



Full wwPDB EM Validation Report ⓘ

May 28, 2026 – 04:47 PM JST

PDB ID : 21KR / pdb_000021kr
EMDB ID : EMD-67778
Title : A Wnt3a/Fzd8-CRD/LRP6-E3E4 complex with FKBP
Authors : Yue, D.; Sun, G.; Zhang, L.; Wang, Z.; Xu, W.
Deposited on : 2025-12-17
Resolution : 2.90 Å (reported)
Based on initial models : 1FAP, 3S8Z, 6AHY

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 : 1.8.5 (274361), CSD as541be (2020)
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

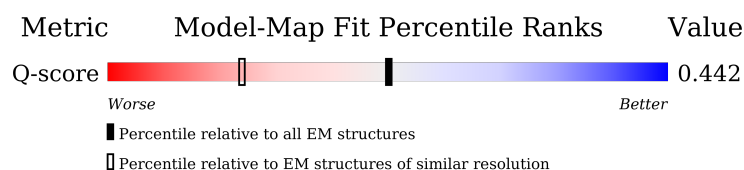
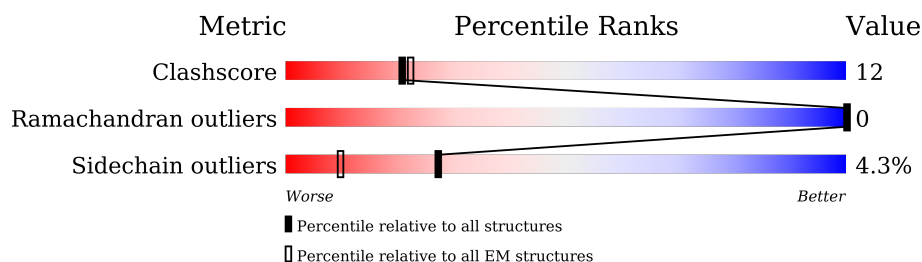
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	334	
1	E	334	
2	B	752	
2	F	752	

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Mol	Chain	Length	Quality of chain
3	C	271	
3	D	271	
3	G	271	
3	H	271	
3	I	271	
4	J	2	
4	K	2	
4	L	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 19900 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 Protein Wnt-3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2611	1615	485	484	27		
1	E	334	Total	C	N	O	S	0	0
			2611	1615	485	484	27		

- Molecule 2 is a protein called Low-density lipoprotein receptor-related protein 6,Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	616	Total	C	N	O	S	0	0
			4903	3075	868	935	25		
2	F	616	Total	C	N	O	S	0	0
			4903	3075	868	935	25		

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	622	ASP	-	expression tag	UNP O75581
B	623	TYR	-	expression tag	UNP O75581
B	624	LYS	-	expression tag	UNP O75581
B	625	ASP	-	expression tag	UNP O75581
B	626	ASP	-	expression tag	UNP O75581
B	627	ASP	-	expression tag	UNP O75581
B	628	ASP	-	expression tag	UNP O75581
B	629	LYS	-	expression tag	UNP O75581
B	1246	GLY	-	linker	UNP O75581
B	1247	GLY	-	linker	UNP O75581
B	1248	GLY	-	linker	UNP O75581
B	1249	GLY	-	linker	UNP O75581
B	1250	SER	-	linker	UNP O75581
B	1251	GLY	-	linker	UNP O75581
B	1252	GLY	-	linker	UNP O75581
B	1253	GLY	-	linker	UNP O75581

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1254	GLY	-	linker	UNP O75581
B	1255	SER	-	linker	UNP O75581
B	1256	GLY	-	linker	UNP O75581
B	1257	GLY	-	linker	UNP O75581
B	1258	GLY	-	linker	UNP O75581
B	1259	GLY	-	linker	UNP O75581
B	1260	SER	-	linker	UNP O75581
B	1261	GLY	-	linker	UNP O75581
B	1262	GLY	-	linker	UNP O75581
B	1263	GLY	-	linker	UNP O75581
B	1264	GLY	-	linker	UNP O75581
B	1265	SER	-	linker	UNP O75581
B	1336	SER	CYS	engineered mutation	UNP A0A8V8TRG9
B	1366	HIS	-	expression tag	UNP A0A8V8TRG9
B	1367	HIS	-	expression tag	UNP A0A8V8TRG9
B	1368	HIS	-	expression tag	UNP A0A8V8TRG9
B	1369	HIS	-	expression tag	UNP A0A8V8TRG9
B	1370	HIS	-	expression tag	UNP A0A8V8TRG9
B	1371	HIS	-	expression tag	UNP A0A8V8TRG9
B	1372	HIS	-	expression tag	UNP A0A8V8TRG9
B	1373	HIS	-	expression tag	UNP A0A8V8TRG9
F	622	ASP	-	expression tag	UNP O75581
F	623	TYR	-	expression tag	UNP O75581
F	624	LYS	-	expression tag	UNP O75581
F	625	ASP	-	expression tag	UNP O75581
F	626	ASP	-	expression tag	UNP O75581
F	627	ASP	-	expression tag	UNP O75581
F	628	ASP	-	expression tag	UNP O75581
F	629	LYS	-	expression tag	UNP O75581
F	1246	GLY	-	linker	UNP O75581
F	1247	GLY	-	linker	UNP O75581
F	1248	GLY	-	linker	UNP O75581
F	1249	GLY	-	linker	UNP O75581
F	1250	SER	-	linker	UNP O75581
F	1251	GLY	-	linker	UNP O75581
F	1252	GLY	-	linker	UNP O75581
F	1253	GLY	-	linker	UNP O75581
F	1254	GLY	-	linker	UNP O75581
F	1255	SER	-	linker	UNP O75581
F	1256	GLY	-	linker	UNP O75581
F	1257	GLY	-	linker	UNP O75581
F	1258	GLY	-	linker	UNP O75581

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1259	GLY	-	linker	UNP O75581
F	1260	SER	-	linker	UNP O75581
F	1261	GLY	-	linker	UNP O75581
F	1262	GLY	-	linker	UNP O75581
F	1263	GLY	-	linker	UNP O75581
F	1264	GLY	-	linker	UNP O75581
F	1265	SER	-	linker	UNP O75581
F	1336	SER	CYS	engineered mutation	UNP A0A8V8TRG9
F	1366	HIS	-	expression tag	UNP A0A8V8TRG9
F	1367	HIS	-	expression tag	UNP A0A8V8TRG9
F	1368	HIS	-	expression tag	UNP A0A8V8TRG9
F	1369	HIS	-	expression tag	UNP A0A8V8TRG9
F	1370	HIS	-	expression tag	UNP A0A8V8TRG9
F	1371	HIS	-	expression tag	UNP A0A8V8TRG9
F	1372	HIS	-	expression tag	UNP A0A8V8TRG9
F	1373	HIS	-	expression tag	UNP A0A8V8TRG9

- Molecule 3 is a protein called Frizzled-8,Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	119	Total	C	N	O	S	0	0
			959	610	159	175	15		
3	D	119	Total	C	N	O	S	0	0
			959	610	159	175	15		
3	G	119	Total	C	N	O	S	0	0
			959	610	159	175	15		
3	H	119	Total	C	N	O	S	0	0
			959	610	159	175	15		
3	I	107	Total	C	N	O	S	0	0
			831	527	146	155	3		

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	expression tag	UNP Q9H461
C	21	HIS	-	expression tag	UNP Q9H461
C	22	HIS	-	expression tag	UNP Q9H461
C	23	HIS	-	expression tag	UNP Q9H461
C	24	HIS	-	expression tag	UNP Q9H461
C	25	HIS	-	expression tag	UNP Q9H461
C	26	HIS	-	expression tag	UNP Q9H461
C	27	HIS	-	expression tag	UNP Q9H461

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	ALA	-	expression tag	UNP Q9H461
C	29	SER	-	expression tag	UNP Q9H461
C	30	ALA	-	expression tag	UNP Q9H461
C	156	GLY	-	linker	UNP Q9H461
C	157	GLY	-	linker	UNP Q9H461
C	158	GLY	-	linker	UNP Q9H461
C	159	GLY	-	linker	UNP Q9H461
C	160	SER	-	linker	UNP Q9H461
C	161	GLY	-	linker	UNP Q9H461
C	162	GLY	-	linker	UNP Q9H461
C	163	GLY	-	linker	UNP Q9H461
C	164	GLY	-	linker	UNP Q9H461
C	165	SER	-	linker	UNP Q9H461
C	166	GLY	-	linker	UNP Q9H461
C	167	GLY	-	linker	UNP Q9H461
C	168	GLY	-	linker	UNP Q9H461
C	169	GLY	-	linker	UNP Q9H461
C	170	SER	-	linker	UNP Q9H461
C	171	GLY	-	linker	UNP Q9H461
C	172	GLY	-	linker	UNP Q9H461
C	173	GLY	-	linker	UNP Q9H461
C	174	GLY	-	linker	UNP Q9H461
C	175	SER	-	linker	UNP Q9H461
C	197	SER	CYS	engineered mutation	UNP P62942
C	283	ASP	-	expression tag	UNP P62942
C	284	TYR	-	expression tag	UNP P62942
C	285	LYS	-	expression tag	UNP P62942
C	286	ASP	-	expression tag	UNP P62942
C	287	ASP	-	expression tag	UNP P62942
C	288	ASP	-	expression tag	UNP P62942
C	289	ASP	-	expression tag	UNP P62942
C	290	LYS	-	expression tag	UNP P62942
D	20	HIS	-	expression tag	UNP Q9H461
D	21	HIS	-	expression tag	UNP Q9H461
D	22	HIS	-	expression tag	UNP Q9H461
D	23	HIS	-	expression tag	UNP Q9H461
D	24	HIS	-	expression tag	UNP Q9H461
D	25	HIS	-	expression tag	UNP Q9H461
D	26	HIS	-	expression tag	UNP Q9H461
D	27	HIS	-	expression tag	UNP Q9H461
D	28	ALA	-	expression tag	UNP Q9H461
D	29	SER	-	expression tag	UNP Q9H461

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	ALA	-	expression tag	UNP Q9H461
D	156	GLY	-	linker	UNP Q9H461
D	157	GLY	-	linker	UNP Q9H461
D	158	GLY	-	linker	UNP Q9H461
D	159	GLY	-	linker	UNP Q9H461
D	160	SER	-	linker	UNP Q9H461
D	161	GLY	-	linker	UNP Q9H461
D	162	GLY	-	linker	UNP Q9H461
D	163	GLY	-	linker	UNP Q9H461
D	164	GLY	-	linker	UNP Q9H461
D	165	SER	-	linker	UNP Q9H461
D	166	GLY	-	linker	UNP Q9H461
D	167	GLY	-	linker	UNP Q9H461
D	168	GLY	-	linker	UNP Q9H461
D	169	GLY	-	linker	UNP Q9H461
D	170	SER	-	linker	UNP Q9H461
D	171	GLY	-	linker	UNP Q9H461
D	172	GLY	-	linker	UNP Q9H461
D	173	GLY	-	linker	UNP Q9H461
D	174	GLY	-	linker	UNP Q9H461
D	175	SER	-	linker	UNP Q9H461
D	197	SER	CYS	engineered mutation	UNP P62942
D	283	ASP	-	expression tag	UNP P62942
D	284	TYR	-	expression tag	UNP P62942
D	285	LYS	-	expression tag	UNP P62942
D	286	ASP	-	expression tag	UNP P62942
D	287	ASP	-	expression tag	UNP P62942
D	288	ASP	-	expression tag	UNP P62942
D	289	ASP	-	expression tag	UNP P62942
D	290	LYS	-	expression tag	UNP P62942
G	20	HIS	-	expression tag	UNP Q9H461
G	21	HIS	-	expression tag	UNP Q9H461
G	22	HIS	-	expression tag	UNP Q9H461
G	23	HIS	-	expression tag	UNP Q9H461
G	24	HIS	-	expression tag	UNP Q9H461
G	25	HIS	-	expression tag	UNP Q9H461
G	26	HIS	-	expression tag	UNP Q9H461
G	27	HIS	-	expression tag	UNP Q9H461
G	28	ALA	-	expression tag	UNP Q9H461
G	29	SER	-	expression tag	UNP Q9H461
G	30	ALA	-	expression tag	UNP Q9H461
G	156	GLY	-	linker	UNP Q9H461

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Chain	Residue	Modelled	Actual	Comment	Reference
G	157	GLY	-	linker	UNP Q9H461
G	158	GLY	-	linker	UNP Q9H461
G	159	GLY	-	linker	UNP Q9H461
G	160	SER	-	linker	UNP Q9H461
G	161	GLY	-	linker	UNP Q9H461
G	162	GLY	-	linker	UNP Q9H461
G	163	GLY	-	linker	UNP Q9H461
G	164	GLY	-	linker	UNP Q9H461
G	165	SER	-	linker	UNP Q9H461
G	166	GLY	-	linker	UNP Q9H461
G	167	GLY	-	linker	UNP Q9H461
G	168	GLY	-	linker	UNP Q9H461
G	169	GLY	-	linker	UNP Q9H461
G	170	SER	-	linker	UNP Q9H461
G	171	GLY	-	linker	UNP Q9H461
G	172	GLY	-	linker	UNP Q9H461
G	173	GLY	-	linker	UNP Q9H461
G	174	GLY	-	linker	UNP Q9H461
G	175	SER	-	linker	UNP Q9H461
G	197	SER	CYS	engineered mutation	UNP P62942
G	283	ASP	-	expression tag	UNP P62942
G	284	TYR	-	expression tag	UNP P62942
G	285	LYS	-	expression tag	UNP P62942
G	286	ASP	-	expression tag	UNP P62942
G	287	ASP	-	expression tag	UNP P62942
G	288	ASP	-	expression tag	UNP P62942
G	289	ASP	-	expression tag	UNP P62942
G	290	LYS	-	expression tag	UNP P62942
H	20	HIS	-	expression tag	UNP Q9H461
H	21	HIS	-	expression tag	UNP Q9H461
H	22	HIS	-	expression tag	UNP Q9H461
H	23	HIS	-	expression tag	UNP Q9H461
H	24	HIS	-	expression tag	UNP Q9H461
H	25	HIS	-	expression tag	UNP Q9H461
H	26	HIS	-	expression tag	UNP Q9H461
H	27	HIS	-	expression tag	UNP Q9H461
H	28	ALA	-	expression tag	UNP Q9H461
H	29	SER	-	expression tag	UNP Q9H461
H	30	ALA	-	expression tag	UNP Q9H461
H	156	GLY	-	linker	UNP Q9H461
H	157	GLY	-	linker	UNP Q9H461
H	158	GLY	-	linker	UNP Q9H461

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Chain	Residue	Modelled	Actual	Comment	Reference
H	159	GLY	-	linker	UNP Q9H461
H	160	SER	-	linker	UNP Q9H461
H	161	GLY	-	linker	UNP Q9H461
H	162	GLY	-	linker	UNP Q9H461
H	163	GLY	-	linker	UNP Q9H461
H	164	GLY	-	linker	UNP Q9H461
H	165	SER	-	linker	UNP Q9H461
H	166	GLY	-	linker	UNP Q9H461
H	167	GLY	-	linker	UNP Q9H461
H	168	GLY	-	linker	UNP Q9H461
H	169	GLY	-	linker	UNP Q9H461
H	170	SER	-	linker	UNP Q9H461
H	171	GLY	-	linker	UNP Q9H461
H	172	GLY	-	linker	UNP Q9H461
H	173	GLY	-	linker	UNP Q9H461
H	174	GLY	-	linker	UNP Q9H461
H	175	SER	-	linker	UNP Q9H461
H	197	SER	CYS	engineered mutation	UNP P62942
H	283	ASP	-	expression tag	UNP P62942
H	284	TYR	-	expression tag	UNP P62942
H	285	LYS	-	expression tag	UNP P62942
H	286	ASP	-	expression tag	UNP P62942
H	287	ASP	-	expression tag	UNP P62942
H	288	ASP	-	expression tag	UNP P62942
H	289	ASP	-	expression tag	UNP P62942
H	290	LYS	-	expression tag	UNP P62942
I	-155	HIS	-	expression tag	UNP Q9H461
I	-154	HIS	-	expression tag	UNP Q9H461
I	-153	HIS	-	expression tag	UNP Q9H461
I	-152	HIS	-	expression tag	UNP Q9H461
I	-151	HIS	-	expression tag	UNP Q9H461
I	-150	HIS	-	expression tag	UNP Q9H461
I	-149	HIS	-	expression tag	UNP Q9H461
I	-148	HIS	-	expression tag	UNP Q9H461
I	-147	ALA	-	expression tag	UNP Q9H461
I	-146	SER	-	expression tag	UNP Q9H461
I	-145	ALA	-	expression tag	UNP Q9H461
I	-19	GLY	-	linker	UNP Q9H461
I	-18	GLY	-	linker	UNP Q9H461
I	-17	GLY	-	linker	UNP Q9H461
I	-16	GLY	-	linker	UNP Q9H461
I	-15	SER	-	linker	UNP Q9H461

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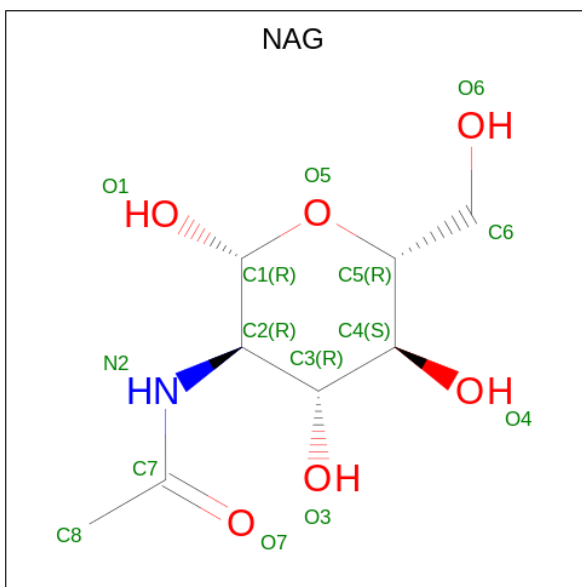
Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	GLY	-	linker	UNP Q9H461
I	-13	GLY	-	linker	UNP Q9H461
I	-12	GLY	-	linker	UNP Q9H461
I	-11	GLY	-	linker	UNP Q9H461
I	-10	SER	-	linker	UNP Q9H461
I	-9	GLY	-	linker	UNP Q9H461
I	-8	GLY	-	linker	UNP Q9H461
I	-7	GLY	-	linker	UNP Q9H461
I	-6	GLY	-	linker	UNP Q9H461
I	-5	SER	-	linker	UNP Q9H461
I	-4	GLY	-	linker	UNP Q9H461
I	-3	GLY	-	linker	UNP Q9H461
I	-2	GLY	-	linker	UNP Q9H461
I	-1	GLY	-	linker	UNP Q9H461
I	0	SER	-	linker	UNP Q9H461
I	22	SER	CYS	engineered mutation	UNP P62942
I	108	ASP	-	expression tag	UNP P62942
I	109	TYR	-	expression tag	UNP P62942
I	110	LYS	-	expression tag	UNP P62942
I	111	ASP	-	expression tag	UNP P62942
I	112	ASP	-	expression tag	UNP P62942
I	113	ASP	-	expression tag	UNP P62942
I	114	ASP	-	expression tag	UNP P62942
I	115	LYS	-	expression tag	UNP P62942

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



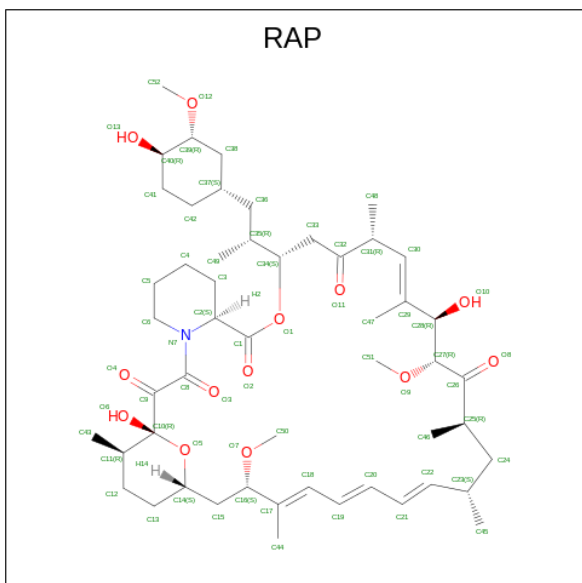
Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0

- Molecule 6 is RAPAMYCIN IMMUNOSUPPRESSANT DRUG (CCD ID: RAP) (formula: $C_{51}H_{79}NO_{13}$) (labeled as "Ligand of Interest" by depositor).

