wwPDB EM Validation Summary Report (i)

Oct 27, 2026 – 10:13 AM EDT

PDB ID	:	9PTT / pdb_00009ptt
EMDB ID	:	EMD-71846
Title	:	Protein Complex(local refinement)
Authors	:	Hu, Q.; Li, D.; Sun, Y.; Li, X.
Deposited on	:	2025-07-29
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

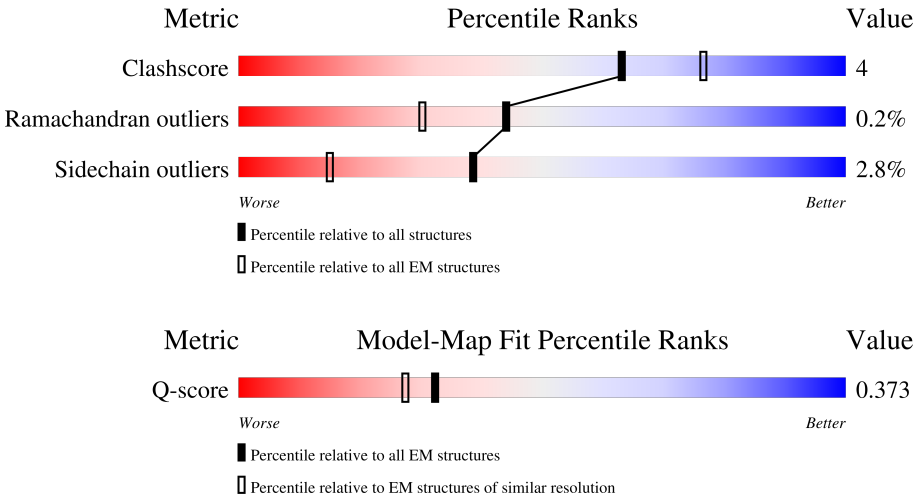
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

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 3.60 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	12797 (3.10 - 4.10)

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 <=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	537	68% 11% • 21%
1	C	537	68% 11% • 21%
2	B	305	67% 14% • 18%
2	D	305	67% 13% • 18%

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Mol	Chain	Length	Quality of chain
3	F	133	60% 8% 32%
3	G	133	57% 9% 34%
3	H	133	59% 8% 34%
3	M	133	61% 8% 32%
4	K	1615	97%
4	P	1615	97%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14410 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 Frizzled-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	425	Total	C	N	O	S	0	0
			3351	2194	529	592	36		
1	C	425	Total	C	N	O	S	0	0
			3351	2194	529	592	36		

- Molecule 2 is a protein called Tetraspanin-12.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	249	Total	C	N	O	S	0	0
			2027	1333	324	346	24		
2	D	249	Total	C	N	O	S	0	0
			2027	1333	324	346	24		

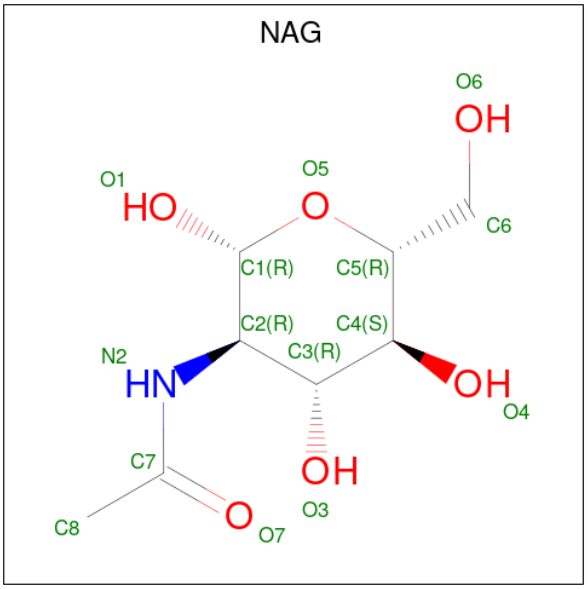
- Molecule 3 is a protein called Norrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	91	Total	C	N	O	S	0	0
			718	434	143	127	14		
3	H	88	Total	C	N	O	S	0	0
			695	421	136	125	13		
3	F	91	Total	C	N	O	S	0	0
			718	434	143	127	14		
3	G	88	Total	C	N	O	S	0	0
			695	421	136	125	13		

- Molecule 4 is a protein called Low-density lipoprotein receptor-related protein 5.

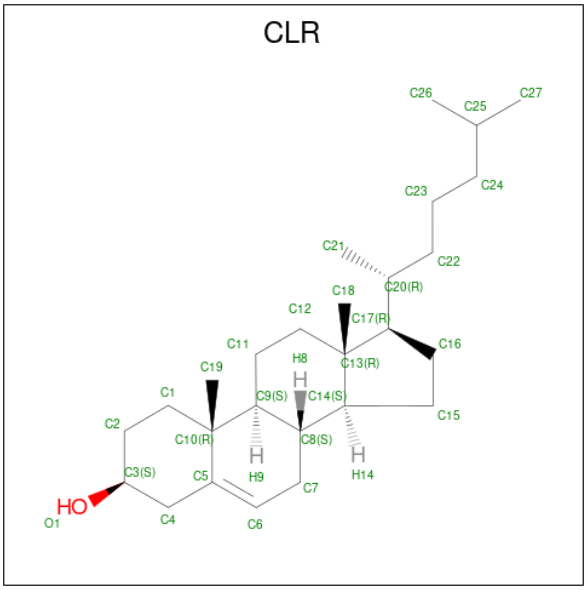
Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	42	Total	C	N	O	S	0	0
			315	194	51	63	7		
4	K	42	Total	C	N	O	S	0	0
			315	194	51	63	7		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			15	8	1	6	
5	C	1	Total	C	N	O	0
			15	8	1	6	

- Molecule 6 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			28	27	1	
6	A	1	Total	C	O	0
			28	27	1	
6	B	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	C	1	Total	C	O	0
			28	27	1	
6	D	1	Total	C	O	0
			28	27	1	

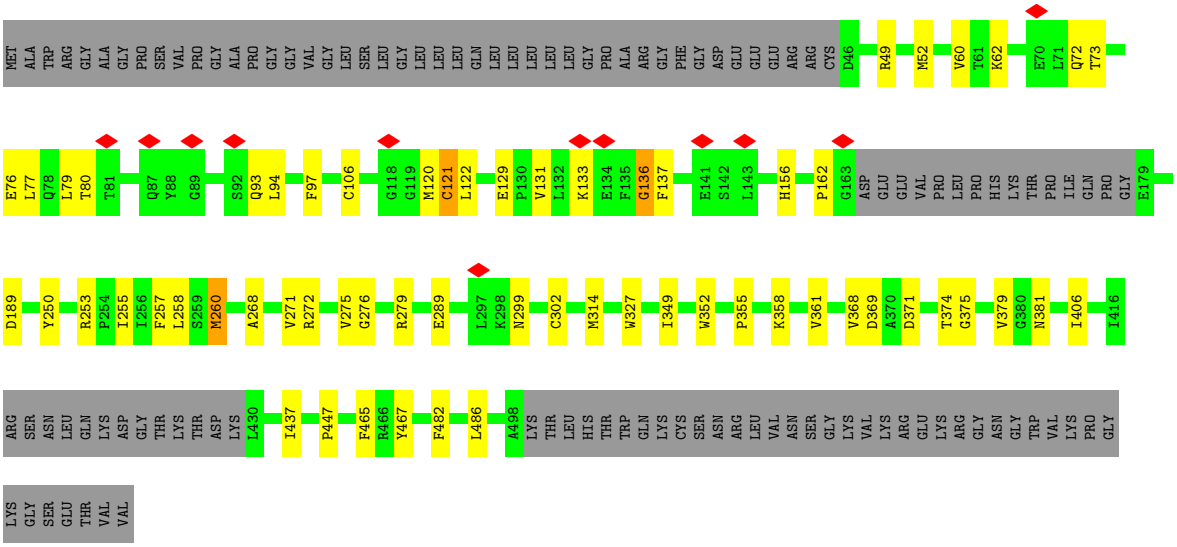
3 Residue-property plots (i)

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: Frizzled-4

Chain A:

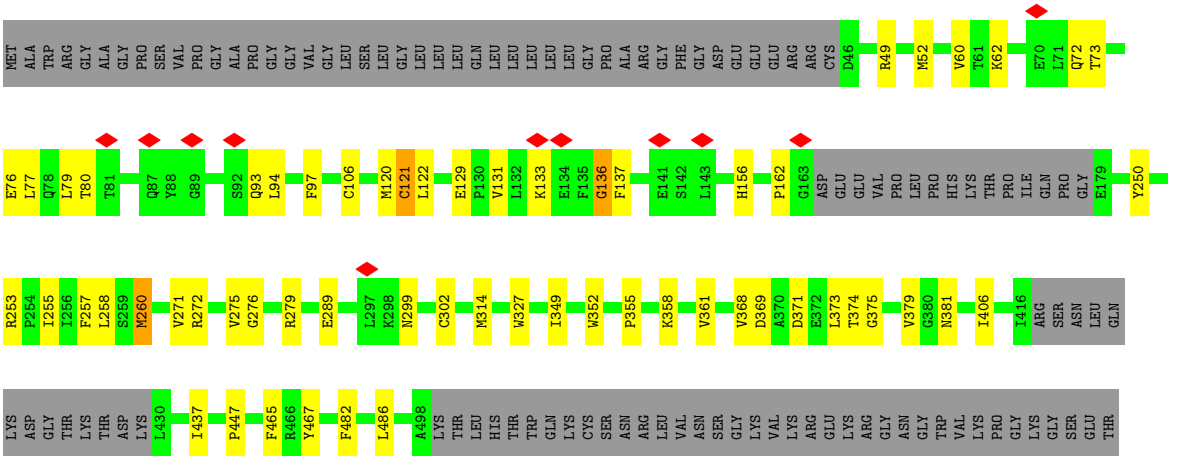




• Molecule 1: Frizzled-4

Chain C:

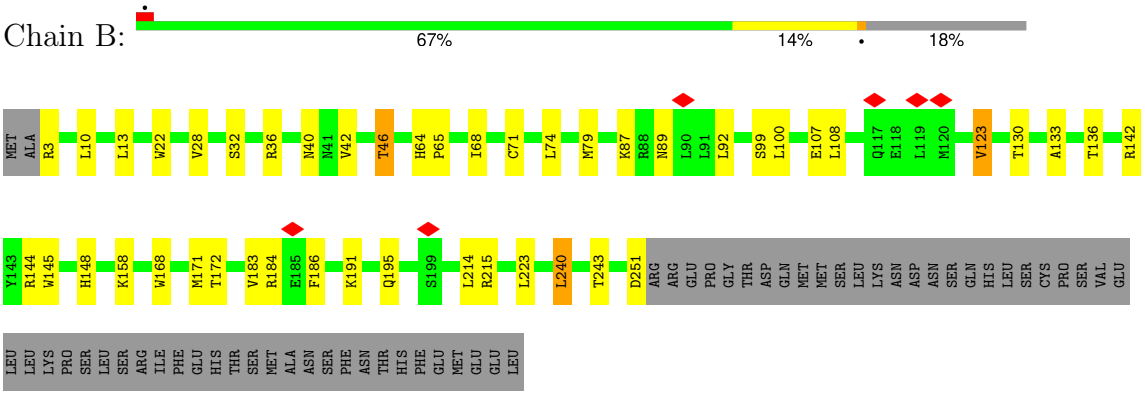






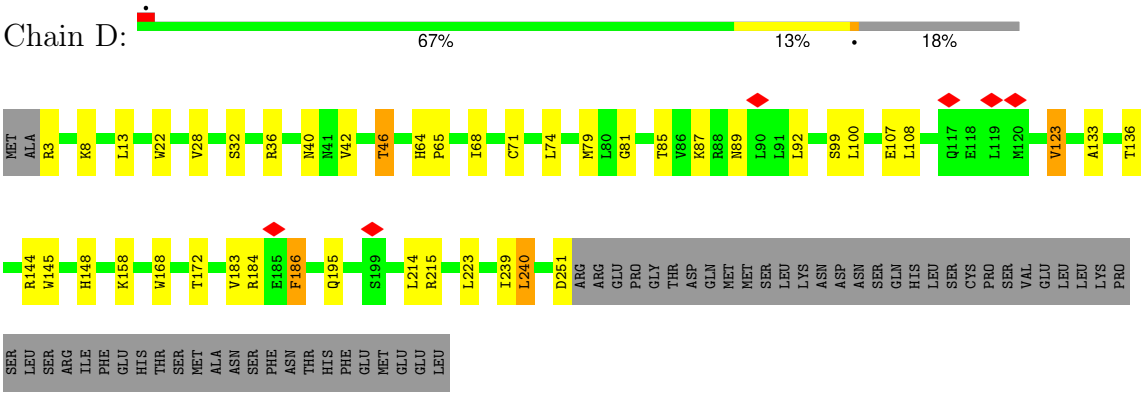
• Molecule 2: Tetraspanin-12

Chain B:



