Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 10:50 PM EDT

PDB ID	:	7TYF
EMDB ID	:	EMD-26178
Title	:	Human Amylin1 Receptor in complex with Gs and rat amylin peptide
Authors	:	Cao, J.; Belousoff, M.J.; Johnson, R.M.; Wootten, D.L.; Sexton, P.M.
Deposited on	:	2022-02-13
Resolution	:	2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

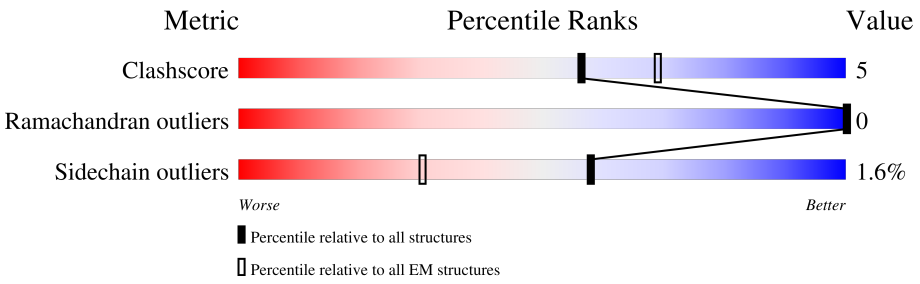
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	394	5%, 51%, 7%, 42%
2	B	350	•, 85%, 12%, •
3	E	149	55%, 64%, 10%, •, 25%
4	G	71	•, 76%, •, 23%
5	N	138	84%, 9%, 7%
6	P	38	45%, 74%, 26%
7	R	501	20%, 61%, 12%, 27%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10331 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	228	1857	1176	336	338	7	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	conflict	UNP P63092
A	226	ALA	GLY	conflict	UNP P63092
A	268	ALA	GLU	conflict	UNP P63092
A	271	LYS	ASN	conflict	UNP P63092
A	274	ASP	LYS	conflict	UNP P63092
A	280	LYS	ARG	conflict	UNP P63092
A	284	ASP	THR	conflict	UNP P63092
A	285	THR	ILE	conflict	UNP P63092
A	366	SER	ALA	engineered mutation	UNP P63092

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	339	2606	1607	468	510	21	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Receptor activity-modifying protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	112	759	495	131	128	5	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	expression tag	UNP O60894
E	1	LYS	-	expression tag	UNP O60894
E	2	THR	-	expression tag	UNP O60894
E	3	ILE	-	expression tag	UNP O60894
E	4	ILE	-	expression tag	UNP O60894
E	5	ALA	-	expression tag	UNP O60894
E	6	LEU	-	expression tag	UNP O60894
E	7	SER	-	expression tag	UNP O60894
E	8	TYR	-	expression tag	UNP O60894
E	9	ILE	-	expression tag	UNP O60894
E	10	PHE	-	expression tag	UNP O60894
E	11	CYS	-	expression tag	UNP O60894
E	12	LEU	-	expression tag	UNP O60894
E	13	VAL	-	expression tag	UNP O60894
E	14	PHE	-	expression tag	UNP O60894
E	15	ALA	-	expression tag	UNP O60894
E	16	ASP	-	expression tag	UNP O60894
E	17	TYR	-	expression tag	UNP O60894
E	18	LYS	-	expression tag	UNP O60894
E	19	ASP	-	expression tag	UNP O60894
E	20	ASP	-	expression tag	UNP O60894
E	21	ASP	-	expression tag	UNP O60894
E	22	ASP	-	expression tag	UNP O60894
E	23	LYS	-	expression tag	UNP O60894
E	24	HIS	-	expression tag	UNP O60894
E	25	GLY	-	expression tag	UNP O60894
E	26	SER	-	expression tag	UNP O60894

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	55	424	266	75	80	3	0	0

- Molecule 5 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	N	128	973	605	170	192	6	0	0

- Molecule 6 is a protein called amylin peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	P	38	285	173	56	54	2	1	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	38	NH2	-	amidation	UNP P12969

- Molecule 7 is a protein called Calcitonin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	367	2982	1973	490	492	27	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-7	MET	-	expression tag	UNP P30988
R	-6	LYS	-	expression tag	UNP P30988
R	-5	THR	-	expression tag	UNP P30988
R	-4	ILE	-	expression tag	UNP P30988
R	-3	ILE	-	expression tag	UNP P30988
R	-2	ALA	-	expression tag	UNP P30988
R	-1	LEU	-	expression tag	UNP P30988
R	0	SER	-	expression tag	UNP P30988
R	1	TYR	-	expression tag	UNP P30988
R	2	ILE	-	expression tag	UNP P30988
R	3	PHE	-	expression tag	UNP P30988

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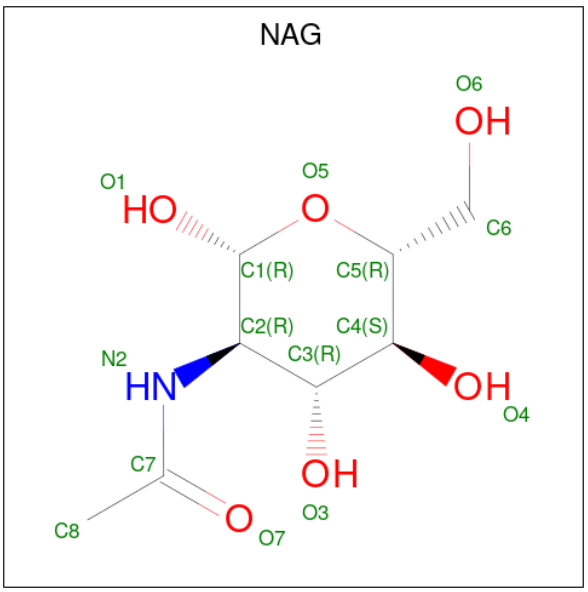
Chain	Residue	Modelled	Actual	Comment	Reference
R	4	CYS	-	expression tag	UNP P30988
R	5	LEU	-	expression tag	UNP P30988
R	6	VAL	-	expression tag	UNP P30988
R	7	PHE	-	expression tag	UNP P30988
R	8	ALA	-	expression tag	UNP P30988
R	9	ASP	-	expression tag	UNP P30988
R	10	TYR	-	expression tag	UNP P30988
R	11	LYS	-	expression tag	UNP P30988
R	12	ASP	-	expression tag	UNP P30988
R	13	ASP	-	expression tag	UNP P30988
R	14	ASP	-	expression tag	UNP P30988
R	15	ASP	-	expression tag	UNP P30988
R	16	LEU	-	expression tag	UNP P30988
R	17	GLU	-	expression tag	UNP P30988
R	18	VAL	-	expression tag	UNP P30988
R	19	LEU	-	expression tag	UNP P30988
R	20	PHE	-	expression tag	UNP P30988
R	21	GLN	-	expression tag	UNP P30988
R	22	GLY	-	expression tag	UNP P30988
R	23	PRO	-	expression tag	UNP P30988
R	24	ALA	-	expression tag	UNP P30988
R	447	LEU	PRO	conflict	UNP P30988
R	475	PRO	-	expression tag	UNP P30988
R	476	ALA	-	expression tag	UNP P30988
R	477	GLY	-	expression tag	UNP P30988
R	478	LEU	-	expression tag	UNP P30988
R	479	GLU	-	expression tag	UNP P30988
R	480	VAL	-	expression tag	UNP P30988
R	481	LEU	-	expression tag	UNP P30988
R	482	PHE	-	expression tag	UNP P30988
R	483	GLN	-	expression tag	UNP P30988
R	484	GLY	-	expression tag	UNP P30988
R	485	PRO	-	expression tag	UNP P30988
R	486	HIS	-	expression tag	UNP P30988
R	487	HIS	-	expression tag	UNP P30988
R	488	HIS	-	expression tag	UNP P30988
R	489	HIS	-	expression tag	UNP P30988
R	490	HIS	-	expression tag	UNP P30988
R	491	HIS	-	expression tag	UNP P30988
R	492	HIS	-	expression tag	UNP P30988
R	493	HIS	-	expression tag	UNP P30988

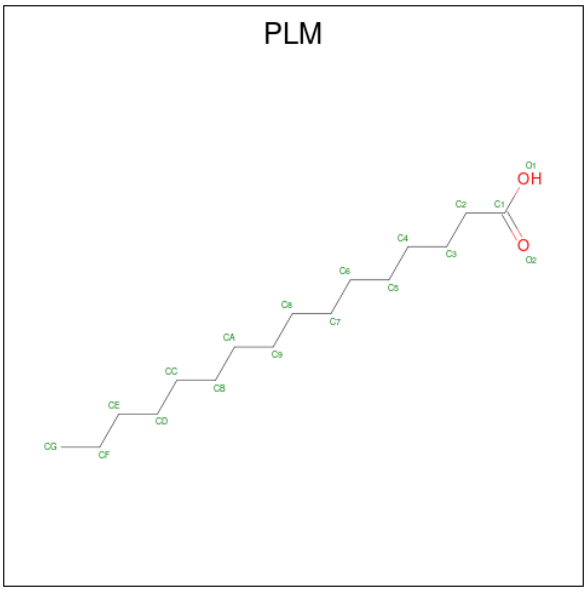
- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

$C_8H_{15}NO_6$).



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

- Molecule 9 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	R	1	18	16	2	0

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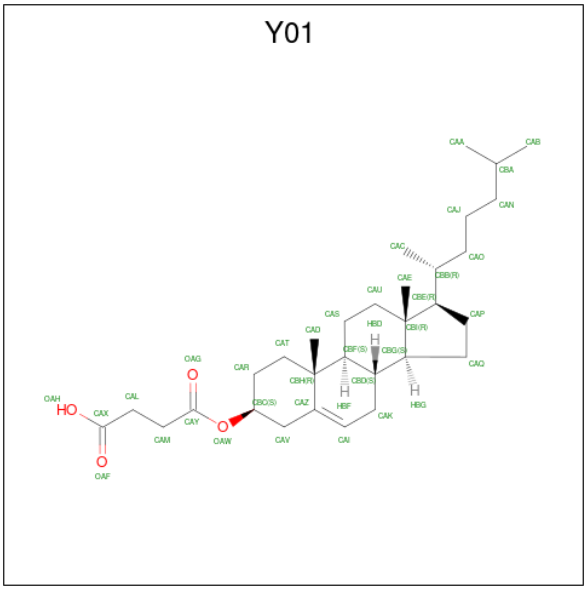
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0
9	R	1	18	16	2	0

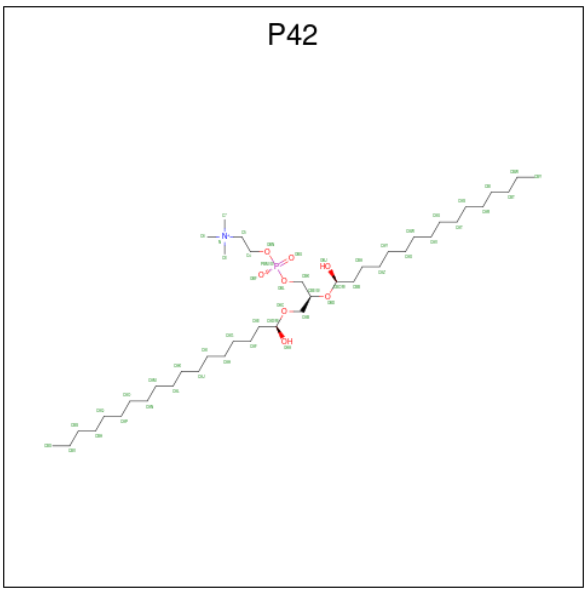
- Molecule 10 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	R	1	35	31	4	0
10	R	1	35	31	4	0

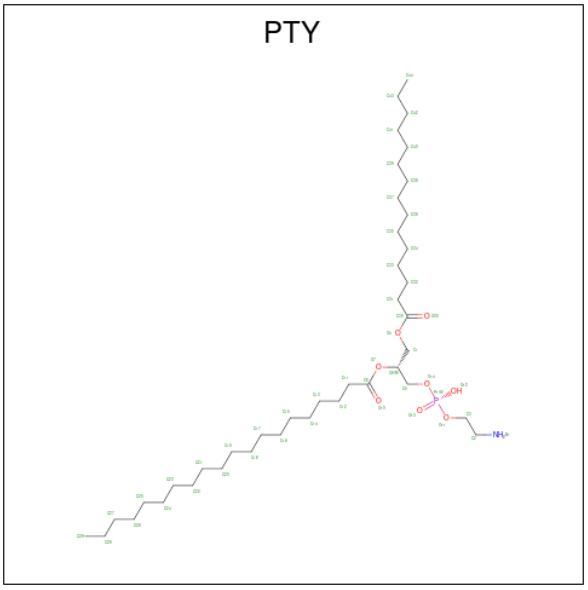
- Molecule 11 is (2S)-2-{[(1R)-1-hydroxyhexadecyl]oxy}-3-{[(1R)-1-hydroxyoctadecyl]oxy}pro

pyl 2-(trimethylammonio)ethyl phosphate (three-letter code: P42) (formula: $C_{42}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
11	R	1	52	42	1	8	1	0

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	R	1	50	40	1	8	1	0

- Molecule 13 is water.