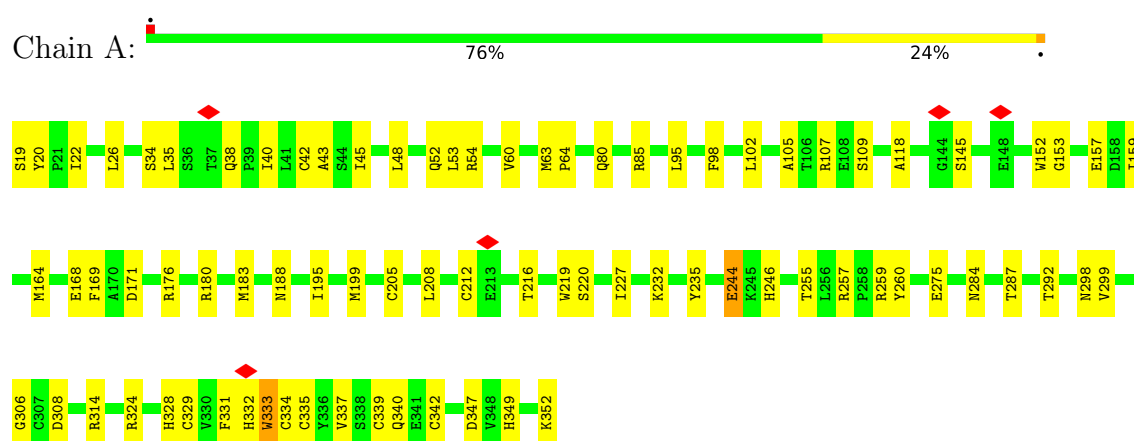


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	I	1	65	51	1	13	0

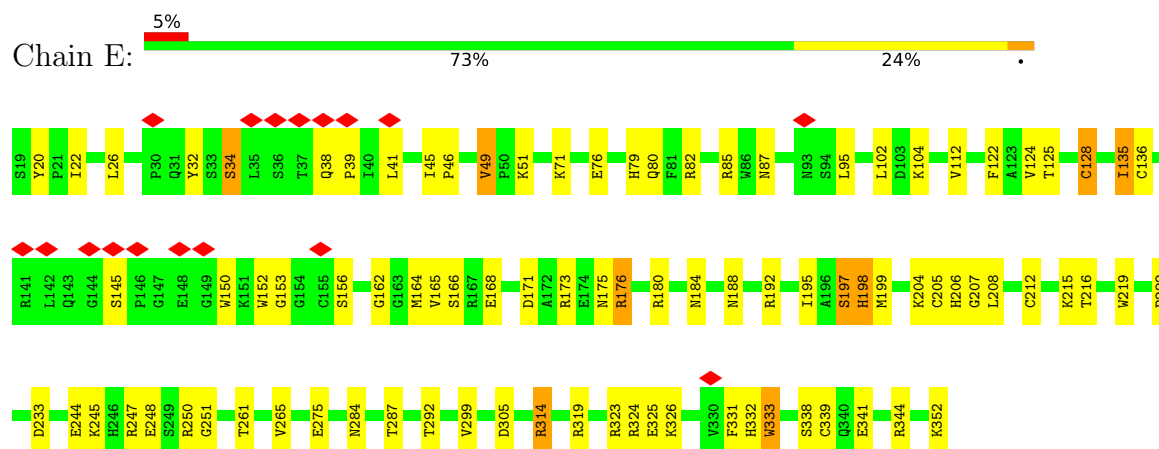
3 Residue-property plots

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.

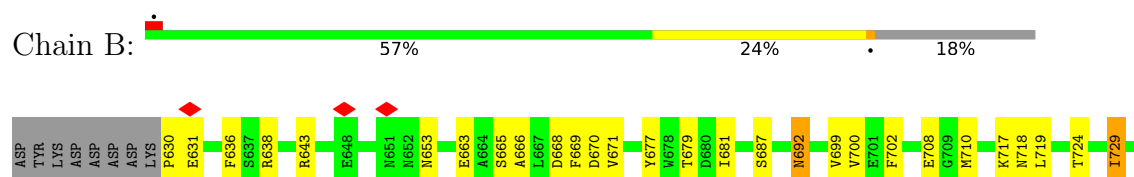
• Molecule 1: Protein Wnt-3a

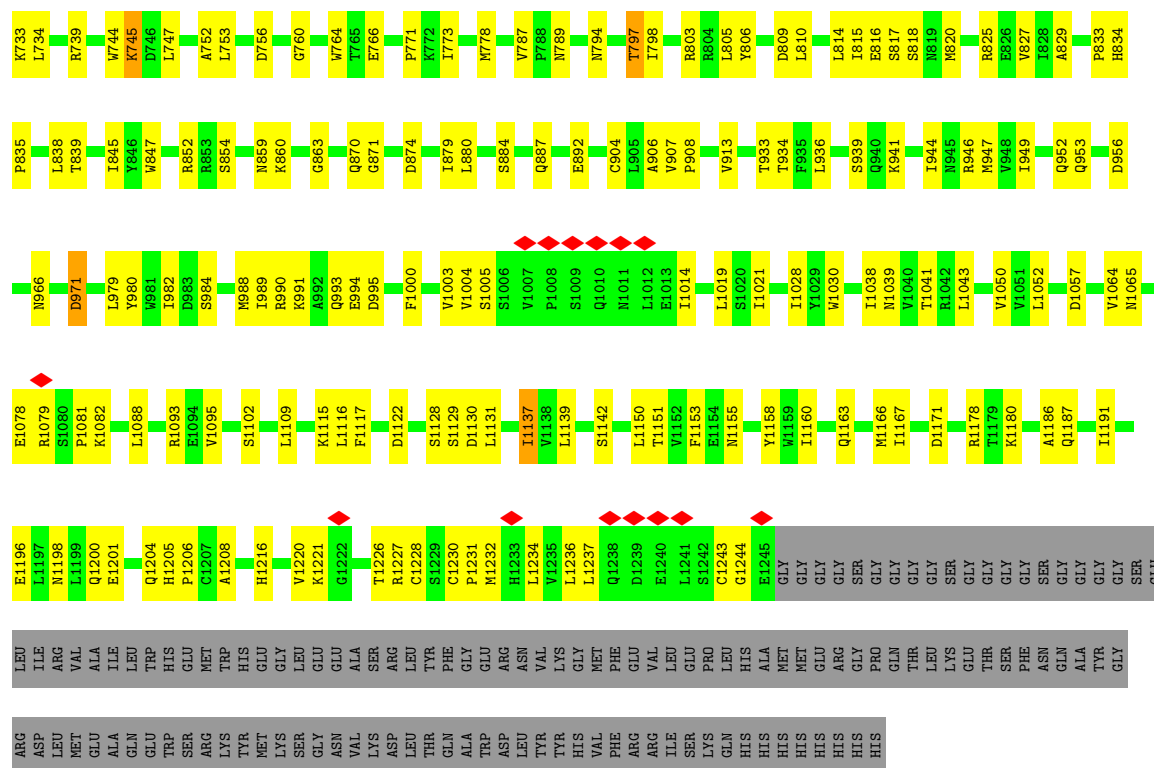


• Molecule 1: Protein Wnt-3a

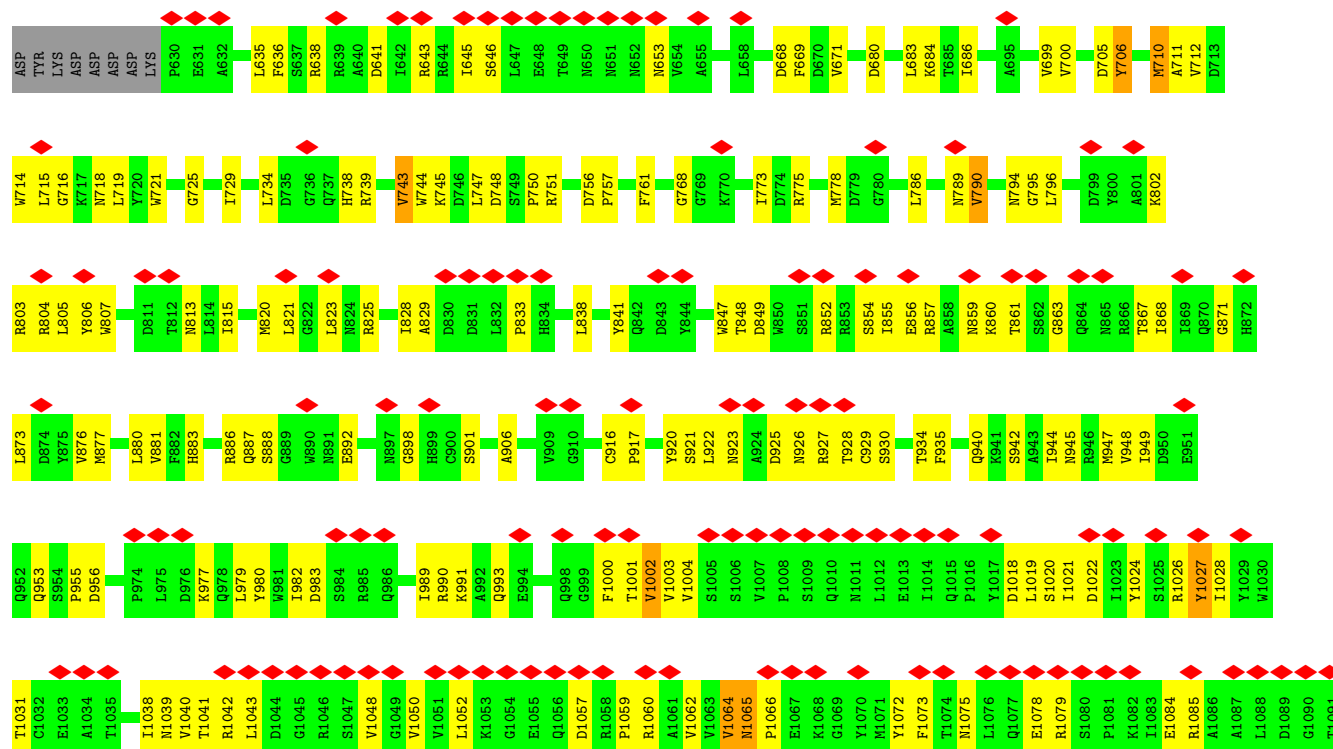


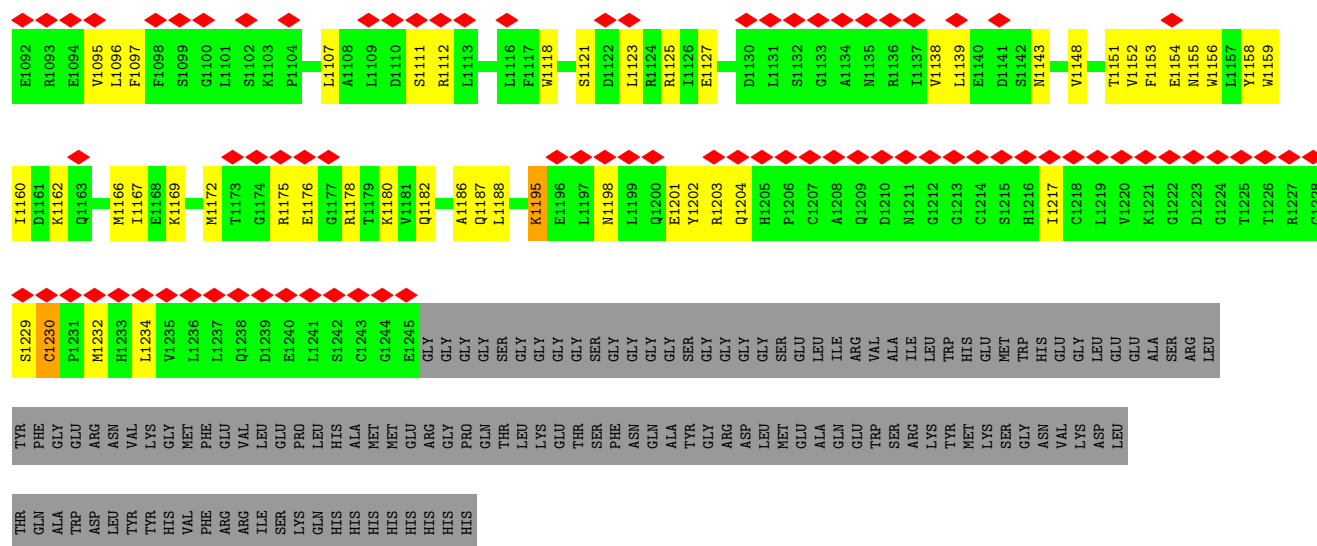
• Molecule 2: Low-density lipoprotein receptor-related protein 6, Serine/threonine-protein kinase mTOR



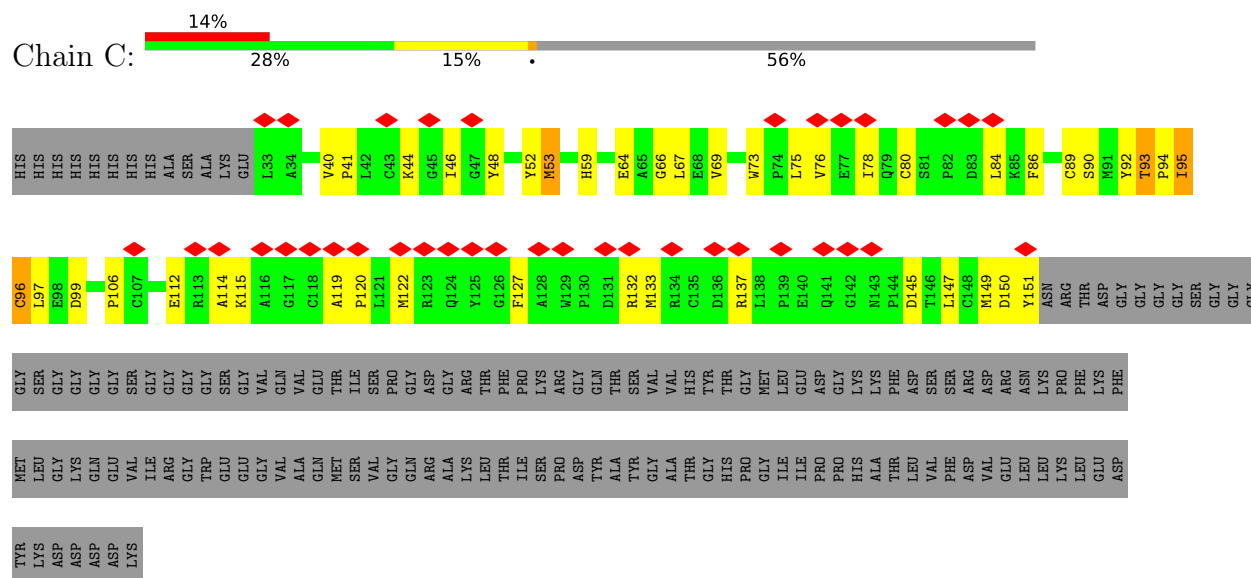


- Molecule 2: Low-density lipoprotein receptor-related protein 6, Serine/threonine-protein kinase mTOR