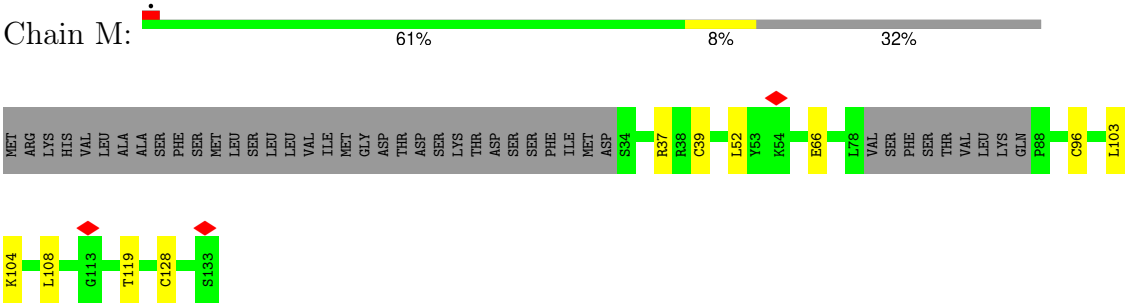
• Molecule 2: Tetraspanin-12

Chain D:



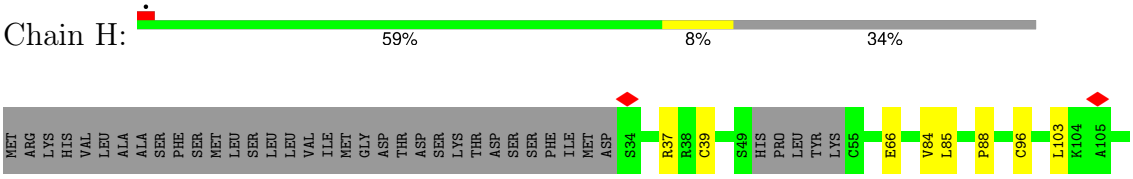
• Molecule 3: Norrin

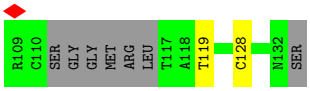
Chain M:



• Molecule 3: Norrin

Chain H:

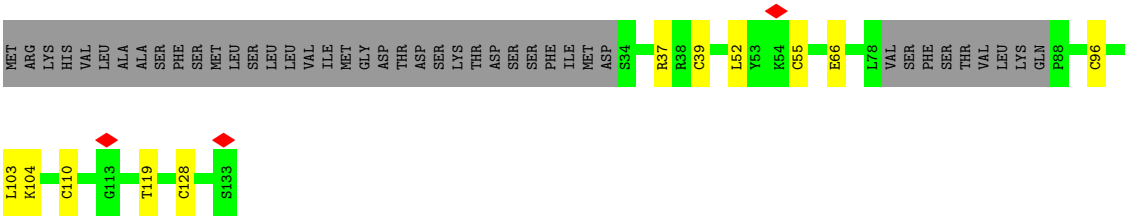




• Molecule 3: Norrin

Chain F:

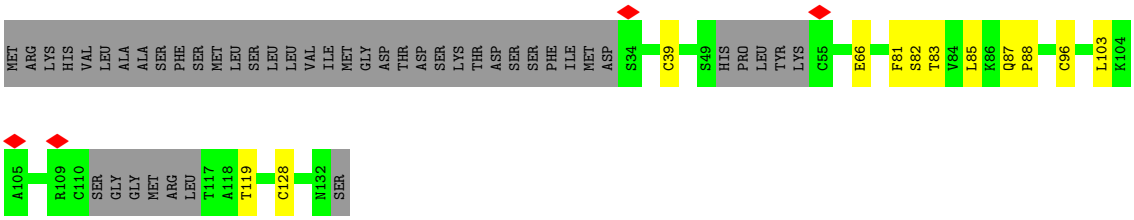




• Molecule 3: Norrin

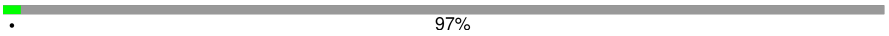
Chain G:

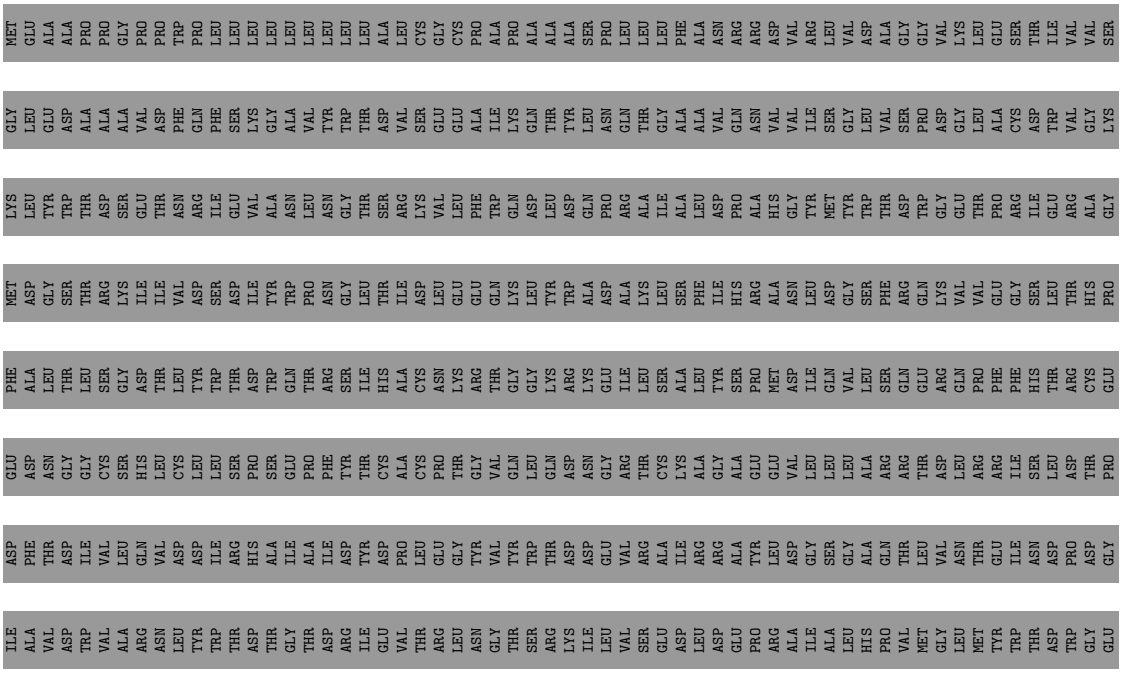


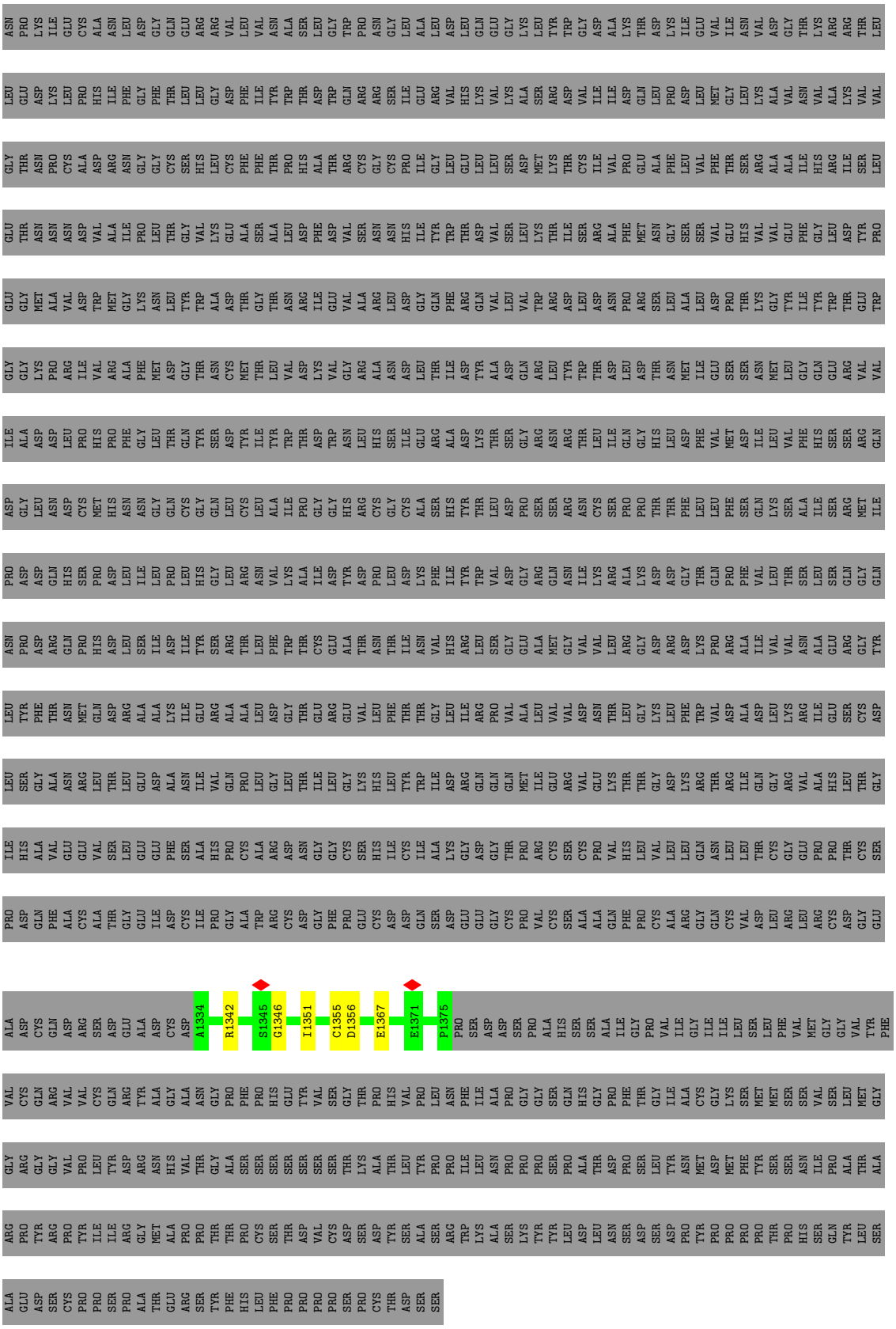


• Molecule 4: Low-density lipoprotein receptor-related protein 5

Chain P:

