Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 05:31 PM EST

PDB ID	:	7SHF
EMDB ID	:	EMD-25126
Title	:	Cryo-EM structure of GPR158 coupled to the RGS7-Gbeta5 complex
Authors	:	Patil, D.N.; Singh, S.; Singh, A.K.; Martemyanov, K.A.
Deposited on	:	2021-10-08
Resolution	:	3.40 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:

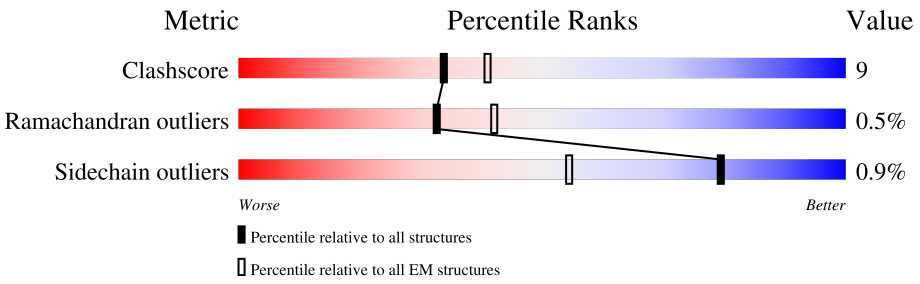
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	C	469	11% 71% 13% 15%
2	D	353	7% 82% 16% •
3	A	781	• 29% 9% • 62%
3	B	781	• 30% 6% 64%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLR	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CLR	A	804	X	-	-	-
4	CLR	A	809	X	-	-	-
4	CLR	B	801	X	-	-	-
5	EIJ	A	813	X	-	-	-
6	PEE	A	814	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11443 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 Isoform 2 of Regulator of G-protein signaling 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	400	3329	2131	564	622	12	1	0

- Molecule 2 is a protein called Guanine nucleotide-binding protein subunit beta-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	346	2660	1653	463	521	23	0	0

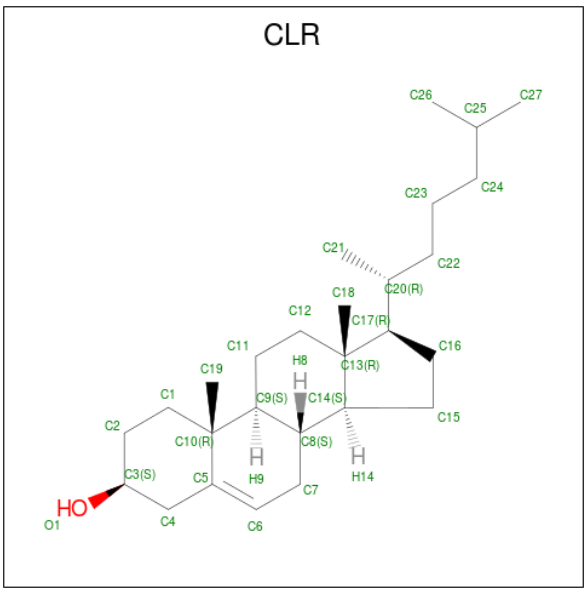
- Molecule 3 is a protein called G-protein coupled receptor 158.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	284	2322	1547	382	377	16	0	0
3	A	296	2412	1603	398	395	16	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	776	LEU	-	expression tag	UNP Q5T848
B	777	GLU	-	expression tag	UNP Q5T848
B	778	VAL	-	expression tag	UNP Q5T848
B	779	LEU	-	expression tag	UNP Q5T848
B	780	PHE	-	expression tag	UNP Q5T848
B	781	GLN	-	expression tag	UNP Q5T848
A	776	LEU	-	expression tag	UNP Q5T848
A	777	GLU	-	expression tag	UNP Q5T848
A	778	VAL	-	expression tag	UNP Q5T848
A	779	LEU	-	expression tag	UNP Q5T848
A	780	PHE	-	expression tag	UNP Q5T848
A	781	GLN	-	expression tag	UNP Q5T848

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	B	1	280	270	10	0
			Total	C	O	
4	A	1	336	324	12	0
			Total	C	O	
4	A	1	336	324	12	0
			Total	C	O	
4	A	1	336	324	12	0

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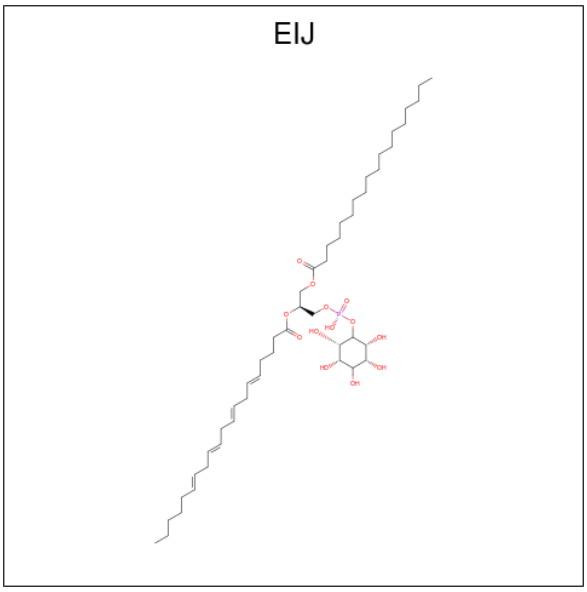
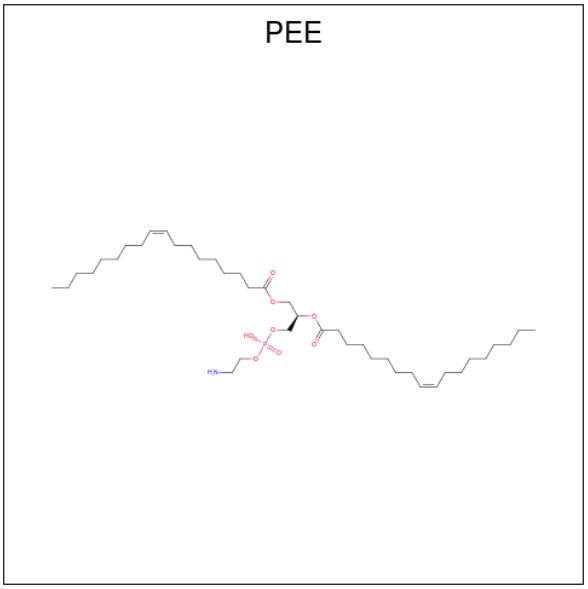
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0
			Total	C	O		
4	A	1	336	324	12		0

- Molecule 5 is (2S)-1-{[(S)-hydroxy{[(1s,2R,3R,4R,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}-3-(octadecanoyloxy)propan-2-yl (5E,8E,11E,14E)-icosa-5,8,11,14-tetraenoate (three-letter code: EIJ) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
5	A	1	55	41	13	1	0

- Molecule 6 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



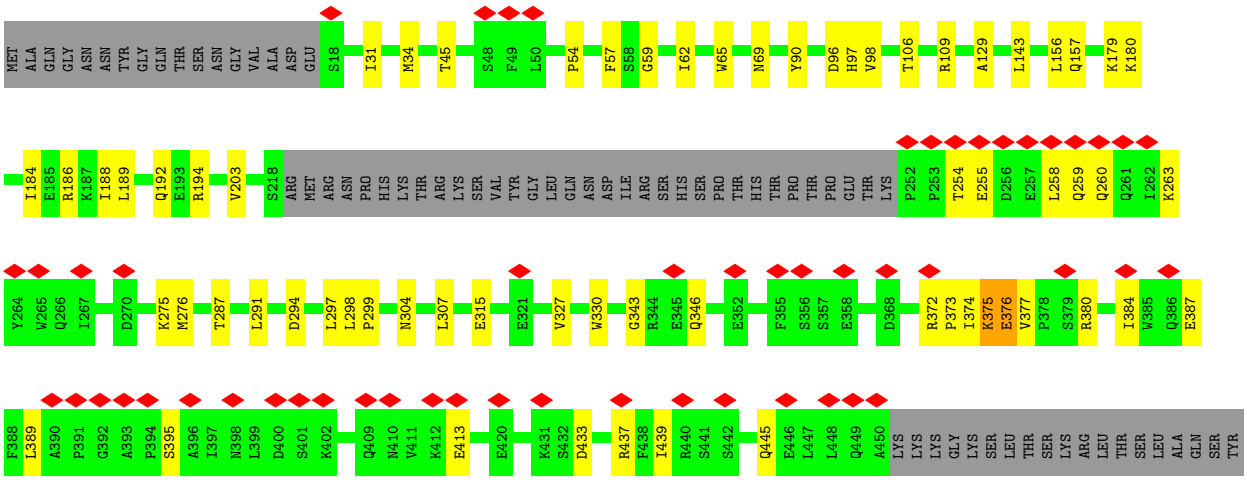
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	A	1	49	39	1	8	1	0