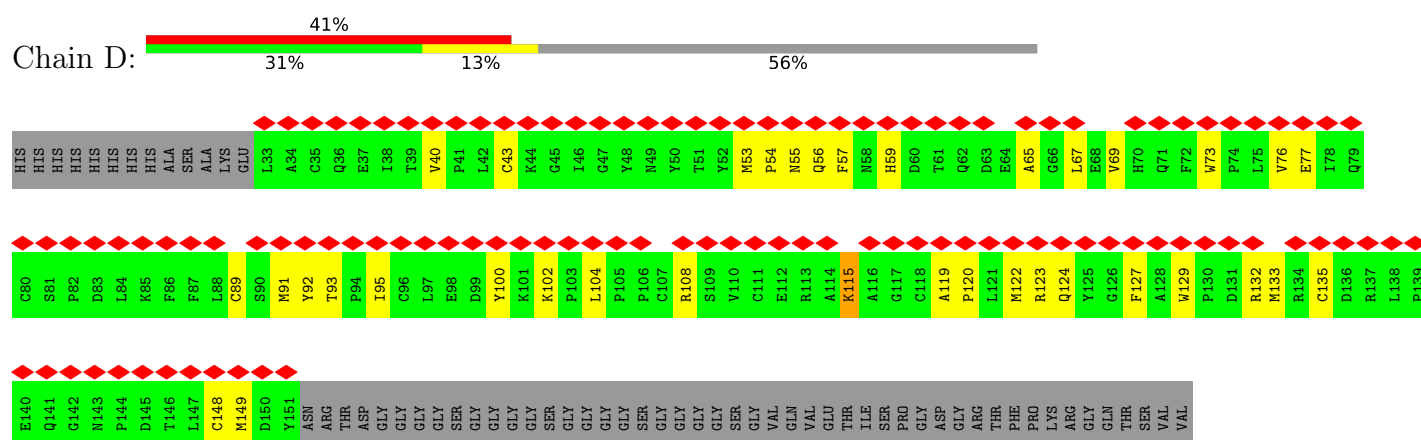


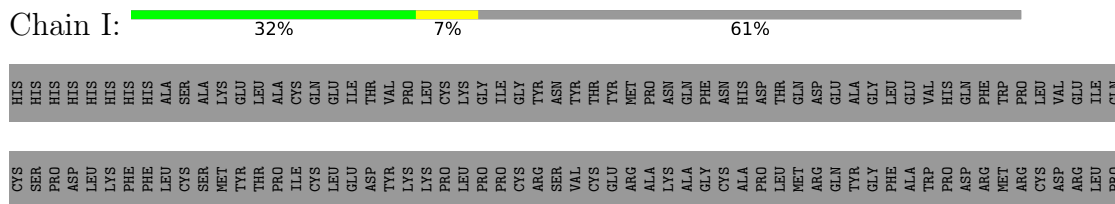
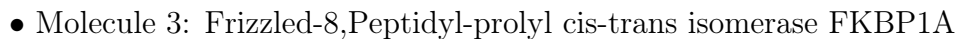
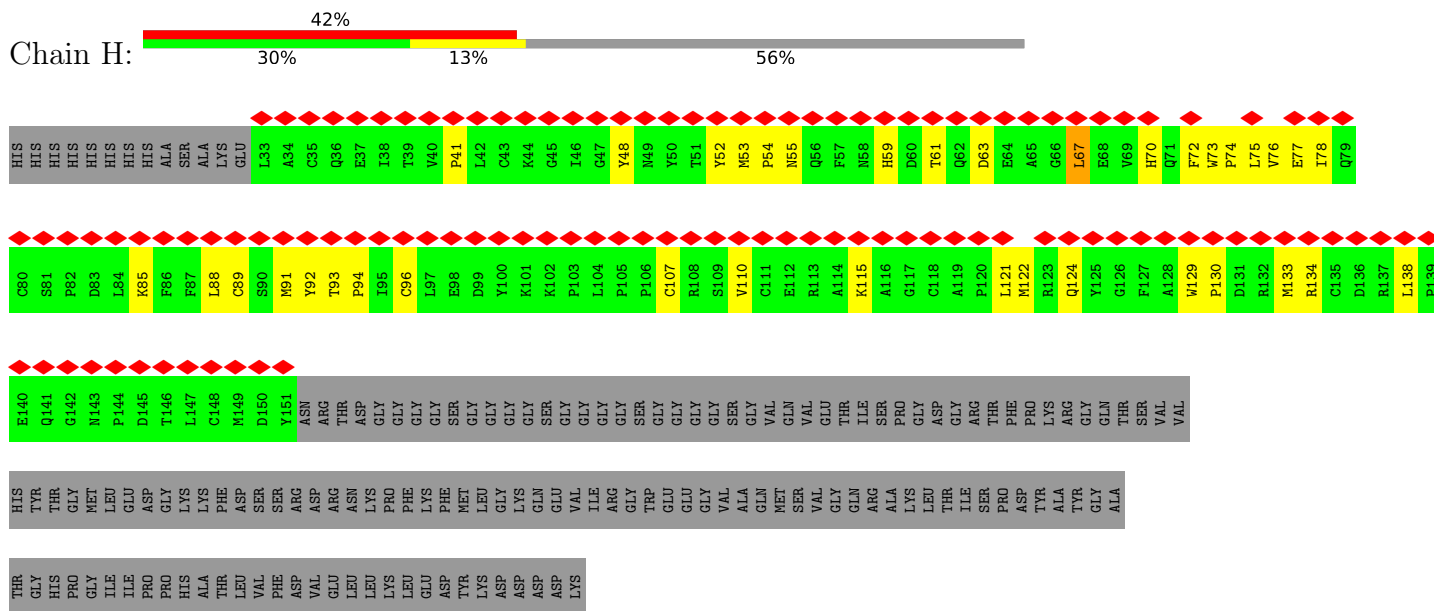
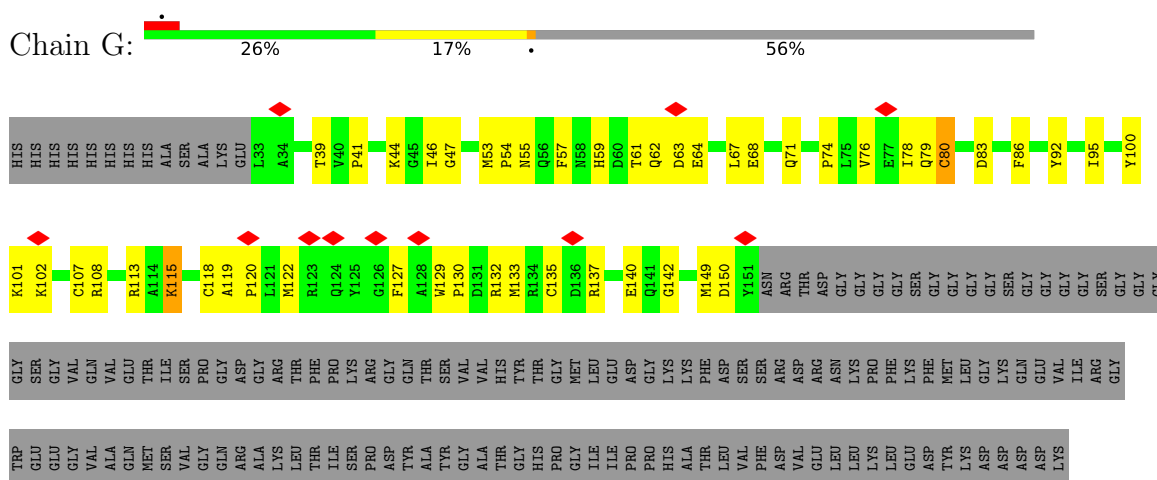
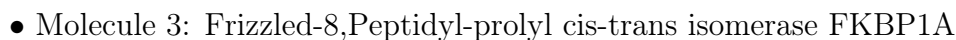
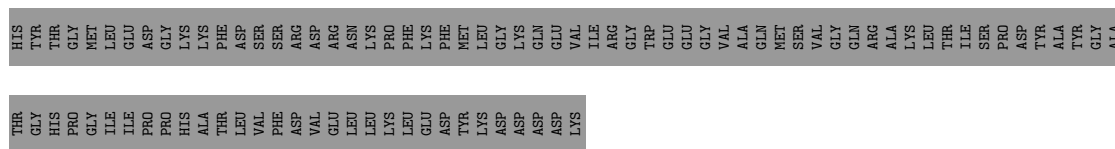


● Molecule 3: Frizzled-8,Peptidyl-prolyl cis-trans isomerase FKBP1A



● Molecule 3: Frizzled-8,Peptidyl-prolyl cis-trans isomerase FKBP1A







- Chain J: 100%



- Chain K:  50% 50%



- Chain L: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	399445	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.791	Depositor
Minimum map value	-1.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.1	Depositor
Map size (\AA)	332.80002, 332.80002, 332.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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	0/2678	0.41	0/3622
1	E	0.19	0/2678	0.37	0/3622
2	B	0.18	0/5007	0.39	1/6796 (0.0%)
2	F	0.15	0/5007	0.36	0/6796
3	C	0.18	0/988	0.49	1/1343 (0.1%)
3	D	0.16	0/988	0.33	0/1343
3	G	0.16	0/988	0.38	0/1343
3	H	0.18	0/988	0.36	0/1343
3	I	0.17	0/850	0.41	0/1146
All	All	0.18	0/20172	0.38	2/27354 (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
1	A	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	92	TYR	N-CA-C	-6.41	104.21	111.14
2	B	939	SER	N-CA-C	5.30	117.61	109.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	TRP	Peptide
1	E	333	TRP	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	A	2611	0	2457	50	0
1	E	2611	0	2457	54	0
2	B	4903	0	4780	108	0
2	F	4903	0	4783	140	0
3	C	959	0	906	34	0
3	D	959	0	906	24	0
3	G	959	0	906	37	0
3	H	959	0	906	24	0
3	I	831	0	831	16	0
4	J	28	0	25	0	0
4	K	28	0	25	1	0
4	L	28	0	25	0	0
5	A	14	0	13	0	0
5	B	42	0	39	1	0
6	I	65	0	79	5	0
All	All	19900	0	19138	470	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 12.