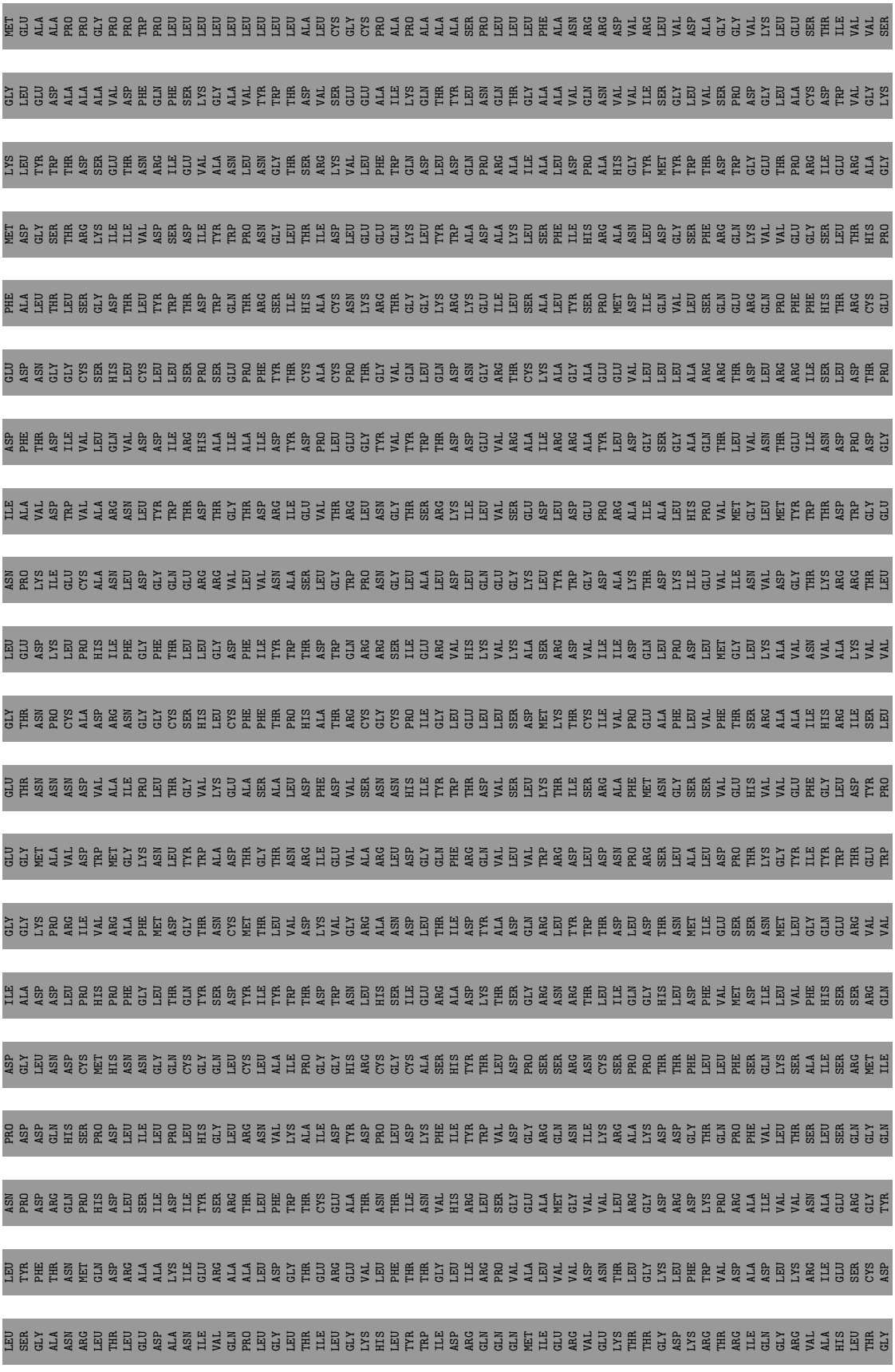


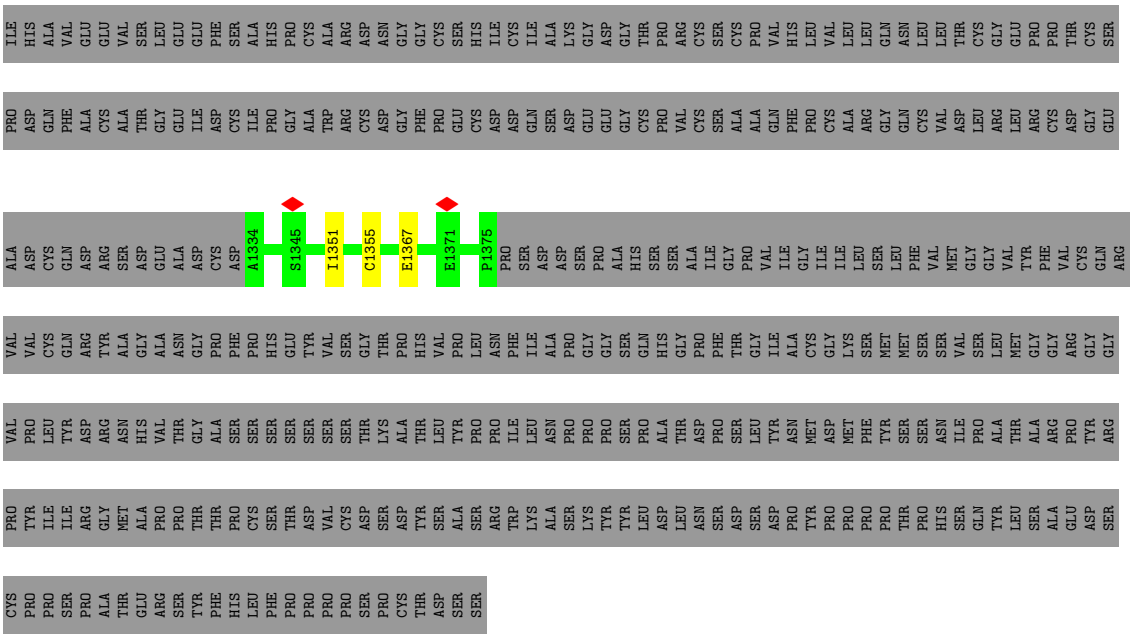




• Molecule 4: Low-density lipoprotein receptor-related protein 5

Chain K: 97%


MET GLU ALA ALA PRO PRO GLY PRO PRO TRP PRO LEU LEU LEU LEU LEU LEU LEU LEU ALA LEU CYS GLY CYS PRO ALA PRO ALA ALA ALA SER PRO LEU LEU LEU PHE ALA ASN ARG ARG ASP VAL ARG LEU VAL ASP ALA GLY GLY VAL LYS LEU GLU SER THR ILE VAL VAL SER
GLY LEU GLU ASP ALA ALA ALA VAL ASP PHE GLN PHE SER LYS GLY ALA VAL TYR TRP THR ASP VAL SER GLU GLU ALA ILE LYS GLN THR TYR LEU ASN GLN THR GLY ALA ALA VAL GLN ASN VAL VAL ILE SER GLY LEU VAL SER PRO ASP GLY LEU ALA CYS ASP TRP VAL GLY LYS
LYS LEU TYR TRP THR ASP SER GLU THR ASN ARG ILE GLU VAL ALA ASN LEU ASN GLY THR SER ARG LYS VAL LEU PHE TRP GLN ASP LEU ASP GLN PRO ARG ALA ILE ALA LEU ASP PRO ALA HIS GLY TYR MET TYR TRP THR ASP TRP GLY GLU THR PRO ARG ILE GLU ARG ALA GLY
MET ASP GLY SER THR ARG LYS ILE ILE VAL ASP SER ASP ILE TYR TRP TRP PRO ASN GLY LEU THR ILE ASP ALA CYS ASP LEU GLU GLU GLN LYS LEU GLY LEU ASP ALA LYS LEU SER PHE ILE HIS ARG ALA ASN LEU ASP GLY SER PHE ARG GLN LYS VAL VAL GLU GLY SER LEU THR HIS PRO
PHE ALA LEU THR LEU SER GLY ASP THR ARG SER ILE HIS ALA CYS ASN LYS ARG THR GLY GLY LYS ARG LYS GLU ILE LEU SER ALA LEU TYR SER PRO MET ASP ILE GLN VAL LEU SER GLN GLU ARG GLN PRO PHE PHE HIS THR ARG CYS GLU
GLU ASP ASN GLY GLY CYS SER HIS LEU CYS LEU LEU LEU SER PRO SER GLU PRO PHE TYR THR CYS ALA CYS PRO THR GLY VAL GLN LEU GLN ASP ASN GLY ARG THR ASP GLU LEU LEU LEU LEU ALA ARG ARG THR ASP LEU ARG ARG ARG ILE SER LEU ASP THR PRO
ASP PHE THR ASP ILE VAL LEU GLN VAL ASP ASP ILE ARG HIS ALA ILE ALA ILE ASP TYR ASP PRO LEU GLU GLY TYR VAL TYR TRP THR ASP ASP GLU VAL ARG ALA ILE ARG ARG ALA GLN THR LEU VAL ASN THR GLU ILE ASP PRO ASP GLY
ILE ALA VAL ASP TRP VAL ALA ARG ASN LEU TYR TRP THR ASP ARG ILE GLU VAL THR ARG LEU ASN GLY THR SER ARG LYS ILE LEU VAL SER GLU ASP LEU ASP GLU PRO ARG ALA ILE ARG ARG ALA ILE LEU HIS PRO VAL MET GLY LEU MET TYR TRP THR ASP TRP GLY GLU
ASN PRO LYS ILE GLU CYS ALA ASN LEU ASP GLY GLN GLU ARG ASN LEU VAL ASN ALA SER LEU GLY GLY TRP PRO ASN GLY LEU GLU ALA LEU ASP LEU GLN LEU GLU GLU PRO ASP ALA LYS THR ASP ILE GLU ILE VAL ILE ASN VAL ASP GLY THR LYS ARG ARG THR LEU
LEU GLU ASP LYS LEU PRO HIS ILE PHE GLY PHE THR LEU LEU GLY ASP PHE ILE TYR TRP THR ASP TRP GLN ARG ARG SER ILE GLU ARG VAL HIS LYS VAL LYS ALA SER ARG ASP VAL ILE ILE ASP GLN LEU PRO ASP LEU MET GLY LEU LYS ALA VAL ASN VAL ALA LYS VAL VAL
GLY THR ASN PRO CYS ALA ASP ARG ASN GLY CYS PHE PHE THR PRO HIS ALA THR ARG CYS GLY CYS PRO ILE GLY LEU GLU LEU GLY SER ASP MET LYS THR CYS ILE VAL PRO GLU ALA PHE LEU VAL PHE THR SER ARG ALA ALA ILE HIS ARG ILE SER LEU
GLU THR ASN ASN ASN ASP VAL ALA ILE PRO LEU THR GLY VAL LYS GLU ALA SER ALA LEU ASP PHE ASP VAL SER ASN ASN HIS ILE TYR TRP THR ASP LYS ILE SER ARG ALA PHE MET ASN GLY SER SER VAL GLU HIS VAL VAL GLU PHE GLY LEU ASP TYR PRO
GLU GLY MET ALA VAL ASP TRP MET GLY LYS ASN LEU TYR TRP ASN ALA ASP GLY THR GLY THR ASN ARG LEU ASP GLY GLN PHE ARG GLN VAL LEU LEU VAL TRP ARG ASP LEU ASP ASN PRO ARG SER LEU ALA LEU ASP PRO THR LYS GLY TYR ILE TYR TRP THR GLU TRP
GLY GLY LYS PRO ARG ILE PHE MET ASP GLY THR ASN ASP LEU THR ILE ASP TYR ALA ASP GLN ARG LEU TYR TRP THR ASP LEU ASP THR ASN MET ILE GLU SER SER ASN MET LEU GLY GLN GLU ARG VAL VAL
ILE ALA ASP ASP LEU PRO HIS PRO PHE GLY LEU THR GLN TYR SER ASP TYR ILE TYR TRP THR ASP TRP ASN LEU HIS SER ILE GLU ARG ALA ASP LYS THR SER GLY ARG ASN ARG THR LEU ILE GLN GLY HIS LEU ASP PHE VAL MET ASP PHE VAL SER ARG GLN
ASP GLY LEU ASN ASP CYS GLN CYS GLY GLN LEU CYS LEU ALA ILE PRO GLY GLY HIS ARG CYS GLY CYS ALA SER HIS TYR THR ASN CYS SER PRO PRO THR THR PHE LEU LEU PHE SER GLN LEU LYS SER ALA ILE SER GLY ARG
PRO ASP ASP GLN HIS SER PRO ASP LEU ILE LEU PRO LEU HIS GLY LEU ARG ASN VAL LYS ALA ILE ASP TYR ASP PRO LEU ASP LYS PHE ILE TYR TRP VAL ASP GLY ARG GLN ASN ILE LYS ARG ALA LYS ASP ASP GLY THR GLN PRO PHE VAL LEU THR SER LEU SER GLN GLY GLN
ASN PRO ASP ARG GLN HIS PRO SER LEU ASP ILE TYR SER THR CYS GLU ALA THR ASN THR ILE ASN VAL HIS ARG LEU PHE TRP GLU ALA ILE ASP VAL GLU VAL LEU ARG GLY ASP ARG ASP LYS PRO ARG ALA ILE VAL VAL ASN ALA GLU ARG GLY TYR
LEU TYR PHE THR ASN MET GLN ASP ARG GLU VAL LEU PHE THR THR GLY LEU ILE ARG GLY PRO VAL ALA ASP VAL ASP ASN THR LEU GLY LYS LEU ASP PHE TRP VAL ASP ALA ILE GLU GLY SER LYS ARG ILE GLU SER CYS ASP
LEU SER GLY ALA GLU THR HIS LEU ASP GLN PRO LEU GLY LYS HIS LEU TYR TRP ILE ASP ARG GLN GLN MET ILE GLU GLU ARG VAL GLU LYS THR THR GLY ASP LYS ARG THR ARG ILE GLN GLY ARG VAL ALA HIS GLU LEU THR GLY


A1334
S1345
I1351
C1355
E1367
E1371
P1375

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	1.448	Depositor
Minimum map value	-0.896	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	357.14297, 357.14297, 357.14297	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9398499, 0.9398499, 0.9398499	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, CLR

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	0.32	0/3440	0.71	3/4678 (0.1%)
1	C	0.31	0/3440	0.71	3/4678 (0.1%)
2	B	0.32	0/2081	0.77	5/2831 (0.2%)
2	D	0.33	0/2081	0.77	5/2831 (0.2%)
3	F	0.28	0/732	0.75	0/978
3	G	0.31	0/706	0.87	2/944 (0.2%)
3	H	0.29	0/706	0.78	0/944
3	M	0.28	0/732	0.75	0/978
4	K	0.31	0/319	0.77	0/429
4	P	0.31	0/319	0.77	0/429
All	All	0.31	0/14556	0.75	18/19720 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	B	0	1
2	D	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	136	GLY	CA-C-N	5.93	132.86	121.54
1	C	136	GLY	C-N-CA	5.93	132.86	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	GLY	CA-C-N	5.91	132.83	121.54
1	A	136	GLY	C-N-CA	5.91	132.83	121.54
3	G	82	SER	CA-C-N	5.72	132.46	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	GLY	Peptide
2	B	107	GLU	Peptide
1	C	136	GLY	Peptide
2	D	107	GLU	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	3351	0	3321	31	0
1	C	3351	0	3321	29	0
2	B	2027	0	2031	24	0
2	D	2027	0	2031	24	0
3	F	718	0	700	5	0
3	G	695	0	678	4	0
3	H	695	0	678	4	0
3	M	718	0	700	5	0
4	K	315	0	296	2	0
4	P	315	0	296	5	0
5	A	15	0	15	0	0
5	C	15	0	15	0	0
6	A	56	0	92	4	0
6	B	28	0	43	1	0
6	C	56	0	92	4	0
6	D	28	0	43	1	0
All	All	14410	0	14352	122	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 4.