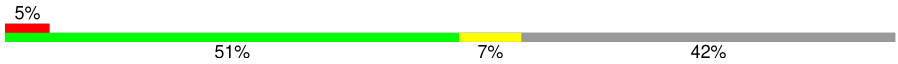
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
13	A	13	13	13	0
13	B	36	36	36	0
13	N	8	8	8	0
13	P	6	6	6	0
13	R	20	20	20	0

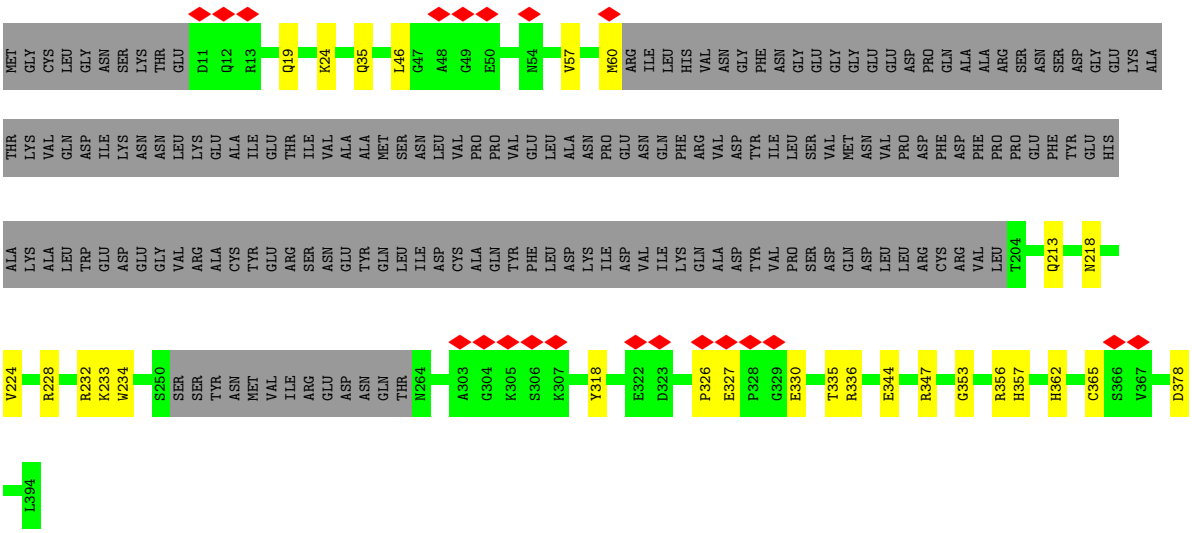
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

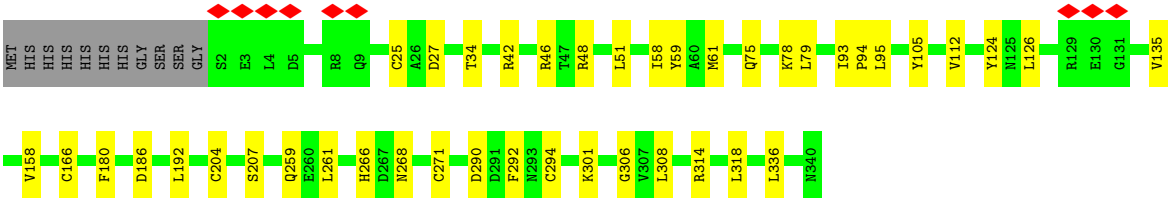
Chain A:





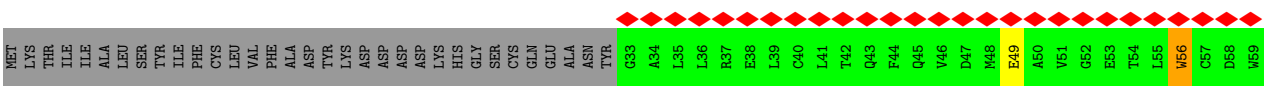
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

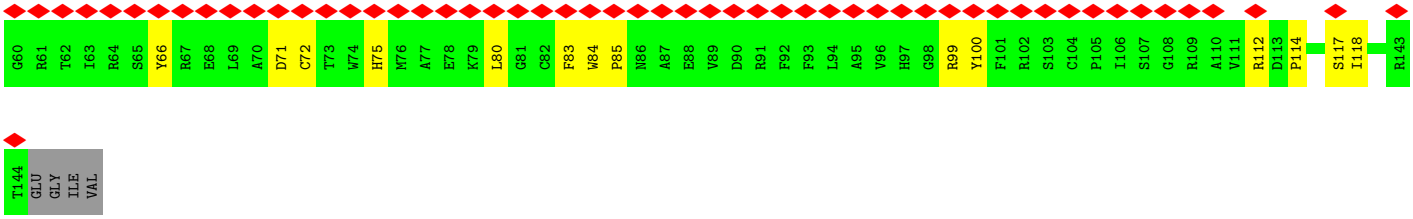
Chain B:



• Molecule 3: Receptor activity-modifying protein 1

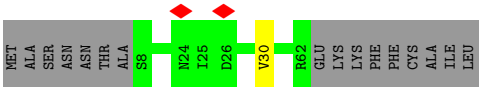
Chain E:





• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

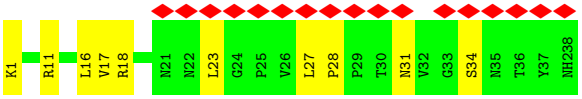


• Molecule 5: Nanobody 35

Chain N:

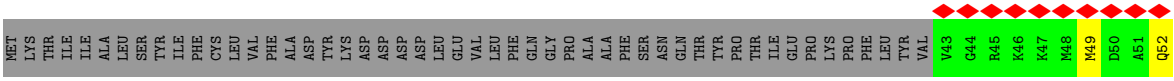
• Molecule 6: amylin peptide

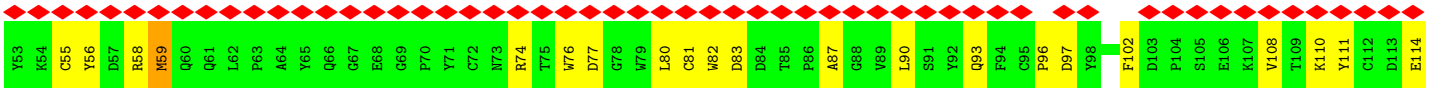
Chain P:

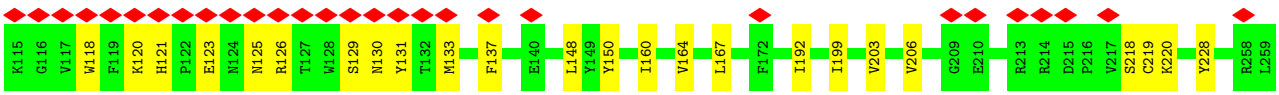


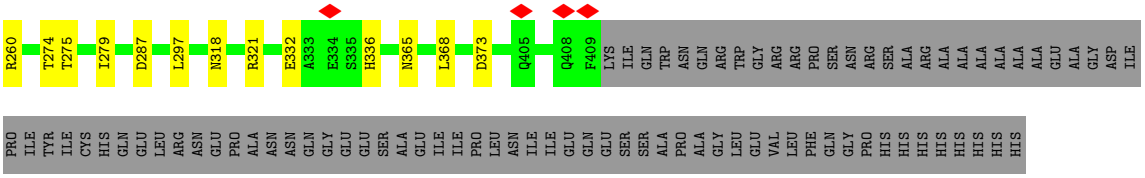
• Molecule 7: Calcitonin receptor

Chain R:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1063000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	65.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.302	Depositor
Minimum map value	-0.178	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	239.04, 239.04, 239.04	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: Y01, NH2, PTY, P42, NAG, PLM

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	0.24	0/1892	0.38	0/2548
2	B	0.25	0/2653	0.48	0/3597
3	E	0.32	0/783	0.40	0/1082
4	G	0.23	0/430	0.35	0/580
5	N	0.26	0/993	0.48	0/1345
6	P	0.25	0/288	0.46	0/393
7	R	0.25	0/3081	0.38	0/4200
All	All	0.25	0/10120	0.42	0/13745

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1857	0	1819	14	0
2	B	2606	0	2510	23	0
3	E	759	0	618	12	0
4	G	424	0	436	1	0
5	N	973	0	938	6	0
6	P	285	0	286	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	R	2982	0	2889	39	0
8	R	28	0	26	0	0
9	R	162	0	279	2	0
10	R	70	0	98	2	0
11	R	52	0	88	2	0
12	R	50	0	79	1	0
13	A	13	0	0	0	0
13	B	36	0	0	0	0
13	N	8	0	0	0	0
13	P	6	0	0	0	0
13	R	20	0	0	0	0
All	All	10331	0	10066	95	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 5.