All (470) 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)
2:F:926:ASN:HB2	2:F:927:ARG:HH21	1.45	0.82
2:F:1027:TYR:OH	2:F:1048:VAL:HG11	1.82	0.80
2:F:1111:SER:HB3	2:F:1112:ARG:HH21	1.47	0.78
2:F:982:ILE:HG12	2:F:989:ILE:HG12	1.67	0.77
2:B:988:MET:HE3	2:B:990:ARG:HB2	1.69	0.75
2:B:699:VAL:HG12	2:B:700:VAL:HG23	1.67	0.75
3:I:24:VAL:HG22	3:I:103:LEU:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:53:MET:SD	3:D:53:MET:N	2.61	0.74
2:F:881:VAL:HG13	2:F:886:ARG:HG3	1.71	0.73
3:G:130:PRO:HG2	3:G:133:MET:HG2	1.69	0.73
1:E:198:HIS:HB3	1:E:222:PRO:HG3	1.73	0.71
2:F:947:MET:HB2	2:F:956:ASP:HB3	1.72	0.71
2:F:1064:VAL:HG23	2:F:1066:PRO:HD3	1.72	0.71
3:C:52:TYR:CZ	3:C:94:PRO:HB2	2.26	0.70
1:E:102:LEU:HD11	1:E:112:VAL:HG11	1.72	0.70
2:F:859:ASN:HB3	2:F:863:GLY:H	1.57	0.70
1:A:98:PHE:CD2	1:A:102:LEU:HD11	2.26	0.70
2:F:715:LEU:HD11	2:F:757:PRO:HB2	1.73	0.69
3:I:23:VAL:HG22	3:I:47:LYS:HG2	1.75	0.68
2:F:745:LYS:HZ2	2:F:953:GLN:HB2	1.58	0.68
3:H:88:LEU:HD22	3:H:91:MET:HE2	1.74	0.68
2:B:745:LYS:HZ3	2:B:953:GLN:HB2	1.59	0.68
1:E:176:ARG:HH12	2:F:768:GLY:HA2	1.58	0.68
2:F:877:MET:HE2	2:F:877:MET:HA	1.76	0.67
2:B:982:ILE:HG12	2:B:989:ILE:HG12	1.75	0.67
2:B:1122:ASP:O	3:I:18:ARG:NH1	2.27	0.67
2:B:1236:LEU:HA	2:B:1243:CYS:HB3	1.77	0.67
2:B:833:PRO:HG2	2:B:852:ARG:HD3	1.75	0.67
2:F:1127:GLU:HG2	2:F:1138:VAL:HA	1.77	0.66
2:F:1024:TYR:HA	2:F:1202:TYR:HE1	1.61	0.65
3:C:149:MET:HA	3:C:149:MET:HE3	1.77	0.65
1:A:314:ARG:NH1	1:A:352:LYS:O	2.28	0.65
3:C:97:LEU:HG	3:C:99:ASP:H	1.60	0.65
2:B:668:ASP:HB2	2:B:710:MET:CE	2.27	0.64
1:E:125:THR:HG23	1:E:162:GLY:HA3	1.80	0.64
2:F:1111:SER:HB3	2:F:1112:ARG:NH2	2.12	0.64
2:F:1160:ILE:HD12	2:F:1188:LEU:HB3	1.80	0.64
3:G:55:ASN:HD21	3:G:59:HIS:HB2	1.62	0.64
3:D:132:ARG:NH2	3:D:133:MET:HG2	2.13	0.63
2:F:1160:ILE:HG22	2:F:1167:ILE:HG12	1.80	0.63
1:E:79:HIS:O	1:E:82:ARG:NH1	2.32	0.63
3:I:102:GLU:HG2	3:I:104:LEU:HD22	1.79	0.63
1:A:26:LEU:HD11	1:A:45:ILE:HG12	1.80	0.63
1:A:299:VAL:HG21	1:A:349:HIS:CE1	2.33	0.63
3:C:52:TYR:HD1	3:C:96:CYS:HB2	1.63	0.63
3:C:122:MET:HE3	3:C:122:MET:HA	1.81	0.63
1:E:85:ARG:HG2	1:E:292:THR:HG21	1.80	0.62
2:F:635:LEU:HD12	2:F:880:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1237:LEU:HG	2:B:1243:CYS:HA	1.81	0.62
1:E:180:ARG:NH1	1:E:184:ASN:OD1	2.32	0.62
2:B:971:ASP:HB3	2:B:1021:ILE:HD13	1.81	0.62
1:A:171:ASP:OD1	1:A:188:ASN:ND2	2.31	0.62
2:F:645:ILE:HD11	2:F:653:ASN:HD22	1.65	0.61
3:I:40:ARG:NH2	3:I:100:ASP:OD1	2.33	0.61
2:B:1160:ILE:HG22	2:B:1167:ILE:HG12	1.81	0.61
2:F:738:HIS:HA	2:F:917:PRO:HG3	1.82	0.61
1:E:122:PHE:HB2	1:E:195:ILE:HD11	1.81	0.61
2:B:944:ILE:HD13	2:B:979:LEU:HD21	1.82	0.61
3:H:52:TYR:HD1	3:H:96:CYS:HB2	1.65	0.61
2:F:1050:VAL:HB	2:F:1232:MET:HE1	1.82	0.61
2:B:1038:ILE:HB	2:B:1052:LEU:HB3	1.82	0.60
2:F:775:ARG:HD3	2:F:786:LEU:HD13	1.83	0.60
3:I:78:PRO:HD3	3:I:96:THR:OG1	2.01	0.60
3:C:48:TYR:OH	3:C:89:CYS:O	2.20	0.60
2:F:856:GLU:HG2	2:F:868:ILE:HG22	1.84	0.60
1:A:98:PHE:CD2	1:A:102:LEU:CD1	2.85	0.60
3:I:71:ARG:HG3	3:I:102:GLU:HB2	1.84	0.60
2:B:1082:LYS:HE3	2:B:1095:VAL:HG11	1.83	0.59
2:F:699:VAL:HG12	2:F:700:VAL:HG23	1.85	0.59
3:C:133:MET:HE2	3:C:133:MET:HA	1.84	0.59
2:B:719:LEU:HB2	2:B:734:LEU:HD23	1.83	0.59
1:E:102:LEU:O	1:E:180:ARG:NH2	2.35	0.59
1:E:326:LYS:HG2	1:E:339:CYS:HB2	1.85	0.59
1:A:153:GLY:HA3	1:A:216:THR:HB	1.85	0.59
3:G:83:ASP:OD2	3:G:113:ARG:NH2	2.36	0.59
2:F:729:ILE:HB	2:F:743:VAL:HG22	1.83	0.59
3:G:46:ILE:HD11	3:G:86:PHE:HA	1.84	0.59
2:F:705:ASP:HB3	2:F:725:GLY:HA3	1.85	0.58
2:B:756:ASP:OD2	2:B:803:ARG:NH2	2.36	0.58
2:F:1065:ASN:OD1	2:F:1065:ASN:N	2.35	0.58
1:E:205:CYS:HB2	1:E:212:CYS:HA	1.85	0.58
2:F:935:PHE:HB3	2:F:948:VAL:HG12	1.84	0.58
2:F:991:LYS:HZ3	2:F:1002:VAL:HG21	1.68	0.58
3:C:106:PRO:HA	3:C:149:MET:HB2	1.85	0.58
3:G:95:ILE:CD1	3:G:149:MET:HE1	2.34	0.57
3:G:80:CYS:SG	3:G:118:CYS:N	2.77	0.57
2:F:1152:VAL:HG23	2:F:1172:MET:HE1	1.85	0.57
3:I:78:PRO:HA	3:I:81:ALA:HB3	1.87	0.57
2:B:859:ASN:HB3	2:B:863:GLY:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:MET:O	1:E:168:GLU:HG2	2.05	0.57
2:B:956:ASP:N	2:B:956:ASP:OD1	2.38	0.56
2:F:1039:ASN:HA	2:F:1050:VAL:HA	1.87	0.56
3:C:84:LEU:HD13	3:C:114:ALA:HB1	1.88	0.56
2:F:1073:PHE:CE1	2:F:1084:GLU:HB2	2.40	0.56
3:G:41:PRO:HA	3:G:44:LYS:HD2	1.88	0.56
2:F:815:ILE:HB	2:F:829:ALA:HB3	1.88	0.56
2:F:719:LEU:HB2	2:F:734:LEU:HD23	1.88	0.55
3:H:130:PRO:HG2	3:H:133:MET:HB3	1.88	0.55
2:B:670:ASP:OD1	2:B:717:LYS:NZ	2.39	0.55
2:F:849:ASP:HB3	2:F:852:ARG:HB2	1.88	0.55
1:A:34:SER:HB2	1:A:38:GLN:HB3	1.87	0.55
1:E:284:ASN:HB3	1:E:287:THR:HG22	1.87	0.55
2:F:671:VAL:HG12	2:F:887:GLN:NE2	2.22	0.55
2:B:638:ARG:NH2	2:B:874:ASP:OD1	2.35	0.55
2:B:933:THR:HB	2:B:1196:GLU:HG3	1.89	0.55
2:B:1064:VAL:HG13	2:B:1088:LEU:HD21	1.89	0.55
3:D:148:CYS:SG	3:D:149:MET:N	2.79	0.55
2:F:901:SER:HB2	2:F:928:THR:HG22	1.88	0.55
1:E:314:ARG:NH1	1:E:352:LYS:O	2.37	0.54
3:D:55:ASN:HD21	3:D:59:HIS:HB2	1.71	0.54
2:F:934:THR:HG22	2:F:1195:LYS:HA	1.88	0.54
1:A:219:TRP:HH2	6:I:201:RAP:H18	1.72	0.54
2:B:671:VAL:HG21	2:B:884:SER:HA	1.89	0.54
2:F:669:PHE:HB3	2:F:880:LEU:HD21	1.88	0.54
3:G:53:MET:HB3	3:G:54:PRO:HD3	1.89	0.54
2:B:934:THR:HG22	2:B:1196:GLU:H	1.72	0.54
1:A:284:ASN:HB3	1:A:287:THR:OG1	2.07	0.54
1:E:171:ASP:OD1	1:E:188:ASN:ND2	2.25	0.54
3:H:88:LEU:O	3:H:91:MET:HG3	2.07	0.54
1:A:22:ILE:HG23	1:A:95:LEU:HB3	1.89	0.54
2:F:778:MET:HB2	2:F:906:ALA:O	2.07	0.54
3:C:132:ARG:O	3:C:137:ARG:NH2	2.39	0.54
3:D:95:ILE:HB	3:D:104:LEU:HD13	1.89	0.54
2:F:944:ILE:HD13	2:F:979:LEU:HD21	1.90	0.54
2:F:922:LEU:HG	2:F:926:ASN:HA	1.88	0.53
1:A:102:LEU:HD22	1:A:109:SER:HA	1.91	0.53
1:A:118:ALA:HA	1:A:195:ILE:HD11	1.91	0.53
3:G:95:ILE:HD11	3:G:149:MET:HE1	1.90	0.53
2:F:789:ASN:O	2:F:825:ARG:NH2	2.34	0.53
2:B:1116:LEU:HB2	2:B:1131:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HB1	2:B:834:HIS:CE1	2.44	0.53
2:B:982:ILE:HG13	2:B:1019:LEU:HD22	1.90	0.53
2:F:1027:TYR:C	2:F:1028:ILE:HD12	2.34	0.53
1:E:208:LEU:HB2	3:H:73:TRP:HE1	1.74	0.53
2:B:1200:GLN:O	2:B:1204:GLN:NE2	2.42	0.53
1:E:38:GLN:NE2	1:E:39:PRO:O	2.38	0.53
1:E:325:GLU:OE2	1:E:344:ARG:NH1	2.41	0.53
2:F:638:ARG:O	2:F:641:ASP:OD1	2.27	0.53
3:C:122:MET:HE2	3:C:127:PHE:CD2	2.44	0.53
2:B:941:LYS:HG3	2:B:966:ASN:HD22	1.73	0.52
2:B:1166:MET:SD	2:B:1180:LYS:HD3	2.50	0.52
2:F:668:ASP:OD2	2:F:712:VAL:HG12	2.08	0.52
2:F:745:LYS:NZ	2:F:953:GLN:HB2	2.24	0.52
3:G:115:LYS:HD2	3:G:119:ALA:HB2	1.90	0.52
2:F:923:ASN:OD1	2:F:930:SER:OG	2.22	0.52
1:A:337:VAL:HG21	3:C:147:LEU:HD22	1.90	0.52
1:A:107:ARG:HB3	1:A:235:TYR:CE1	2.45	0.52
1:A:164:MET:O	1:A:168:GLU:HG2	2.10	0.52
2:F:813:ASN:ND2	2:F:833:PRO:O	2.40	0.52
3:H:76:VAL:HG21	3:H:85:LYS:HB2	1.90	0.52
2:B:1155:ASN:ND2	2:B:1171:ASP:OD1	2.43	0.52
2:B:692:ASN:HB3	5:B:1401:NAG:O5	2.10	0.52
2:B:991:LYS:HG2	2:B:1000:PHE:HB3	1.90	0.52
2:F:989:ILE:HB	2:F:1003:VAL:HB	1.92	0.52
3:H:55:ASN:HD21	3:H:59:HIS:HB2	1.75	0.52
1:A:246:HIS:ND1	2:B:1180:LYS:HD2	2.25	0.51
2:B:702:PHE:O	2:B:739:ARG:NH1	2.26	0.51
2:F:747:LEU:HD21	2:F:750:PRO:HG3	1.92	0.51
2:F:821:LEU:HD22	2:F:823:LEU:HD21	1.91	0.51
2:F:926:ASN:CB	2:F:927:ARG:HH21	2.19	0.51
2:F:857:ARG:NH2	2:F:867:THR:OG1	2.42	0.51
2:F:686:ILE:CG2	2:F:700:VAL:HB	2.40	0.51
2:F:855:ILE:HG22	2:F:873:LEU:HD12	1.92	0.51
3:G:132:ARG:C	3:G:133:MET:HE2	2.35	0.51
2:B:817:SER:OG	2:B:818:SER:N	2.43	0.51
1:E:26:LEU:HD11	1:E:45:ILE:HG23	1.92	0.51
1:E:332:HIS:CE1	1:E:338:SER:HG	2.27	0.51
2:F:847:TRP:CZ3	2:F:856:GLU:HB2	2.45	0.51
3:D:73:TRP:HA	3:D:76:VAL:HG22	1.93	0.51
2:B:946:ARG:NH1	2:B:994:GLU:OE1	2.37	0.51
3:C:67:LEU:HA	3:D:67:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:860:LYS:HG3	2:F:861:THR:HG23	1.92	0.51
2:F:1084:GLU:HG2	2:F:1095:VAL:HG22	1.93	0.51
2:B:752:ALA:O	2:B:764:TRP:HA	2.10	0.51
1:E:207:GLY:O	3:G:71:GLN:NE2	2.32	0.51
2:F:636:PHE:CE1	2:F:643:ARG:HB2	2.46	0.51
2:F:859:ASN:HB3	2:F:863:GLY:N	2.23	0.51
1:A:35:LEU:HB3	1:A:64:PRO:HB3	1.93	0.51
3:D:120:PRO:O	3:D:124:GLN:NE2	2.44	0.51
2:F:1175:ARG:HG3	2:F:1176:GLU:HG2	1.92	0.51
1:E:22:ILE:HG23	1:E:95:LEU:HB3	1.92	0.50
3:H:74:PRO:HA	3:H:77:GLU:HB2	1.92	0.50
2:B:816:GLU:HG3	2:B:827:VAL:HG22	1.93	0.50
3:C:52:TYR:CE1	3:C:94:PRO:HB2	2.46	0.50
2:B:653:ASN:HD22	2:B:870:GLN:HE22	1.60	0.50
2:B:1078:GLU:OE2	2:B:1079:ARG:NE	2.44	0.50
2:F:712:VAL:HG23	2:F:734:LEU:HD21	1.94	0.50
2:F:1039:ASN:OD1	2:F:1040:VAL:N	2.41	0.50
1:A:26:LEU:HD21	1:A:45:ILE:HD13	1.93	0.50
3:C:46:ILE:HD11	3:C:86:PHE:HD1	1.77	0.50
1:E:305:ASP:OD1	1:E:305:ASP:N	2.40	0.50
2:B:1166:MET:HG3	2:B:1167:ILE:N	2.28	0.49
2:F:806:TYR:CE2	2:F:828:ILE:HG13	2.47	0.49
2:B:966:ASN:OD1	2:B:984:SER:OG	2.30	0.49
2:B:744:TRP:HE1	2:B:745:LYS:NZ	2.11	0.49
1:E:49:VAL:HG23	1:E:51:LYS:H	1.78	0.49
3:G:67:LEU:HD21	3:H:41:PRO:HG3	1.93	0.49
1:A:259:ARG:NH2	1:A:260:TYR:OH	2.46	0.49
1:E:205:CYS:CB	1:E:212:CYS:HA	2.43	0.49
2:B:773:ILE:HB	2:B:787:VAL:HB	1.95	0.49
1:E:22:ILE:HG22	1:E:46:PRO:HB2	1.94	0.49
2:F:1057:ASP:HA	2:F:1075:ASN:HD21	1.77	0.49
2:B:798:ILE:HG23	2:B:820:MET:HE1	1.95	0.49
2:F:715:LEU:HD12	2:F:716:GLY:N	2.28	0.49
2:F:980:TYR:HE2	2:F:1021:ILE:HD12	1.78	0.49
2:B:789:ASN:O	2:B:825:ARG:NH1	2.45	0.48
2:F:710:MET:HG3	2:F:711:ALA:N	2.28	0.48
1:A:244:GLU:OE2	1:A:257:ARG:HB2	2.12	0.48
2:B:989:ILE:HB	2:B:1003:VAL:HB	1.94	0.48
3:G:41:PRO:HG3	3:H:67:LEU:HD21	1.94	0.48
2:B:766:GLU:O	2:B:771:PRO:HA	2.12	0.48
3:C:41:PRO:HA	3:C:44:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1030:TRP:NE1	2:B:1041:THR:OG1	2.39	0.48
2:F:805:LEU:HB2	2:F:820:MET:HE1	1.95	0.48
2:B:729:ILE:HG13	2:B:747:LEU:HD21	1.95	0.48
2:B:1206:PRO:HG2	2:B:1220:VAL:HG22	1.95	0.48
1:A:157:GLU:HG3	1:A:220:SER:HA	1.95	0.48
2:B:1128:SER:HB3	2:B:1139:LEU:CD1	2.44	0.48
2:F:714:TRP:CD2	2:F:887:GLN:HB2	2.48	0.48
3:I:24:VAL:HG13	3:I:102:GLU:O	2.14	0.48
1:A:105:ALA:HB1	1:A:183:MET:SD	2.54	0.48
2:F:714:TRP:NE1	2:F:888:SER:O	2.36	0.48
3:G:149:MET:HB2	3:G:149:MET:HE2	1.58	0.48
2:B:907:VAL:HG21	2:B:913:VAL:HG13	1.95	0.47
3:I:23:VAL:HG13	3:I:45:PRO:HB2	1.96	0.47
1:A:48:LEU:HB3	1:A:53:LEU:HD12	1.96	0.47
2:B:665:SER:OG	2:B:681:ILE:HG13	2.14	0.47
1:E:156:SER:HB3	1:E:219:TRP:HB2	1.96	0.47
2:F:977:LYS:O	2:F:993:GLN:NE2	2.44	0.47
2:B:677:TYR:CZ	2:B:734:LEU:HD22	2.50	0.47
2:B:794:ASN:HB2	2:B:810:LEU:HD11	1.96	0.47
1:A:331:PHE:CG	1:A:332:HIS:N	2.81	0.47
2:B:936:LEU:HD21	2:B:1191:ILE:HD11	1.97	0.47
2:F:1027:TYR:HE1	2:F:1048:VAL:HG21	1.80	0.47
3:I:53:GLN:NE2	6:I:201:RAP:H522	2.29	0.47
2:F:743:VAL:HG23	2:F:747:LEU:HD22	1.95	0.47
2:F:1198:ASN:HB3	2:F:1201:GLU:HB3	1.97	0.47
3:H:48:TYR:OH	3:H:89:CYS:O	2.33	0.47
2:B:1057:ASP:OD1	2:B:1093:ARG:NH2	2.36	0.47
2:B:1057:ASP:CG	2:B:1093:ARG:HH22	2.20	0.47
2:B:1216:HIS:HB2	2:B:1230:CYS:HB3	1.97	0.47
1:A:85:ARG:HG2	1:A:292:THR:HG21	1.97	0.47
2:B:1230:CYS:HB2	2:B:1231:PRO:HD2	1.96	0.47
3:D:56:GLN:O	3:D:56:GLN:HG2	2.14	0.47
1:E:197:SER:O	1:E:197:SER:OG	2.31	0.47
1:A:52:GLN:NE2	1:A:169:PHE:O	2.46	0.47
3:D:57:PHE:CE2	3:D:92:TYR:CD1	3.03	0.47
1:A:208:LEU:HB2	3:D:73:TRP:NE1	2.30	0.46
1:A:329:CYS:HB3	1:A:337:VAL:CG1	2.44	0.46
2:B:669:PHE:O	2:B:887:GLN:NE2	2.49	0.46
2:B:806:TYR:HB3	2:B:838:LEU:HD21	1.98	0.46
2:B:1005:SER:HB2	2:B:1014:ILE:HB	1.97	0.46
3:G:57:PHE:HD1	3:G:132:ARG:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:123:ARG:NH1	3:D:127:PHE:O	2.40	0.46
2:F:920:TYR:HB3	2:F:929:CYS:HB3	1.97	0.46
6:I:201:RAP:H422	6:I:201:RAP:H35	1.61	0.46
1:A:333:TRP:CE3	3:C:151:TYR:HA	2.51	0.46
3:C:78:ILE:HD11	3:C:80:CYS:HB3	1.98	0.46
3:D:40:VAL:HG12	3:D:43:CYS:H	1.80	0.46
1:E:150:TRP:HB3	1:E:215:LYS:HB3	1.96	0.46
2:F:847:TRP:CH2	2:F:856:GLU:HB2	2.51	0.46
3:C:86:PHE:O	3:C:90:SER:HB3	2.16	0.46
2:B:669:PHE:CD1	2:B:880:LEU:HD21	2.51	0.46
2:B:1117:PHE:CD2	2:B:1128:SER:HB2	2.51	0.46
3:I:14:THR:O	3:I:14:THR:OG1	2.34	0.46
1:E:247:ARG:NH1	1:E:251:GLY:HA2	2.31	0.46
3:G:61:THR:HG22	3:G:64:GLU:HG3	1.96	0.46
3:D:57:PHE:CE1	3:D:132:ARG:HD3	2.51	0.46
2:B:1151:THR:HG22	2:B:1158:TYR:HB2	1.97	0.45
3:D:57:PHE:HE2	3:D:92:TYR:HA	1.80	0.45
2:F:773:ILE:HG13	2:F:790:VAL:HG11	1.99	0.45
2:F:1027:TYR:CE1	2:F:1048:VAL:HG21	2.51	0.45
3:C:73:TRP:HA	3:C:76:VAL:HG22	1.97	0.45
2:F:881:VAL:CG1	2:F:886:ARG:HG3	2.45	0.45
3:G:39:THR:N	3:G:62:GLN:OE1	2.50	0.45
1:A:42:CYS:CB	1:A:45:ILE:HD12	2.46	0.45
3:C:53:MET:HB3	3:C:53:MET:HE3	1.67	0.45
2:B:1186:ALA:C	2:B:1187:GLN:HG2	2.41	0.45
1:E:331:PHE:HE2	1:E:333:TRP:HE3	1.62	0.45
2:F:841:TYR:CG	2:F:881:VAL:HG21	2.51	0.45
2:F:982:ILE:HD11	2:F:1019:LEU:HB2	1.98	0.45
3:G:74:PRO:O	3:G:78:ILE:HG23	2.16	0.45
2:B:797:THR:HG21	2:B:838:LEU:HG	1.99	0.45
3:C:66:GLY:HA2	3:C:69:VAL:HG12	1.98	0.45
2:F:796:LEU:HD12	2:F:807:TRP:HB3	1.97	0.45
2:F:1065:ASN:HD21	2:F:1072:TYR:HE1	1.64	0.45
2:F:1078:GLU:OE2	2:F:1079:ARG:NE	2.48	0.45
3:H:122:MET:HE1	3:H:129:TRP:HA	1.98	0.45
1:A:80:GLN:HB3	1:A:232:LYS:HD3	1.98	0.45
1:E:331:PHE:CG	1:E:332:HIS:N	2.85	0.45
2:F:940:GLN:NE2	2:F:1186:ALA:O	2.35	0.45
3:H:72:PHE:HB3	3:H:75:LEU:HD12	1.99	0.45
2:B:1180:LYS:HB2	2:B:1180:LYS:HE3	1.60	0.45
2:F:1019:LEU:CD1	2:F:1028:ILE:HG23	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLU:OE2	1:A:255:THR:HG22	2.17	0.45
2:B:815:ILE:HB	2:B:829:ALA:HB3	1.99	0.45
3:C:53:MET:H	3:C:53:MET:HG2	1.45	0.45
2:F:1143:ASN:HB3	2:F:1178:ARG:NH1	2.32	0.45
1:E:166:SER:OG	1:E:192:ARG:HD3	2.17	0.45
3:G:95:ILE:HD11	3:G:149:MET:CE	2.47	0.45
1:A:45:ILE:HG22	1:A:48:LEU:HD13	1.99	0.44
2:B:1039:ASN:HA	2:B:1050:VAL:HA	1.99	0.44
2:B:1232:MET:H	2:B:1232:MET:HG2	1.49	0.44
3:H:107:CYS:O	3:H:110:VAL:HG12	2.17	0.44
1:A:54:ARG:HE	2:B:663:GLU:CD	2.25	0.44
1:A:60:VAL:HA	1:A:63:MET:HG2	1.99	0.44
2:B:814:LEU:HD23	2:B:814:LEU:N	2.31	0.44
3:C:75:LEU:HD11	3:C:80:CYS:SG	2.58	0.44
1:E:333:TRP:HZ3	3:G:149:MET:HG3	1.82	0.44
3:G:133:MET:HE2	3:G:133:MET:N	2.32	0.44
3:H:115:LYS:HD2	3:H:134:ARG:NH2	2.32	0.44
2:F:804:ARG:HD3	2:F:804:ARG:HA	1.85	0.44
2:F:1166:MET:SD	2:F:1180:LYS:HD2	2.57	0.44
2:F:1186:ALA:C	2:F:1187:GLN:HG2	2.41	0.44
2:B:630:PRO:HB2	2:B:631:GLU:H	1.62	0.44
3:H:61:THR:HG23	3:H:63:ASP:H	1.81	0.44
3:C:59:HIS:ND1	3:C:64:GLU:HB2	2.33	0.44
3:C:112:GLU:HA	3:C:115:LYS:HG2	2.00	0.44
3:G:108:ARG:HG3	3:G:108:ARG:HH11	1.82	0.44
1:A:19:SER:HA	1:A:102:LEU:HD12	1.99	0.44
2:F:991:LYS:HG3	2:F:1002:VAL:HG22	1.99	0.44
1:A:195:ILE:HG12	1:A:227:ILE:HD13	1.99	0.44
2:B:988:MET:HB2	2:B:1004:VAL:HG23	1.99	0.44
3:C:150:ASP:N	3:C:150:ASP:OD1	2.50	0.44
2:F:1022:ASP:O	2:F:1026:ARG:N	2.50	0.44
2:B:835:PRO:HB3	2:B:847:TRP:CD1	2.52	0.44
3:D:122:MET:HE1	3:D:129:TRP:HA	2.00	0.44
3:H:115:LYS:HD2	3:H:134:ARG:HH22	1.82	0.44
2:B:666:ALA:HB3	2:B:679:THR:HG23	2.00	0.44
1:E:247:ARG:CZ	2:F:953:GLN:HE22	2.30	0.44
2:F:1107:LEU:HD12	2:F:1118:TRP:HB3	1.99	0.44
2:F:1123:LEU:HB3	2:F:1125:ARG:NH1	2.33	0.44
3:H:52:TYR:HD2	3:H:54:PRO:HD2	1.83	0.44
2:F:1072:TYR:CD2	2:F:1085:ARG:HB3	2.53	0.43
2:F:1148:VAL:HG21	2:F:1162:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:715:LEU:HD12	2:F:716:GLY:H	1.84	0.43
3:I:24:VAL:CG2	3:I:103:LEU:HD12	2.44	0.43
1:A:246:HIS:CE1	2:B:1180:LYS:HD2	2.53	0.43
3:C:145:ASP:OD1	3:C:145:ASP:N	2.52	0.43
2:F:989:ILE:O	2:F:1002:VAL:HG23	2.18	0.43
2:F:1230:CYS:HB2	2:F:1234:LEU:HB2	2.01	0.43
1:E:34:SER:HB3	1:E:38:GLN:HB3	2.00	0.43
2:B:718:ASN:ND2	2:B:904:CYS:O	2.47	0.43
2:F:1038:ILE:HB	2:F:1052:LEU:HB3	2.01	0.43
2:F:1059:PRO:O	2:F:1060:ARG:NH1	2.50	0.43
2:F:1159:TRP:HZ2	2:F:1178:ARG:HH21	1.67	0.43
2:B:1065:ASN:HD22	2:B:1109:LEU:HD13	1.84	0.43
1:E:76:GLU:OE2	1:E:80:GLN:NE2	2.52	0.43
3:G:61:THR:HG23	3:G:63:ASP:H	1.83	0.43
2:F:1019:LEU:HD11	2:F:1028:ILE:HG23	2.01	0.43
2:F:1085:ARG:HD2	2:F:1096:LEU:HD13	1.99	0.43
1:A:105:ALA:HB3	1:A:275:GLU:HG3	2.01	0.43
1:E:32:TYR:CZ	1:E:71:LYS:HD3	2.54	0.43
1:E:331:PHE:CE2	1:E:333:TRP:HE3	2.36	0.43
2:F:756:ASP:OD1	2:F:761:PHE:HB2	2.19	0.43
3:H:138:LEU:HD23	3:H:138:LEU:HA	1.86	0.43
2:B:1142:SER:O	2:B:1178:ARG:NH1	2.42	0.43
2:B:1198:ASN:HB3	2:B:1201:GLU:HB3	2.00	0.43
3:D:100:TYR:CZ	3:D:102:LYS:HB2	2.54	0.43
2:B:760:GLY:O	2:B:908:PRO:HD3	2.19	0.43
2:B:1128:SER:OG	2:B:1129:SER:N	2.51	0.43
1:E:247:ARG:HA	1:E:247:ARG:HD3	1.83	0.43
3:H:91:MET:HE3	3:H:92:TYR:HB2	2.01	0.43
1:A:328:HIS:HB2	1:A:340:GLN:NE2	2.34	0.42
1:E:128:CYS:HB2	1:E:136:CYS:HB3	1.46	0.42
3:C:40:VAL:HG11	3:C:69:VAL:HG11	2.01	0.42
3:D:115:LYS:NZ	3:D:135:CYS:SG	2.88	0.42
1:E:247:ARG:NE	2:F:953:GLN:HE22	2.18	0.42
2:F:1018:ASP:OD2	2:F:1062:VAL:N	2.45	0.42
2:F:1203:ARG:HD3	2:F:1204:GLN:N	2.34	0.42
6:I:201:RAP:H471	6:I:201:RAP:H31	1.75	0.42
2:B:947:MET:HB3	2:B:956:ASP:HB3	2.01	0.42
2:F:892:GLU:HG3	2:F:898:GLY:HA2	2.02	0.42
3:G:46:ILE:HG13	3:G:47:GLY:H	1.84	0.42
3:H:48:TYR:OH	3:H:93:THR:O	2.23	0.42
3:D:89:CYS:O	3:D:93:THR:N	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1042:ARG:HH11	2:F:1043:LEU:HB2	1.84	0.42
3:G:95:ILE:HD12	3:G:149:MET:HE1	2.01	0.42
3:G:140:GLU:HG2	3:G:142:GLY:H	1.85	0.42
2:B:636:PHE:CE2	2:B:643:ARG:HB2	2.54	0.42
2:F:806:TYR:HB3	2:F:838:LEU:HD21	2.01	0.42
3:H:121:LEU:HD12	3:H:121:LEU:HA	1.91	0.42
1:E:199:MET:HE2	1:E:199:MET:HA	2.01	0.42
2:F:990:ARG:HD2	2:F:1001:THR:HA	2.01	0.42
3:G:76:VAL:O	3:G:79:GLN:NE2	2.52	0.42
2:B:980:TYR:CZ	2:B:1043:LEU:HD22	2.55	0.42
2:B:1205:HIS:HB3	2:B:1208:ALA:HB2	2.02	0.42
1:E:145:SER:HB2	1:E:152:TRP:CH2	2.55	0.42
1:E:331:PHE:HE2	1:E:333:TRP:CE3	2.36	0.42
2:F:925:ASP:O	2:F:927:ARG:NE	2.46	0.42
2:B:753:LEU:HD12	2:B:764:TRP:HB3	2.00	0.42
2:B:845:ILE:HG23	2:B:860:LYS:HB3	2.02	0.42
2:B:854:SER:OG	2:B:871:GLY:HA2	2.20	0.42
1:E:324:ARG:NH1	1:E:341:GLU:OE2	2.52	0.42
2:F:794:ASN:OD1	2:F:795:GLY:N	2.52	0.42
2:F:854:SER:OG	2:F:871:GLY:HA2	2.19	0.42
2:F:1151:THR:HG22	2:F:1158:TYR:HB2	2.02	0.42
3:G:68:GLU:HG2	3:G:92:TYR:CE1	2.55	0.42
3:D:53:MET:HB2	3:D:54:PRO:HD3	2.02	0.42
3:G:57:PHE:CD1	3:G:132:ARG:HD3	2.55	0.42
3:G:107:CYS:SG	3:G:150:ASP:HB2	2.59	0.42
3:H:92:TYR:O	3:H:94:PRO:HD3	2.20	0.42
3:C:64:GLU:HA	3:C:67:LEU:HD12	2.02	0.42
2:F:751:ARG:HD3	2:F:751:ARG:C	2.44	0.42
2:F:1024:TYR:HD1	2:F:1202:TYR:CE1	2.38	0.42
3:H:75:LEU:O	3:H:78:ILE:HG22	2.19	0.42
3:C:115:LYS:HB2	3:C:115:LYS:HE3	1.83	0.41
3:D:73:TRP:O	3:D:77:GLU:HB2	2.21	0.41
2:F:680:ASP:O	2:F:684:LYS:N	2.52	0.41
3:D:119:ALA:HB3	3:D:120:PRO:HD3	2.02	0.41
1:E:204:LYS:HB3	1:E:204:LYS:HE2	1.90	0.41
2:F:949:ILE:HD13	2:F:1153:PHE:CE2	2.55	0.41
2:F:1217:ILE:HB	2:F:1229:SER:C	2.45	0.41
1:A:102:LEU:O	1:A:180:ARG:NH2	2.54	0.41
1:A:145:SER:O	1:A:152:TRP:NE1	2.48	0.41
1:A:208:LEU:HB2	3:D:73:TRP:CE2	2.55	0.41
2:B:733:LYS:HA	2:B:733:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1097:PHE:HE2	2:F:1118:TRP:CH2	2.38	0.41
3:G:115:LYS:HE2	3:G:129:TRP:CD1	2.55	0.41
3:C:89:CYS:O	3:C:93:THR:HG23	2.20	0.41
2:F:803:ARG:HG3	2:F:820:MET:HG2	2.03	0.41
2:F:1156:TRP:CE3	2:F:1169:LYS:HD2	2.56	0.41
3:G:132:ARG:C	3:G:137:ARG:HH22	2.28	0.41
1:A:159:ILE:HG21	1:A:199:MET:SD	2.61	0.41
2:B:934:THR:HG22	2:B:1196:GLU:N	2.35	0.41
2:F:802:LYS:HG3	2:F:804:ARG:HB2	2.02	0.41
2:F:983:ASP:OD1	2:F:983:ASP:N	2.51	0.41
3:I:29:MET:HA	3:I:35:LYS:HA	2.03	0.41
6:I:201:RAP:H19	6:I:201:RAP:H441	1.84	0.41
1:A:54:ARG:CZ	2:B:681:ILE:HG22	2.51	0.41
2:F:744:TRP:CE2	2:F:955:PRO:HD3	2.56	0.41
2:F:1153:PHE:CD2	2:F:1154:GLU:HG3	2.56	0.41
2:B:1028:ILE:HD11	2:B:1043:LEU:HD23	2.02	0.41
1:E:51:LYS:HG3	2:F:706:TYR:CE1	2.55	0.41
2:F:841:TYR:HH	2:F:883:HIS:CE1	2.38	0.41
3:G:108:ARG:HG3	3:G:108:ARG:NH1	2.35	0.41
3:G:119:ALA:HB3	3:G:120:PRO:HD3	2.03	0.41
3:D:65:ALA:O	3:D:69:VAL:HG13	2.20	0.41
3:G:122:MET:HB2	3:G:127:PHE:HB2	2.02	0.41
1:A:205:CYS:HB3	1:A:212:CYS:HA	2.03	0.41
2:B:778:MET:HB2	2:B:906:ALA:O	2.21	0.41
2:B:892:GLU:H	2:B:892:GLU:HG2	1.74	0.41
1:E:104:LYS:HG3	1:E:275:GLU:OE1	2.21	0.41
1:E:124:VAL:HG21	1:E:165:VAL:HG11	2.03	0.41
2:F:1019:LEU:HD12	2:F:1020:SER:N	2.36	0.41
3:G:100:TYR:CE2	3:G:102:LYS:HB2	2.55	0.41
2:B:1081:PRO:HG3	2:B:1102:SER:O	2.21	0.41
2:B:1234:LEU:HD22	2:B:1244:GLY:HA2	2.02	0.41
3:C:48:TYR:CD2	3:C:95:ILE:HG23	2.56	0.41
3:C:119:ALA:HB3	3:C:120:PRO:HD3	2.03	0.41
2:F:680:ASP:HB3	2:F:683:LEU:HB3	2.03	0.41
2:B:805:LEU:HD12	2:B:820:MET:HA	2.02	0.40
1:E:76:GLU:O	1:E:80:GLN:HG2	2.21	0.40
2:F:925:ASP:OD1	2:F:925:ASP:N	2.53	0.40
3:I:57:ARG:HD2	3:I:57:ARG:HA	1.84	0.40
1:A:334:CYS:HA	1:A:335:CYS:HA	1.73	0.40
2:B:708:GLU:HG3	2:B:724:THR:OG1	2.21	0.40
2:B:814:LEU:HD12	2:B:827:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:949:ILE:HD13	2:B:1153:PHE:CE2	2.55	0.40
2:F:947:MET:HE3	2:F:947:MET:HB3	1.85	0.40
3:I:7:ILE:HD11	3:I:73:LYS:HB2	2.03	0.40
1:E:87:ASN:HB3	4:K:1:NAG:H2	2.02	0.40
1:E:153:GLY:HA3	1:E:216:THR:HB	2.03	0.40
2:B:1221:LYS:HE2	2:B:1227:ARG:HB3	2.03	0.40
1:E:135:ILE:H	1:E:135:ILE:HG13	1.53	0.40
1:A:298:ASN:O	1:A:306:GLY:HA2	2.22	0.40
2:B:1137:ILE:O	2:B:1137:ILE:HG12	2.21	0.40
2:F:721:TRP:HZ2	2:F:739:ARG:HH11	1.70	0.40
2:F:848:THR:HG21	2:F:876:VAL:HB	2.02	0.40
2:F:1042:ARG:NH1	2:F:1043:LEU:HB2	2.36	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	332/334 (99%)	323 (97%)	9 (3%)	0	100	100
1	E	332/334 (99%)	321 (97%)	11 (3%)	0	100	100
2	B	614/752 (82%)	575 (94%)	39 (6%)	0	100	100
2	F	614/752 (82%)	577 (94%)	37 (6%)	0	100	100
3	C	117/271 (43%)	113 (97%)	4 (3%)	0	100	100
3	D	117/271 (43%)	112 (96%)	5 (4%)	0	100	100
3	G	117/271 (43%)	107 (92%)	10 (8%)	0	100	100
3	H	117/271 (43%)	117 (100%)	0	0	100	100
3	I	105/271 (39%)	102 (97%)	3 (3%)	0	100	100
All	All	2465/3527 (70%)	2347 (95%)	118 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/282 (99%)	271 (97%)	9 (3%)	34	68
1	E	280/282 (99%)	257 (92%)	23 (8%)	10	32
2	B	538/646 (83%)	519 (96%)	19 (4%)	32	66
2	F	538/646 (83%)	513 (95%)	25 (5%)	24	57
3	C	107/223 (48%)	103 (96%)	4 (4%)	30	64
3	D	107/223 (48%)	104 (97%)	3 (3%)	38	72
3	G	107/223 (48%)	103 (96%)	4 (4%)	30	64
3	H	107/223 (48%)	103 (96%)	4 (4%)	30	64
3	I	89/223 (40%)	88 (99%)	1 (1%)	65	88
All	All	2153/2971 (72%)	2061 (96%)	92 (4%)	27	60