The worst 5 of 122 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:39:CYS:HA	3:F:66:GLU:O	1.88	0.74
3:H:39:CYS:HA	3:H:66:GLU:O	1.88	0.73
3:M:39:CYS:HA	3:M:66:GLU:O	1.88	0.73
3:G:39:CYS:HA	3:G:66:GLU:O	1.88	0.73
2:D:28:VAL:O	2:D:32:SER:HB2	1.89	0.73

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	A	419/537 (78%)	389 (93%)	29 (7%)	1 (0%)	43 72
1	C	419/537 (78%)	389 (93%)	29 (7%)	1 (0%)	43 72
2	B	247/305 (81%)	232 (94%)	15 (6%)	0	100 100
2	D	247/305 (81%)	232 (94%)	15 (6%)	0	100 100
3	F	87/133 (65%)	81 (93%)	6 (7%)	0	100 100
3	G	82/133 (62%)	77 (94%)	4 (5%)	1 (1%)	10 41
3	H	82/133 (62%)	78 (95%)	4 (5%)	0	100 100
3	M	87/133 (65%)	82 (94%)	5 (6%)	0	100 100
4	K	40/1615 (2%)	37 (92%)	3 (8%)	0	100 100
4	P	40/1615 (2%)	37 (92%)	3 (8%)	0	100 100
All	All	1750/5446 (32%)	1634 (93%)	113 (6%)	3 (0%)	44 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	PHE
1	C	137	PHE
3	G	83	THR

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/459 (80%)	358 (98%)	9 (2%)	42	63
1	C	367/459 (80%)	357 (97%)	10 (3%)	39	61
2	B	223/276 (81%)	216 (97%)	7 (3%)	35	59
2	D	223/276 (81%)	217 (97%)	6 (3%)	39	61
3	F	84/123 (68%)	81 (96%)	3 (4%)	31	56
3	G	83/123 (68%)	80 (96%)	3 (4%)	31	56
3	H	83/123 (68%)	80 (96%)	3 (4%)	31	56
3	M	84/123 (68%)	81 (96%)	3 (4%)	31	56
4	K	38/1383 (3%)	38 (100%)	0	100	100
4	P	38/1383 (3%)	38 (100%)	0	100	100
All	All	1590/4728 (34%)	1546 (97%)	44 (3%)	38	60

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	379	VAL
2	D	186	PHE
1	C	406	ILE
2	D	64	HIS
2	D	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
4	K	1353	GLN

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Mol	Chain	Res	Type
3	G	42	HIS
3	G	87	GLN
3	H	42	HIS
2	D	40	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)

8 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	C	601	-	15,15,15	0.57	0	21,21,21	0.96	1 (4%)
6	CLR	C	602	-	31,31,31	0.47	0	48,48,48	1.05	3 (6%)
6	CLR	C	603	-	31,31,31	0.45	0	48,48,48	0.96	1 (2%)
6	CLR	B	801	-	31,31,31	0.46	0	48,48,48	0.97	3 (6%)
6	CLR	A	602	-	31,31,31	0.46	0	48,48,48	1.05	3 (6%)
6	CLR	A	603	-	31,31,31	0.45	0	48,48,48	0.96	1 (2%)
6	CLR	D	801	-	31,31,31	0.47	0	48,48,48	0.96	3 (6%)
5	NAG	A	601	-	15,15,15	0.57	0	21,21,21	0.96	1 (4%)

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	C	601	-	-	1/6/26/26	0/1/1/1
6	CLR	C	602	-	-	6/10/68/68	0/4/4/4
6	CLR	C	603	-	-	1/10/68/68	0/4/4/4
6	CLR	B	801	-	-	1/10/68/68	0/4/4/4
6	CLR	A	602	-	-	6/10/68/68	0/4/4/4
6	CLR	A	603	-	-	1/10/68/68	0/4/4/4
6	CLR	D	801	-	-	1/10/68/68	0/4/4/4
5	NAG	A	601	-	-	1/6/26/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	602	CLR	C21-C20-C17	3.40	117.99	112.88
6	C	602	CLR	C21-C20-C17	3.40	117.98	112.88
6	C	602	CLR	C13-C17-C20	2.94	124.04	119.50
6	A	602	CLR	C13-C17-C20	2.90	123.98	119.50
6	B	801	CLR	C21-C20-C17	2.59	116.77	112.88

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	602	CLR	C17-C20-C22-C23
6	C	602	CLR	C17-C20-C22-C23
6	A	602	CLR	C21-C20-C22-C23
6	C	602	CLR	C21-C20-C22-C23
6	B	801	CLR	C22-C23-C24-C25

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	602	CLR	4	0
6	C	603	CLR	2	0
6	B	801	CLR	1	0
6	A	602	CLR	4	0

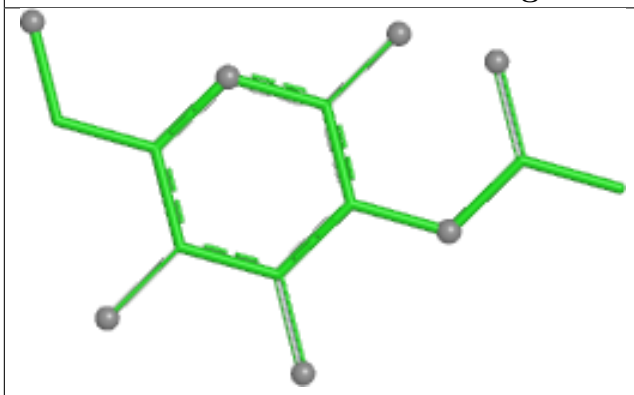
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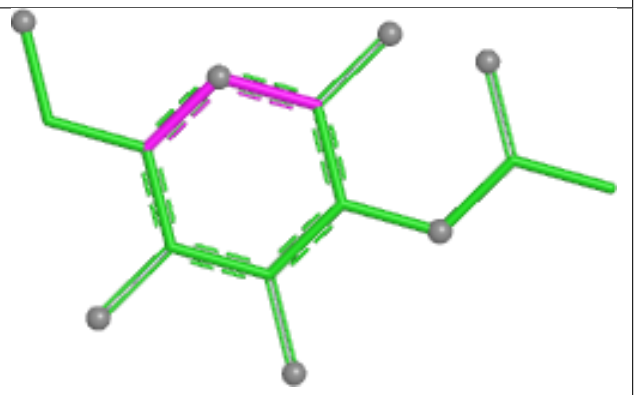
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	CLR	2	0
6	D	801	CLR	1	0