3 Residue-property plots (i)

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

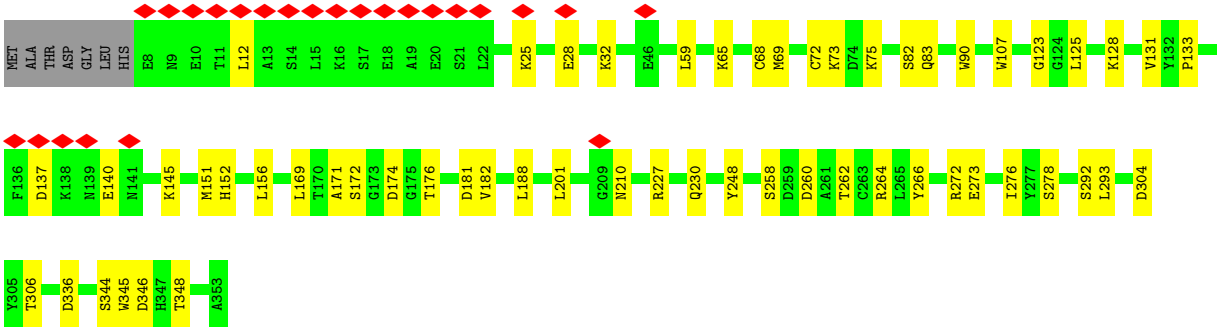
• Molecule 1: Isoform 2 of Regulator of G-protein signaling 7

Chain C:



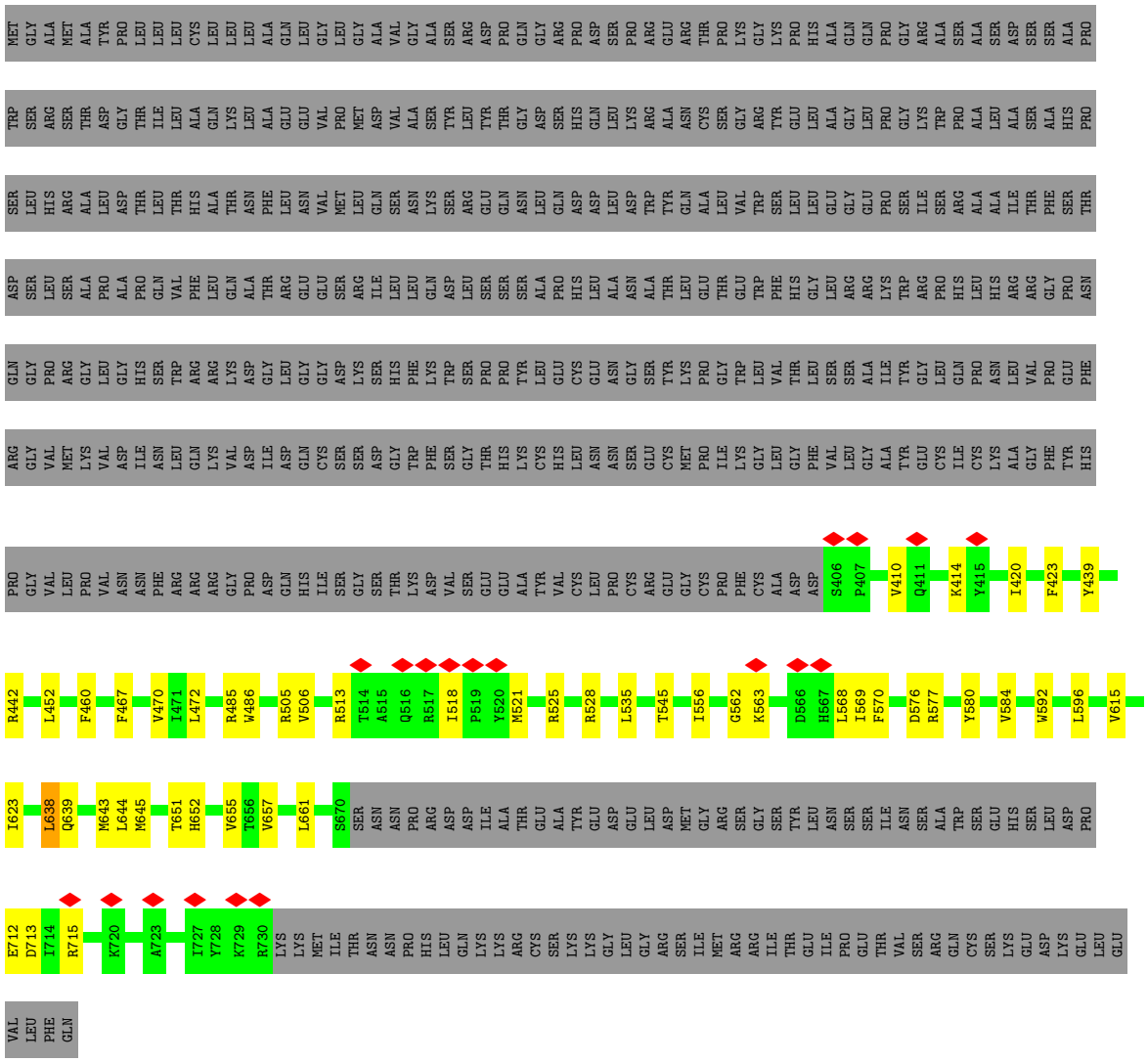
• Molecule 2: Guanine nucleotide-binding protein subunit beta-5

Chain D:



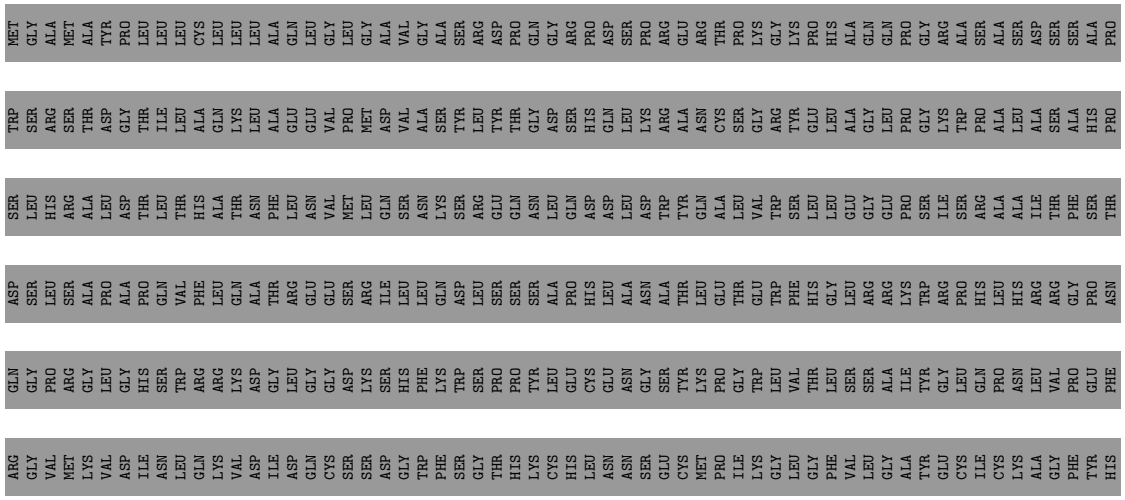
• Molecule 3: G-protein coupled receptor 158

