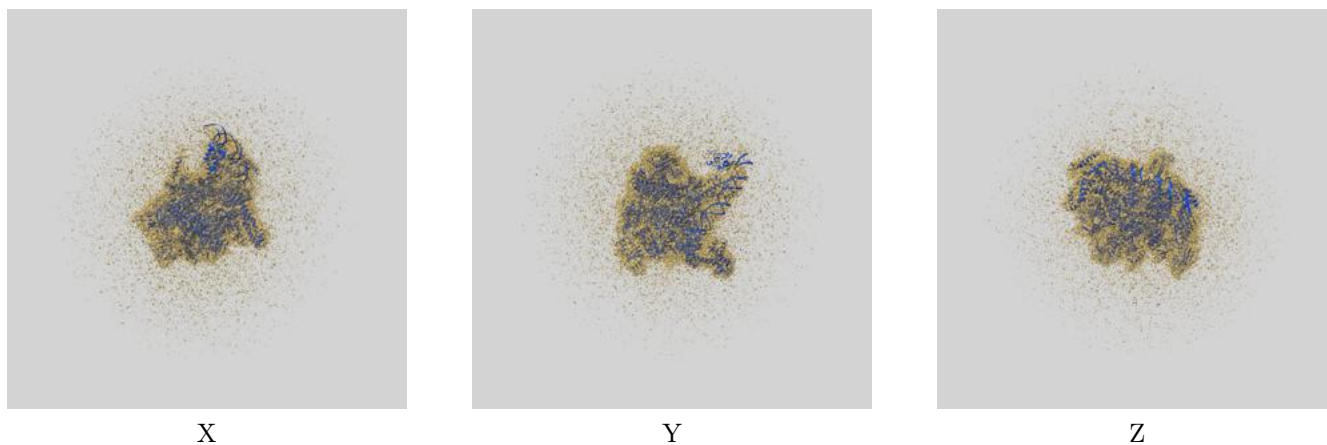
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	3.96	3.53
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

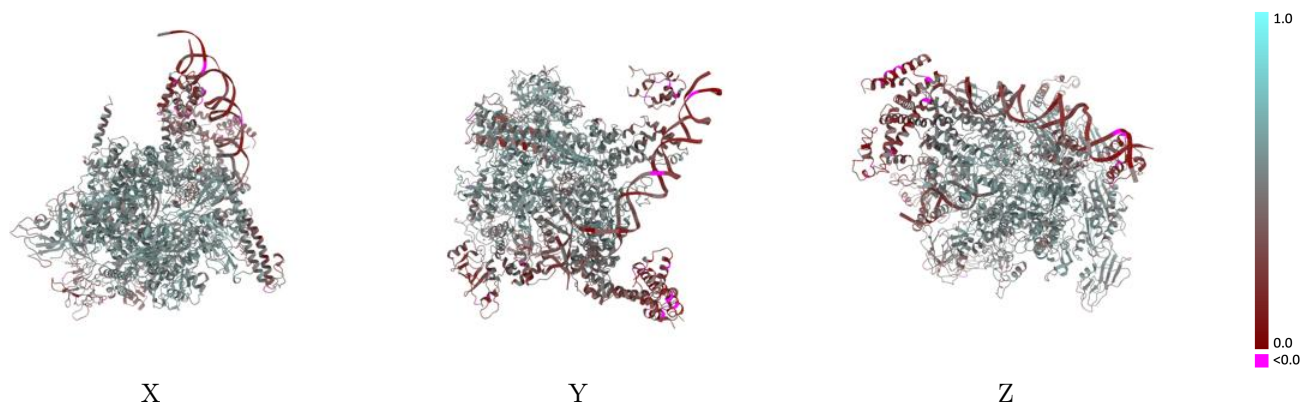
This section contains information regarding the fit between EMDB map EMD-20465 and PDB model 6PSV. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



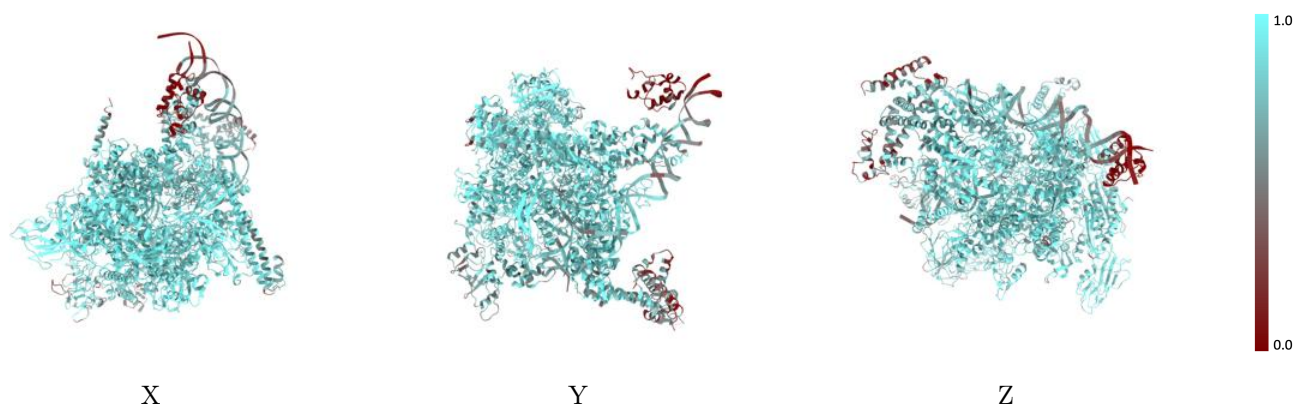
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