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

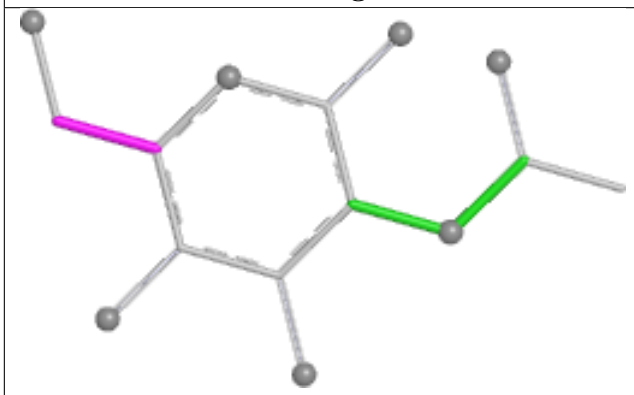
Ligand NAG C 601



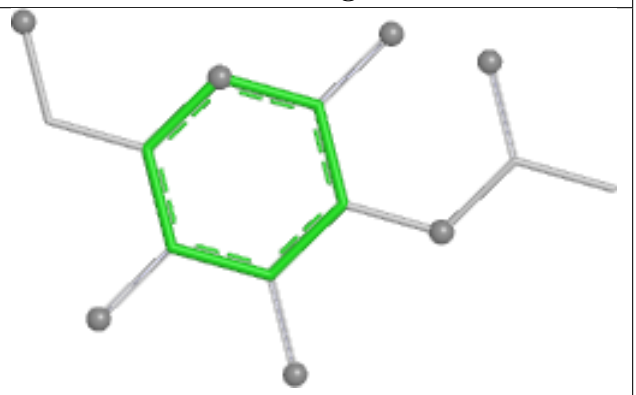
Bond lengths



Bond angles

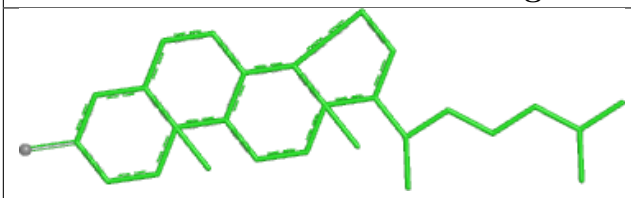


Torsions

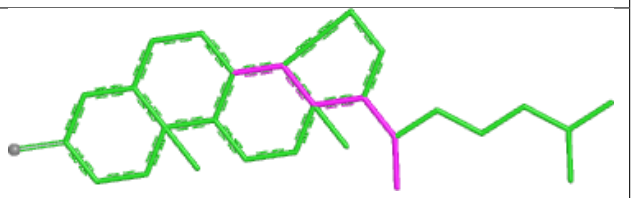


Rings

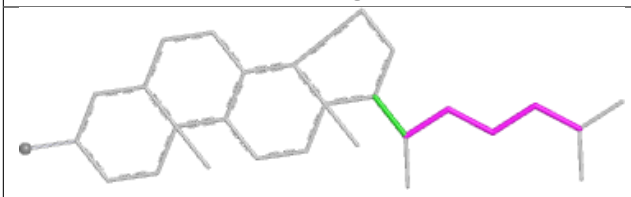
Ligand CLR C 602



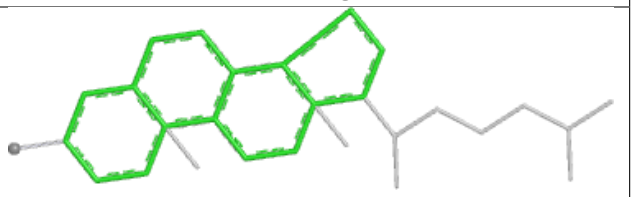
Bond lengths



Bond angles

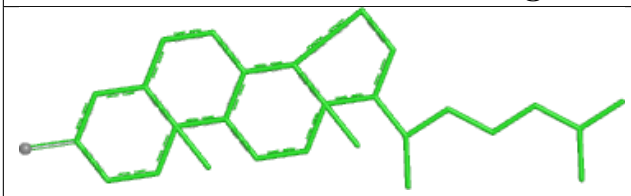


Torsions

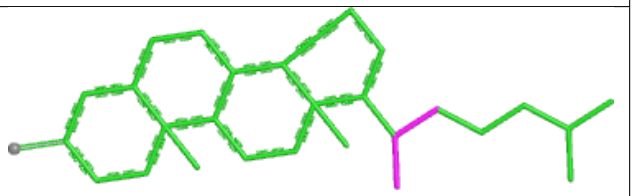


Rings

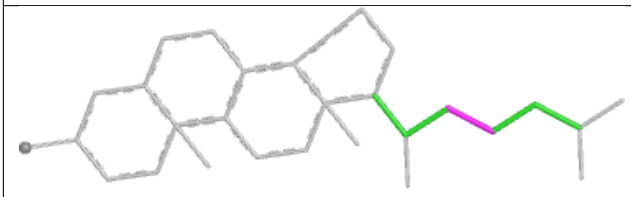
Ligand CLR C 603



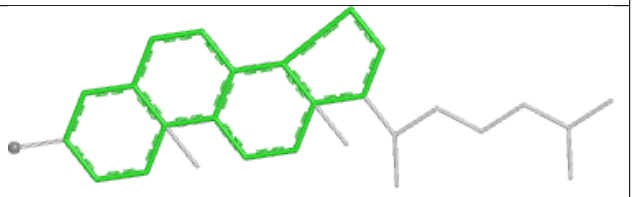
Bond lengths



Bond angles

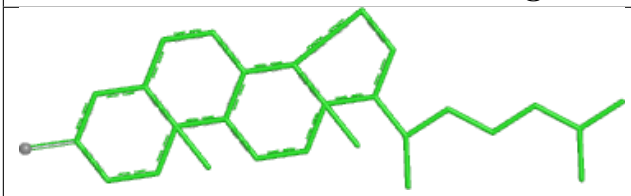


Torsions

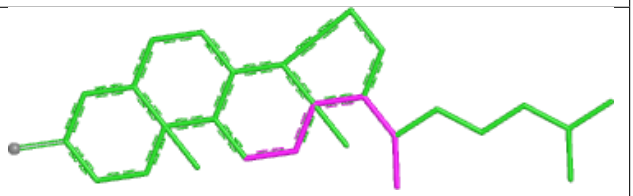


Rings

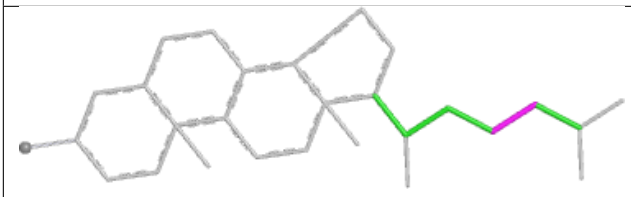
Ligand CLR B 801



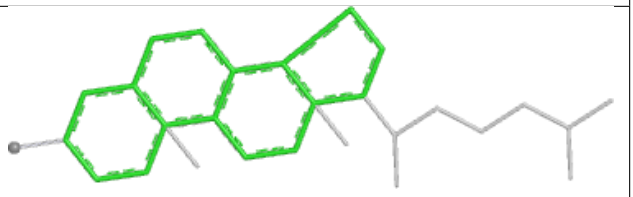
Bond lengths



Bond angles

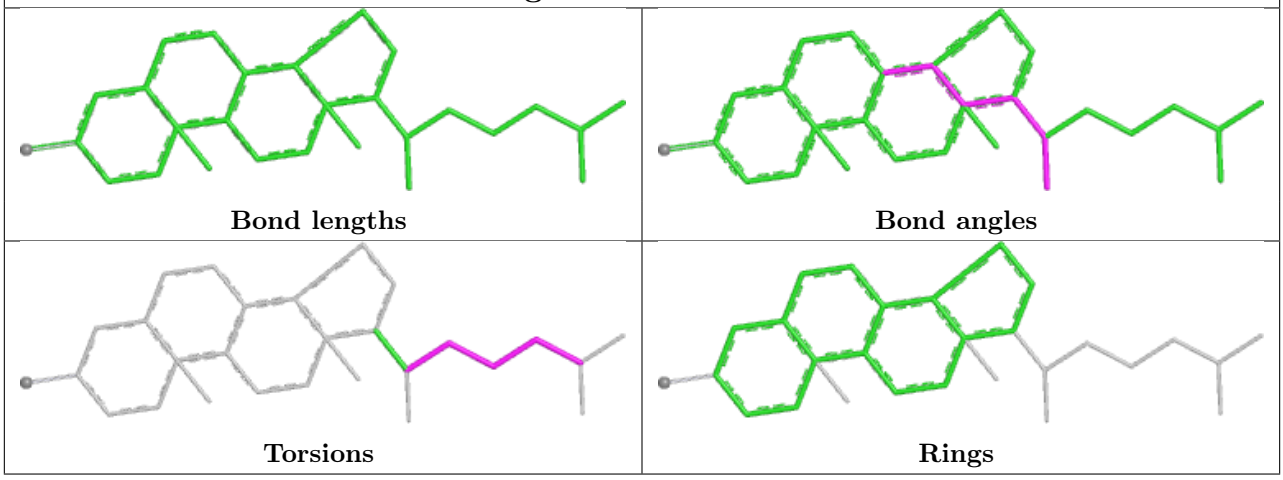


Torsions

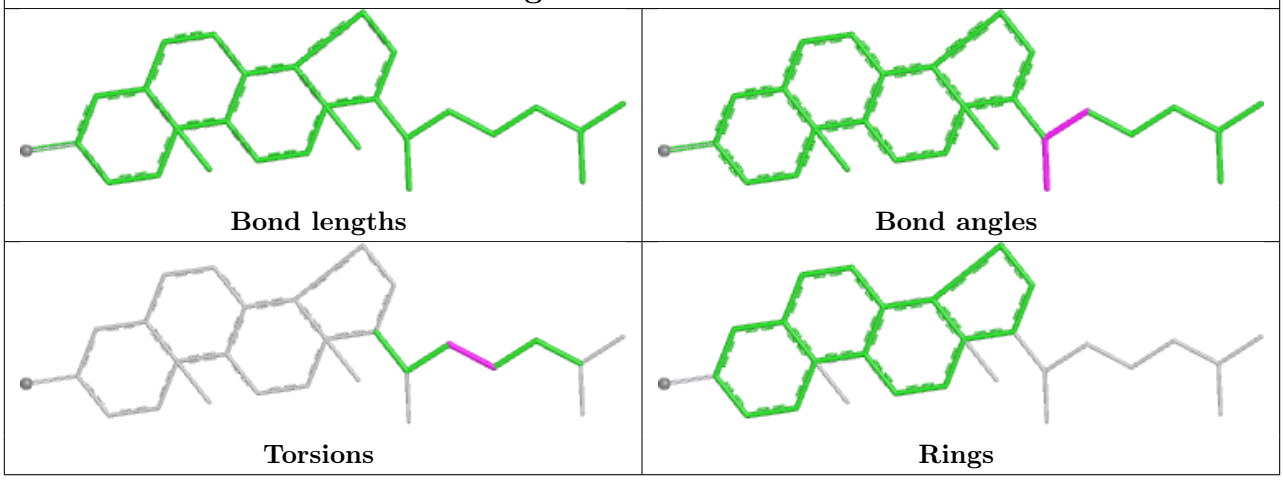


Rings

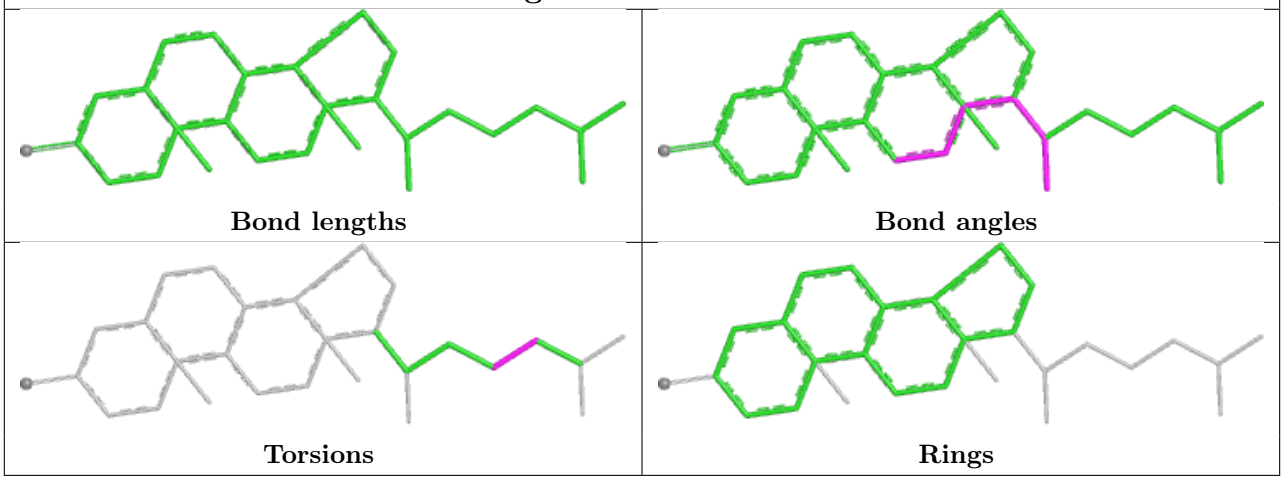
Ligand CLR A 602



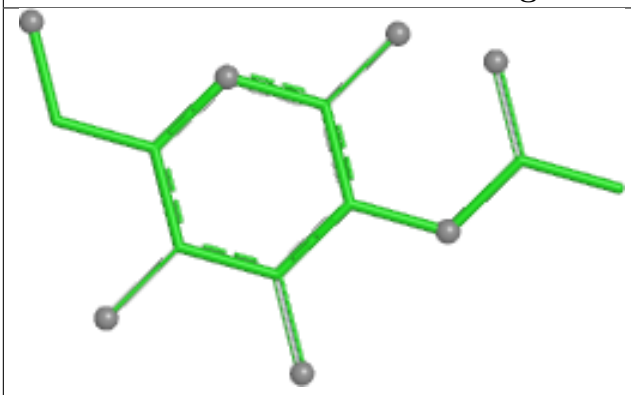
Ligand CLR A 603



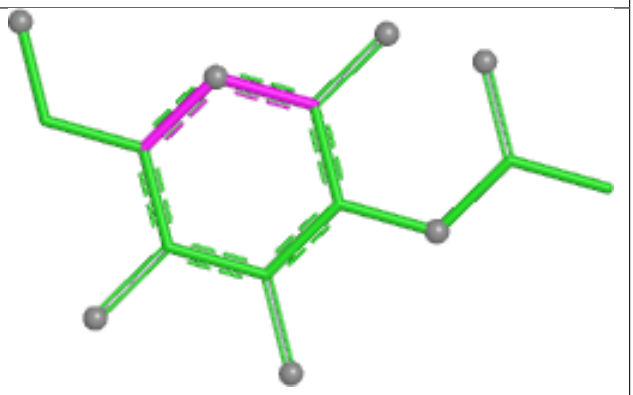
Ligand CLR D 801



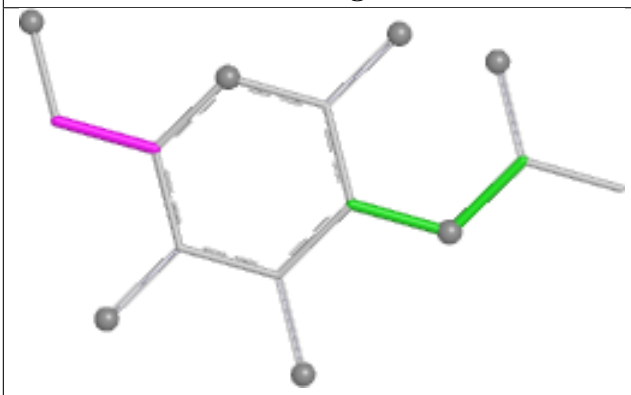
Ligand NAG A 601



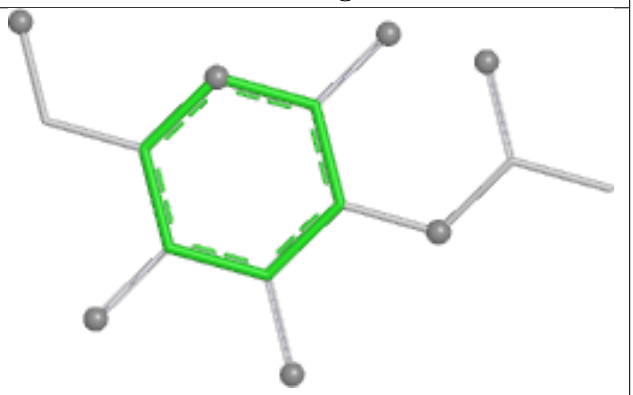
Bond lengths



Bond angles



Torsions



Rings

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.

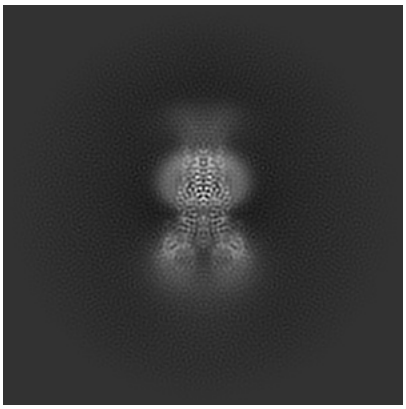
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71846. These allow visual inspection of the internal detail of the map and identification of artifacts.