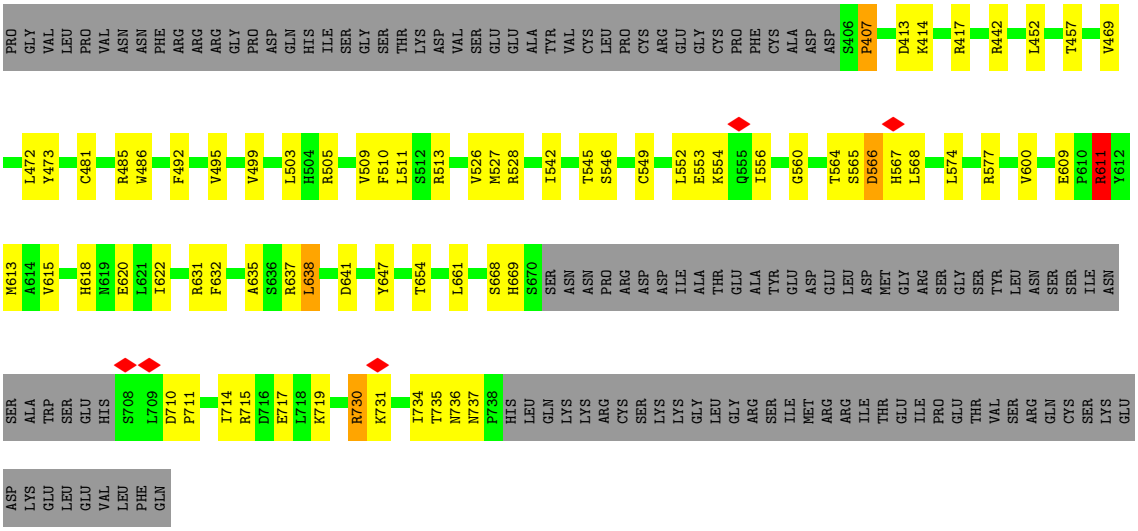
Chain B:



- Molecule 3: G-protein coupled receptor 158

Chain A:




PRO GLY VAL LEU PRO VAL ASN ASN PHE ARG ARG ARG GLY PRO ASP GLN HIS ILE SER GLY SER THR LYS ASP VAL SER GLU GLU ALA TYR VAL CYS LEU PRO CYS ARG GLU GLY CYS PRO PHE CYS ALA ASP ASP S406 P407 D413 K414 R417 R442 L452 T457 V469
L472 Y473 C481 R485 W486 F492 V495 V499 L503 H504 R505 V509 F510 L511 S512 R513 V526 M527 R528 I542 T545 S546 C549 L552 E553 K554 Q555 I556 G560 T564 S565 D566 H567 L568 L574 R577 V600 E609 P610 R611 Y612
M613 A614 V615 H618 N619 E620 L621 I622 R631 F632 A635 S636 R637 L638 D641 Y647 T654 L661 S668 H669 S670 SER ASN ASN PRO ARG ASP ASP ILE ALA THR GLU ALA TYR GLU ASP GLU LEU ASP MET GLY ARG SER GLY SER TYR LEU ASN SER SER ILE ASN
SER ALA TRP SER GLU HIS S708 L709 D710 P711 I714 R715 D716 E717 L718 K719 R730 K731 I734 T735 N736 N737 P738 HIS LEU GLN LYS LYS ARG CYS SER LYS LYS GLY LEU GLY ARG SER ILE MET ARG ARG ILE THR GLU ILE PRO GLU THR VAL SER ARG GLN CYS SER LYS GLU
ASP LYS GLU LEU GLU VAL LEU PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151954	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.320	Depositor
Minimum map value	-2.164	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.359	Depositor
Map size (Å)	349.2, 349.2, 349.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.873, 0.873, 0.873	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: EIJ, PEE, 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	C	0.28	0/3417	0.50	0/4623
2	D	0.29	0/2713	0.51	0/3666
3	A	0.32	0/2471	0.57	2/3350 (0.1%)
3	B	0.29	0/2380	0.53	0/3227
All	All	0.29	0/10981	0.53	2/14866 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	407	PRO	N-CA-CB	6.68	111.32	103.30
3	A	611	ARG	CB-CA-C	-5.30	99.80	110.40

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	C	3329	0	3260	43	0
2	D	2660	0	2562	33	0
3	A	2412	0	2507	60	0
3	B	2322	0	2417	46	0
4	A	336	0	552	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	280	0	459	28	0
5	A	55	0	0	1	0
6	A	49	0	71	2	0
All	All	11443	0	11828	210	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 9.