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	40	ILE
1	A	176	ARG
1	A	244	GLU
1	A	308	ASP
1	A	324	ARG
1	A	339	CYS
1	A	342	CYS
1	A	347	ASP
2	B	687	SER
2	B	692	ASN
2	B	729	ILE
2	B	745	LYS
2	B	797	THR
2	B	809	ASP

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Mol	Chain	Res	Type
2	B	839	THR
2	B	879	ILE
2	B	952	GLN
2	B	971	ASP
2	B	993	GLN
2	B	995	ASP
2	B	1115	LYS
2	B	1130	ASP
2	B	1137	ILE
2	B	1150	LEU
2	B	1163	GLN
2	B	1226	THR
2	B	1228	CYS
3	C	53	MET
3	C	93	THR
3	C	95	ILE
3	C	96	CYS
3	D	91	MET
3	D	108	ARG
3	D	115	LYS
1	E	20	TYR
1	E	34	SER
1	E	41	LEU
1	E	49	VAL
1	E	128	CYS
1	E	135	ILE
1	E	173	ARG
1	E	175	ASN
1	E	176	ARG
1	E	197	SER
1	E	198	HIS
1	E	206	HIS
1	E	233	ASP
1	E	244	GLU
1	E	245	LYS
1	E	248	GLU
1	E	250	ARG
1	E	261	THR
1	E	265	VAL
1	E	299	VAL
1	E	314	ARG
1	E	319	ARG

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Mol	Chain	Res	Type
1	E	323	ARG
2	F	646	SER
2	F	706	TYR
2	F	710	MET
2	F	718	ASN
2	F	743	VAL
2	F	748	ASP
2	F	790	VAL
2	F	916	CYS
2	F	921	SER
2	F	942	SER
2	F	945	ASN
2	F	1000	PHE
2	F	1002	VAL
2	F	1004	VAL
2	F	1027	TYR
2	F	1031	THR
2	F	1041	THR
2	F	1064	VAL
2	F	1065	ASN
2	F	1121	SER
2	F	1139	LEU
2	F	1155	ASN
2	F	1182	GLN
2	F	1195	LYS
2	F	1230	CYS
3	G	80	CYS
3	G	101	LYS
3	G	115	LYS
3	G	135	CYS
3	H	53	MET
3	H	67	LEU
3	H	70	HIS
3	H	124	GLN
3	I	96	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	HIS
1	A	284	ASN
1	A	340	GLN

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Mol	Chain	Res	Type
2	B	737	GLN
2	B	966	ASN
3	C	79	GLN
3	D	124	GLN
1	E	79	HIS
1	E	80	GLN
1	E	246	HIS
1	E	317	ASN
2	F	650	ASN
2	F	738	HIS
2	F	966	ASN
2	F	1198	ASN
3	G	59	HIS
3	G	79	GLN
3	H	62	GLN
3	H	124	GLN
3	I	3	GLN
3	I	25	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 ⓘ

6 monosaccharides are modelled in this entry.

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	$\# Z > 2$
4	NAG	J	1	4,1	14,14,15	0.18	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	J	2	4	14,14,15	0.18	0	17,19,21	0.45	0
4	NAG	K	1	4,1	14,14,15	0.36	0	17,19,21	0.60	0
4	NAG	K	2	4	14,14,15	0.43	0	17,19,21	0.44	0
4	NAG	L	1	4,1	14,14,15	0.28	0	17,19,21	0.51	0
4	NAG	L	2	4	14,14,15	0.24	0	17,19,21	0.41	0

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
4	NAG	J	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

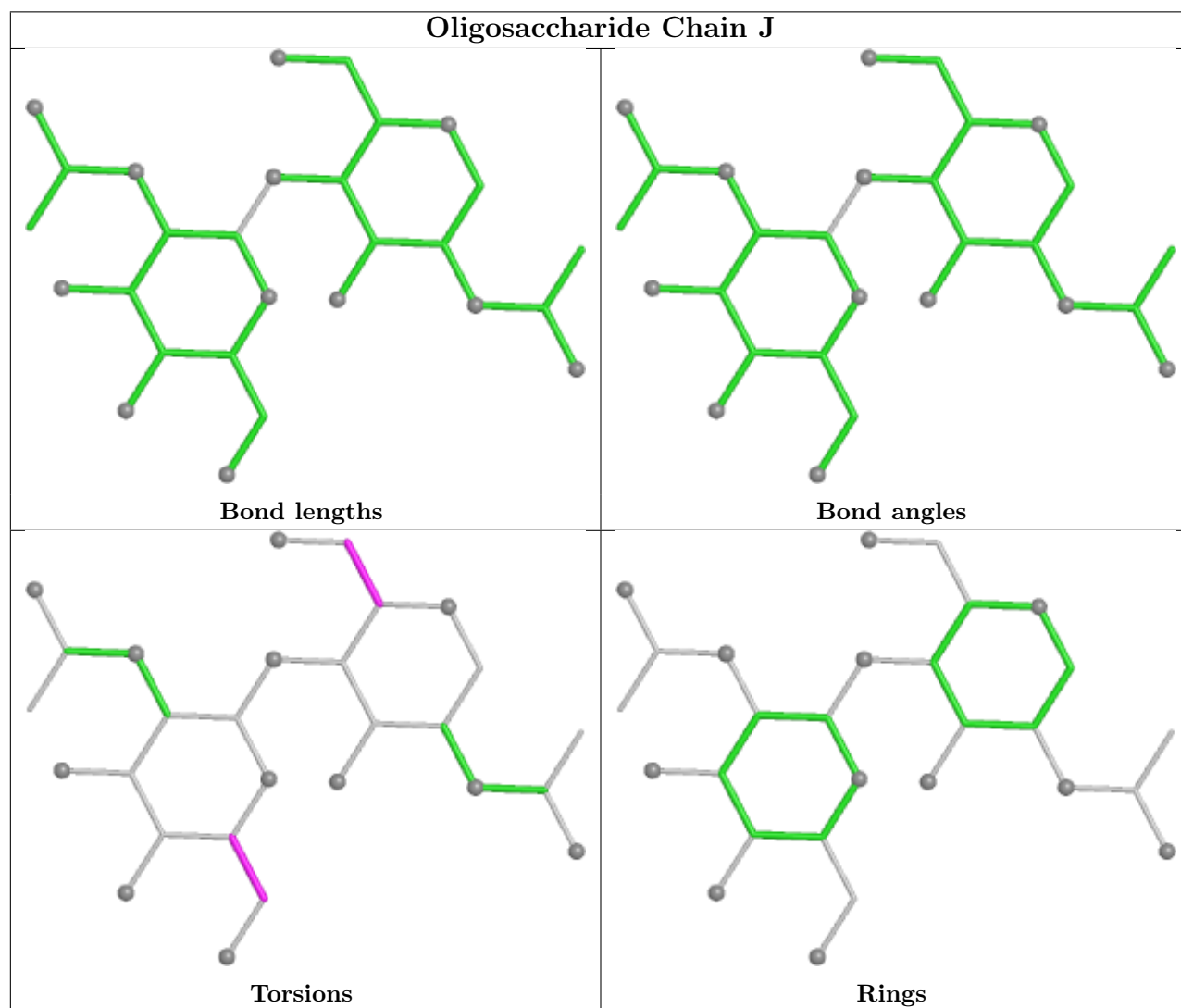
Mol	Chain	Res	Type	Atoms
4	K	1	NAG	C4-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2
4	L	1	NAG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	J	1	NAG	C4-C5-C6-O6

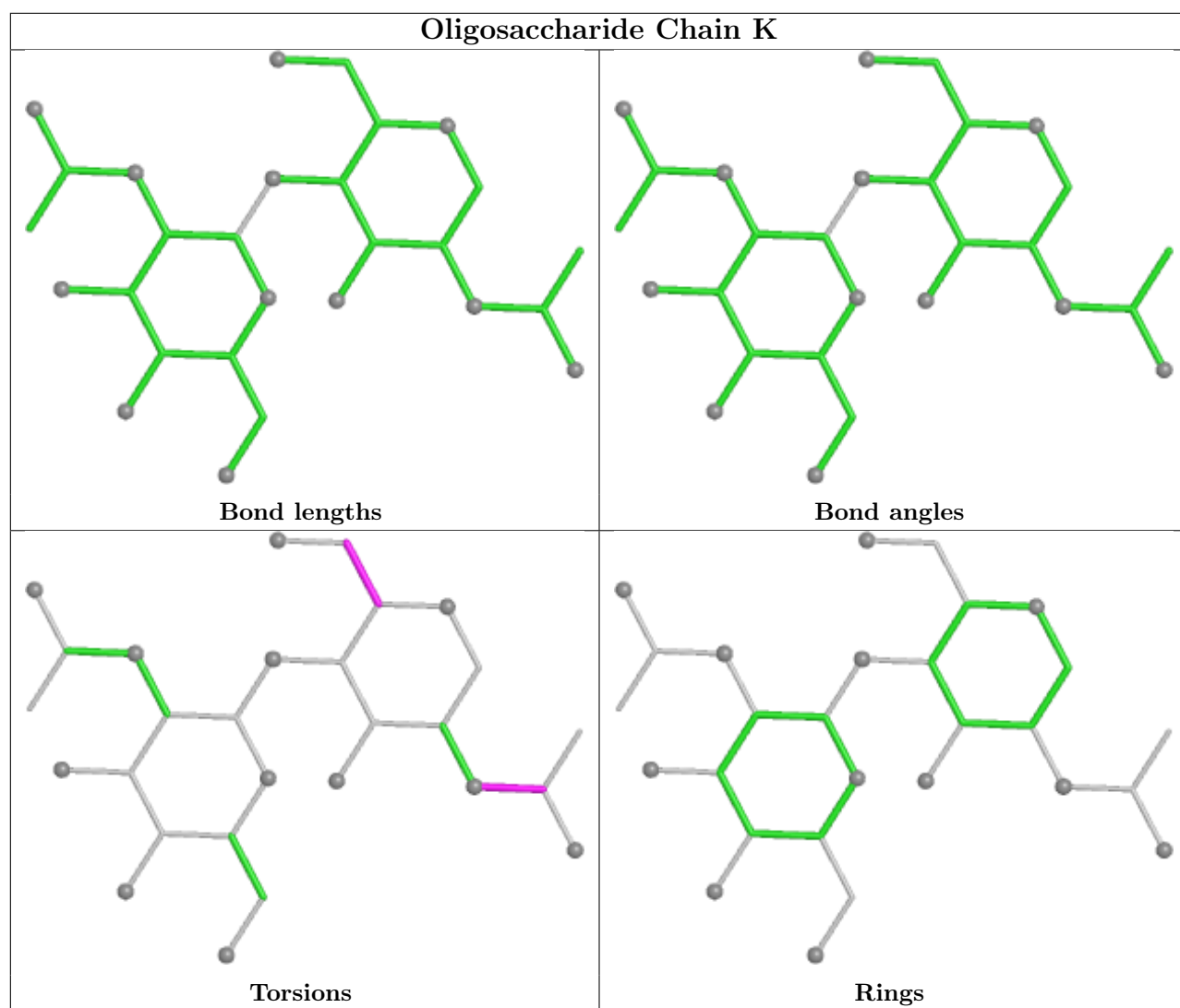
There are no ring outliers.