All (95) 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)
7:R:365:ASN:HD22	7:R:368:LEU:HB2	1.37	0.89
7:R:74:ARG:HG2	7:R:83:ASP:HA	1.71	0.70
7:R:76:TRP:HE3	7:R:81:CYS:HB3	1.58	0.69
3:E:49:GLU:HA	3:E:56:TRP:HE1	1.56	0.68
1:A:318:TYR:O	1:A:336:ARG:NH1	2.29	0.66
1:A:228:ARG:NH2	2:B:186:ASP:OD1	2.30	0.65
2:B:46:ARG:HH11	2:B:48:ARG:HH12	1.46	0.63
1:A:327:GLU:HB2	1:A:330:GLU:HB2	1.83	0.61
1:A:344:GLU:OE1	1:A:347:ARG:NH2	2.34	0.60
5:N:22:CYS:HB3	5:N:79:LEU:HB3	1.86	0.57
6:P:1:LYS:HE2	6:P:11:ARG:HD2	1.86	0.57
7:R:93:GLN:N	7:R:108:VAL:O	2.33	0.56
7:R:133:MET:HE3	7:R:137:PHE:HE2	1.70	0.56
7:R:199:ILE:O	7:R:203:VAL:HG22	2.06	0.56
2:B:25:CYS:SG	2:B:259:GLN:NE2	2.81	0.54
7:R:129:SER:HB2	7:R:131:TYR:CE2	2.43	0.53
7:R:160:ILE:O	7:R:164:VAL:HG23	2.08	0.53
7:R:80:LEU:HD11	7:R:96:PRO:HD3	1.91	0.52
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.91	0.52
6:P:34:SER:HB3	7:R:123:GLU:OE2	2.10	0.52
1:A:213:GLN:HE21	1:A:218:ASN:HD21	1.57	0.51
2:B:58:ILE:HD13	2:B:336:LEU:HG	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.93	0.51
7:R:93:GLN:O	7:R:108:VAL:N	2.38	0.51
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.92	0.50
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.93	0.50
2:B:79:LEU:HB2	2:B:93:ILE:HB	1.94	0.49
7:R:260:ARG:HH11	10:R:506:Y01:HAM2	1.78	0.49
1:A:224:VAL:HG11	1:A:234:TRP:CZ3	2.48	0.49
3:E:99:ARG:HG2	3:E:100:TYR:CE1	2.48	0.49
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.48	0.49
7:R:150:TYR:HE1	9:R:507:PLM:H42	1.78	0.48
7:R:275:THR:O	7:R:279:ILE:HG13	2.14	0.48
12:R:514:PTY:H422	12:R:514:PTY:H261	1.94	0.48
7:R:133:MET:HE3	7:R:137:PHE:CE2	2.48	0.48
3:E:99:ARG:HG2	3:E:100:TYR:CZ	2.48	0.48
7:R:55:CYS:O	7:R:58:ARG:HB3	2.14	0.47
2:B:290:ASP:OD1	2:B:314:ARG:NE	2.45	0.47
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.96	0.47
3:E:71:ASP:O	3:E:75:HIS:ND1	2.34	0.47
6:P:31:ASN:OD1	6:P:31:ASN:N	2.48	0.47
6:P:16:LEU:HB3	6:P:23:LEU:HD11	1.97	0.47
5:N:52:SER:HB3	5:N:57:SER:HB3	1.95	0.46
7:R:110:LYS:HG2	7:R:118:TRP:CE3	2.50	0.46
7:R:228:TYR:HA	7:R:274:THR:HG21	1.98	0.46
7:R:150:TYR:HB3	11:R:510:P42:HBBA	1.98	0.46
2:B:34:THR:O	2:B:301:LYS:NZ	2.49	0.45
2:B:261:LEU:HD22	4:G:30:VAL:HG13	1.98	0.45
2:B:266:HIS:ND1	2:B:268:ASN:OD1	2.49	0.45
1:A:326:PRO:HB3	1:A:335:THR:HG21	1.97	0.45
7:R:220:LYS:NZ	7:R:287:ASP:O	2.50	0.45
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.99	0.45
6:P:18[A]:ARG:NH1	7:R:102:PHE:O	2.50	0.45
1:A:232:ARG:NH2	2:B:204:CYS:HB3	2.32	0.44
3:E:114:PRO:HB2	3:E:118:ILE:HG23	1.99	0.44
7:R:121:HIS:CE1	7:R:123:GLU:HG2	2.52	0.44
6:P:27:LEU:HD13	6:P:28:PRO:HD2	1.98	0.44
7:R:77:ASP:OD1	7:R:82:TRP:NE1	2.49	0.44
2:B:27:ASP:N	2:B:27:ASP:OD1	2.50	0.44
5:N:83:MET:HB3	5:N:86:LEU:HD21	2.00	0.44
11:R:510:P42:HABA	11:R:510:P42:HBC	1.70	0.44
7:R:56:TYR:HA	7:R:59:MET:HG3	1.99	0.43
7:R:121:HIS:O	7:R:125:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:112:ARG:HD2	3:E:112:ARG:HA	1.82	0.43
5:N:39:GLN:HB2	5:N:45:LEU:HD23	2.00	0.43
2:B:78:LYS:HD2	2:B:94:PRO:HA	2.01	0.42
1:A:213:GLN:HE21	1:A:218:ASN:ND2	2.17	0.42
7:R:148:LEU:HD11	7:R:373:ASP:HB3	2.02	0.42
6:P:17:VAL:HG22	7:R:206:VAL:HA	2.01	0.42
7:R:87:ALA:HB1	7:R:114:GLU:HA	2.02	0.42
7:R:167:LEU:HD12	7:R:192:ILE:HD12	2.01	0.42
1:A:57:VAL:O	1:A:60:MET:HG2	2.20	0.42
1:A:233:LYS:HD3	1:A:233:LYS:HA	1.87	0.42
1:A:353:GLY:O	1:A:356:ARG:HG2	2.19	0.42
3:E:84:TRP:HB3	3:E:85:PRO:HD3	2.02	0.42
2:B:268:ASN:OD1	2:B:268:ASN:N	2.46	0.41
3:E:114:PRO:HD2	7:R:297:LEU:HD11	2.01	0.41
3:E:66:TYR:HE2	7:R:52:GLN:HG3	1.85	0.41
5:N:88:PRO:HA	5:N:126:VAL:HB	2.01	0.41
2:B:42:ARG:CZ	2:B:306:GLY:HA2	2.50	0.41
2:B:292:PHE:N	2:B:292:PHE:CD1	2.88	0.41
3:E:80:LEU:HD23	3:E:80:LEU:HA	1.89	0.41
7:R:49:MET:HA	7:R:52:GLN:OE1	2.20	0.41
7:R:90:LEU:HG	7:R:111:TYR:HD1	1.86	0.41
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.86	0.41
1:A:362:HIS:NE2	1:A:378:ASP:OD2	2.48	0.41
5:N:37:VAL:HG12	5:N:47:TRP:HA	2.02	0.41
7:R:97:ASP:N	7:R:97:ASP:OD1	2.52	0.41
7:R:218:SER:HB2	9:R:503:PLM:H81	2.03	0.40
7:R:260:ARG:HB3	10:R:506:Y01:HAL1	2.03	0.40
2:B:158:VAL:HG11	2:B:192:LEU:HD21	2.02	0.40
3:E:83:PHE:CD2	7:R:126:ARG:HG3	2.57	0.40
7:R:318:ASN:ND2	7:R:321:ARG:HH11	2.19	0.40
7:R:332:GLU:OE1	7:R:336:HIS:ND1	2.54	0.40
3:E:72:CYS:HA	3:E:75:HIS:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/394 (56%)	219 (99%)	3 (1%)	0	100	100
2	B	337/350 (96%)	332 (98%)	5 (2%)	0	100	100
3	E	110/149 (74%)	107 (97%)	3 (3%)	0	100	100
4	G	53/71 (75%)	51 (96%)	2 (4%)	0	100	100
5	N	126/138 (91%)	125 (99%)	1 (1%)	0	100	100
6	P	37/38 (97%)	35 (95%)	2 (5%)	0	100	100
7	R	365/501 (73%)	359 (98%)	6 (2%)	0	100	100
All	All	1250/1641 (76%)	1228 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	195/350 (56%)	190 (97%)	5 (3%)	41	54
2	B	282/291 (97%)	276 (98%)	6 (2%)	48	63
3	E	57/129 (44%)	55 (96%)	2 (4%)	31	41
4	G	45/58 (78%)	45 (100%)	0	100	100
5	N	106/115 (92%)	106 (100%)	0	100	100
6	P	33/32 (103%)	33 (100%)	0	100	100
7	R	315/445 (71%)	311 (99%)	4 (1%)	65	78
All	All	1033/1420 (73%)	1016 (98%)	17 (2%)	58	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	24	LYS
1	A	35	GLN
1	A	357	HIS
1	A	365	CYS
2	B	59	TYR
2	B	61	MET
2	B	75	GLN
2	B	105	TYR
2	B	207	SER
2	B	318	LEU
3	E	56	TRP
3	E	117	SER
7	R	59	MET
7	R	120	LYS
7	R	130	ASN
7	R	219	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
2	B	16	ASN
2	B	75	GLN
2	B	259	GLN
5	N	3	GLN
5	N	13	GLN
6	P	22	ASN
7	R	144	ASN
7	R	201	HIS
7	R	318	ASN
7	R	365	ASN
7	R	396	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)

15 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	$\#\|Z\| > 2$
12	PTY	R	514	-	49,49,49	0.31	0	52,54,54	0.31	0
9	PLM	R	508	-	17,17,17	0.53	0	17,17,17	0.50	0
8	NAG	R	502	7	14,14,15	0.38	0	17,19,21	0.39	0
9	PLM	R	503	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	511	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	512	-	17,17,17	0.54	0	17,17,17	0.49	0
9	PLM	R	515	-	17,17,17	0.55	0	17,17,17	0.52	0
11	P42	R	510	-	51,51,51	0.35	0	53,59,59	0.36	0
10	Y01	R	506	-	38,38,38	0.45	0	57,57,57	0.63	0
9	PLM	R	513	-	17,17,17	0.54	0	17,17,17	0.49	0
10	Y01	R	505	-	38,38,38	0.47	0	57,57,57	0.53	0
9	PLM	R	504	-	17,17,17	0.53	0	17,17,17	0.50	0
9	PLM	R	509	-	17,17,17	0.53	0	17,17,17	0.50	0
8	NAG	R	501	7	14,14,15	0.44	0	17,19,21	0.70	1 (5%)
9	PLM	R	507	-	17,17,17	0.52	0	17,17,17	0.49	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
12	PTY	R	514	-	-	8/53/53/53	-
9	PLM	R	508	-	-	2/15/15/15	-
8	NAG	R	502	7	-	2/6/23/26	0/1/1/1
9	PLM	R	503	-	-	0/15/15/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	PLM	R	511	-	-	2/15/15/15	-
9	PLM	R	512	-	-	3/15/15/15	-
9	PLM	R	515	-	-	0/15/15/15	-
11	P42	R	510	-	-	7/55/55/55	-
10	Y01	R	506	-	-	7/19/77/77	0/4/4/4
9	PLM	R	513	-	-	2/15/15/15	-
10	Y01	R	505	-	-	6/19/77/77	0/4/4/4
9	PLM	R	504	-	-	2/15/15/15	-
9	PLM	R	509	-	-	2/15/15/15	-
8	NAG	R	501	7	-	0/6/23/26	0/1/1/1
9	PLM	R	507	-	-	2/15/15/15	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	501	NAG	C1-O5-C5	2.36	115.35	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	514	PTY	C3-O11-P1-O14
10	R	506	Y01	CAV-CBC-OAW-CAY
8	R	502	NAG	O5-C5-C6-O6
8	R	502	NAG	C4-C5-C6-O6
12	R	514	PTY	C31-C30-O4-C1
12	R	514	PTY	O30-C30-O4-C1
12	R	514	PTY	C20-C21-C22-C23
10	R	506	Y01	CAL-CAM-CAY-OAW
10	R	505	Y01	CAO-CBB-CBE-CBI
10	R	505	Y01	CAC-CBB-CBE-CBI
10	R	505	Y01	CAO-CBB-CBE-CAP
10	R	506	Y01	CAM-CAY-OAW-CBC
11	R	510	P42	C5-C4-OBN-PBM
11	R	510	P42	OBN-C4-C5-N
10	R	505	Y01	CAC-CBB-CBE-CAP
12	R	514	PTY	O14-C5-C6-O7
11	R	510	P42	CAB-CBE-OBD-CBC

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Mol	Chain	Res	Type	Atoms
11	R	510	P42	CBK-CBE-OBD-CBC
12	R	514	PTY	C3-O11-P1-O13
10	R	506	Y01	OAG-CAY-OAW-CBC
9	R	507	PLM	O2-C1-C2-C3
9	R	504	PLM	O2-C1-C2-C3
10	R	506	Y01	CAM-CAL-CAX-OAF
9	R	512	PLM	O1-C1-C2-C3
9	R	508	PLM	O1-C1-C2-C3
11	R	510	P42	OAA-CAD-CAE-CAF
10	R	505	Y01	CAM-CAL-CAX-OAH
9	R	504	PLM	O1-C1-C2-C3
10	R	506	Y01	CAM-CAL-CAX-OAH
9	R	509	PLM	O1-C1-C2-C3
9	R	511	PLM	O1-C1-C2-C3
9	R	512	PLM	O2-C1-C2-C3
9	R	507	PLM	O1-C1-C2-C3
9	R	513	PLM	O1-C1-C2-C3
10	R	505	Y01	CAM-CAL-CAX-OAF
9	R	508	PLM	O2-C1-C2-C3
9	R	512	PLM	C2-C3-C4-C5
9	R	513	PLM	O2-C1-C2-C3
9	R	511	PLM	O2-C1-C2-C3
9	R	509	PLM	O2-C1-C2-C3
12	R	514	PTY	O14-C5-C6-C1
12	R	514	PTY	C13-C14-C15-C16
11	R	510	P42	CAZ-CBA-CBB-CBC
11	R	510	P42	OAA-CAD-OAC-CAB
10	R	506	Y01	CAL-CAM-CAY-OAG

There are no ring outliers.