All (210) 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:B:460:PHE:CE2	4:B:803:CLR:H231	1.43	1.50
4:A:811:CLR:C18	4:A:812:CLR:C21	1.92	1.46
4:A:811:CLR:C18	4:A:812:CLR:H212	1.48	1.42
3:B:460:PHE:HE2	4:B:803:CLR:C23	1.56	1.18
3:B:460:PHE:CE2	4:B:803:CLR:C23	2.26	1.18
4:A:811:CLR:H181	4:A:812:CLR:H213	1.32	1.10
3:B:460:PHE:CD2	4:B:803:CLR:H231	1.89	1.07
4:A:811:CLR:H183	4:A:812:CLR:C21	1.82	1.07
4:A:811:CLR:H182	4:A:812:CLR:H212	1.09	1.03
4:A:811:CLR:H181	4:A:812:CLR:C21	1.82	0.97
3:B:623:ILE:HB	4:B:808:CLR:C26	1.99	0.91
3:B:460:PHE:CE2	4:B:803:CLR:C22	2.59	0.85
4:A:811:CLR:C18	4:A:812:CLR:H213	1.89	0.84
1:C:372:ARG:HD3	1:C:373:PRO:HD2	1.62	0.80
3:A:486:TRP:HE1	3:A:545:THR:HG21	1.48	0.79
4:A:811:CLR:H183	4:A:812:CLR:H212	1.52	0.79
3:B:460:PHE:CD2	4:B:803:CLR:C23	2.61	0.77
4:A:811:CLR:H183	4:A:812:CLR:H211	1.64	0.77
3:B:460:PHE:CE2	4:B:803:CLR:H222	2.19	0.77
4:A:811:CLR:H182	4:A:812:CLR:C21	1.88	0.76
3:A:481:CYS:O	3:A:485:ARG:NH1	2.25	0.69
3:B:623:ILE:HB	4:B:808:CLR:H263	1.74	0.68
3:A:715:ARG:O	3:A:719:LYS:NZ	2.25	0.68
1:C:275:LYS:NZ	2:D:32:LYS:O	2.28	0.67
3:A:527:MET:HG2	4:A:809:CLR:H191	1.75	0.67
1:C:439:ILE:O	1:C:445:GLN:NE2	2.29	0.66
3:A:730:ARG:O	3:A:737:ASN:ND2	2.27	0.66
2:D:72:CYS:SG	2:D:73:LYS:N	2.69	0.66
3:A:549:CYS:SG	4:A:812:CLR:H22	2.36	0.65
3:A:566:ASP:OD1	3:A:567:HIS:N	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:460:PHE:HE2	4:B:803:CLR:H231	0.88	0.64
1:C:189:LEU:HD21	3:A:730:ARG:HA	1.79	0.63
2:D:262:THR:HG22	2:D:278:SER:HB2	1.81	0.62
3:A:413:ASP:OD1	3:A:414:LYS:N	2.33	0.62
3:A:661:LEU:HD21	4:A:804:CLR:H151	1.81	0.62
2:D:264:ARG:HG2	2:D:276:ILE:HG12	1.81	0.61
1:C:129:ALA:HB2	1:C:156:LEU:HD23	1.84	0.60
1:C:375:LYS:HG2	1:C:376:GLU:HG2	1.83	0.60
3:B:460:PHE:CE2	4:B:803:CLR:H272	2.36	0.60
1:C:179:LYS:HA	1:C:186:ARG:HH12	1.68	0.59
4:B:801:CLR:H152	4:A:802:CLR:H71	1.82	0.59
3:A:542:ILE:HG12	4:A:812:CLR:H222	1.84	0.59
1:C:276:MET:SD	2:D:272:ARG:NH1	2.76	0.58
3:B:472:LEU:HD11	3:B:643:MET:HG3	1.85	0.58
2:D:75:LYS:HD3	2:D:336:ASP:HB3	1.86	0.58
3:B:442:ARG:HG3	3:B:452:LEU:HD22	1.85	0.58
3:A:714:ILE:HA	3:A:717:GLU:HG2	1.86	0.58
2:D:304:ASP:OD2	2:D:306:THR:OG1	2.20	0.58
3:A:577:ARG:HH11	4:A:807:CLR:H192	1.69	0.58
2:D:210:ASN:HD21	2:D:227:ARG:HE	1.49	0.58
2:D:123:GLY:HA3	2:D:156:LEU:HD23	1.86	0.57
3:B:562:GLY:O	3:B:570:PHE:N	2.35	0.57
1:C:34:MET:HG2	1:C:65:TRP:CZ3	2.39	0.57
3:A:457:THR:HG22	4:A:810:CLR:H183	1.85	0.57
3:B:661:LEU:HD23	4:B:810:CLR:H111	1.87	0.57
3:A:710:ASP:HB2	3:A:711:PRO:HD3	1.86	0.57
3:A:730:ARG:HD3	3:A:731:LYS:HB2	1.87	0.57
4:A:804:CLR:H152	4:A:805:CLR:H8	1.87	0.57
3:B:623:ILE:HB	4:B:808:CLR:H261	1.85	0.56
3:A:565:SER:HB3	3:A:568:LEU:HD12	1.87	0.56
3:B:423:PHE:HE2	3:B:652:HIS:CE1	2.24	0.56
4:B:801:CLR:H181	4:A:802:CLR:H14	1.87	0.56
3:A:552:LEU:HA	3:A:556:ILE:O	2.07	0.55
3:A:632:PHE:HD2	4:A:806:CLR:H213	1.72	0.55
1:C:304:ASN:HB3	1:C:307:LEU:HB2	1.89	0.54
3:B:513:ARG:HH22	3:B:518:ILE:HB	1.71	0.54
1:C:157:GLN:NE2	3:A:513:ARG:O	2.40	0.54
2:D:346:ASP:OD1	2:D:348:THR:OG1	2.19	0.53
3:B:615:VAL:HG21	4:B:809:CLR:H8	1.91	0.53
3:A:564:THR:O	3:A:568:LEU:HB2	2.09	0.52
3:B:563:LYS:HA	3:B:569:ILE:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ASP:O	1:C:194:ARG:NH1	2.43	0.52
2:D:65:LYS:NZ	2:D:83:GLN:OE1	2.39	0.52
2:D:181:ASP:HB2	2:D:188:LEU:HD11	1.92	0.52
3:B:410:VAL:HG22	3:B:568:LEU:HD13	1.92	0.52
3:A:560:GLY:HA3	3:A:574:LEU:HD21	1.92	0.52
3:B:715:ARG:NH1	3:A:710:ASP:OD1	2.37	0.51
1:C:260:GLN:HA	1:C:263:LYS:HE3	1.92	0.51
2:D:258:SER:OG	2:D:260:ASP:OD1	2.29	0.51
1:C:31:ILE:HG13	1:C:90:TYR:HD2	1.76	0.51
2:D:171:ALA:HB2	2:D:201:LEU:HD23	1.93	0.51
2:D:137:ASP:HB2	2:D:140:GLU:HG2	1.93	0.51
1:C:374:ILE:O	1:C:377:VAL:HG12	2.12	0.50
3:A:486:TRP:NE1	3:A:545:THR:HG21	2.23	0.50
5:A:813:EIJ:O54	6:A:814:PEE:O4P	2.29	0.50
3:A:486:TRP:CZ2	4:A:812:CLR:H211	2.47	0.50
3:A:618:HIS:HB3	4:A:803:CLR:H112	1.94	0.50
3:B:528:ARG:HG2	4:B:801:CLR:H71	1.94	0.50
3:A:549:CYS:SG	4:A:812:CLR:H192	2.51	0.50
1:C:65:TRP:NE1	1:C:69:ASN:OD1	2.45	0.50
3:A:469:VAL:HG22	3:A:647:TYR:HB3	1.94	0.50
1:C:380:ARG:HH22	1:C:384:ILE:HD11	1.75	0.50
3:B:592:TRP:O	3:B:596:LEU:HD23	2.11	0.50
3:A:668:SER:OG	3:A:669:HIS:ND1	2.44	0.50
2:D:82:SER:OG	2:D:83:GLN:N	2.44	0.49
3:A:417:ARG:NH2	3:A:641:ASP:OD1	2.32	0.49
3:A:528:ARG:NE	4:A:808:CLR:H11	2.28	0.49
3:A:615:VAL:HG23	4:A:803:CLR:H12	1.93	0.49
1:C:59:GLY:N	1:C:106:THR:O	2.45	0.49
1:C:180:LYS:HD3	1:C:180:LYS:O	2.13	0.49
1:C:98:VAL:HG22	1:C:203:VAL:HG11	1.96	0.48
2:D:59:LEU:HD23	2:D:90:TRP:CD2	2.49	0.48
2:D:174:ASP:OD1	2:D:176:THR:OG1	2.28	0.48
3:B:576:ASP:OD1	3:B:577:ARG:N	2.46	0.48
1:C:327:VAL:O	1:C:330:TRP:HB2	2.13	0.48
2:D:68:CYS:SG	2:D:69:MET:N	2.87	0.48
2:D:128:LYS:HG2	2:D:151:MET:HG2	1.95	0.48
3:A:637:ARG:HG3	3:A:638:LEU:H	1.78	0.48
3:B:460:PHE:HE2	4:B:803:CLR:C22	2.10	0.48
3:B:467:PHE:HA	3:B:470:VAL:HG22	1.96	0.47