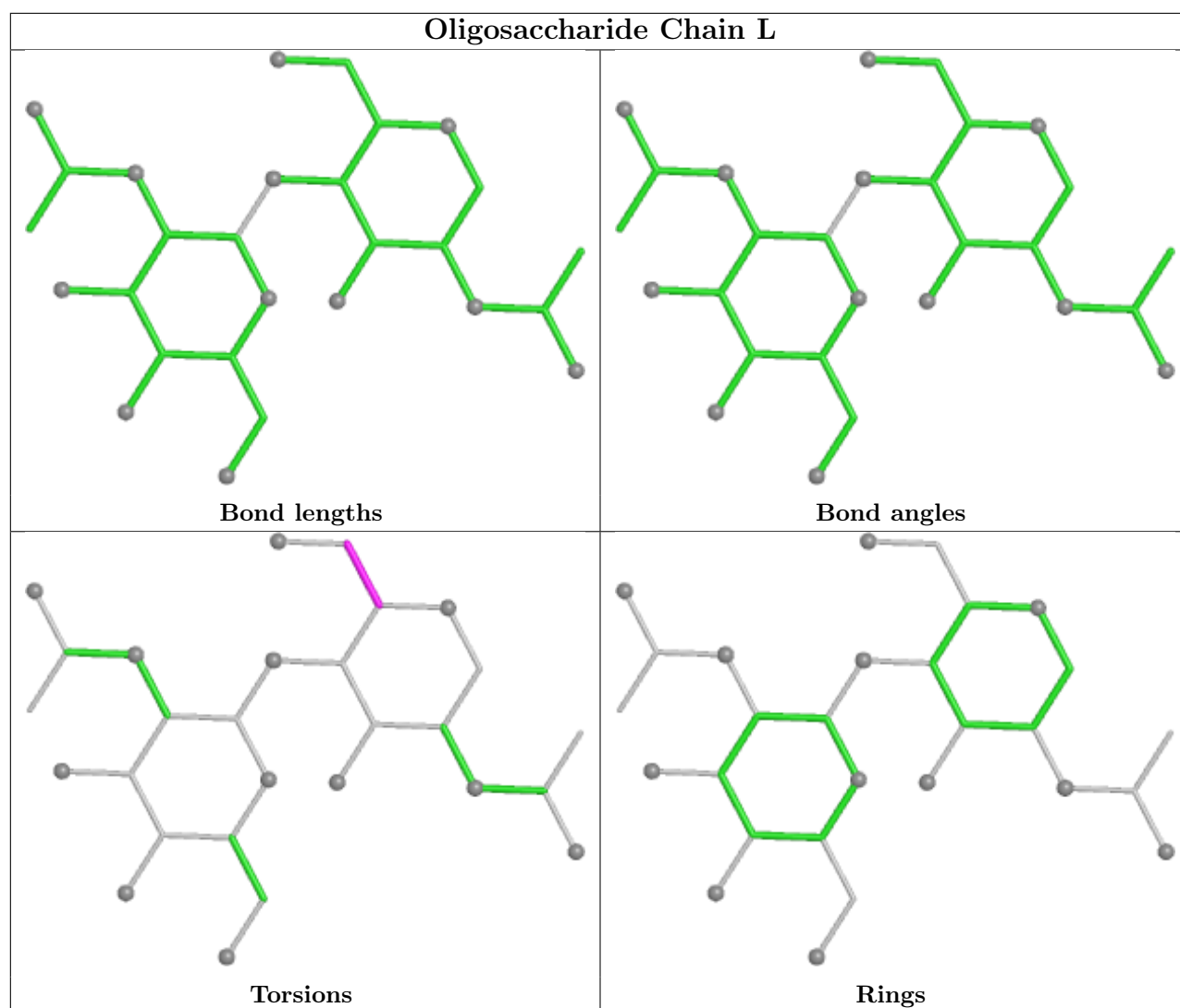
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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	$\# Z > 2$
5	NAG	B	1402	2	14,14,15	0.27	0	17,19,21	1.11	1 (5%)
5	NAG	B	1401	2	14,14,15	0.20	0	17,19,21	0.39	0
5	NAG	B	1403	2	14,14,15	0.73	1 (7%)	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	RAP	I	201	-	65,68,68	1.11	4 (6%)	73,96,96	1.60	10 (13%)
5	NAG	A	401	1	14,14,15	0.89	1 (7%)	17,19,21	0.48	0

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
5	NAG	B	1402	2	-	2/6/23/26	0/1/1/1
5	NAG	B	1401	2	-	4/6/23/26	0/1/1/1
5	NAG	B	1403	2	-	3/6/23/26	0/1/1/1
6	RAP	I	201	-	-	11/81/124/124	1/3/4/4
5	NAG	A	401	1	-	3/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	201	RAP	C8-C9	-5.35	1.46	1.53
6	I	201	RAP	O1-C1	4.87	1.45	1.34
5	A	401	NAG	O5-C1	-3.24	1.38	1.43
5	B	1403	NAG	O5-C1	-2.58	1.39	1.43
6	I	201	RAP	C31-C32	-2.54	1.50	1.53
6	I	201	RAP	O6-C10	2.35	1.43	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	201	RAP	C15-C16-C17	-5.59	105.73	113.50
6	I	201	RAP	C19-C18-C17	-5.24	119.62	127.32
6	I	201	RAP	O1-C1-C2	4.51	120.71	110.78
6	I	201	RAP	C34-O1-C1	-4.11	111.73	117.89
5	B	1402	NAG	C1-O5-C5	3.33	116.71	112.19
6	I	201	RAP	C44-C17-C18	-2.99	120.34	124.03
6	I	201	RAP	C20-C19-C18	-2.89	117.55	123.47
6	I	201	RAP	O1-C1-O2	-2.76	118.79	123.94
6	I	201	RAP	O3-C8-C9	2.24	119.97	116.28
6	I	201	RAP	C44-C17-C16	2.15	120.03	115.07
6	I	201	RAP	C25-C24-C23	-2.07	109.95	114.67

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1403	NAG	O5-C5-C6-O6
5	B	1402	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	B	1401	NAG	C8-C7-N2-C2
5	B	1401	NAG	O7-C7-N2-C2
5	B	1401	NAG	C4-C5-C6-O6
6	I	201	RAP	O5-C14-C15-C16
6	I	201	RAP	C13-C14-C15-C16
6	I	201	RAP	C49-C35-C36-C37
5	B	1401	NAG	O5-C5-C6-O6
5	A	401	NAG	O5-C5-C6-O6
6	I	201	RAP	C21-C22-C23-C24
6	I	201	RAP	C34-C35-C36-C37
5	B	1403	NAG	C3-C2-N2-C7
6	I	201	RAP	C17-C18-C19-C20
6	I	201	RAP	C32-C33-C34-O1
6	I	201	RAP	C21-C22-C23-C45
6	I	201	RAP	O10-C28-C29-C47
6	I	201	RAP	C32-C33-C34-C35
6	I	201	RAP	C46-C25-C26-C27

All (1) ring outliers are listed below:

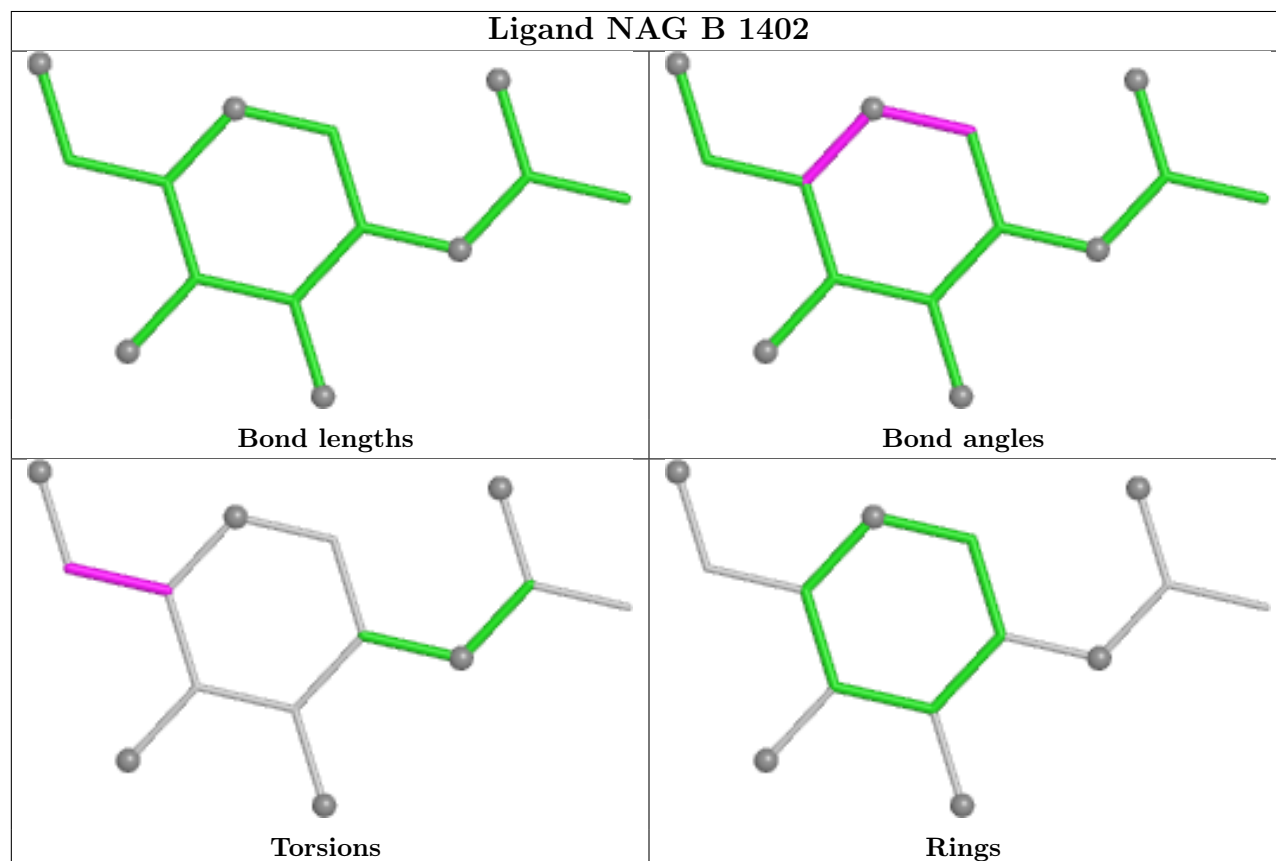
Mol	Chain	Res	Type	Atoms
6	I	201	RAP	C37-C38-C39-C40-C41-C42

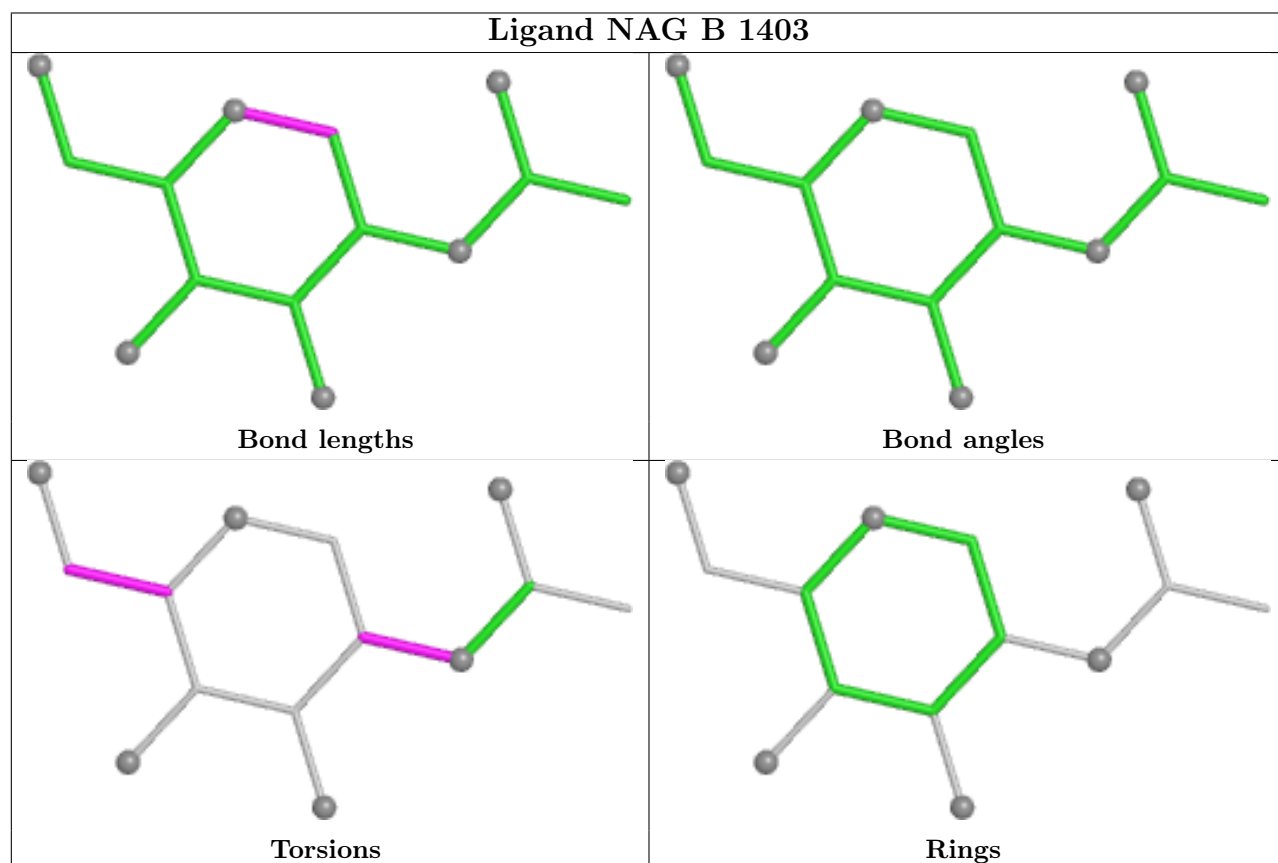
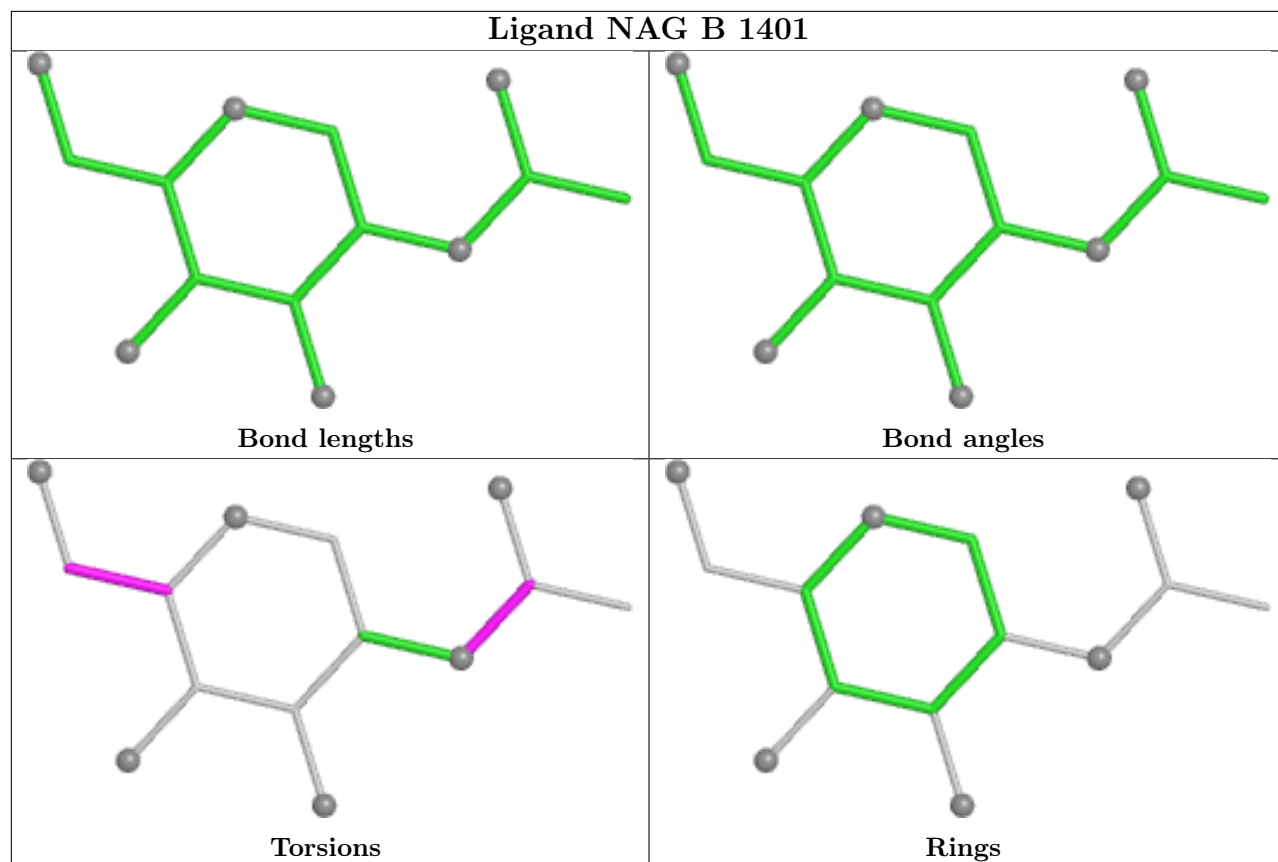
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1401	NAG	1	0
6	I	201	RAP	5	0

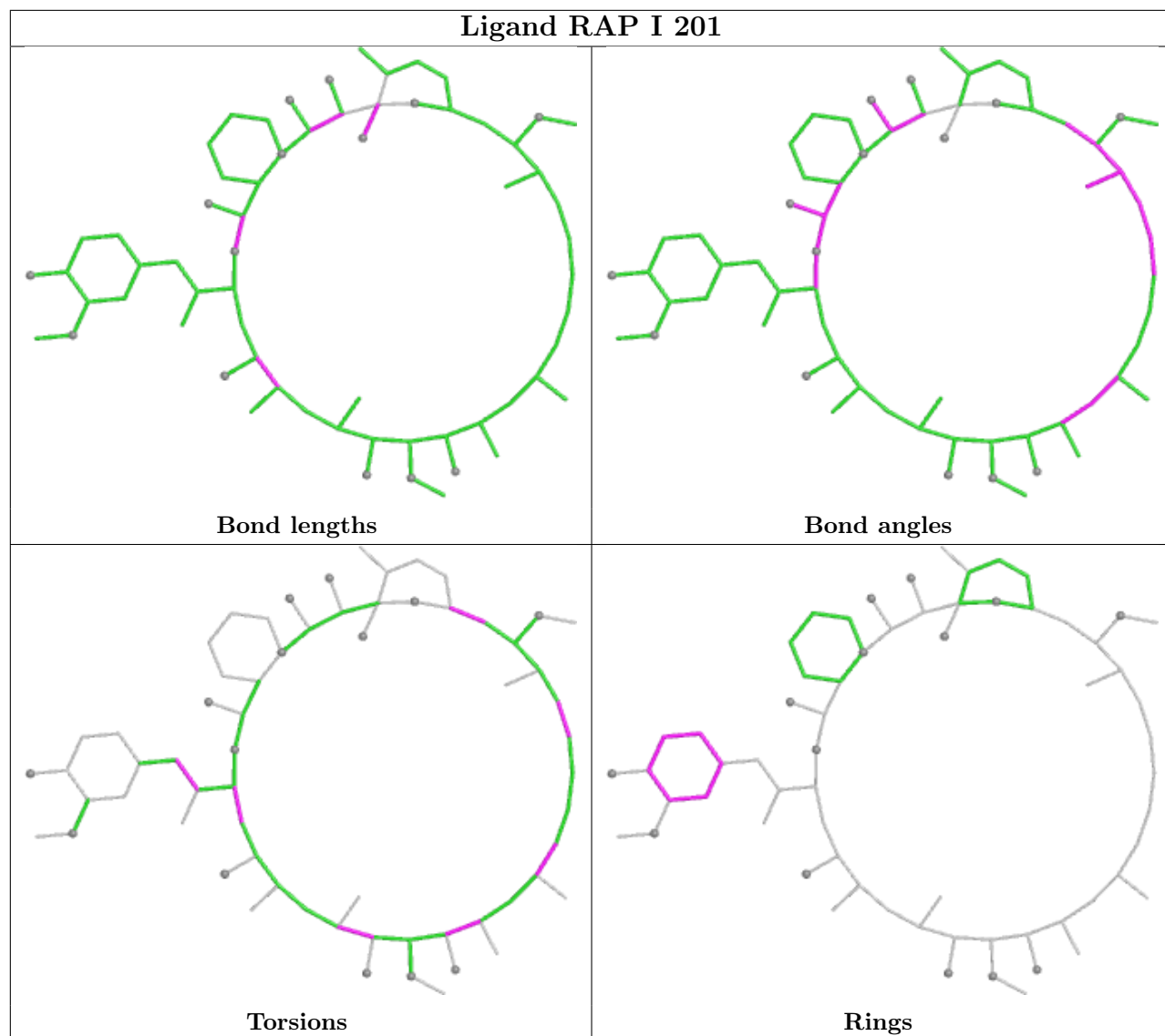
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

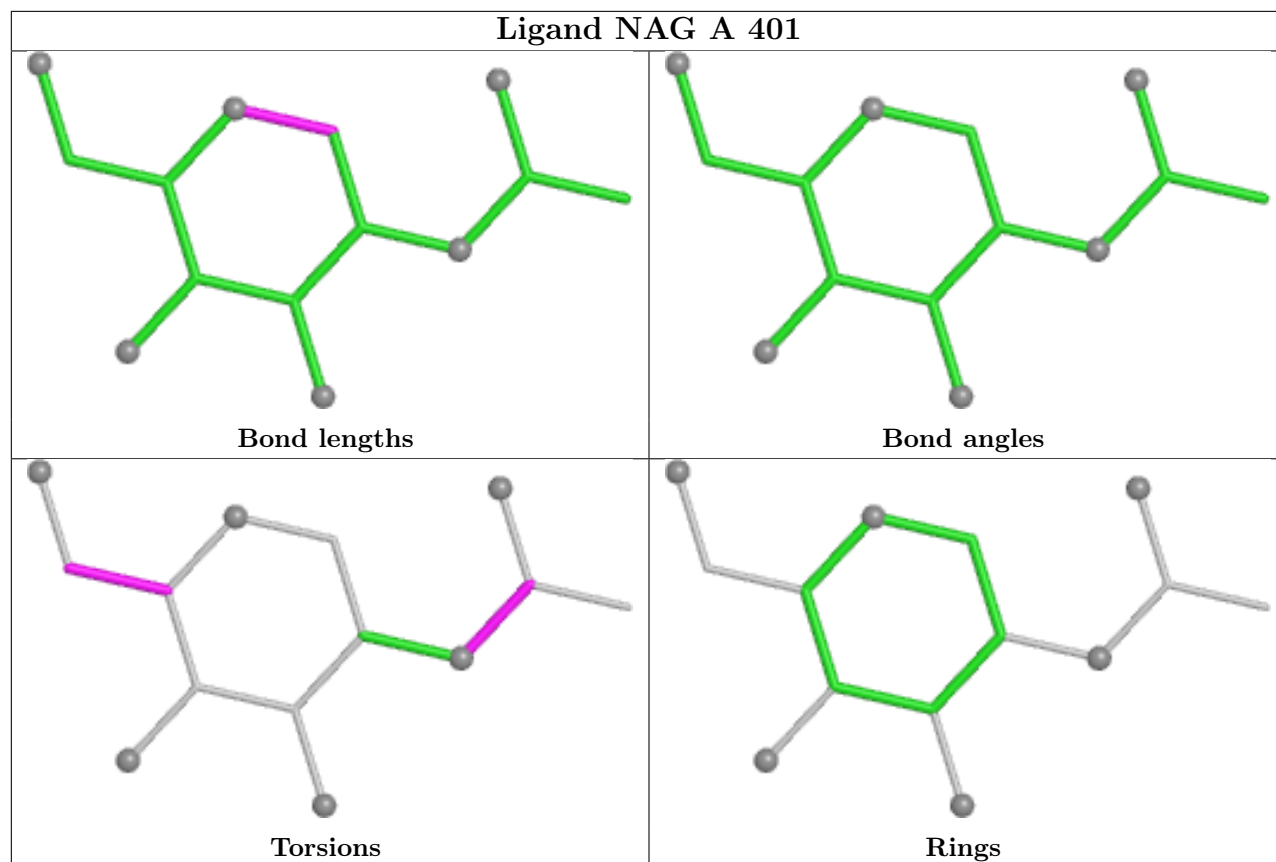
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.