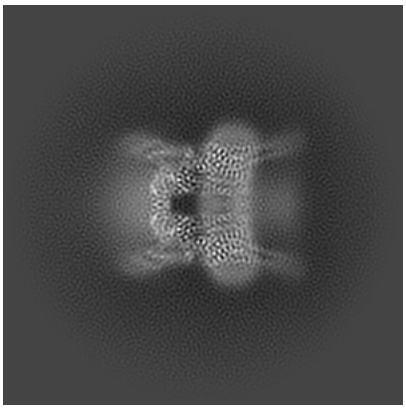
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

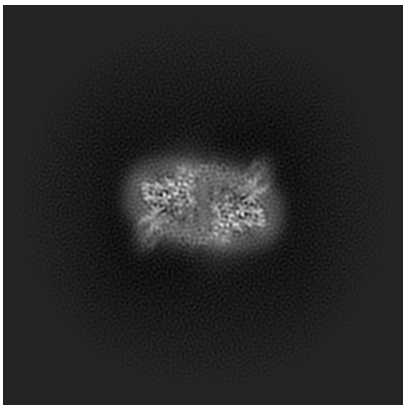
6.1.1 Primary map



X

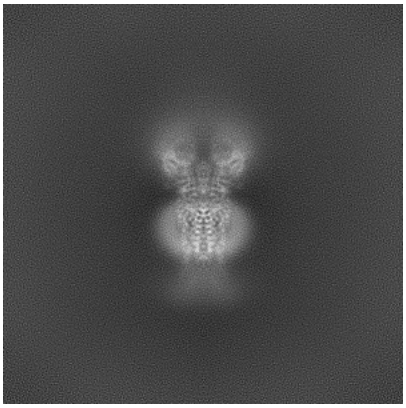


Y

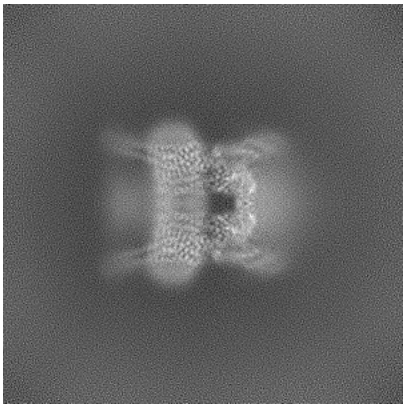


Z

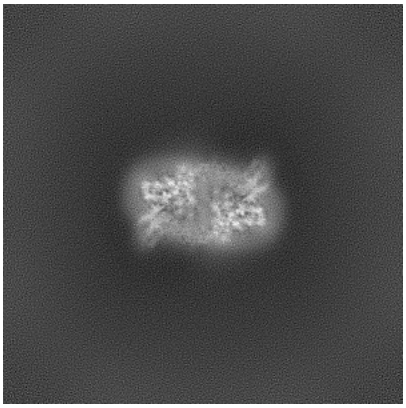
6.1.2 Raw map



X



Y

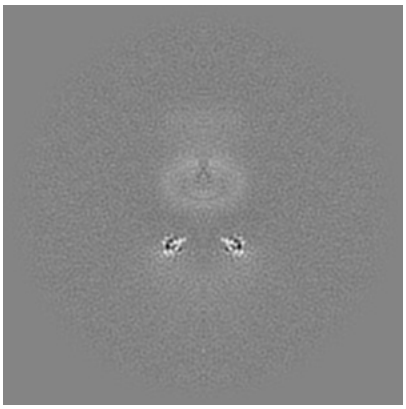


Z

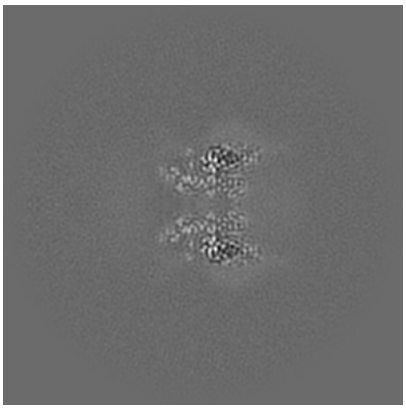
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

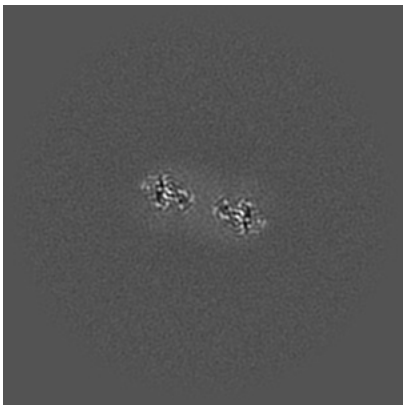
6.2.1 Primary map



X Index: 190

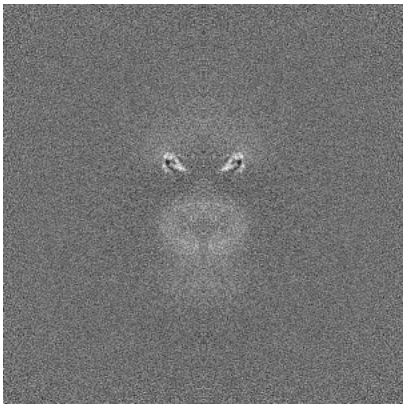


Y Index: 190

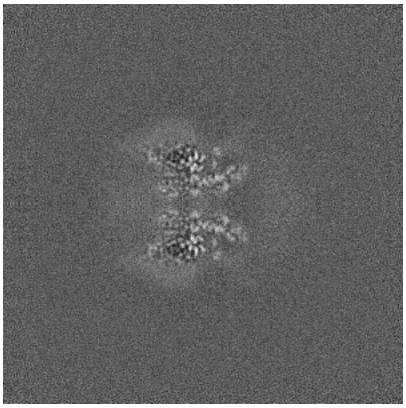


Z Index: 190

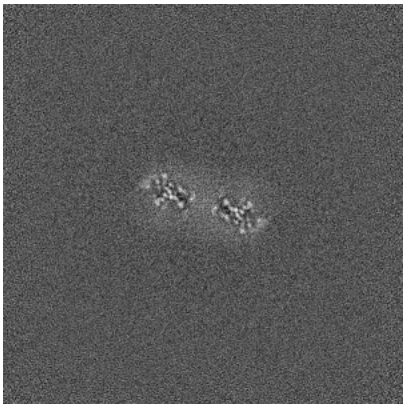
6.2.2 Raw map



X Index: 190



Y Index: 190

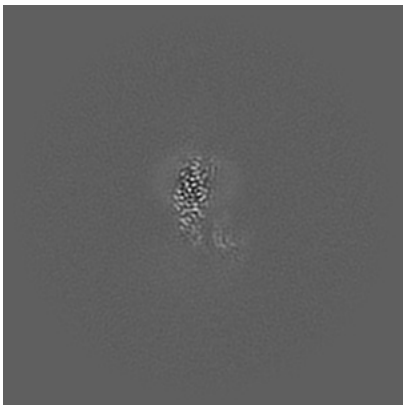


Z Index: 190

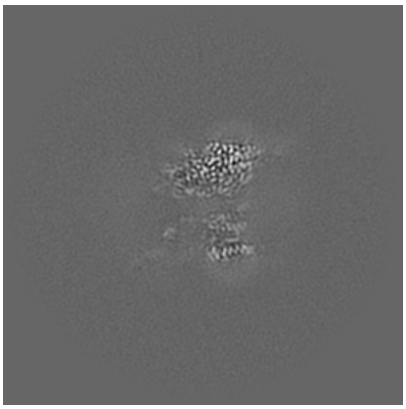
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

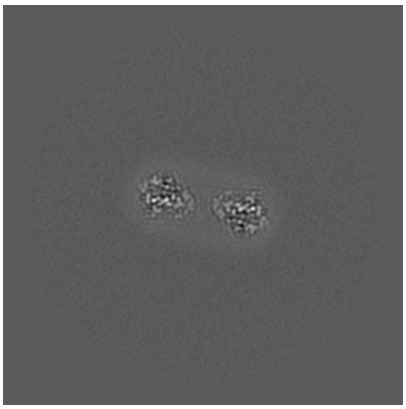
6.3.1 Primary map



X Index: 226

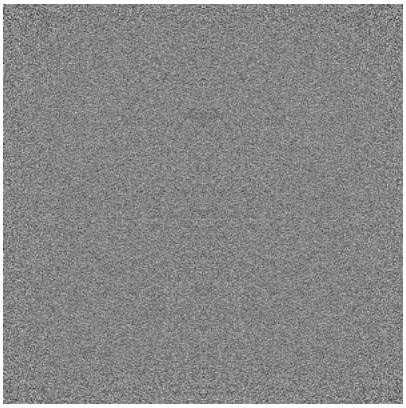


Y Index: 184

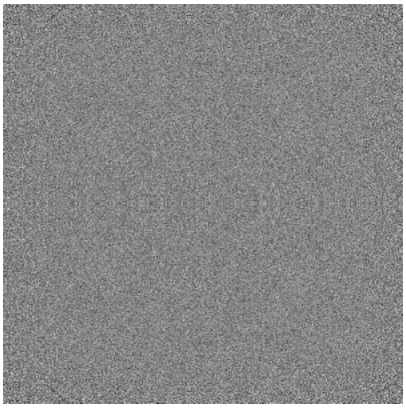


Z Index: 200

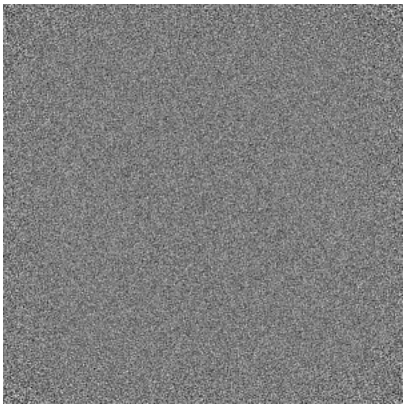
6.3.2 Raw map



X Index: 0



Y Index: 0

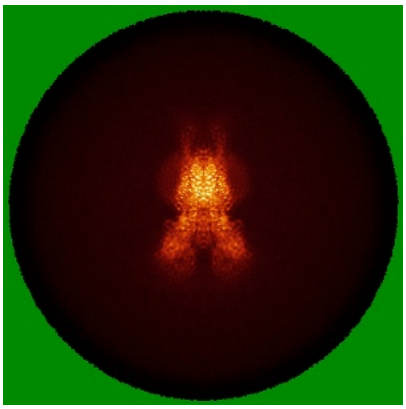


Z Index: 0

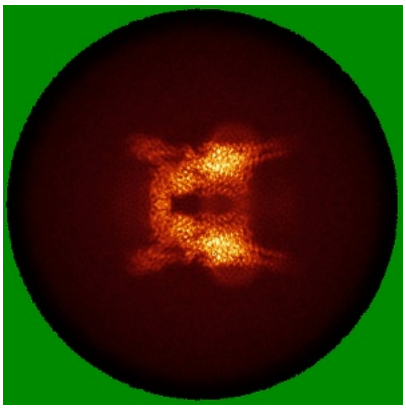
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

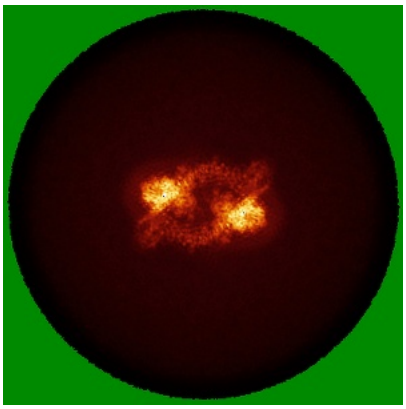
6.4.1 Primary map



X

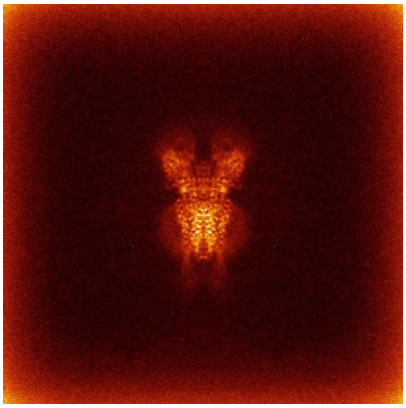


Y

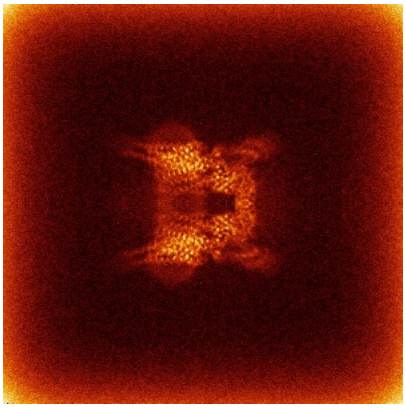


Z

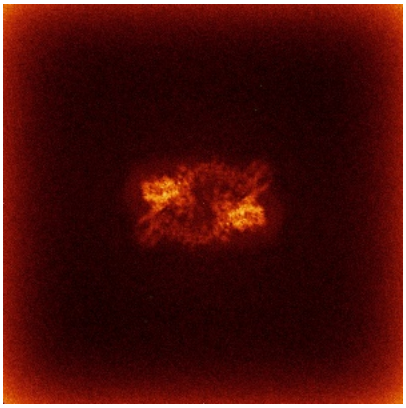
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