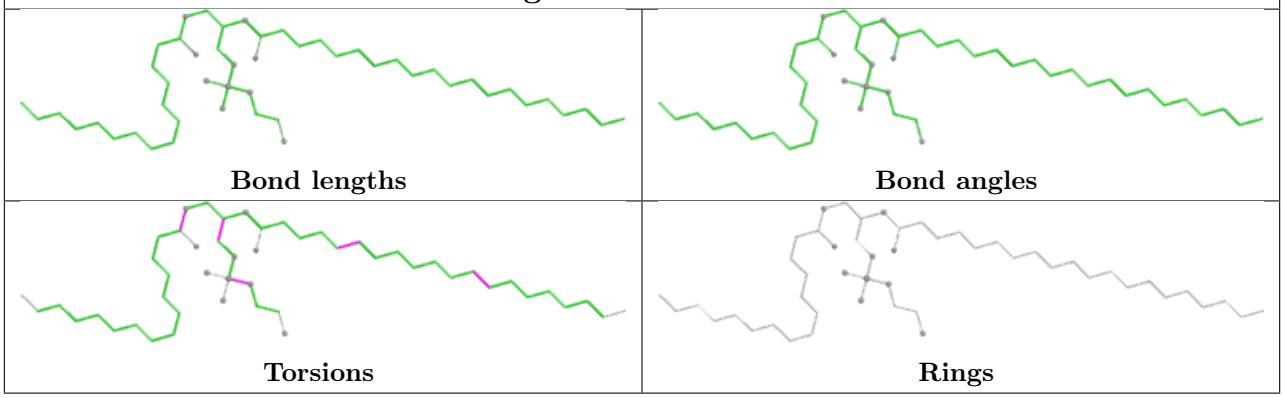
5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	514	PTY	1	0
9	R	503	PLM	1	0
11	R	510	P42	2	0
10	R	506	Y01	2	0
9	R	507	PLM	1	0

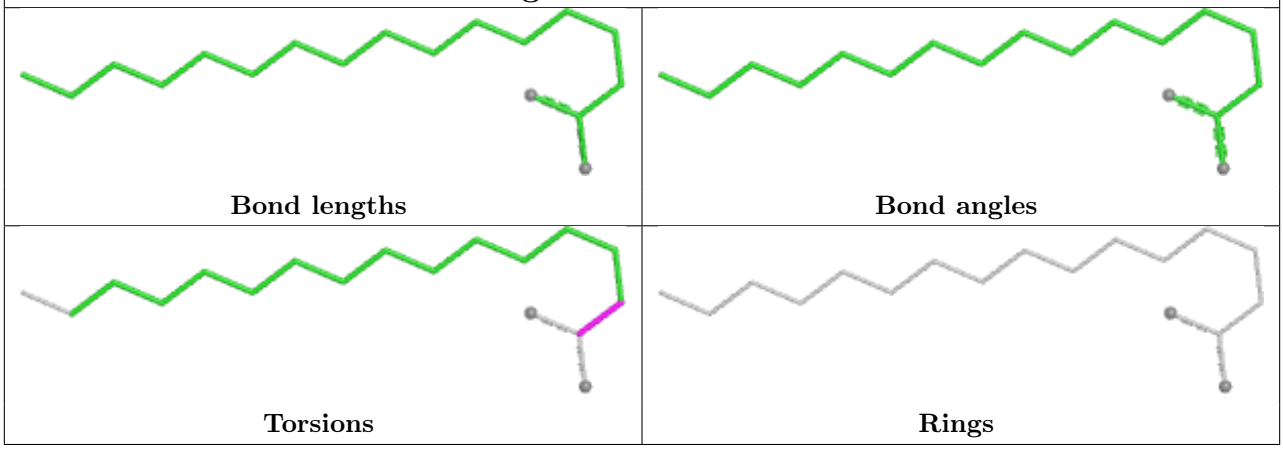
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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 PTY R 514



Ligand PLM R 508



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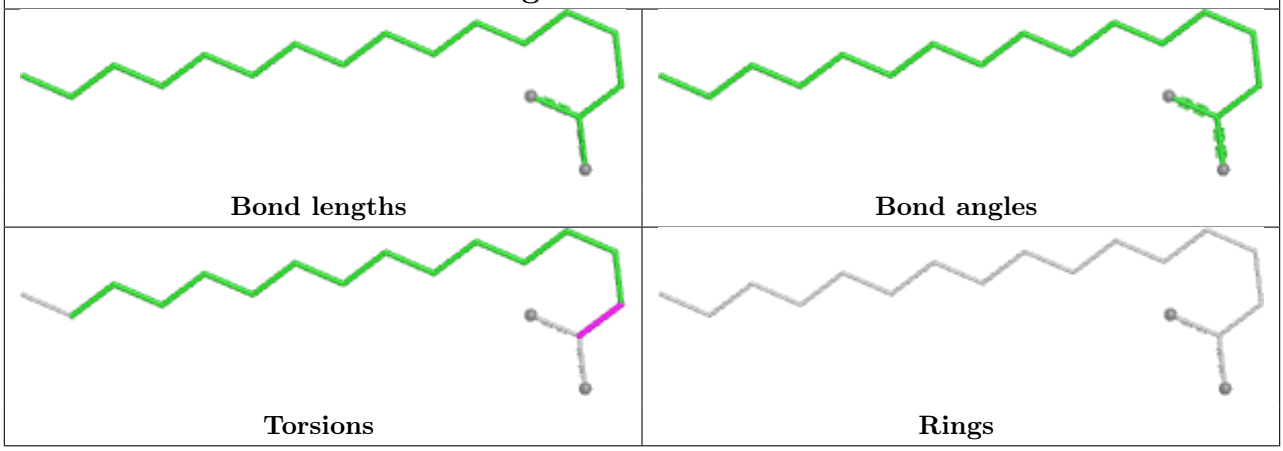

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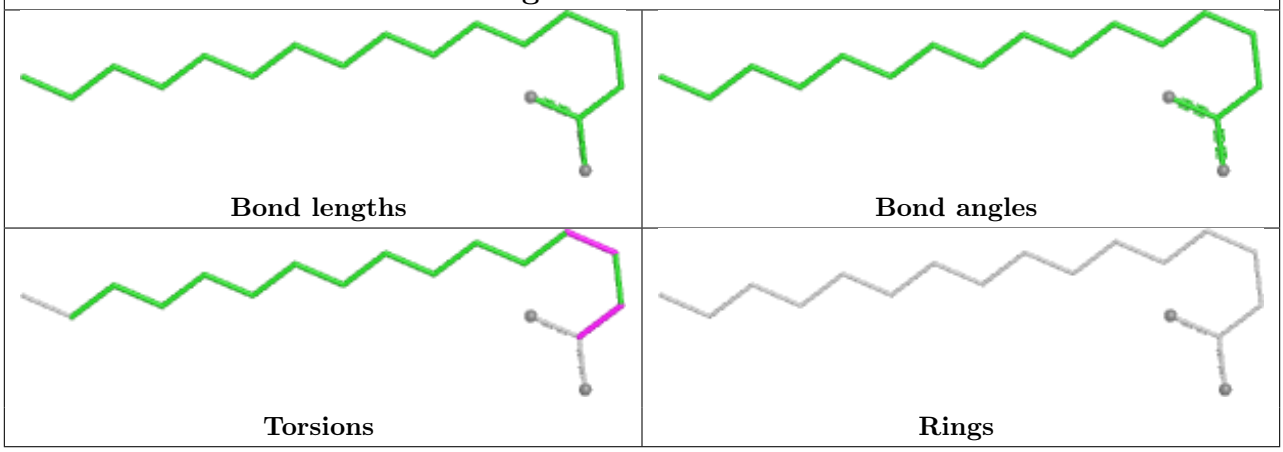
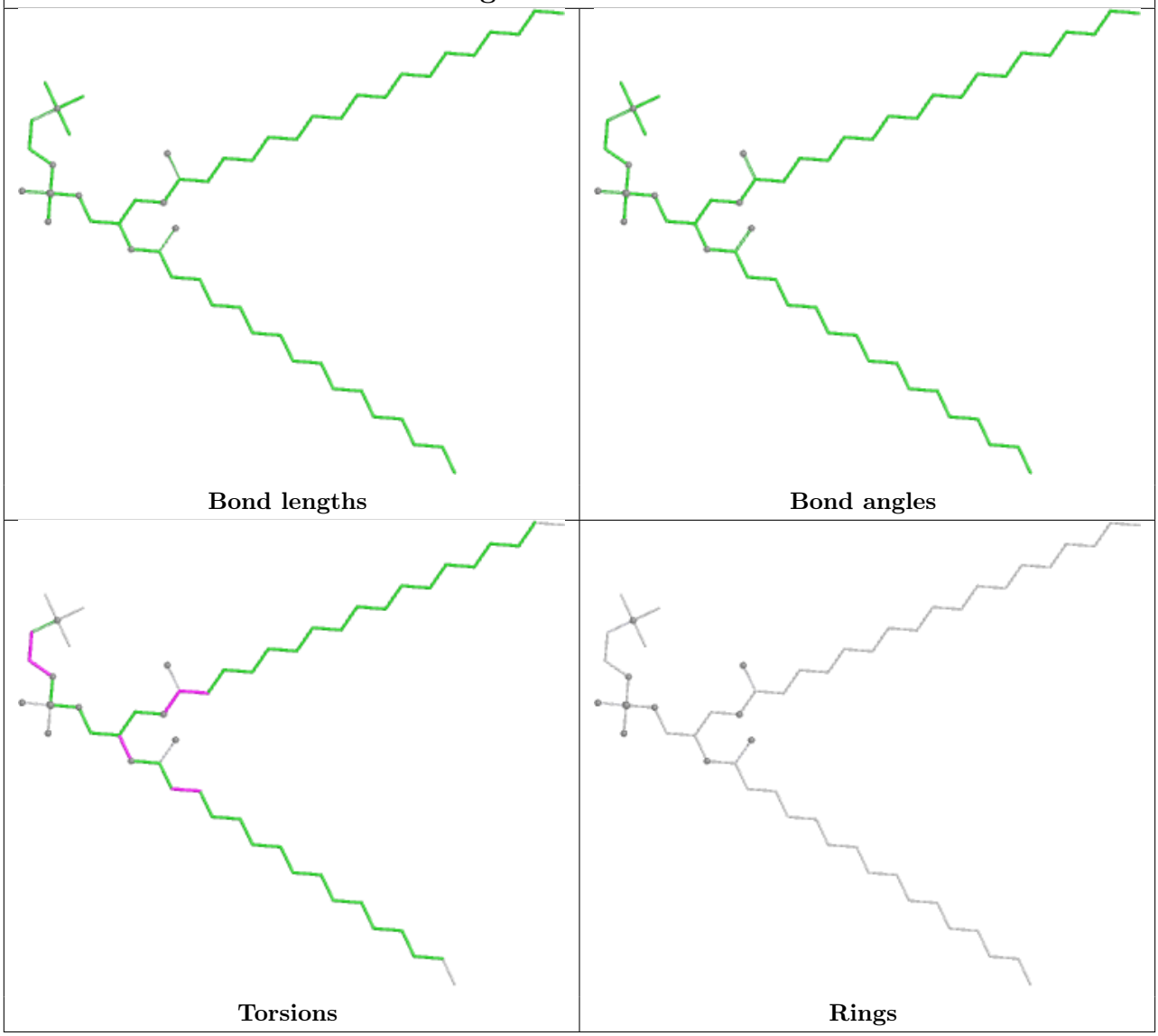
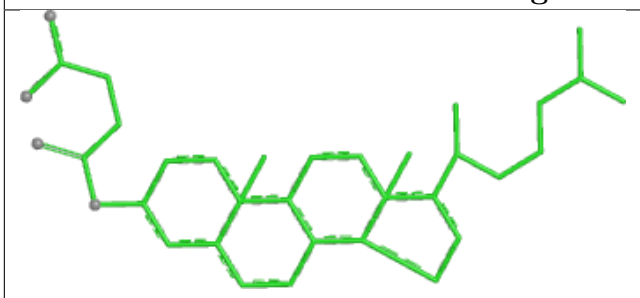
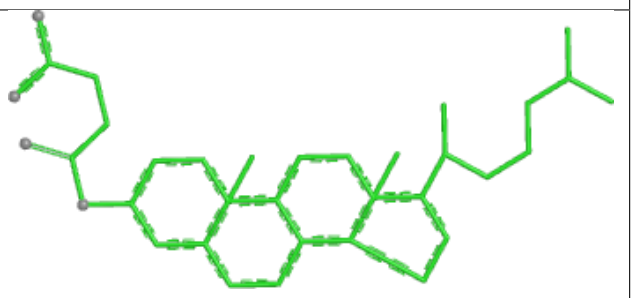
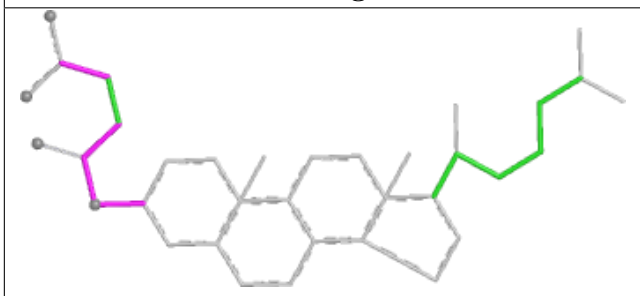
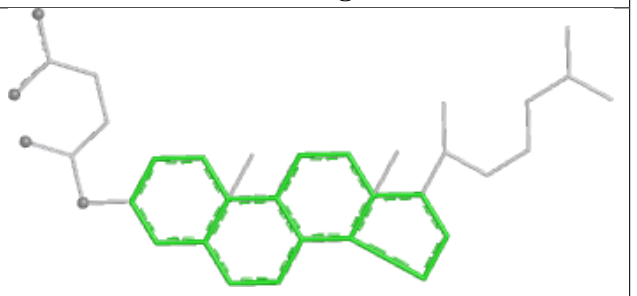
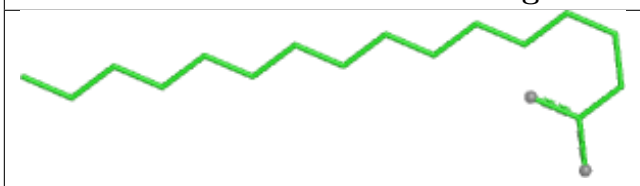
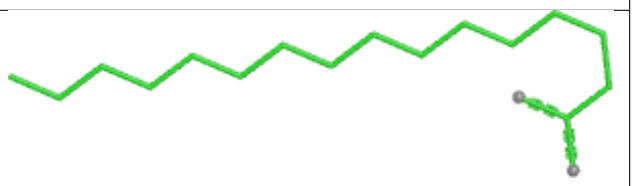
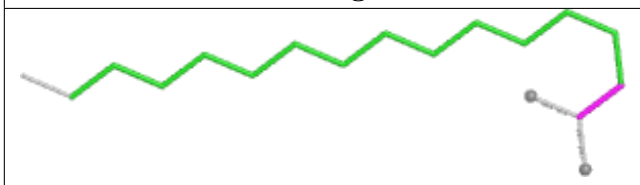