Ligand RAP I 201





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.

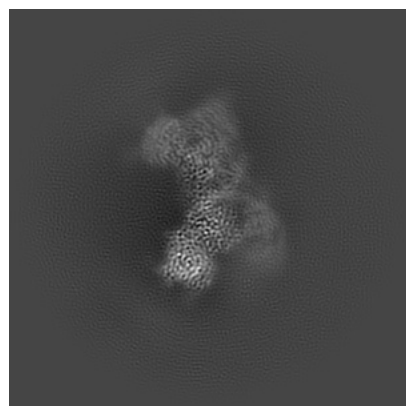
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67778. These allow visual inspection of the internal detail of the map and identification of artifacts.

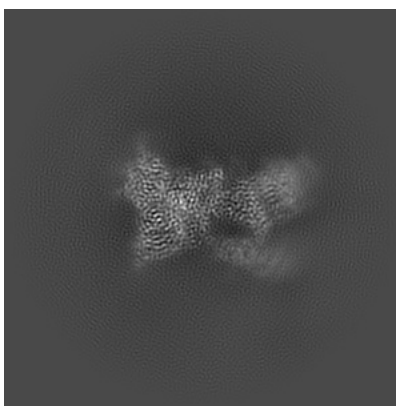
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

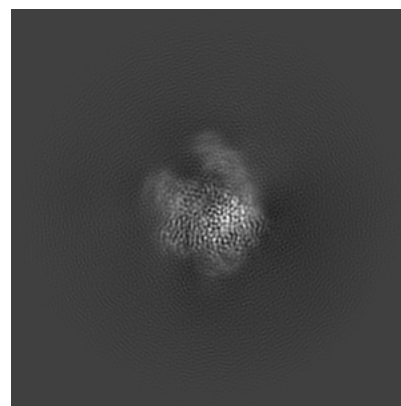
6.1.1 Primary map



X

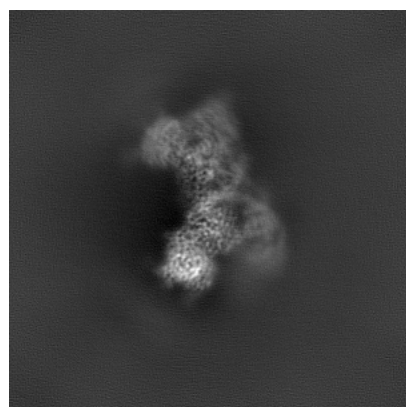


Y

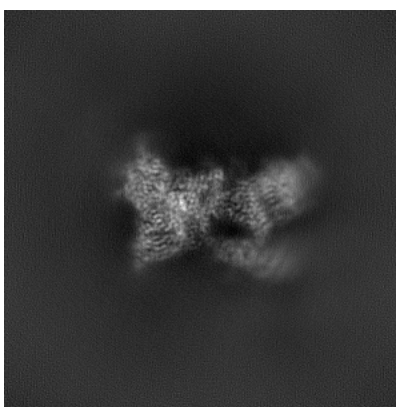


Z

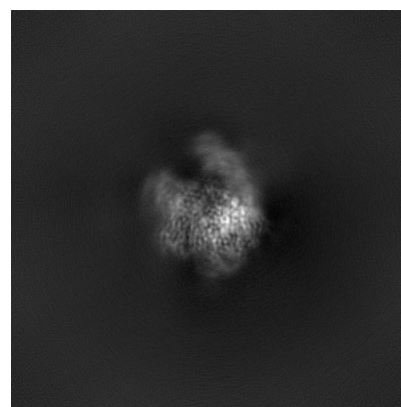
6.1.2 Raw map



X



Y

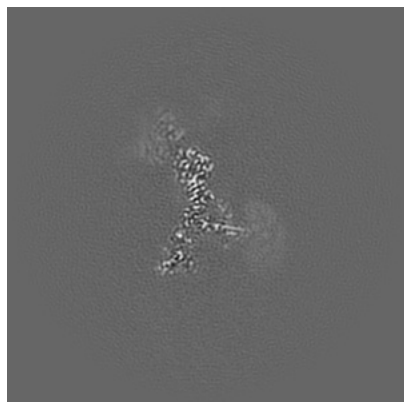


Z

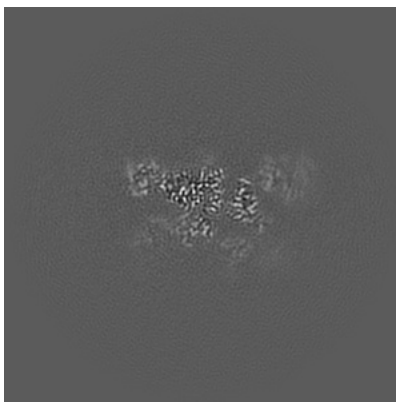
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

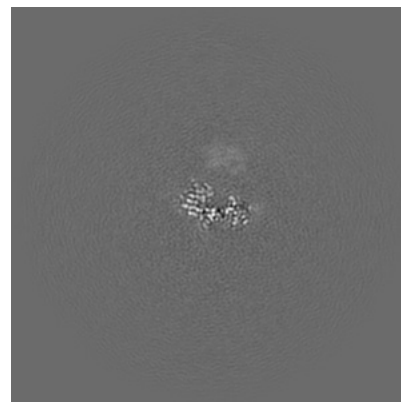
6.2.1 Primary map



X Index: 200

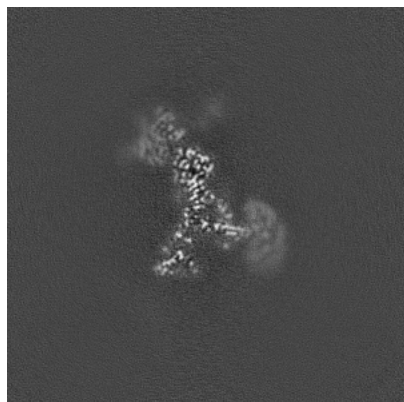


Y Index: 200

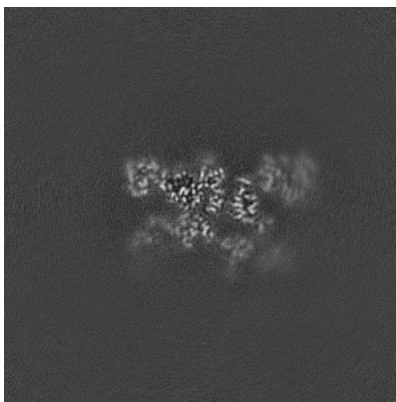


Z Index: 200

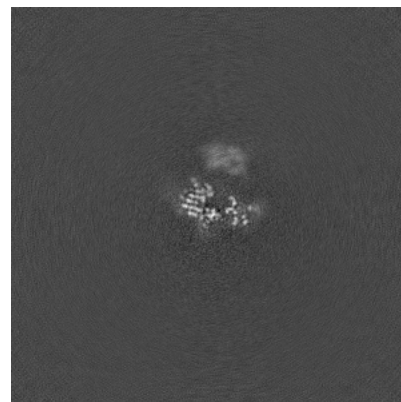
6.2.2 Raw map



X Index: 200



Y Index: 200

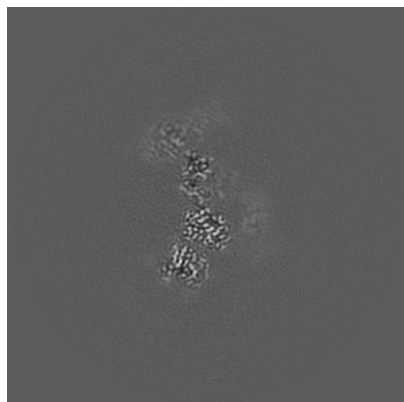


Z Index: 200

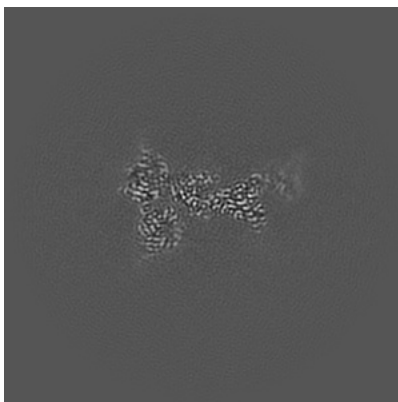
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

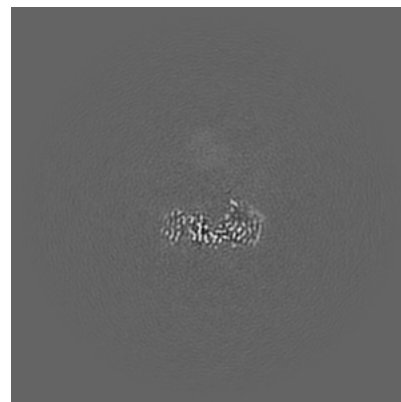
6.3.1 Primary map



X Index: 213

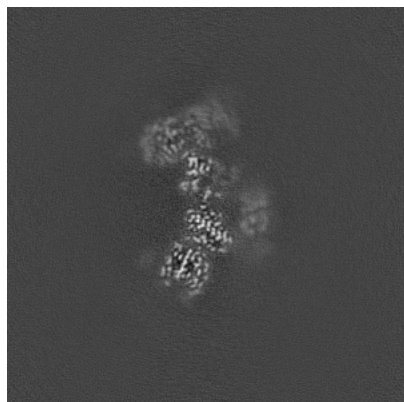


Y Index: 187

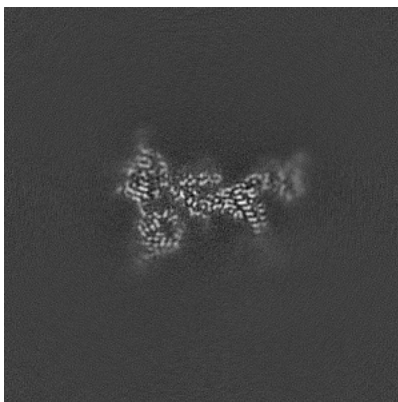


Z Index: 154

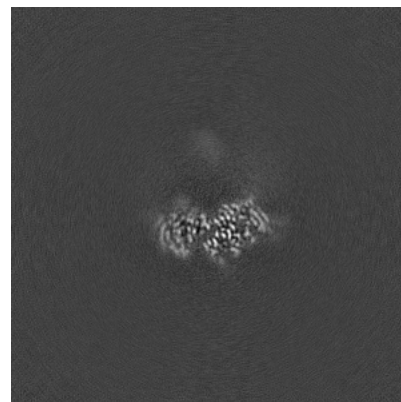
6.3.2 Raw map



X Index: 216



Y Index: 188

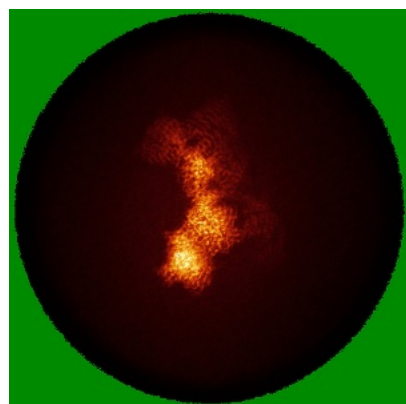


Z Index: 141

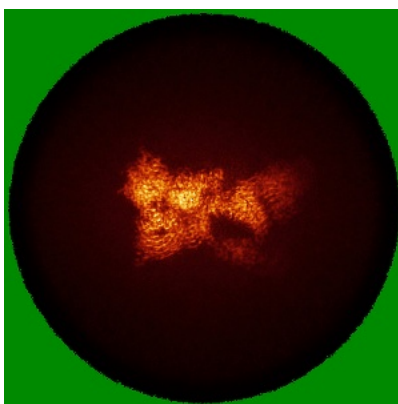
The images above show the largest variance slices of the map in three orthogonal directions.

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

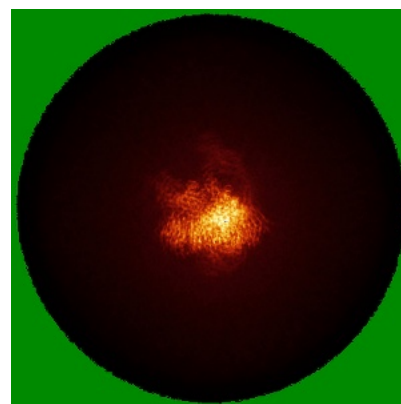
6.4.1 Primary map



X

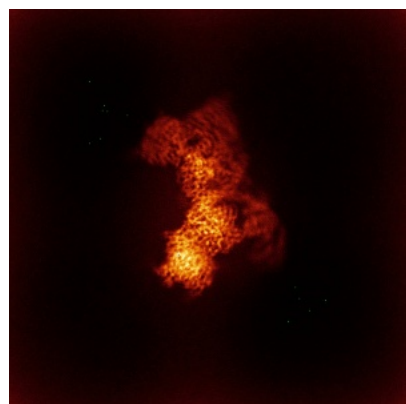


Y

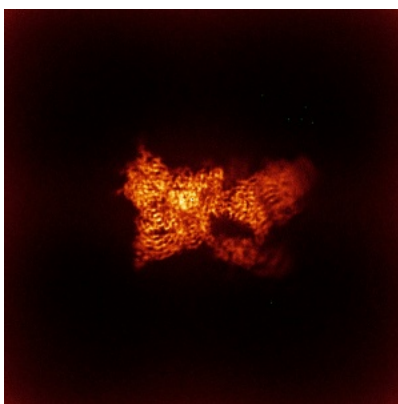


Z

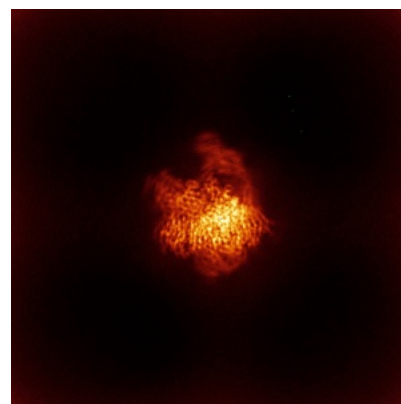
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

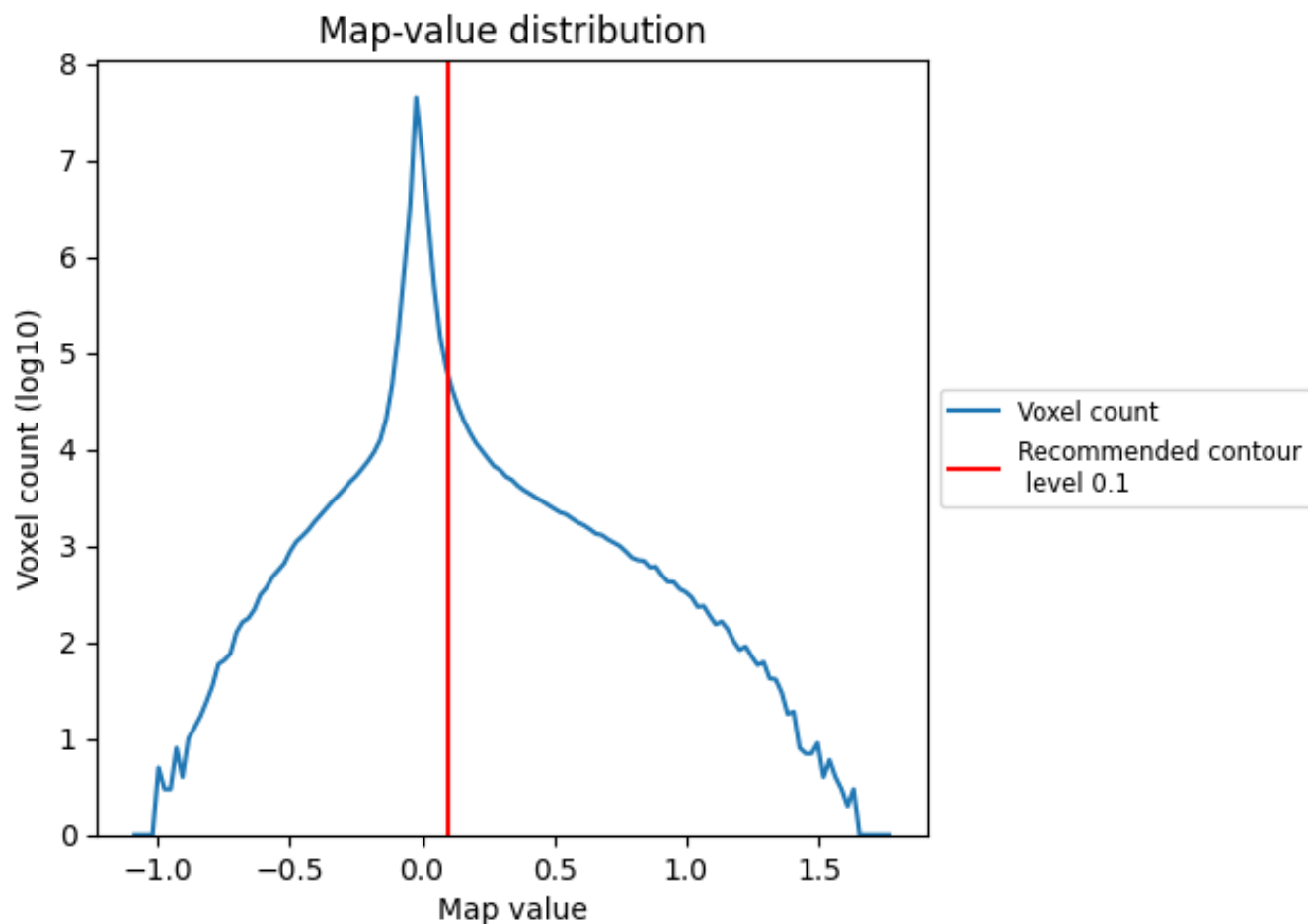
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