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

6.5.2 Raw map



X Y Z

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

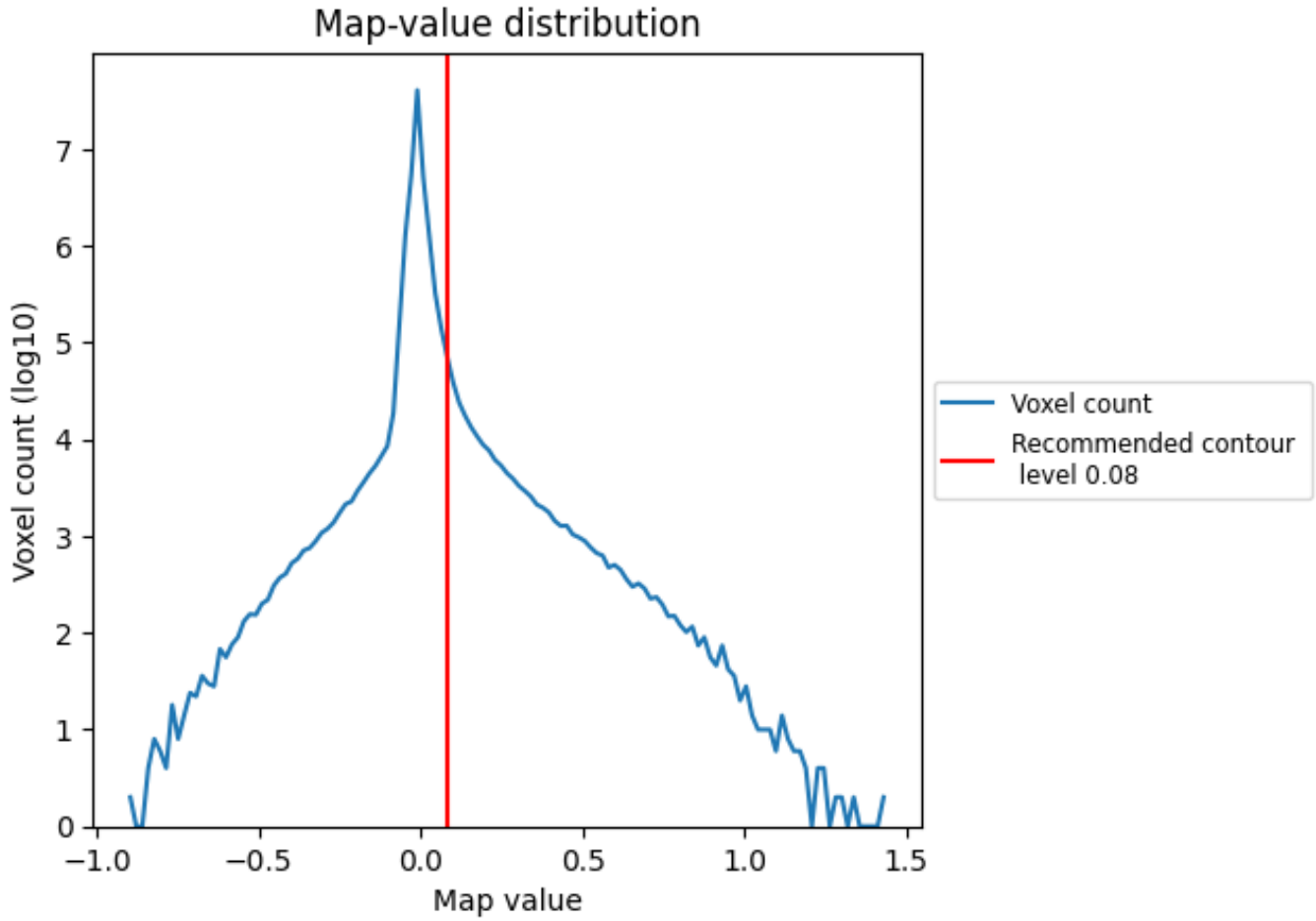
6.6 Mask visualisation (i)

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

7 Map analysis

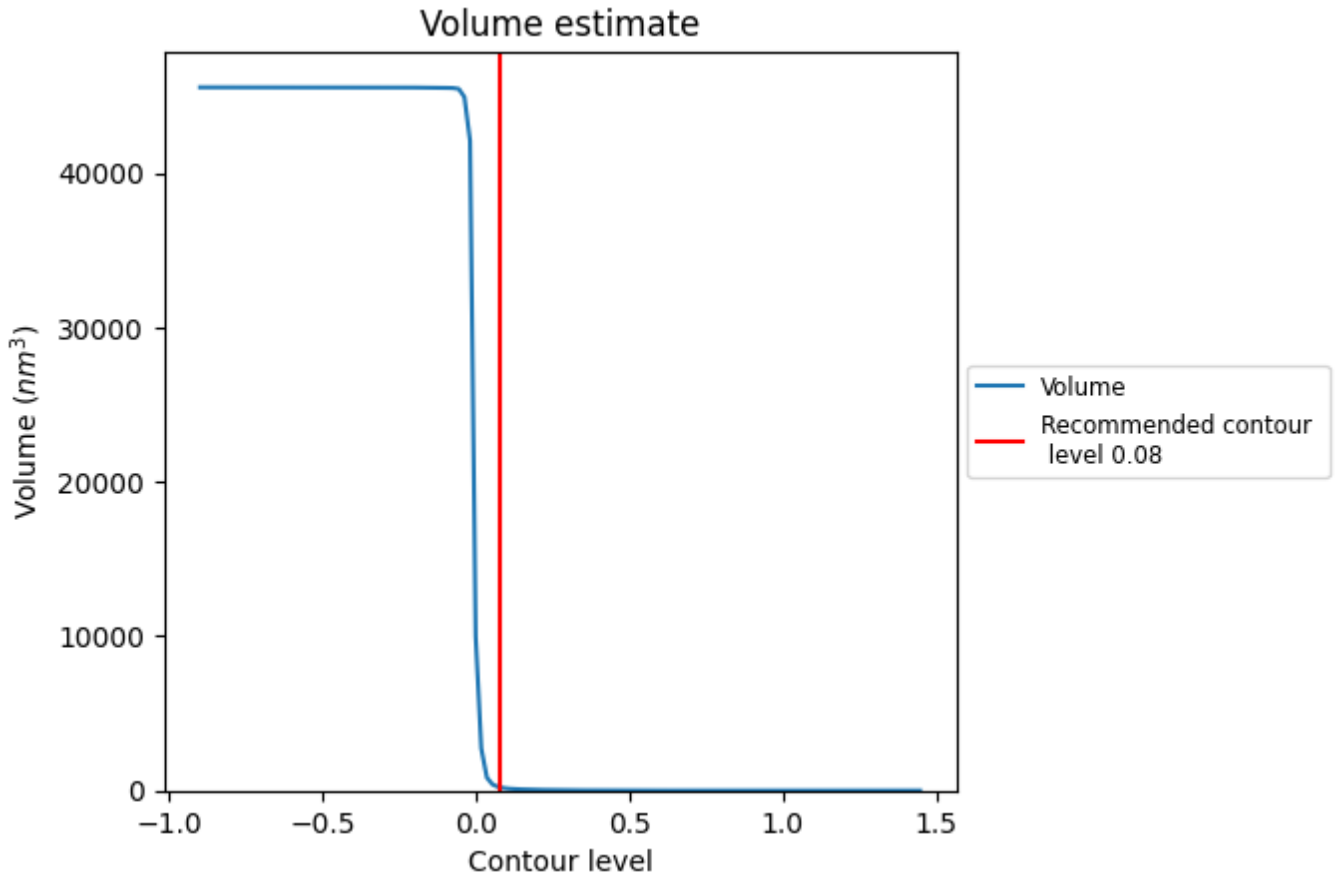
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

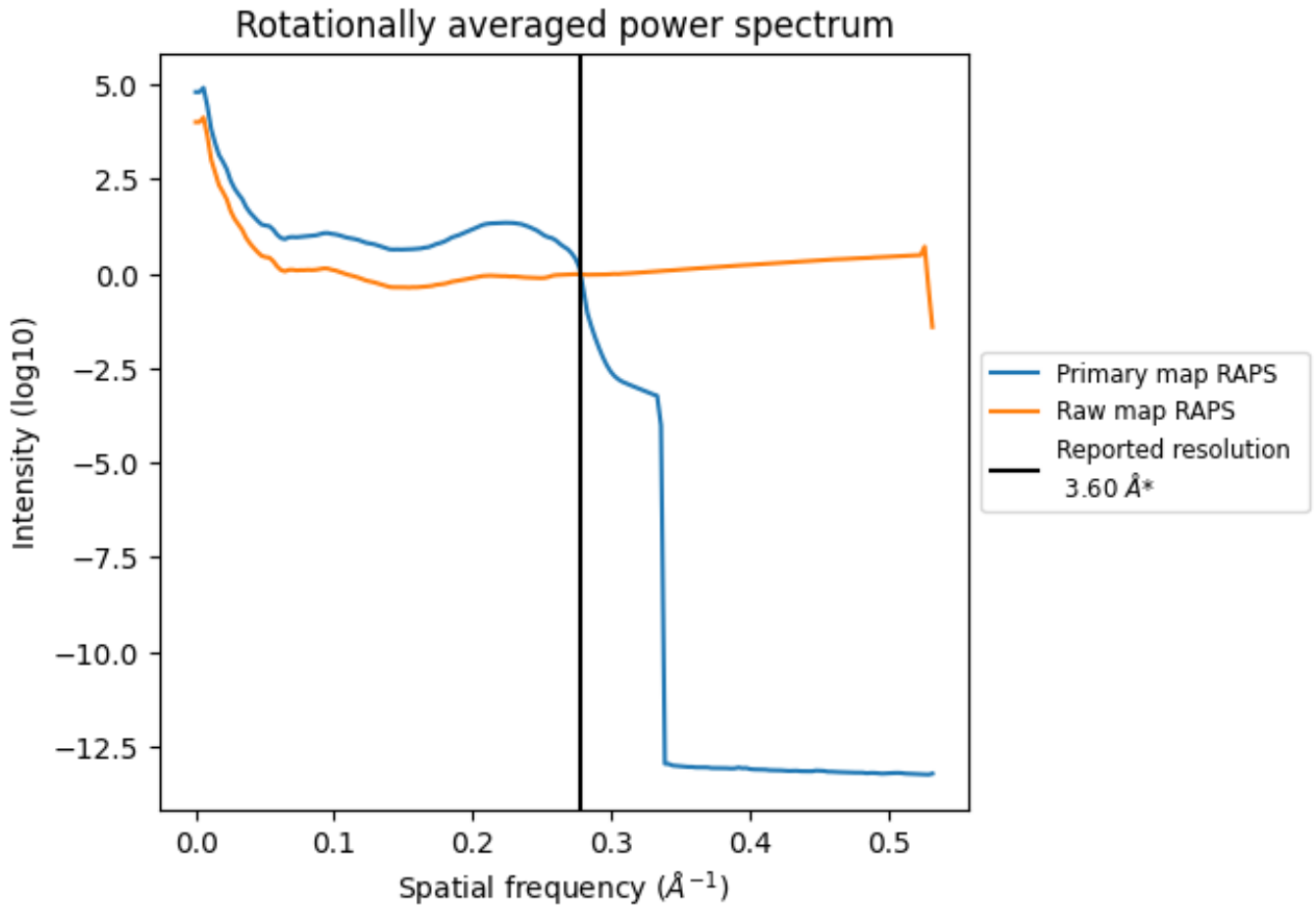
7.2 Volume estimate (i)



The volume at the recommended contour level is 214 nm^3; this corresponds to an approximate mass of 193 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)