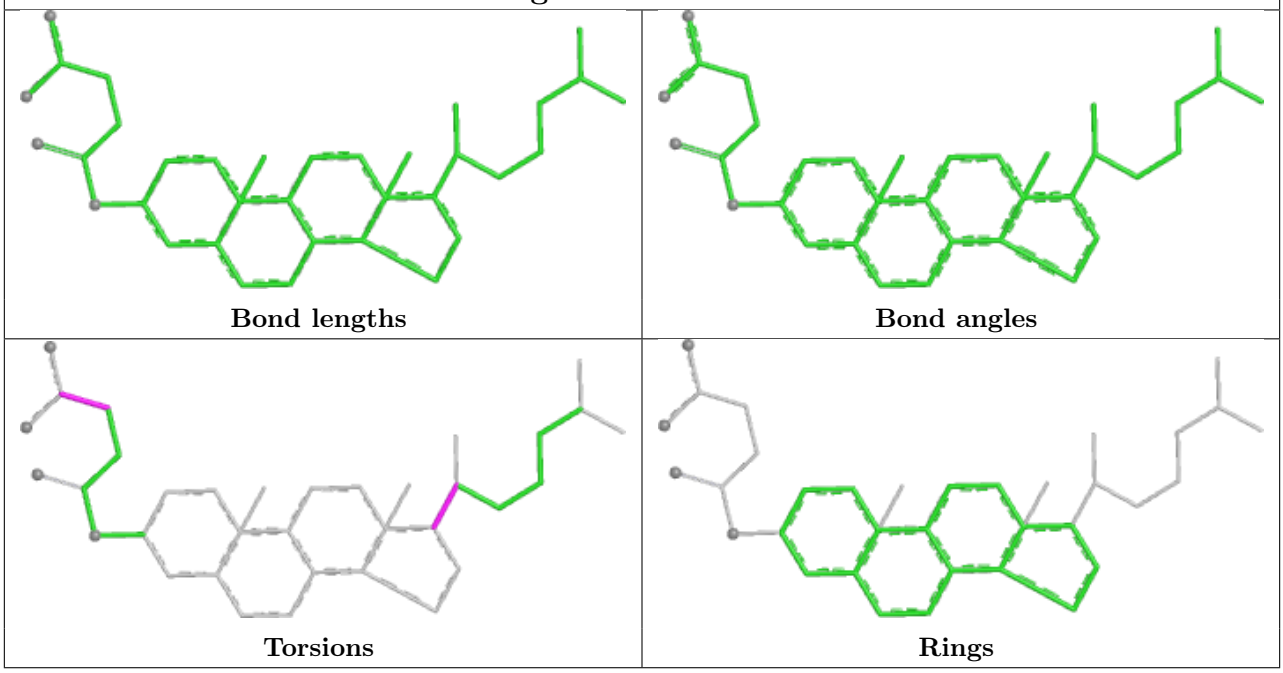
Ligand P42 R 510



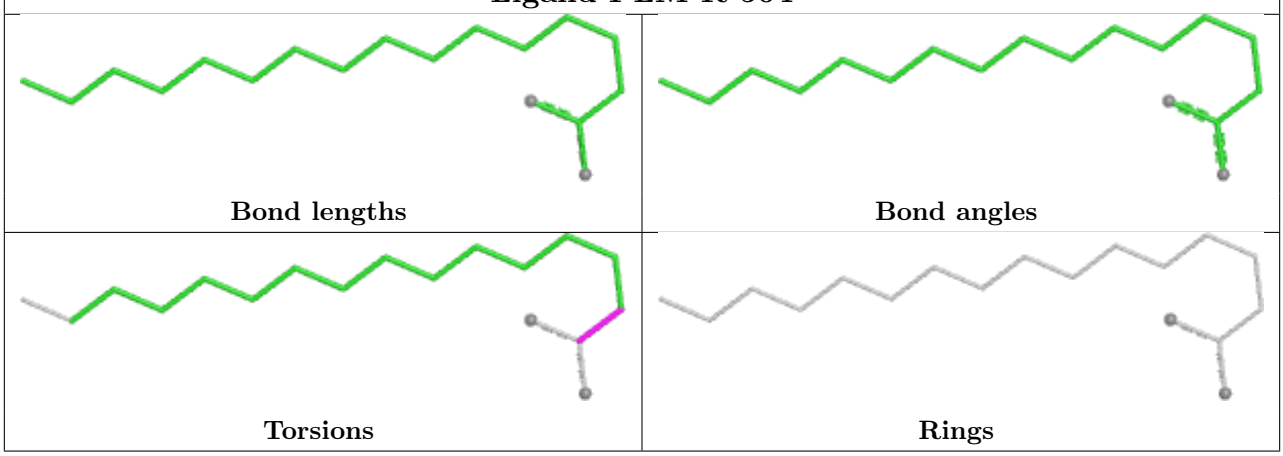
Ligand Y01 R 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PLM R 513	
 Bond lengths	 Bond angles
 Torsions	Rings

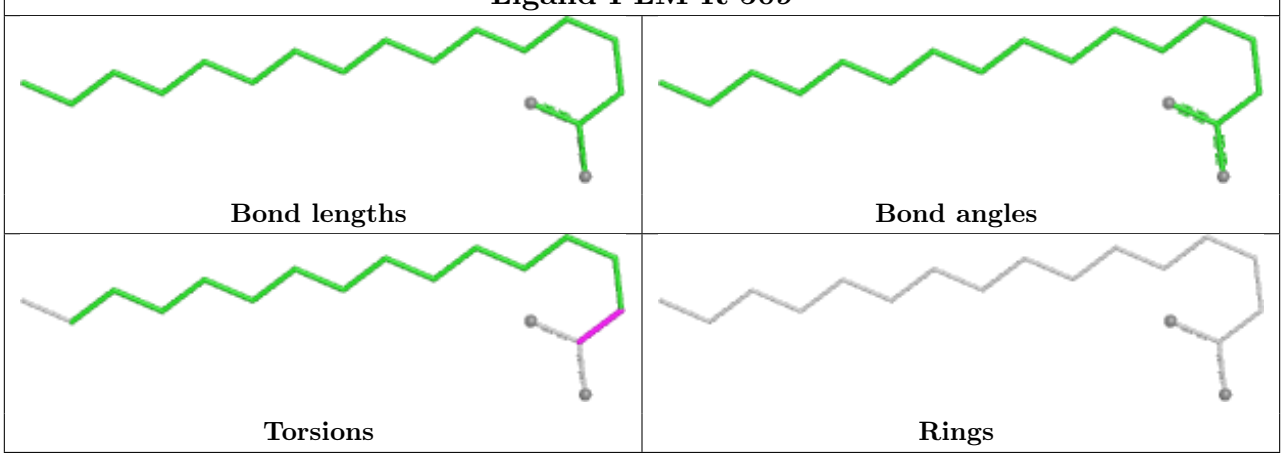
Ligand Y01 R 505

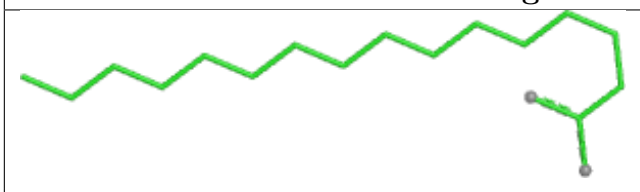
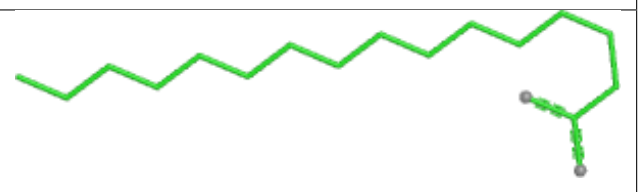
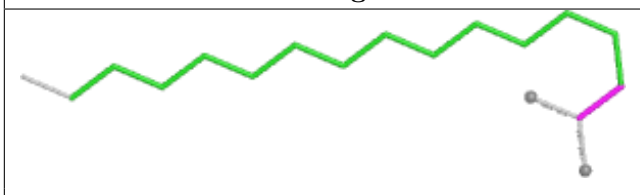
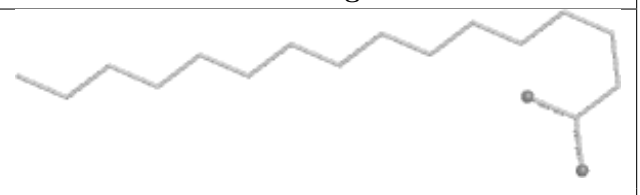


Ligand PLM R 504



Ligand PLM R 509



Ligand PLM R 507	
 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.

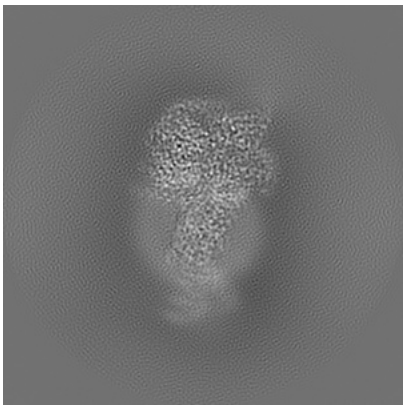
6 Map visualisation (i)

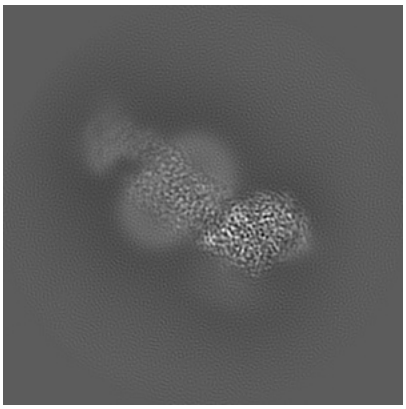
This section contains visualisations of the EMDB entry EMD-26178. These allow visual inspection of the internal detail of the map and identification of artifacts.