2:D:25:LYS:O	2:D:28:GLU:HG3	2.15	0.47
1:C:330:TRP:CH2	1:C:343:GLY:HA2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:503:LEU:HD13	3:A:613:MET:HE2	1.97	0.47
4:A:808:CLR:H211	4:A:808:CLR:H231	1.72	0.47
4:B:807:CLR:H212	4:A:801:CLR:H151	1.97	0.47
1:C:387:GLU:O	1:C:395:SER:OG	2.29	0.47
3:B:486:TRP:HE1	3:B:545:THR:HG21	1.78	0.46
3:A:528:ARG:CZ	4:A:808:CLR:H11	2.45	0.46
1:C:143:LEU:HD12	3:A:511:LEU:HD21	1.97	0.46
3:B:513:ARG:NE	3:B:513:ARG:HA	2.31	0.46
4:A:811:CLR:H273	4:A:811:CLR:H232	1.81	0.46
3:A:495:VAL:O	3:A:499:VAL:HG23	2.15	0.46
1:C:413:GLU:N	1:C:413:GLU:OE2	2.49	0.46
3:B:521:MET:SD	3:B:525:ARG:HG2	2.56	0.46
3:A:546:SER:HA	4:A:812:CLR:H193	1.98	0.45
4:B:808:CLR:H222	4:B:808:CLR:H162	1.46	0.45
4:B:804:CLR:H242	4:B:805:CLR:H213	1.97	0.45
4:A:808:CLR:H262	4:A:809:CLR:H232	1.99	0.45
2:D:230:GLN:N	2:D:230:GLN:OE1	2.49	0.45
3:B:513:ARG:NH2	3:B:518:ILE:HB	2.32	0.45
3:B:638:LEU:O	3:B:639:GLN:HG3	2.17	0.45
3:B:460:PHE:CD2	4:B:803:CLR:H222	2.50	0.45
1:C:254:THR:HG23	2:D:12:LEU:HD11	1.99	0.45
1:C:259:GLN:NE2	1:C:260:GLN:HG3	2.31	0.45
3:B:439:TYR:O	3:B:442:ARG:HB2	2.17	0.45
3:B:615:VAL:HG13	3:B:661:LEU:HD13	1.99	0.45
4:A:803:CLR:H222	4:A:803:CLR:H162	1.42	0.45
4:A:811:CLR:H191	4:A:812:CLR:H122	1.98	0.44
2:D:133:PRO:HD2	2:D:145:LYS:HB3	2.00	0.44
4:A:806:CLR:H211	4:A:806:CLR:H231	1.65	0.44
1:C:433:ASP:OD1	1:C:437:ARG:NH2	2.51	0.44
1:C:294:ASP:OD2	2:D:292:SER:OG	2.34	0.44
1:C:57:PHE:CD2	1:C:62:ILE:HD11	2.52	0.44
3:B:506:VAL:HG12	3:B:506:VAL:O	2.18	0.44
3:A:472:LEU:HD12	3:A:472:LEU:HA	1.86	0.44
3:A:553:GLU:HB2	3:A:554:LYS:NZ	2.32	0.44
3:A:613:MET:HB3	3:A:613:MET:HE3	1.71	0.44
4:A:802:CLR:H273	4:A:802:CLR:H232	1.80	0.44
2:D:152:HIS:ND1	2:D:172:SER:OG	2.38	0.43
1:C:287:THR:OG1	2:D:248:TYR:OH	2.36	0.43
3:A:613:MET:HE2	3:A:613:MET:HB2	1.66	0.43
3:A:609:GLU:C	3:A:611:ARG:H	2.21	0.43
3:A:620:GLU:HG2	3:A:654:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:811:CLR:C19	4:A:812:CLR:H112	2.49	0.43
1:C:143:LEU:O	1:C:143:LEU:HD23	2.18	0.43
1:C:96:ASP:OD1	1:C:97:HIS:N	2.51	0.43
4:B:806:CLR:H152	4:A:808:CLR:H161	2.00	0.43
1:C:315:GLU:HA	1:C:315:GLU:OE1	2.19	0.43
2:D:107:TRP:HB2	2:D:125:LEU:HD13	2.01	0.43
1:C:255:GLU:HA	1:C:258:LEU:HD12	2.01	0.43
3:B:420:ILE:HD11	3:B:645:MET:SD	2.59	0.43
3:B:638:LEU:HD13	3:B:643:MET:CE	2.48	0.43
3:A:622:ILE:HD12	4:A:803:CLR:H121	2.01	0.43
4:A:804:CLR:H17	4:A:804:CLR:H231	1.52	0.43
3:A:632:PHE:HB3	4:A:806:CLR:H122	2.01	0.42
4:A:804:CLR:H213	4:A:804:CLR:H161	1.77	0.42
3:A:542:ILE:HG23	4:A:812:CLR:H181	2.02	0.42
4:A:811:CLR:H232	4:A:811:CLR:H211	1.83	0.42
4:B:804:CLR:H222	4:B:804:CLR:H162	1.34	0.42
1:C:192:GLN:HE22	3:A:736:ASN:HD22	1.68	0.42
1:C:389:LEU:H	1:C:389:LEU:HD23	1.85	0.42
4:B:810:CLR:H162	4:B:810:CLR:H221	1.50	0.42
3:A:631:ARG:O	3:A:635:ALA:HB2	2.19	0.42
2:D:131:VAL:HG21	2:D:182:VAL:HG23	2.02	0.42
3:A:505:ARG:O	3:A:509:VAL:HG23	2.18	0.42
3:B:486:TRP:HE1	3:B:545:THR:CG2	2.33	0.42
3:B:505:ARG:HD2	3:B:521:MET:O	2.19	0.41
4:A:812:CLR:H213	4:A:812:CLR:H232	1.93	0.41
1:C:45:THR:HG23	1:C:54:PRO:HA	2.02	0.41
1:C:143:LEU:HD11	3:A:510:PHE:CD2	2.55	0.41
4:A:810:CLR:H231	4:A:810:CLR:H211	1.74	0.41
3:B:580:TYR:O	3:B:584:VAL:HG23	2.20	0.41
3:A:417:ARG:HG2	3:A:473:TYR:HE2	1.84	0.41
3:A:505:ARG:HD3	3:A:526:VAL:HG21	2.01	0.41
3:A:577:ARG:NH1	4:A:807:CLR:H192	2.32	0.41
4:A:805:CLR:H221	4:A:805:CLR:H162	1.27	0.41
3:B:651:THR:O	3:B:655:VAL:HG12	2.21	0.41
4:A:802:CLR:H221	4:A:802:CLR:H162	1.51	0.41
4:A:812:CLR:H162	4:A:812:CLR:H221	1.61	0.41
4:A:802:CLR:H232	4:A:802:CLR:H213	1.79	0.41
2:D:266:TYR:HA	2:D:273:GLU:HA	2.03	0.41
2:D:292:SER:OG	2:D:293:LEU:N	2.53	0.41
3:B:420:ILE:HD13	3:B:644:LEU:HB3	2.03	0.41
4:B:810:CLR:H211	4:B:810:CLR:H231	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:509:VAL:O	3:A:513:ARG:HG2	2.20	0.41
4:A:803:CLR:H262	4:A:803:CLR:H231	1.76	0.41
1:C:330:TRP:HH2	1:C:346:GLN:HG3	1.86	0.41
2:D:169:LEU:HD23	2:D:169:LEU:HA	1.90	0.41
3:A:442:ARG:HG3	3:A:452:LEU:HD21	2.03	0.41
1:C:192:GLN:NE2	3:A:736:ASN:HD22	2.18	0.41
2:D:344:SER:OG	2:D:345:TRP:N	2.54	0.41
3:B:452:LEU:HD12	3:B:452:LEU:HA	1.93	0.41
3:B:535:LEU:HD13	4:B:801:CLR:H242	2.03	0.41
3:A:492:PHE:HD2	6:A:814:PEE:H44	1.85	0.41
1:C:54:PRO:HG3	1:C:184:ILE:HD12	2.03	0.40
1:C:109:ARG:HD3	1:C:188:ILE:HG23	2.03	0.40
3:A:600:VAL:O	3:A:600:VAL:HG12	2.20	0.40
3:A:734:ILE:O	3:A:735:THR:OG1	2.32	0.40
3:B:657:VAL:HG11	4:B:809:CLR:H20	2.03	0.40
4:A:809:CLR:H162	4:A:810:CLR:H213	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	C	397/469 (85%)	376 (95%)	20 (5%)	1 (0%)	41 72
2	D	344/353 (98%)	326 (95%)	18 (5%)	0	100 100
3	A	292/781 (37%)	262 (90%)	27 (9%)	3 (1%)	15 46
3	B	280/781 (36%)	249 (89%)	28 (10%)	3 (1%)	14 44
All	All	1313/2384 (55%)	1213 (92%)	93 (7%)	7 (0%)	32 61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	638	LEU
3	A	407	PRO
3	A	566	ASP
3	A	638	LEU
3	B	414	LYS
3	B	556	ILE
1	C	299	PRO