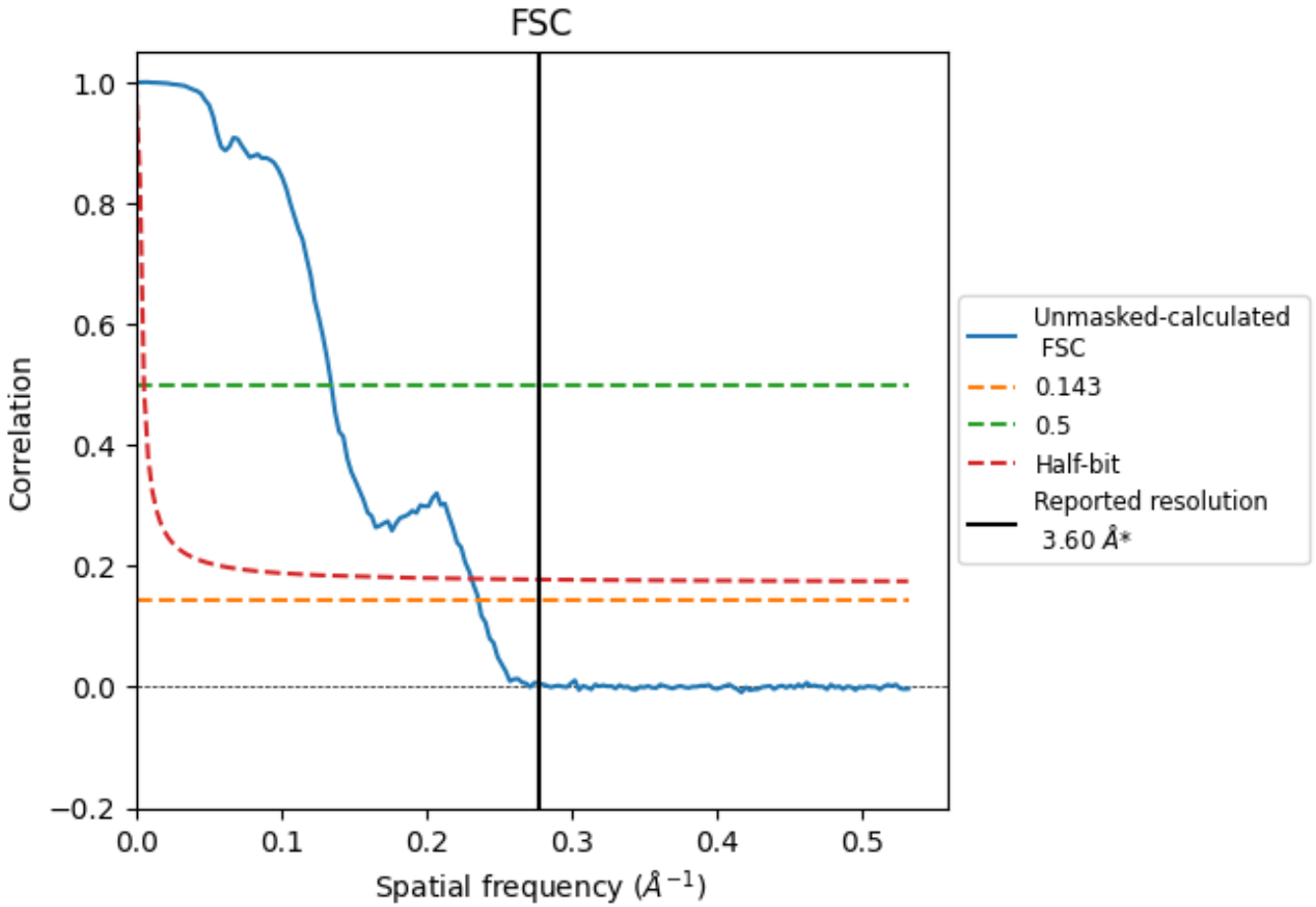


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

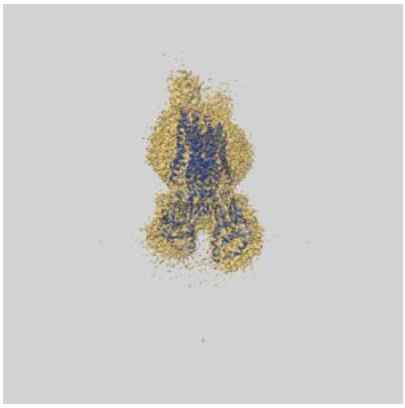
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.43	4.33

*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 4.24 differs from the reported value 3.6 by more than 10 %

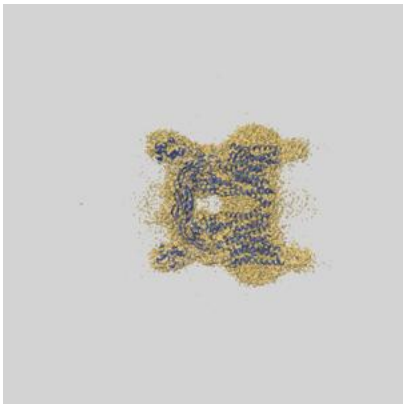
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71846 and PDB model 9PTT. Per-residue inclusion information can be found in section 3 on page 7.

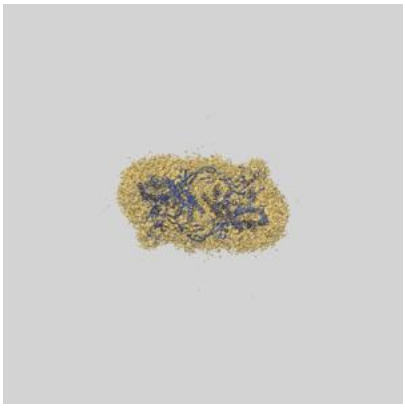
9.1 Map-model overlay



X



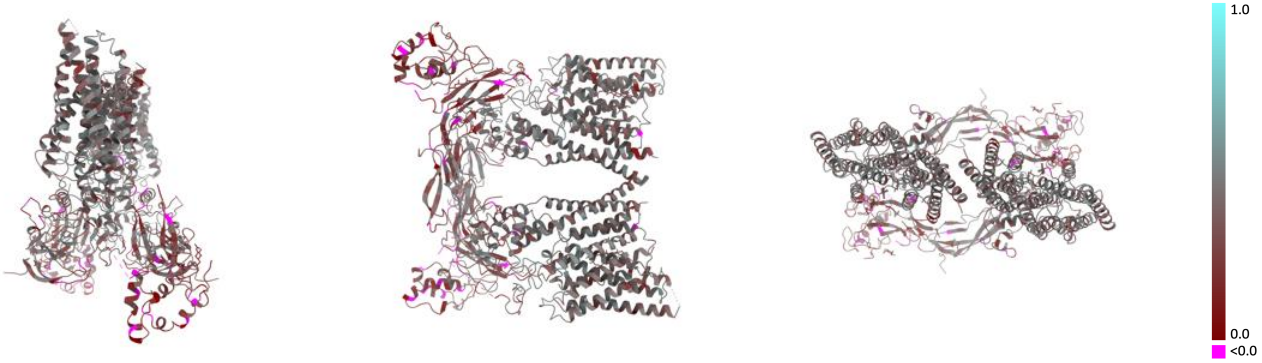
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

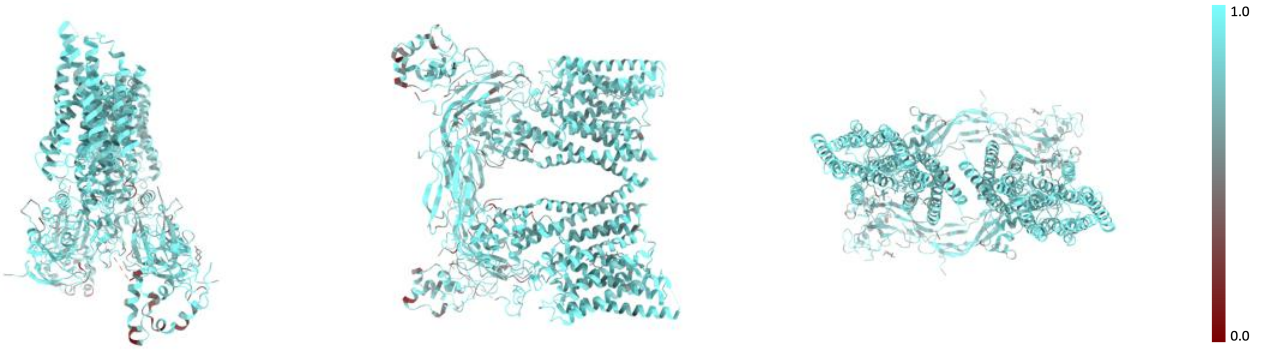
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

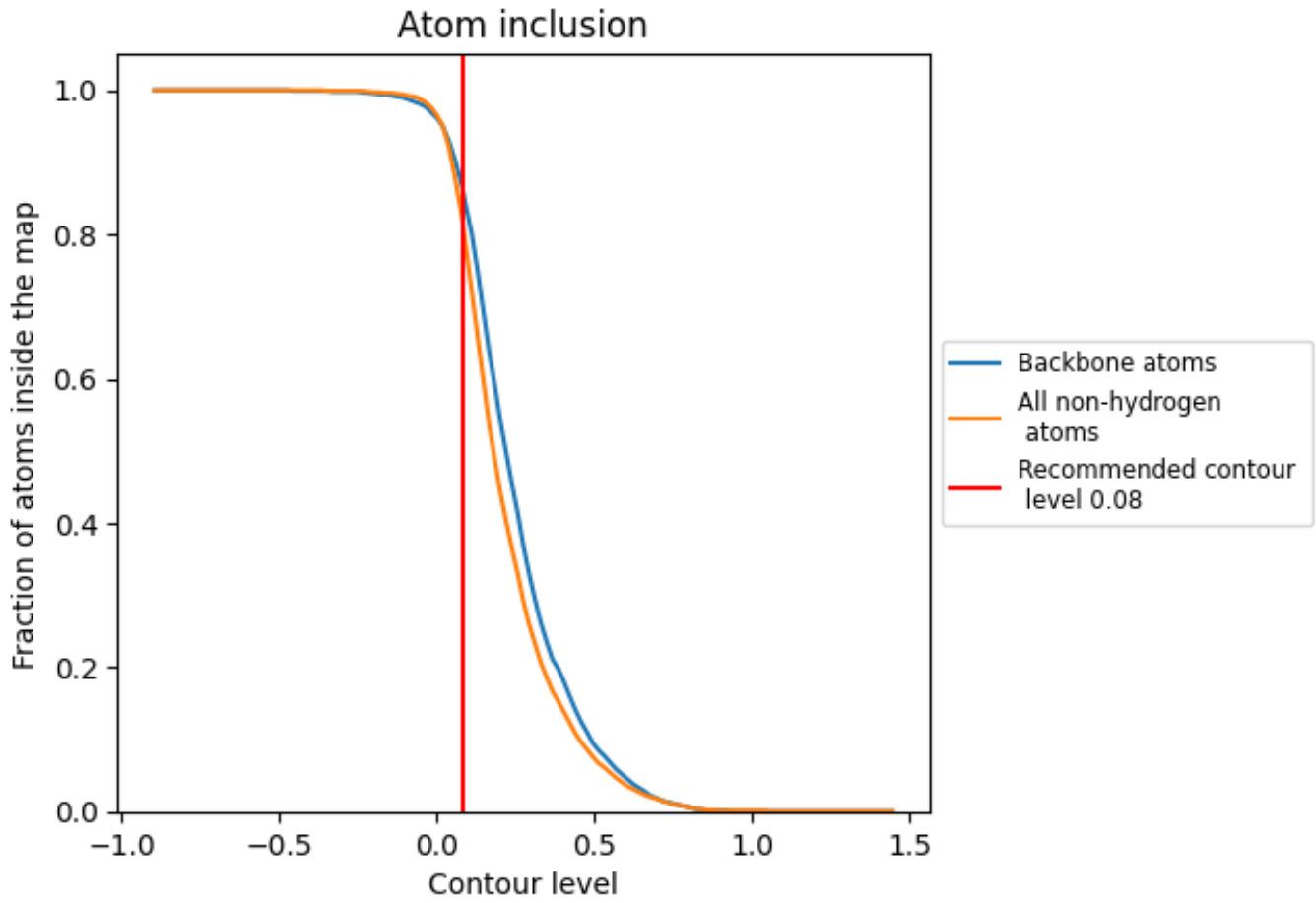
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 87% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.3730
A	0.8350	0.3760
B	0.8280	0.4100
C	0.8370	0.3750
D	0.8290	0.4110
F	0.8350	0.3430
G	0.7680	0.2770
H	0.7600	0.2750
K	0.7640	0.3910
M	0.8350	0.3420
P	0.7640	0.3890