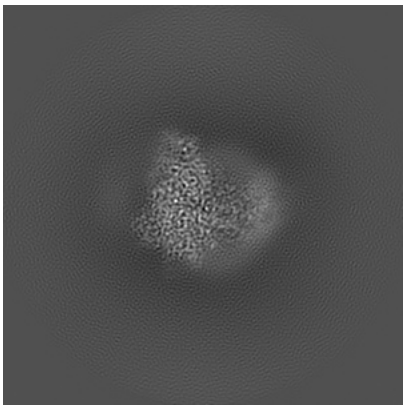
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

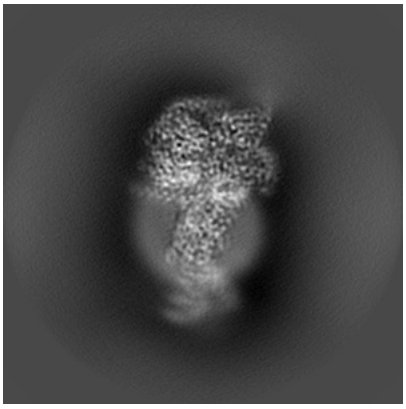
6.1.1 Primary map

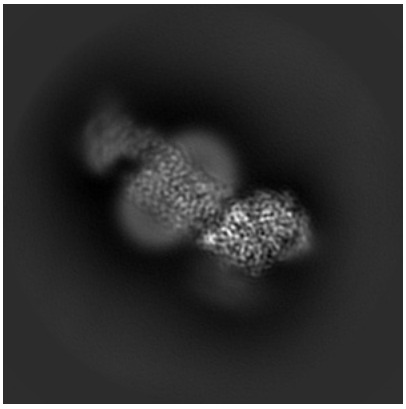

X

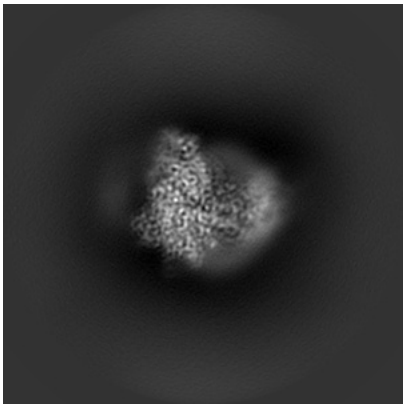

Y


Z

6.1.2 Raw map


X


Y

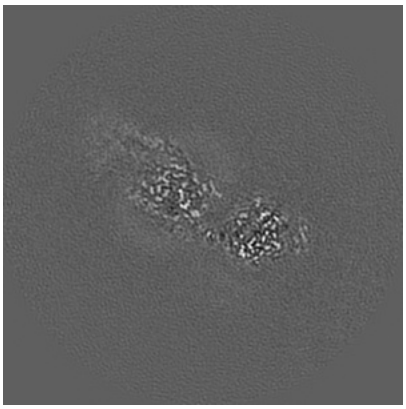

Z

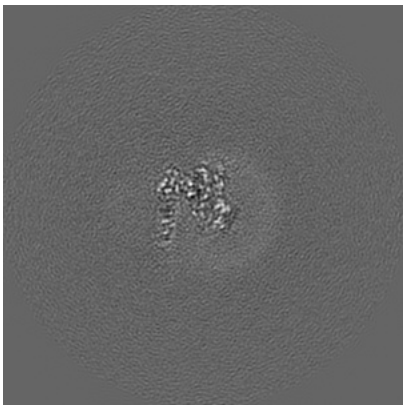
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

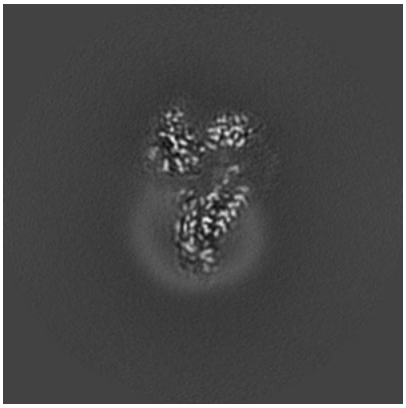
6.2.1 Primary map

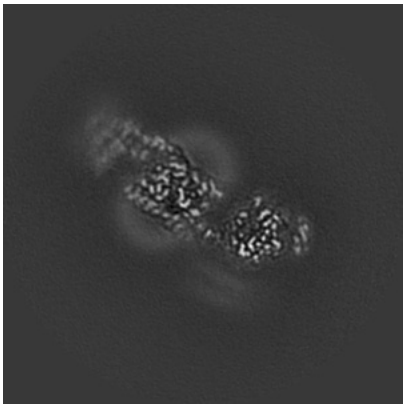
X Index: 144

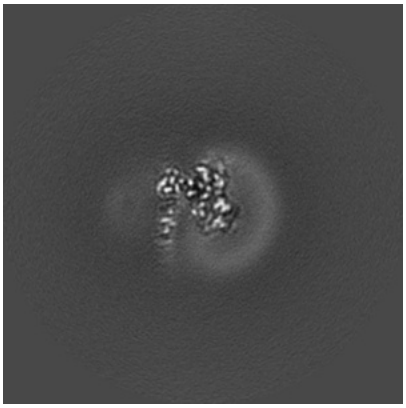

Y Index: 144


Z Index: 144

6.2.2 Raw map


X Index: 144

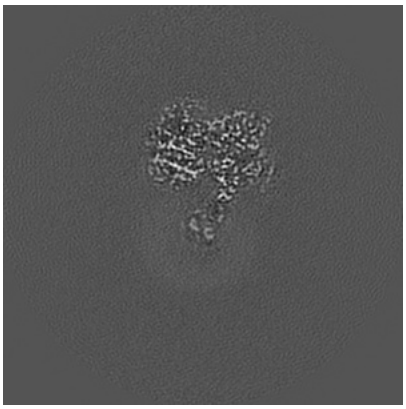

Y Index: 144

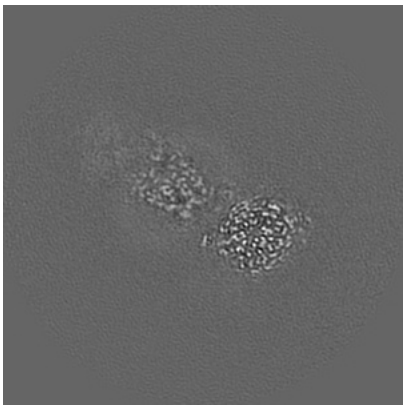

Z Index: 144

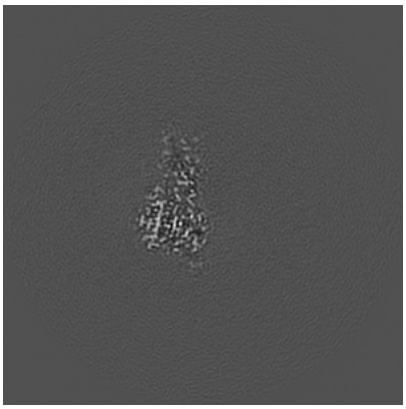
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

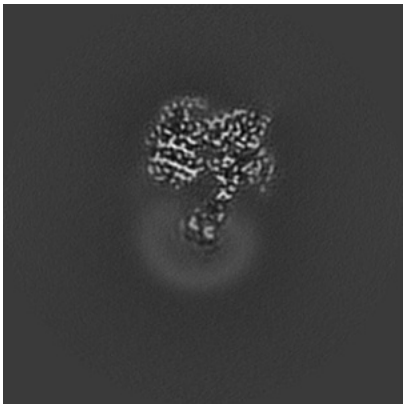
6.3.1 Primary map

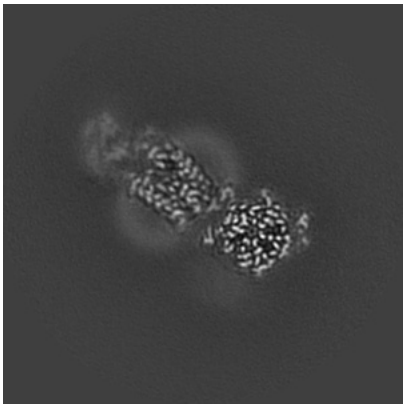

X Index: 132

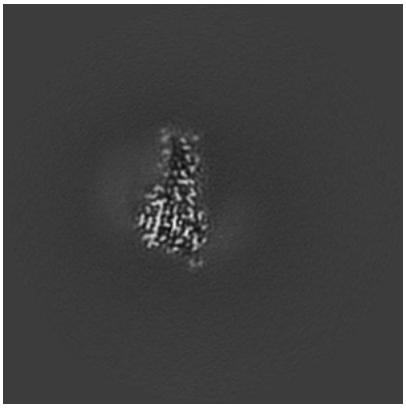

Y Index: 132


Z Index: 172

6.3.2 Raw map


X Index: 132

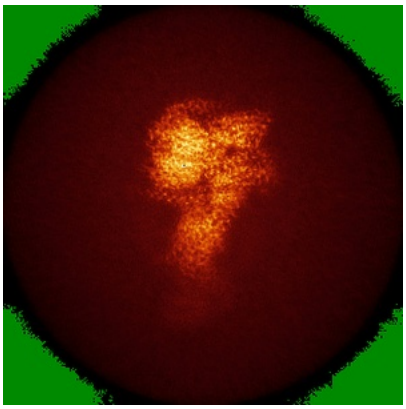

Y Index: 134

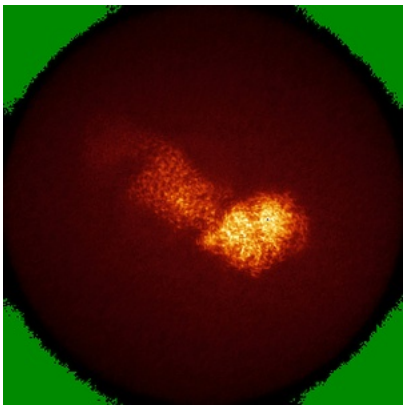

Z Index: 172

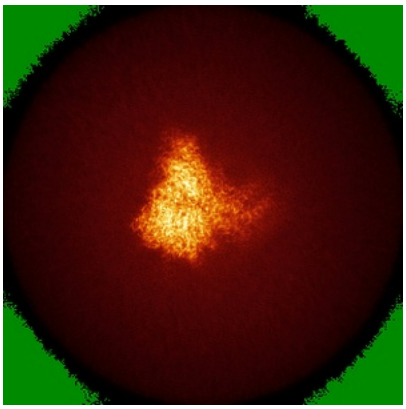
The images above show the largest variance slices of the map in three orthogonal directions.

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

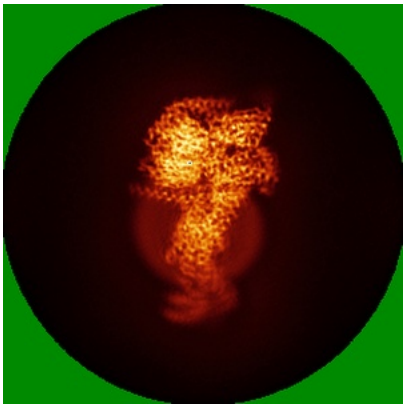
6.4.1 Primary map

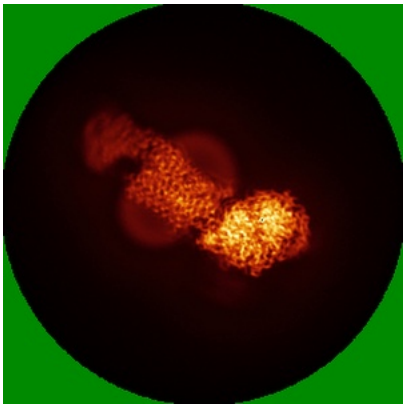

X

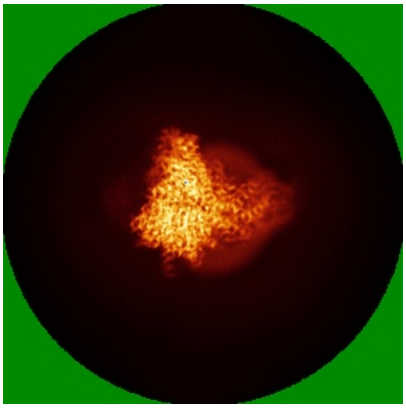

Y


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 0.029. 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.