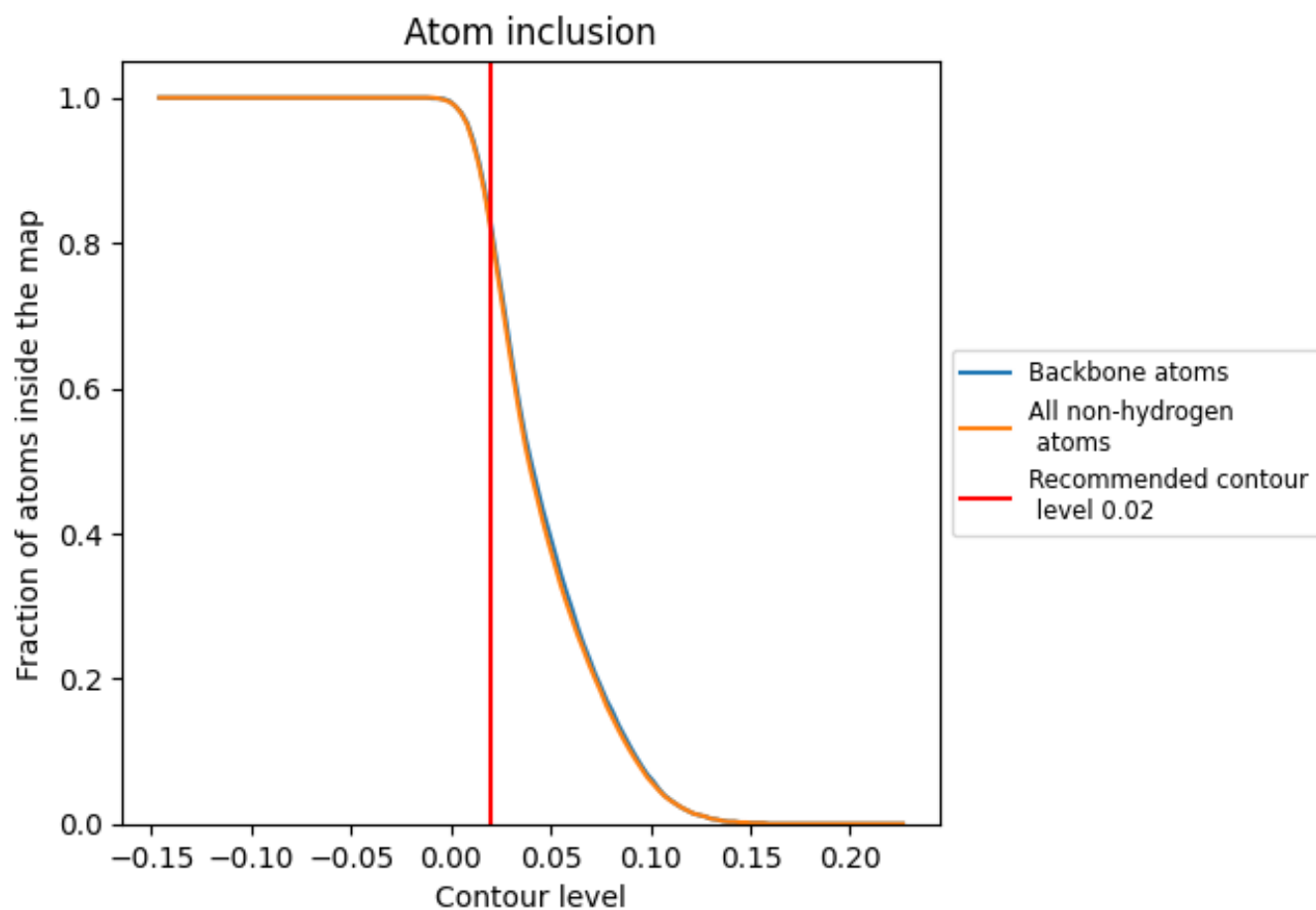
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).























9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8190	 0.4680
G	 0.8980	 0.5330
H	 0.8990	 0.5120
I	 0.8720	 0.5020
J	 0.8750	 0.5050
K	 0.7690	 0.5000
L	 0.7030	 0.3630
M	 0.0890	 0.2660
N	 0.8760	 0.5060
O	 0.6300	 0.2580
P	 0.5790	 0.2620