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	C	365/425 (86%)	360 (99%)	5 (1%)	67	83
2	D	290/295 (98%)	290 (100%)	0	100	100
3	A	263/677 (39%)	261 (99%)	2 (1%)	81	91
3	B	253/677 (37%)	250 (99%)	3 (1%)	71	85
All	All	1171/2074 (56%)	1161 (99%)	10 (1%)	79	90

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	291	LEU
1	C	297	LEU
1	C	298	LEU
1	C	375	LYS
1	C	376	GLU
3	B	485	ARG
3	B	712	GLU
3	B	713	ASP
3	A	611	ARG
3	A	730	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	669	HIS
3	A	618	HIS
3	A	736	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
4	CLR	B	807	-	31,31,31	0.28	0	48,48,48	0.71	1 (2%)
4	CLR	A	806	-	31,31,31	0.31	0	48,48,48	0.89	3 (6%)
4	CLR	B	801	-	31,31,31	0.44	0	48,48,48	1.91	11 (22%)
4	CLR	A	802	-	31,31,31	0.29	0	48,48,48	0.45	0
4	CLR	A	808	-	31,31,31	0.28	0	48,48,48	0.85	0
5	EIJ	A	813	-	55,55,61	1.58	11 (20%)	65,67,73	1.46	3 (4%)
4	CLR	A	807	-	31,31,31	0.31	0	48,48,48	0.59	0
4	CLR	B	810	-	31,31,31	0.29	0	48,48,48	0.58	0
4	CLR	A	801	-	31,31,31	0.33	0	48,48,48	0.47	0
4	CLR	B	804	-	31,31,31	0.29	0	48,48,48	0.46	0
4	CLR	A	812	-	31,31,31	0.29	0	48,48,48	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	CLR	B	802	-	31,31,31	0.30	0	48,48,48	0.46	0
4	CLR	A	810	-	31,31,31	0.34	0	48,48,48	0.79	0
6	PEE	A	814	-	48,48,50	1.71	11 (22%)	51,53,55	1.57	4 (7%)
4	CLR	A	803	-	31,31,31	0.34	0	48,48,48	1.25	5 (10%)
4	CLR	A	805	-	31,31,31	0.33	0	48,48,48	0.60	0
4	CLR	B	806	-	31,31,31	0.28	0	48,48,48	0.48	0
4	CLR	A	811	-	31,31,31	0.28	0	48,48,48	0.69	1 (2%)
4	CLR	B	805	-	31,31,31	0.28	0	48,48,48	0.43	0
4	CLR	A	809	-	31,31,31	0.33	0	48,48,48	0.50	0
4	CLR	A	804	-	31,31,31	0.32	0	48,48,48	0.61	0
4	CLR	B	803	-	31,31,31	0.27	0	48,48,48	0.69	1 (2%)
4	CLR	B	808	-	31,31,31	0.28	0	48,48,48	0.49	0
4	CLR	B	809	-	31,31,31	0.29	0	48,48,48	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	B	807	-	-	8/10/68/68	0/4/4/4
4	CLR	A	806	-	-	2/10/68/68	0/4/4/4
4	CLR	B	801	-	2/2/10/11	6/10/68/68	0/4/4/4
4	CLR	A	802	-	-	10/10/68/68	0/4/4/4
4	CLR	A	808	-	-	10/10/68/68	0/4/4/4
5	EIJ	A	813	-	2/2/10/18	19/50/74/80	0/1/1/1
4	CLR	A	807	-	-	5/10/68/68	0/4/4/4
4	CLR	B	810	-	-	10/10/68/68	0/4/4/4
4	CLR	A	801	-	-	7/10/68/68	0/4/4/4
4	CLR	B	804	-	-	8/10/68/68	0/4/4/4
4	CLR	A	812	-	-	9/10/68/68	0/4/4/4
4	CLR	B	802	-	-	9/10/68/68	0/4/4/4
4	CLR	A	810	-	-	4/10/68/68	0/4/4/4
6	PEE	A	814	-	1/1/4/8	27/52/52/54	-
4	CLR	A	803	-	1/1/10/11	7/10/68/68	0/4/4/4
4	CLR	A	805	-	-	9/10/68/68	0/4/4/4
4	CLR	B	806	-	-	6/10/68/68	0/4/4/4
4	CLR	A	811	-	-	9/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CLR	B	805	-	-	7/10/68/68	0/4/4/4
4	CLR	A	809	-	1/1/10/11	7/10/68/68	0/4/4/4
4	CLR	A	804	-	1/1/10/11	8/10/68/68	0/4/4/4
4	CLR	B	803	-	-	8/10/68/68	0/4/4/4
4	CLR	B	808	-	-	9/10/68/68	0/4/4/4
4	CLR	B	809	-	-	7/10/68/68	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	814	PEE	O3-C30	4.44	1.46	1.33
5	A	813	EIJ	C10-C09	4.03	1.55	1.31
5	A	813	EIJ	C13-C12	3.93	1.54	1.31
5	A	813	EIJ	C07-C06	3.89	1.54	1.31
6	A	814	PEE	O2-C10	3.89	1.45	1.34
6	A	814	PEE	C39-C38	3.68	1.53	1.31
6	A	814	PEE	C24-C25	-3.43	1.32	1.51
5	A	813	EIJ	C04-C03	3.22	1.53	1.29
5	A	813	EIJ	O19-C17	3.19	1.43	1.34
5	A	813	EIJ	O22-C23	2.95	1.41	1.33
6	A	814	PEE	C21-C22	-2.89	1.35	1.51
6	A	814	PEE	C31-C30	2.84	1.59	1.50
5	A	813	EIJ	P42-O45	2.77	1.67	1.60
6	A	814	PEE	O2-C2	-2.65	1.40	1.46
6	A	814	PEE	C3-C2	2.59	1.58	1.50
5	A	813	EIJ	O19-C20	-2.55	1.40	1.46
5	A	813	EIJ	C05-C06	-2.47	1.33	1.51
6	A	814	PEE	P-O3P	2.37	1.68	1.59
6	A	814	PEE	C11-C10	2.37	1.57	1.50
5	A	813	EIJ	C08-C09	-2.35	1.34	1.51
6	A	814	PEE	P-O4P	2.17	1.68	1.59
5	A	813	EIJ	P42-O41	2.05	1.67	1.59

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	813	EIJ	C09-C08-C07	8.47	153.73	112.02
6	A	814	PEE	C21-C22-C23	7.55	152.74	114.42
4	B	801	CLR	C7-C8-C9	6.21	117.23	109.71
4	B	801	CLR	C10-C9-C8	4.62	119.66	112.73
4	B	801	CLR	C13-C17-C20	4.56	126.63	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	814	PEE	O2-C10-C11	4.34	120.85	111.50
5	A	813	EIJ	O19-C17-C16	4.21	120.58	111.50
4	B	801	CLR	C12-C11-C9	3.84	119.77	113.11
4	A	803	CLR	C7-C8-C9	3.72	114.22	109.71
6	A	814	PEE	C20-C19-C18	3.59	152.27	124.73
4	A	803	CLR	C14-C8-C9	3.32	113.53	109.09
4	B	801	CLR	C14-C8-C9	3.22	113.40	109.09
4	A	803	CLR	C13-C14-C8	2.99	118.81	114.38
4	B	801	CLR	C18-C13-C17	-2.98	106.16	111.71
5	A	813	EIJ	O22-C23-C25	2.79	120.66	111.91
6	A	814	PEE	O3-C30-C31	2.79	120.65	111.91
4	B	801	CLR	C16-C17-C13	2.77	107.17	103.84
4	B	801	CLR	C13-C14-C8	2.51	118.10	114.38
4	B	801	CLR	C9-C10-C5	2.49	113.55	109.65
4	A	803	CLR	C7-C6-C5	-2.47	120.51	125.06
4	B	803	CLR	C16-C17-C13	-2.36	101.00	103.84
4	A	803	CLR	C1-C2-C3	2.34	113.48	110.47
4	A	806	CLR	C13-C14-C8	2.32	117.81	114.38
4	B	801	CLR	C16-C15-C14	-2.31	100.56	105.13
4	A	806	CLR	C15-C14-C13	-2.22	101.17	103.84
4	B	801	CLR	C11-C12-C13	2.14	116.44	112.78
4	A	806	CLR	C13-C17-C20	2.09	122.77	119.49
4	A	811	CLR	C16-C17-C13	-2.09	101.33	103.84
4	B	807	CLR	C16-C17-C13	-2.02	101.41	103.84

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	801	CLR	C8
4	B	801	CLR	C17
4	A	803	CLR	C8
4	A	804	CLR	C17
4	A	809	CLR	C17
5	A	813	EIJ	C47
5	A	813	EIJ	C55
6	A	814	PEE	C2