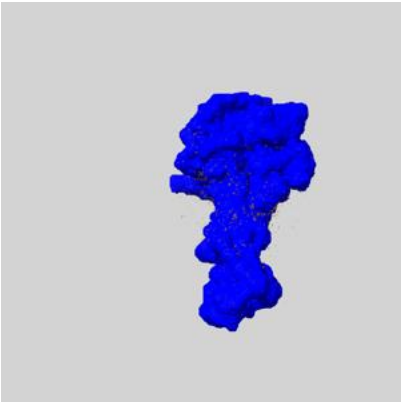
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

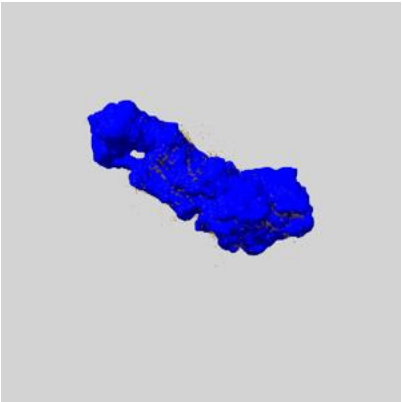
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

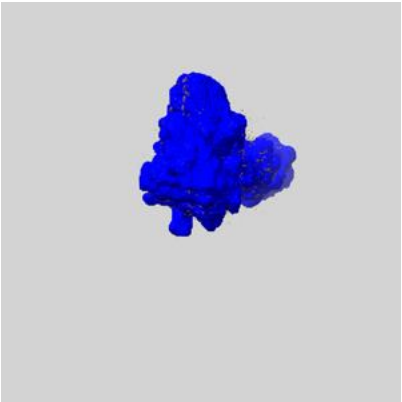
6.6.1 emd_26178_msk_1.map (i)



X



Y

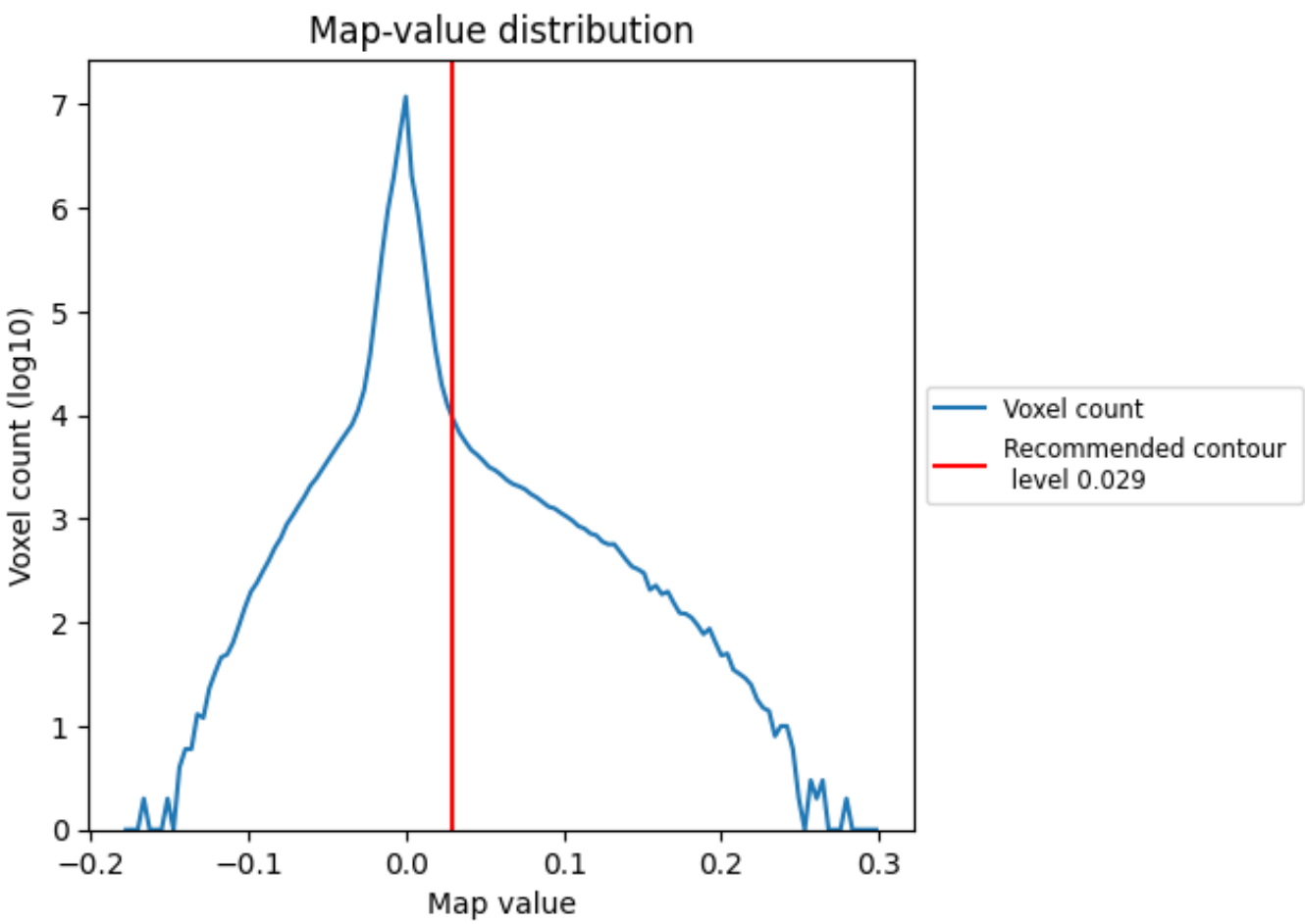


Z

7 Map analysis (i)

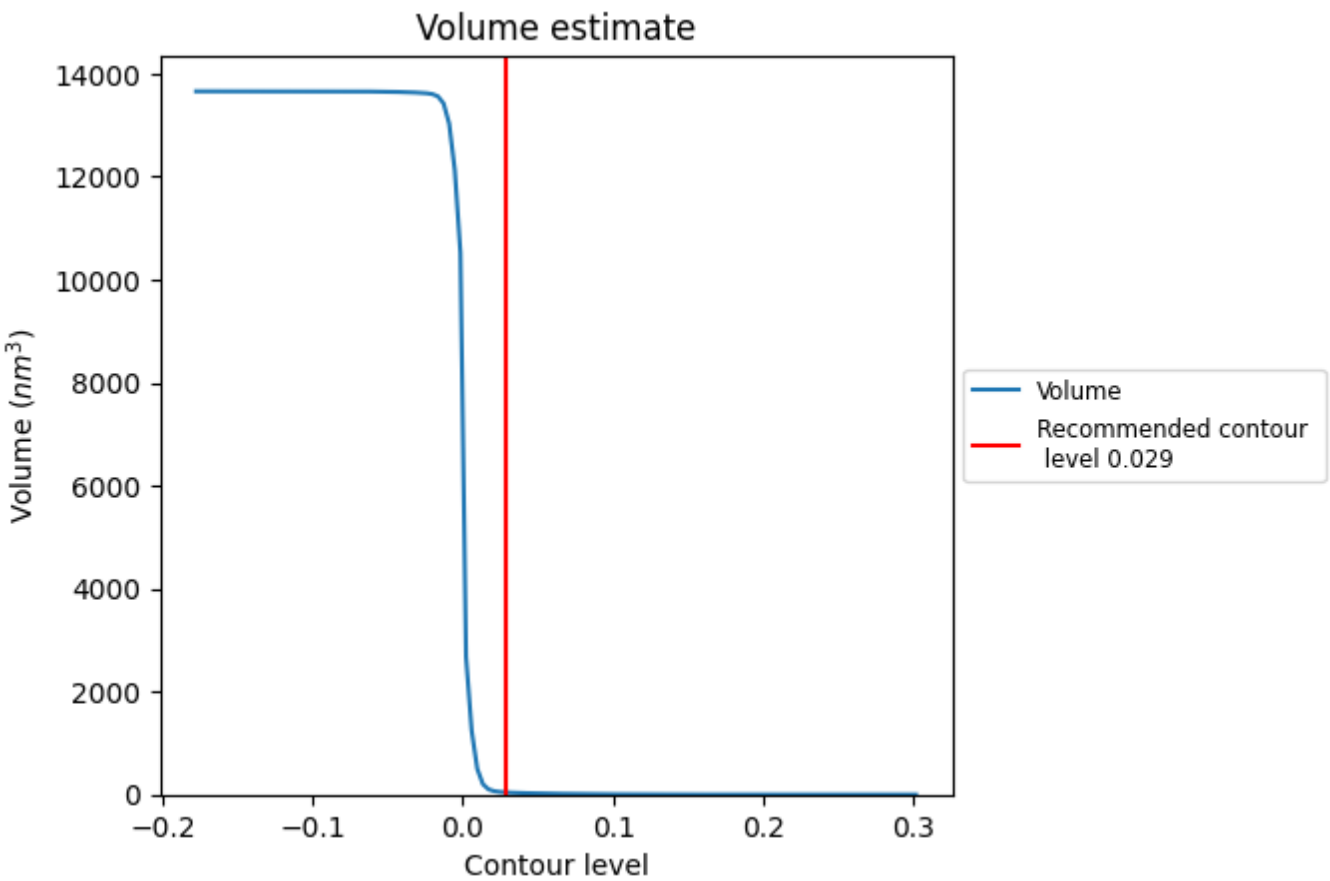
This section contains the results of statistical analysis of the map.

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.

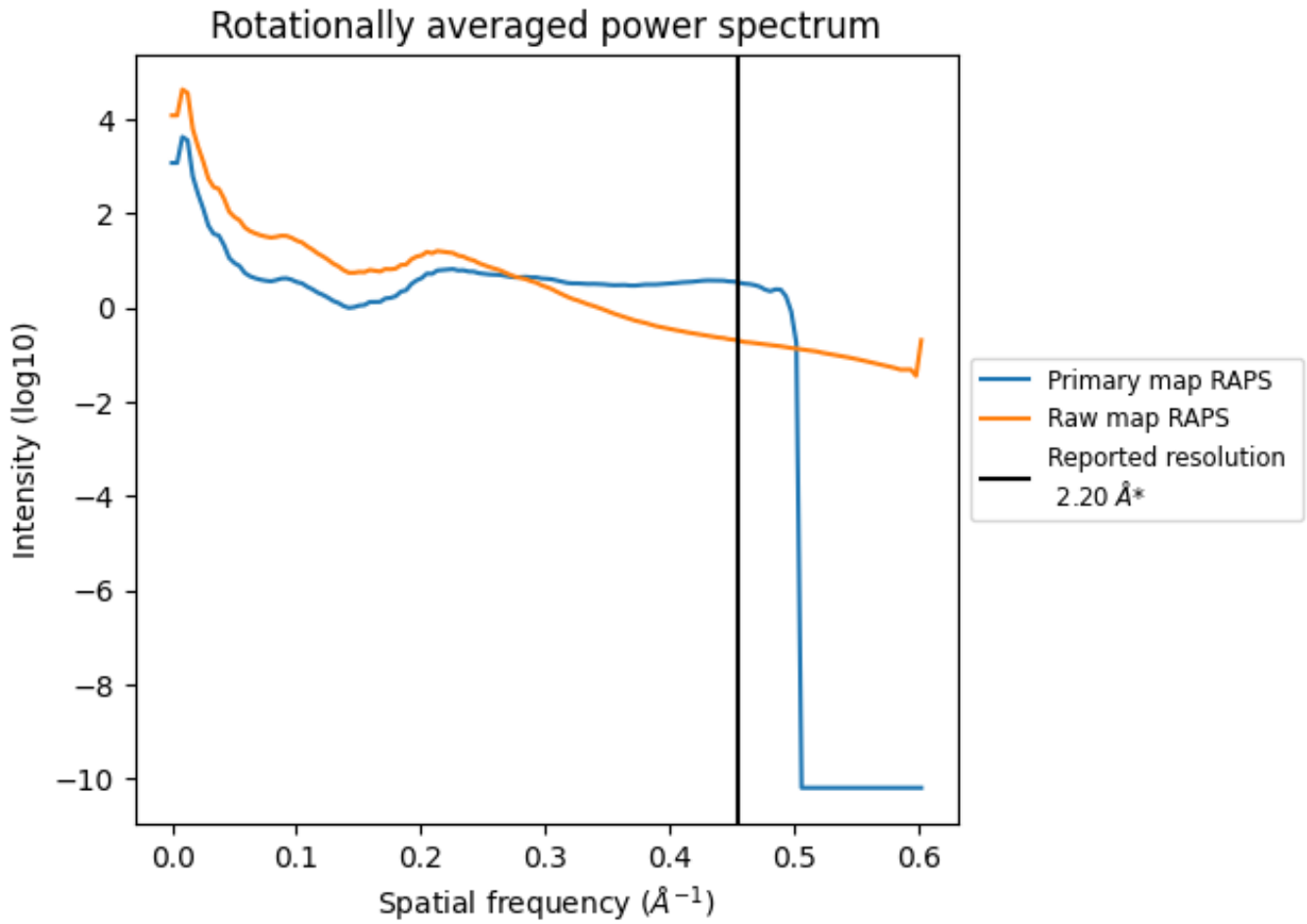
7.2 Volume estimate (i)



The volume at the recommended contour level is 42 nm^3; this corresponds to an approximate mass of 38 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)