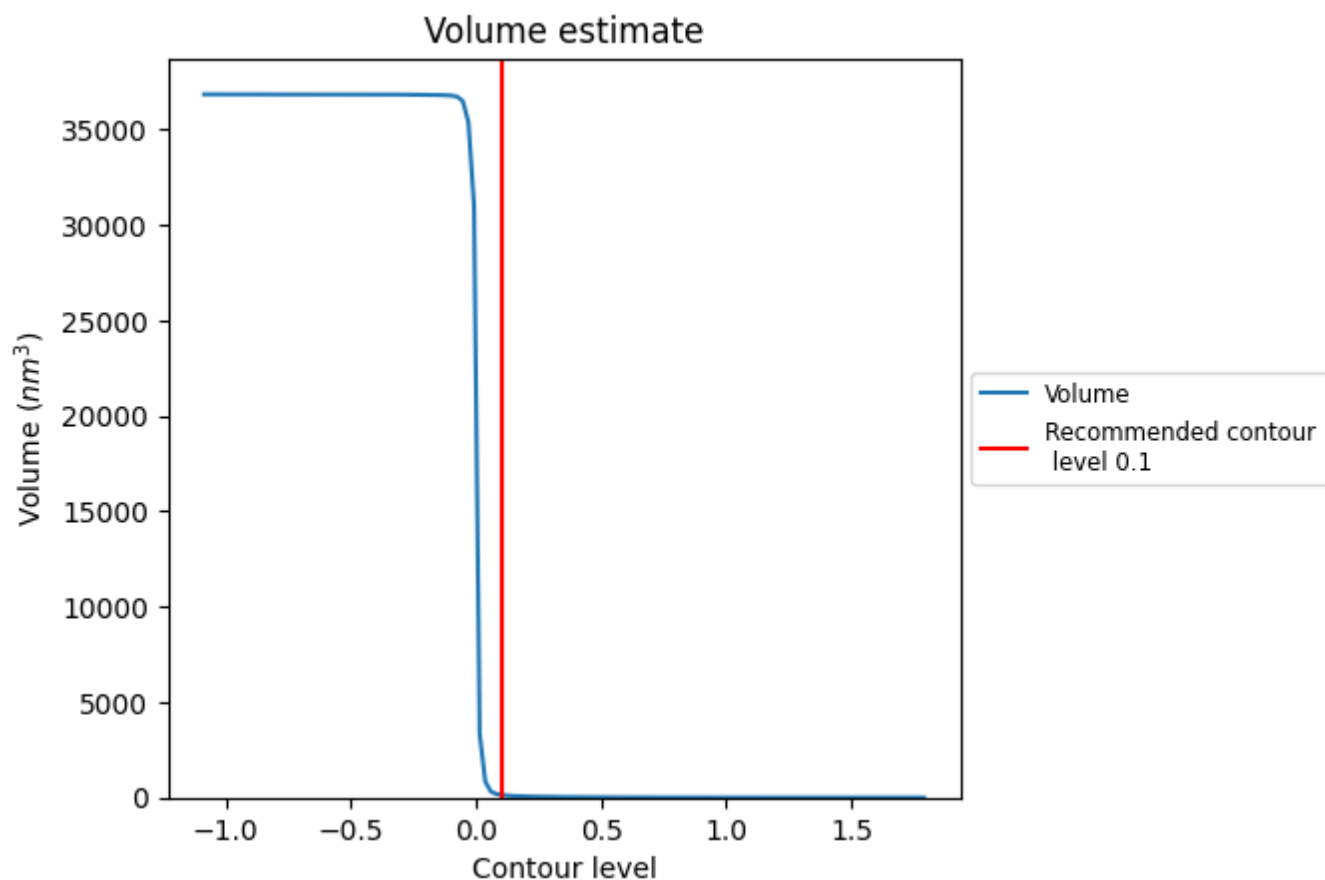
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

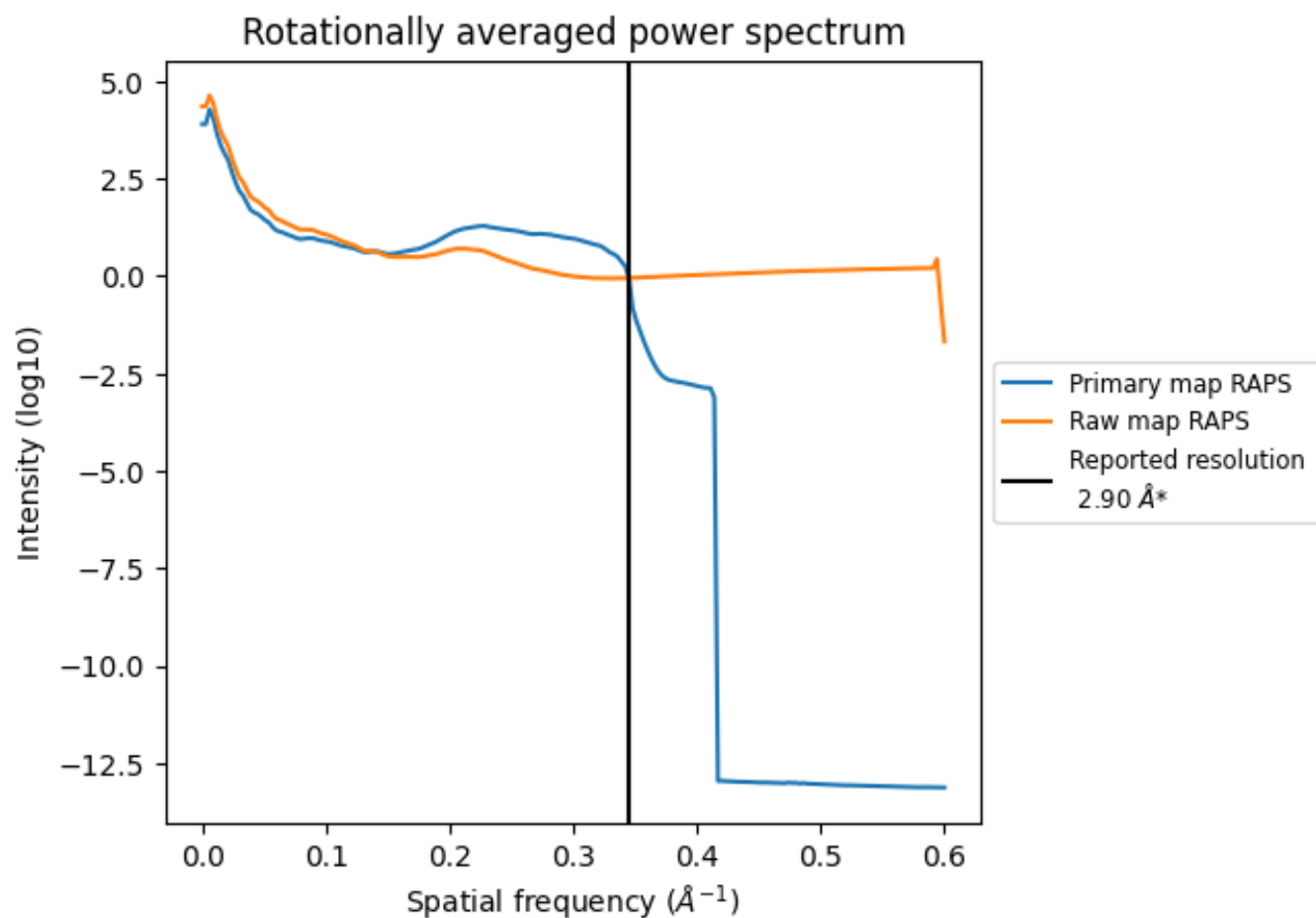
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm³; this corresponds to an approximate mass of 128 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 ⓘ

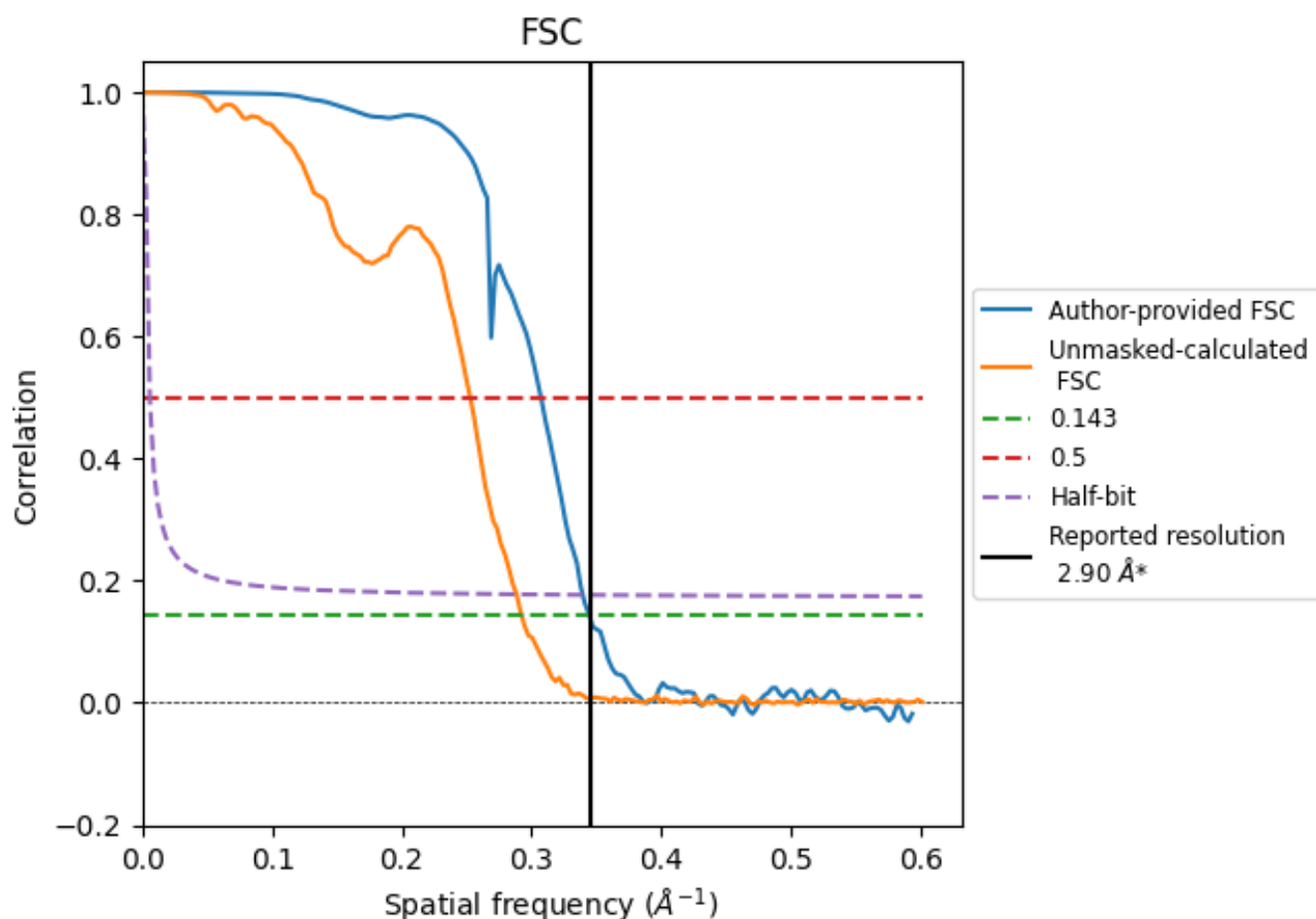


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

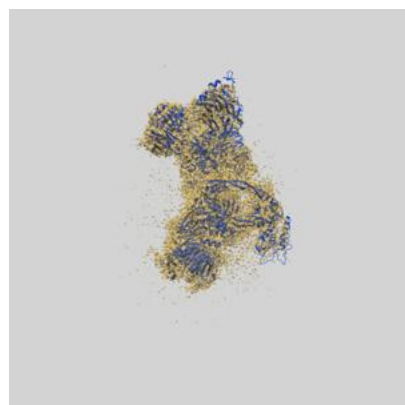
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.25	2.95
Unmasked-calculated*	3.42	3.96	3.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.42 differs from the reported value 2.9 by more than 10 %

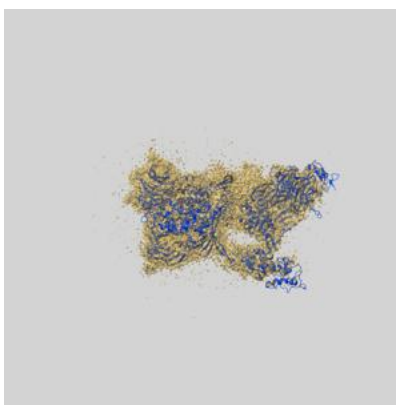
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67778 and PDB model 21KR. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

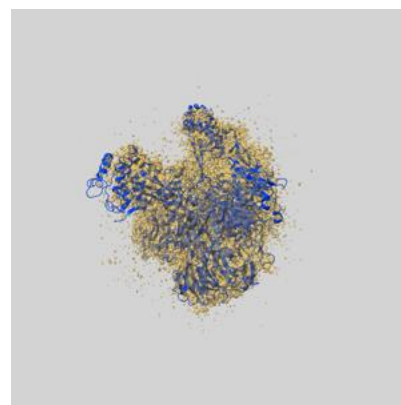
9.1 Map-model overlay [i](#)



X



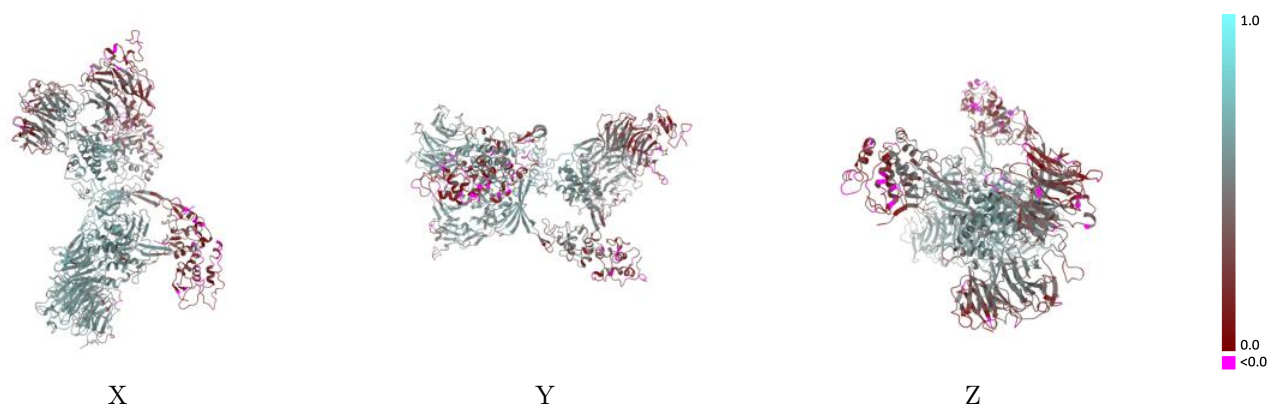
Y



Z

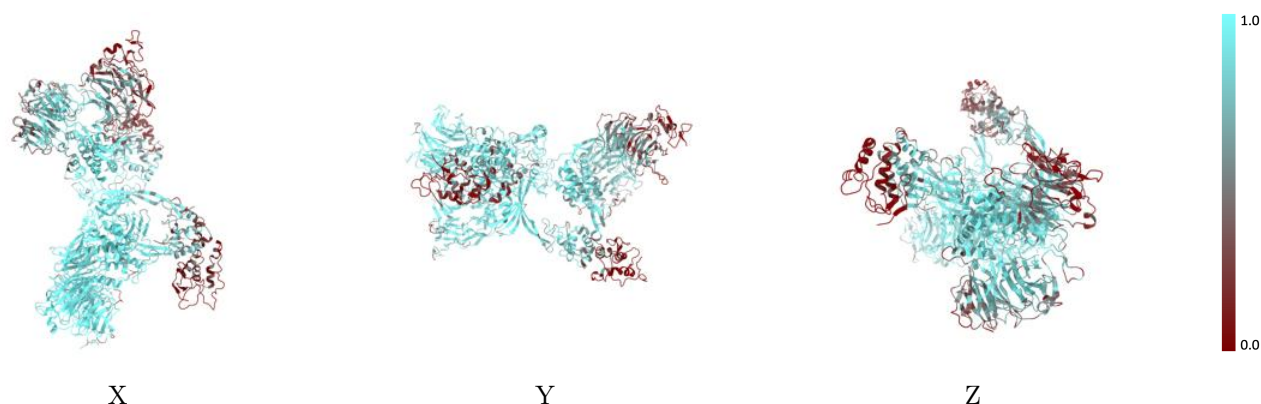
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



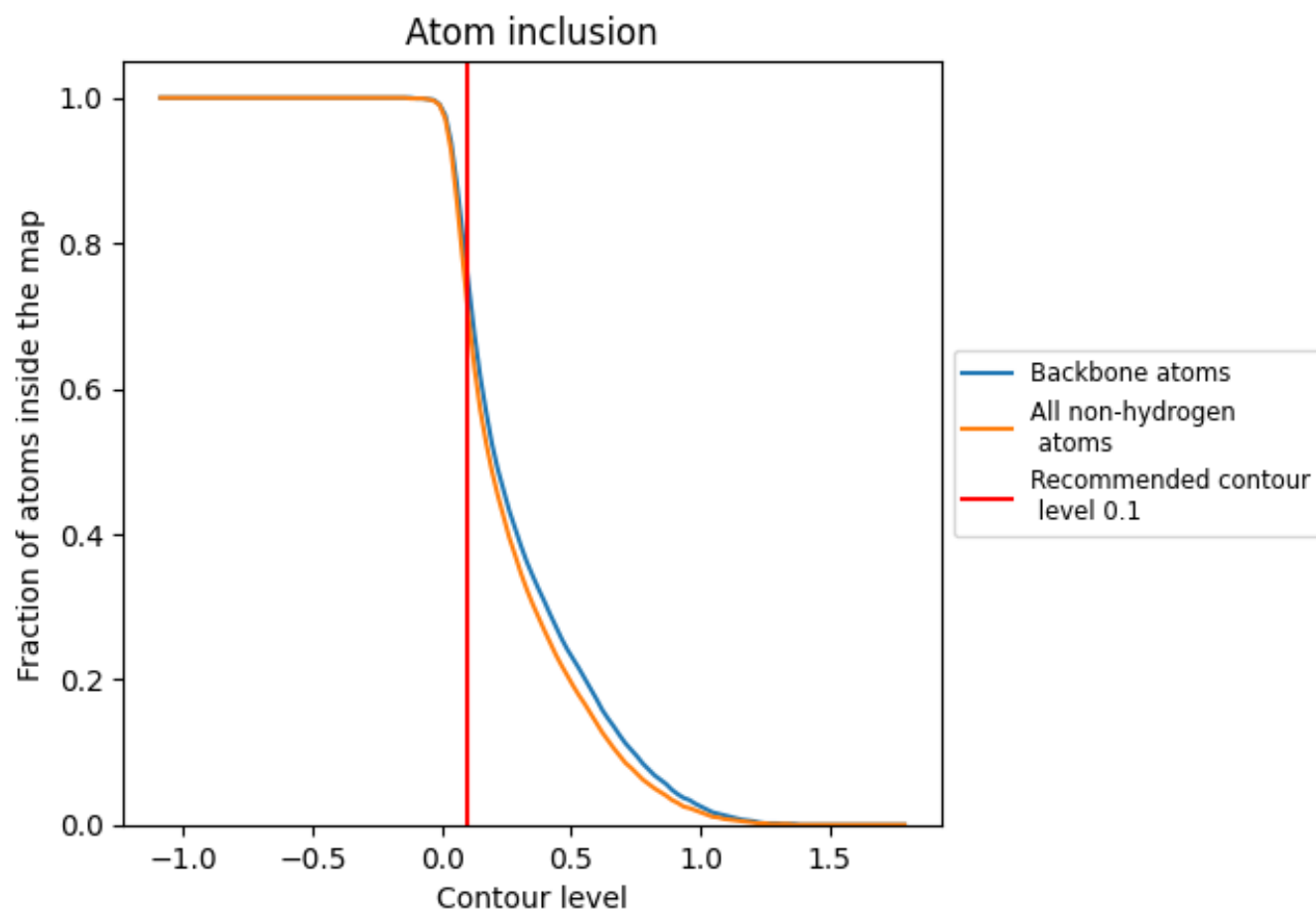
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 71% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7110	<div></div> 0.4420
A	<div></div> 0.9170	<div></div> 0.5520
B	<div></div> 0.9130	<div></div> 0.5550
C	<div></div> 0.5600	<div></div> 0.2630
D	<div></div> 0.1310	<div></div> 0.1340
E	<div></div> 0.8720	<div></div> 0.5410
F	<div></div> 0.5330	<div></div> 0.3480
G	<div></div> 0.7260	<div></div> 0.4270
H	<div></div> 0.0820	<div></div> 0.1820
I	<div></div> 0.9250	<div></div> 0.5430
J	<div></div> 0.8210	<div></div> 0.5350
K	<div></div> 0.8570	<div></div> 0.3880
L	<div></div> 0.8570	<div></div> 0.5610