All (211) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	804	CLR	C13-C17-C20-C21
4	B	804	CLR	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
4	B	804	CLR	C16-C17-C20-C22
4	B	808	CLR	C13-C17-C20-C21
4	B	808	CLR	C16-C17-C20-C21
4	B	809	CLR	C13-C17-C20-C21
4	B	810	CLR	C13-C17-C20-C21
4	B	810	CLR	C16-C17-C20-C22
4	A	803	CLR	C13-C17-C20-C21
4	A	804	CLR	C16-C17-C20-C21
4	A	804	CLR	C17-C20-C22-C23
4	A	805	CLR	C13-C17-C20-C21
4	A	805	CLR	C16-C17-C20-C22
4	A	807	CLR	C13-C17-C20-C21
4	A	807	CLR	C16-C17-C20-C22
4	A	809	CLR	C13-C17-C20-C21
4	A	809	CLR	C13-C17-C20-C22
4	A	809	CLR	C16-C17-C20-C21
5	A	813	EIJ	C16-C17-O19-C20
6	A	814	PEE	O3P-C1-C2-O2
6	A	814	PEE	C4-O4P-P-O1P
4	B	802	CLR	C21-C20-C22-C23
4	A	808	CLR	C21-C20-C22-C23
4	B	804	CLR	C16-C17-C20-C21
4	B	809	CLR	C16-C17-C20-C21
4	B	810	CLR	C16-C17-C20-C21
4	A	805	CLR	C16-C17-C20-C21
4	A	807	CLR	C16-C17-C20-C21
4	A	808	CLR	C16-C17-C20-C21
4	B	803	CLR	C13-C17-C20-C21
4	A	802	CLR	C13-C17-C20-C21
4	A	804	CLR	C13-C17-C20-C21
4	A	808	CLR	C13-C17-C20-C21
4	A	812	CLR	C13-C17-C20-C21
4	B	808	CLR	C16-C17-C20-C22
4	A	804	CLR	C16-C17-C20-C22
4	A	809	CLR	C16-C17-C20-C22
4	B	808	CLR	C13-C17-C20-C22
4	B	810	CLR	C13-C17-C20-C22
4	A	805	CLR	C13-C17-C20-C22
4	A	807	CLR	C13-C17-C20-C22
5	A	813	EIJ	O18-C17-O19-C20
4	B	805	CLR	C21-C20-C22-C23
4	B	810	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
4	A	802	CLR	C21-C20-C22-C23
4	A	805	CLR	C21-C20-C22-C23
4	A	812	CLR	C21-C20-C22-C23
5	A	813	EIJ	O24-C23-O22-C21
4	B	803	CLR	C16-C17-C20-C21
4	B	806	CLR	C16-C17-C20-C21
4	B	807	CLR	C16-C17-C20-C21
4	A	802	CLR	C16-C17-C20-C21
4	A	803	CLR	C16-C17-C20-C21
4	A	812	CLR	C16-C17-C20-C21
4	B	806	CLR	C13-C17-C20-C21
4	B	807	CLR	C13-C17-C20-C21
4	B	809	CLR	C16-C17-C20-C22
4	A	803	CLR	C16-C17-C20-C22
4	A	812	CLR	C16-C17-C20-C22
4	B	803	CLR	C13-C17-C20-C22
4	B	805	CLR	C13-C17-C20-C22
4	B	806	CLR	C13-C17-C20-C22
4	B	809	CLR	C13-C17-C20-C22
4	A	802	CLR	C13-C17-C20-C22
4	A	803	CLR	C13-C17-C20-C22
4	A	804	CLR	C13-C17-C20-C22
4	A	808	CLR	C13-C17-C20-C22
4	A	812	CLR	C13-C17-C20-C22
6	A	814	PEE	C20-C21-C22-C23
5	A	813	EIJ	C25-C23-O22-C21
5	A	813	EIJ	C11-C12-C13-C14
4	B	809	CLR	C21-C20-C22-C23
4	B	805	CLR	C13-C17-C20-C21
4	B	806	CLR	C16-C17-C20-C22
4	B	807	CLR	C16-C17-C20-C22
4	A	802	CLR	C16-C17-C20-C22
4	A	808	CLR	C16-C17-C20-C22
4	B	807	CLR	C13-C17-C20-C22
4	A	805	CLR	C17-C20-C22-C23
4	B	805	CLR	C16-C17-C20-C21
4	B	805	CLR	C17-C20-C22-C23
4	A	812	CLR	C17-C20-C22-C23
5	A	813	EIJ	C20-C40-O41-P42
4	A	801	CLR	C21-C20-C22-C23
6	A	814	PEE	C22-C23-C24-C25
4	B	803	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
4	A	801	CLR	C17-C20-C22-C23
4	A	806	CLR	C21-C20-C22-C23
4	A	810	CLR	C21-C20-C22-C23
4	A	809	CLR	C17-C20-C22-C23
5	A	813	EIJ	C30-C31-C32-C33
4	B	807	CLR	C21-C20-C22-C23
4	B	801	CLR	C13-C17-C20-C22
6	A	814	PEE	C10-C11-C12-C13
4	B	802	CLR	C17-C20-C22-C23
4	B	804	CLR	C17-C20-C22-C23
4	A	802	CLR	C17-C20-C22-C23
4	A	804	CLR	C21-C20-C22-C23
4	B	806	CLR	C22-C23-C24-C25
4	B	808	CLR	C22-C23-C24-C25
4	A	811	CLR	C20-C22-C23-C24
4	B	810	CLR	C22-C23-C24-C25
4	A	809	CLR	C20-C22-C23-C24
4	B	805	CLR	C16-C17-C20-C22
6	A	814	PEE	C30-C31-C32-C33
4	A	807	CLR	C22-C23-C24-C25
6	A	814	PEE	C11-C10-O2-C2
4	B	802	CLR	C20-C22-C23-C24
4	A	806	CLR	C20-C22-C23-C24
4	B	807	CLR	C22-C23-C24-C25
4	A	808	CLR	C22-C23-C24-C25
4	A	808	CLR	C20-C22-C23-C24
4	B	802	CLR	C13-C17-C20-C22
6	A	814	PEE	O4-C10-O2-C2
4	A	803	CLR	C22-C23-C24-C25
4	B	801	CLR	C22-C23-C24-C25
4	A	801	CLR	C22-C23-C24-C25
6	A	814	PEE	C13-C14-C15-C16
5	A	813	EIJ	C29-C30-C31-C32
5	A	813	EIJ	C26-C27-C28-C29
4	B	804	CLR	C21-C20-C22-C23
4	A	804	CLR	C23-C24-C25-C27
4	A	808	CLR	C23-C24-C25-C26
6	A	814	PEE	C14-C15-C16-C17
4	A	811	CLR	C13-C17-C20-C22
4	B	802	CLR	C23-C24-C25-C26
5	A	813	EIJ	C28-C29-C30-C31
6	A	814	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
4	A	803	CLR	C23-C24-C25-C27
4	A	804	CLR	C23-C24-C25-C26
4	A	811	CLR	C23-C24-C25-C26
4	B	806	CLR	C20-C22-C23-C24
4	A	802	CLR	C23-C24-C25-C26
4	A	811	CLR	C13-C17-C20-C21
5	A	813	EIJ	C27-C28-C29-C30
4	B	810	CLR	C20-C22-C23-C24
4	A	805	CLR	C22-C23-C24-C25
4	A	812	CLR	C20-C22-C23-C24
6	A	814	PEE	C24-C25-C26-C27
6	A	814	PEE	C12-C13-C14-C15
4	A	802	CLR	C20-C22-C23-C24
4	B	802	CLR	C13-C17-C20-C21
4	B	807	CLR	C23-C24-C25-C26
4	A	808	CLR	C23-C24-C25-C27
4	B	802	CLR	C23-C24-C25-C27
4	B	801	CLR	C20-C22-C23-C24
5	A	813	EIJ	C40-O41-P42-O45
6	A	814	PEE	C4-O4P-P-O3P
4	A	810	CLR	C20-C22-C23-C24
4	A	811	CLR	C22-C23-C24-C25
6	A	814	PEE	O3P-C1-C2-C3
4	B	803	CLR	C17-C20-C22-C23
4	B	802	CLR	C16-C17-C20-C21
4	B	802	CLR	C16-C17-C20-C22
4	A	811	CLR	C16-C17-C20-C21
6	A	814	PEE	C39-C40-C41-C42
5	A	813	EIJ	C33-C34-C35-C36
4	B	801	CLR	C23-C24-C25-C27
4	B	808	CLR	C23-C24-C25-C26
4	B	803	CLR	C21-C20-C22-C23
4	A	809	CLR	C22-C23-C24-C25
4	B	810	CLR	C17-C20-C22-C23
4	A	811	CLR	C16-C17-C20-C22
5	A	813	EIJ	C34-C35-C36-C37
4	B	803	CLR	C20-C22-C23-C24
4	B	804	CLR	C22-C23-C24-C25
4	A	801	CLR	C20-C22-C23-C24
6	A	814	PEE	C21-C22-C23-C24
6	A	814	PEE	C1-C2-C3-O3
4	B	809	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
5	A	813	EIJ	C04-C05-C06-C07
5	A	813	EIJ	C06-C07-C08-C09
5	A	813	EIJ	C07-C08-C09-C10
5	A	813	EIJ	C09-C10-C11-C12
4	A	811	CLR	C23-C24-C25-C27
4	B	808	CLR	C17-C20-C22-C23
4	B	807	CLR	C23-C24-C25-C27
4	A	803	CLR	C23-C24-C25-C26
4	B	810	CLR	C23-C24-C25-C27
6	A	814	PEE	C32-C33-C34-C35
4	B	801	CLR	C17-C20-C22-C23
4	A	802	CLR	C22-C23-C24-C25
4	A	802	CLR	C23-C24-C25-C27
4	B	804	CLR	C20-C22-C23-C24
4	B	801	CLR	C23-C24-C25-C26
4	B	808	CLR	C23-C24-C25-C27
4	B	805	CLR	C23-C24-C25-C26
5	A	813	EIJ	C40-O41-P42-O44
6	A	814	PEE	C4-O4P-P-O2P
4	A	810	CLR	C23-C24-C25-C26
6	A	814	PEE	C11-C12-C13-C14
4	A	805	CLR	C23-C24-C25-C26
4	B	803	CLR	C22-C23-C24-C25
4	B	810	CLR	C23-C24-C25-C26
4	B	808	CLR	C21-C20-C22-C23
4	A	810	CLR	C23-C24-C25-C27
4	A	801	CLR	C16-C17-C20-C22
4	A	808	CLR	C17-C20-C22-C23
4	A	812	CLR	C23-C24-C25-C26
6	A	814	PEE	C38-C39-C40-C41
4	A	805	CLR	C23-C24-C25-C27
6	A	814	PEE	C40-C41-C42-C43
4	A	801	CLR	C13-C17-C20-C21
6	A	814	PEE	O2-C2-C3-O3
6	A	814	PEE	C16-C17-C18-C19
4	A	801	CLR	C16-C17-C20-C21
4	A	811	CLR	C21-C20-C22-C23
4	B	809	CLR	C23-C24-C25-C26
6	A	814	PEE	C36-C37-C38-C39
4	A	812	CLR	C23-C24-C25-C27
6	A	814	PEE	C1-O3P-P-O1P