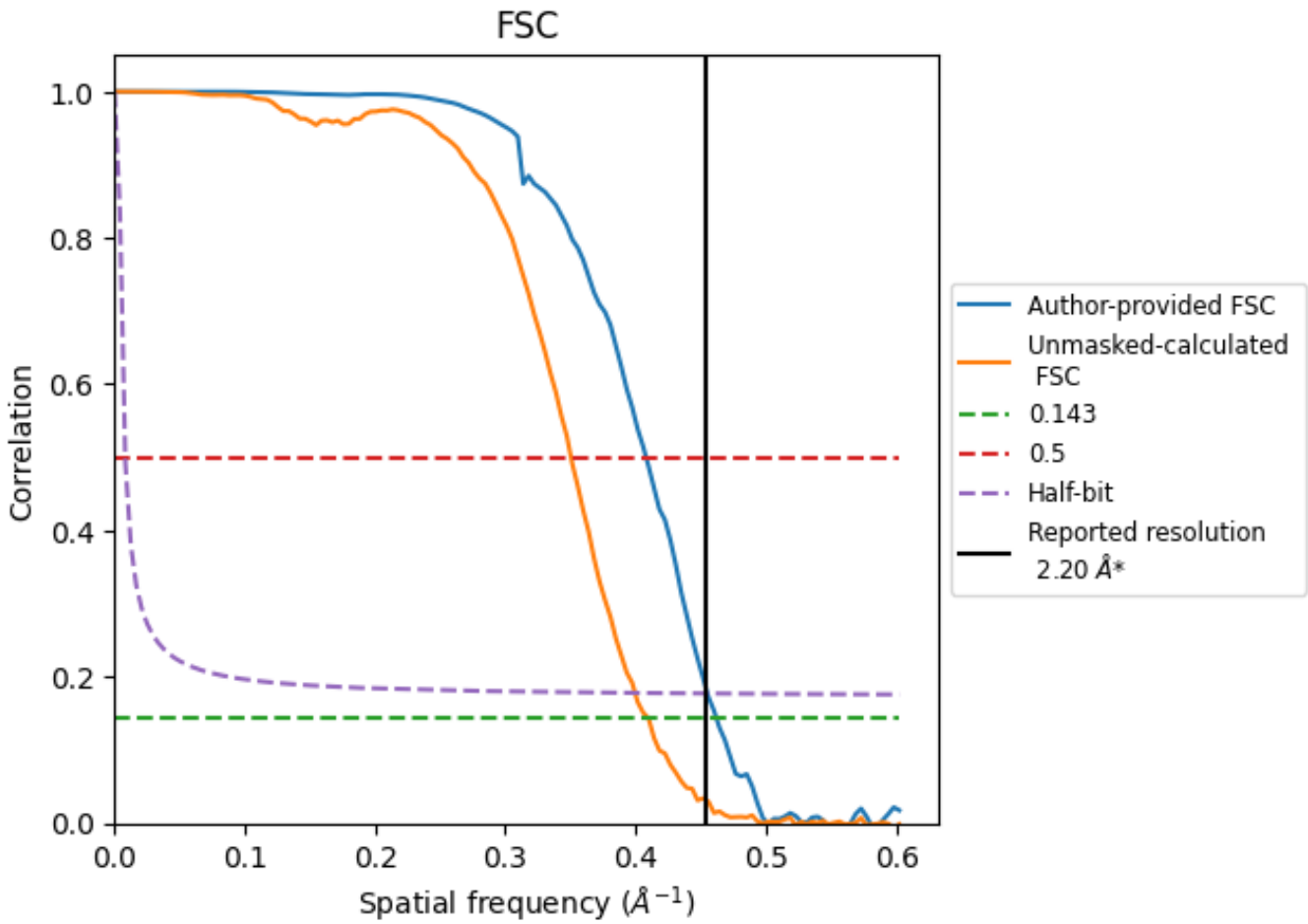


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

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 0.455 Å^{-1}

8.2 Resolution estimates (i)

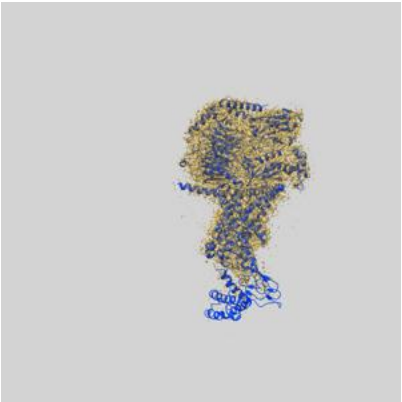
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.16	2.45	2.20
Unmasked-calculated*	2.44	2.85	2.50

*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 2.44 differs from the reported value 2.2 by more than 10 %

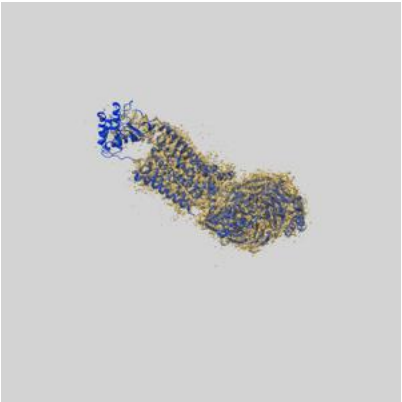
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26178 and PDB model 7TYF. Per-residue inclusion information can be found in section 3 on page 11.

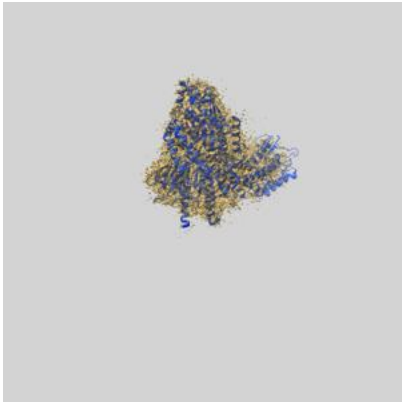
9.1 Map-model overlay (i)



X



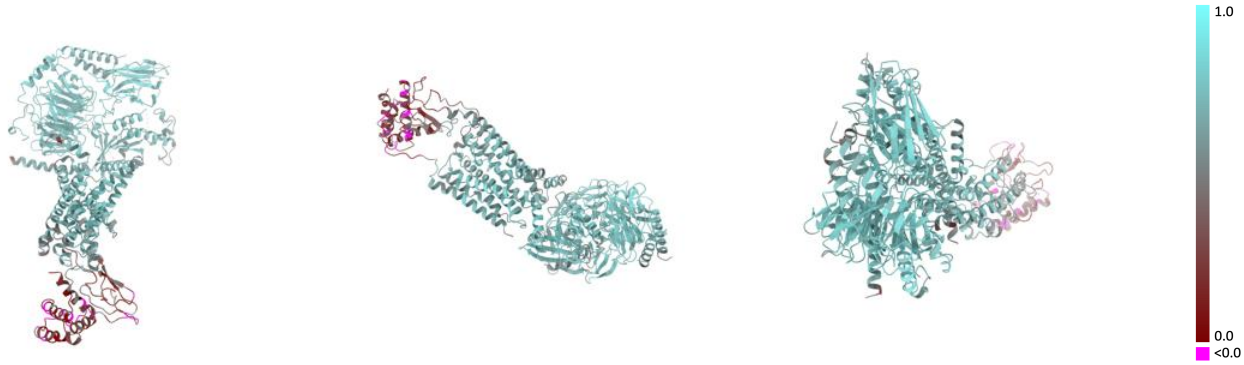
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.029 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.

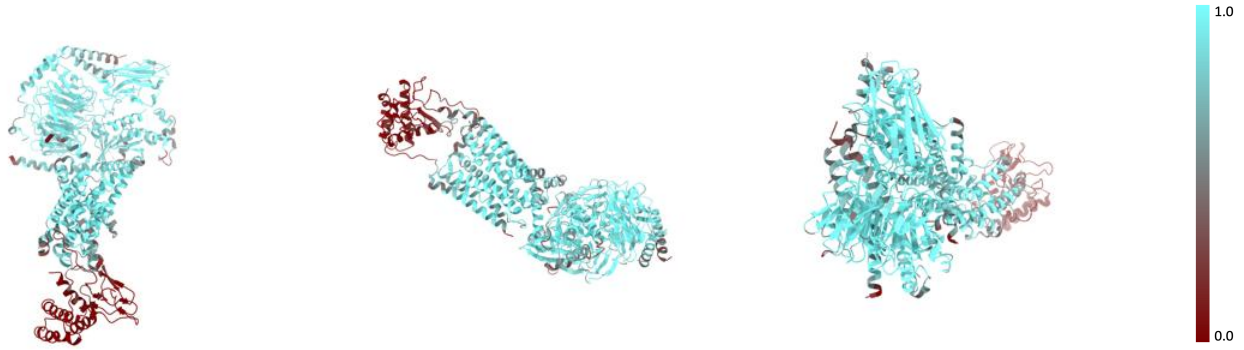
9.2 Q-score mapped to coordinate model (i)



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.

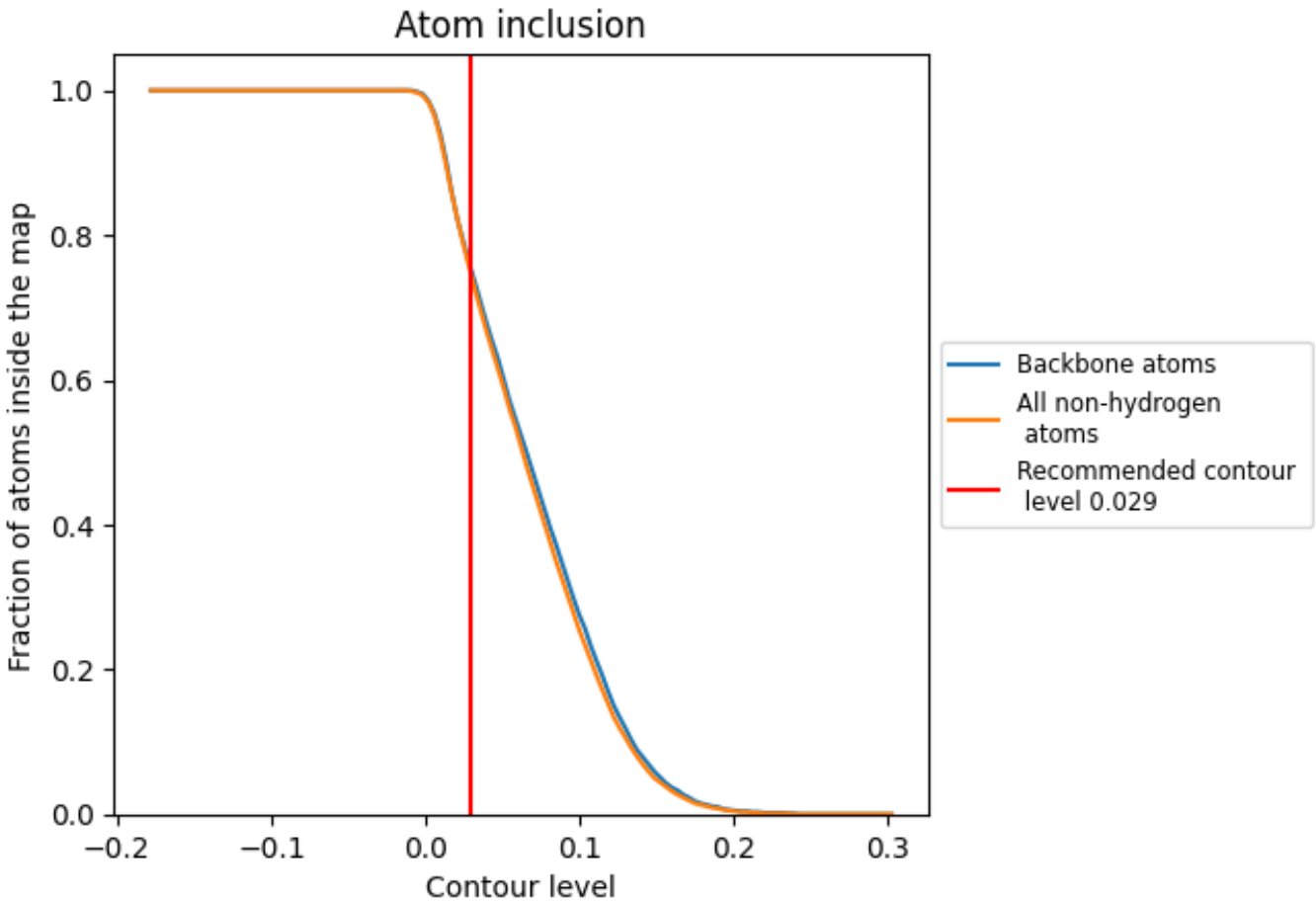
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.029).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7500	0.6310
A	0.8430	0.6850
B	0.9390	0.7390
E	0.2650	0.3420
G	0.7910	0.6840
N	0.9550	0.7320
P	0.5580	0.5250
R	0.6250	0.5550