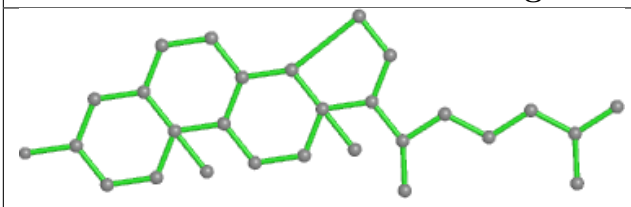
There are no ring outliers.

23 monomers are involved in 78 short contacts:

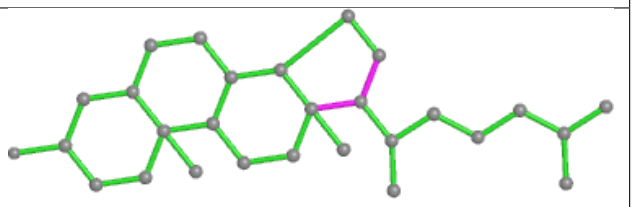
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	807	CLR	1	0
4	A	806	CLR	3	0
4	B	801	CLR	4	0
4	A	802	CLR	5	0
4	A	808	CLR	5	0
5	A	813	EIJ	1	0
4	A	807	CLR	2	0
4	B	810	CLR	3	0
4	A	801	CLR	1	0
4	B	804	CLR	2	0
4	A	812	CLR	20	0
4	A	810	CLR	3	0
6	A	814	PEE	2	0
4	A	803	CLR	5	0
4	A	805	CLR	2	0
4	B	806	CLR	1	0
4	A	811	CLR	14	0
4	B	805	CLR	1	0
4	A	809	CLR	3	0
4	A	804	CLR	4	0
4	B	803	CLR	11	0
4	B	808	CLR	4	0
4	B	809	CLR	2	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.

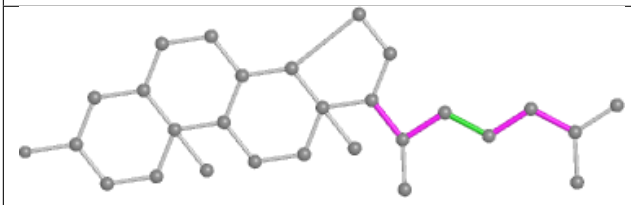
Ligand CLR B 807



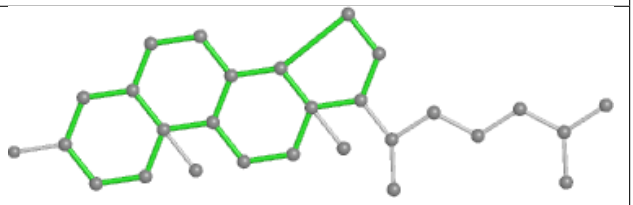
Bond lengths



Bond angles

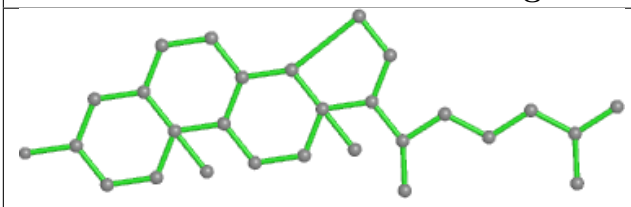


Torsions

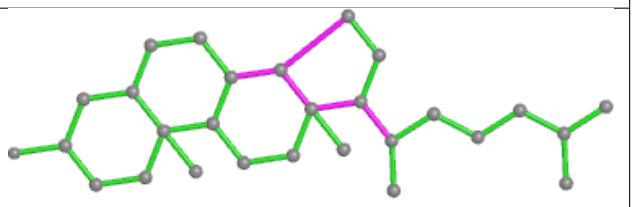


Rings

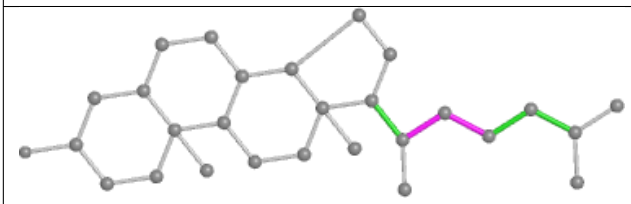
Ligand CLR A 806



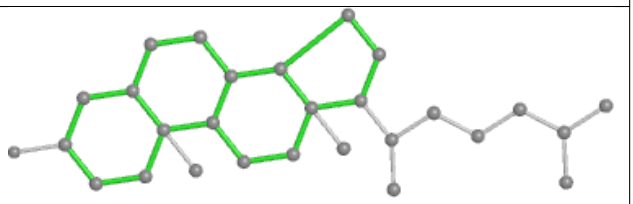
Bond lengths



Bond angles

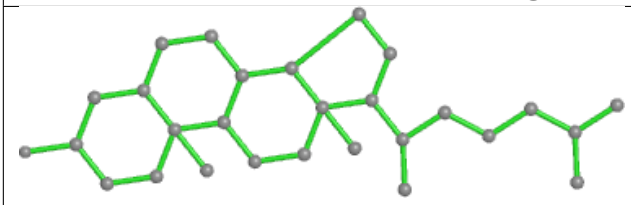


Torsions

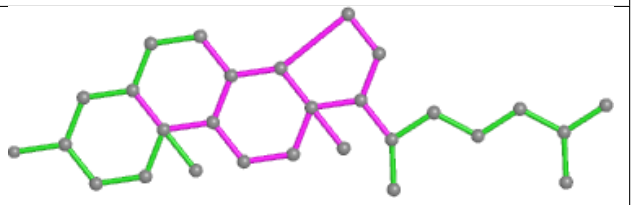


Rings

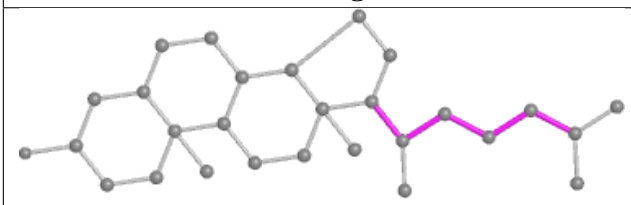
Ligand CLR B 801



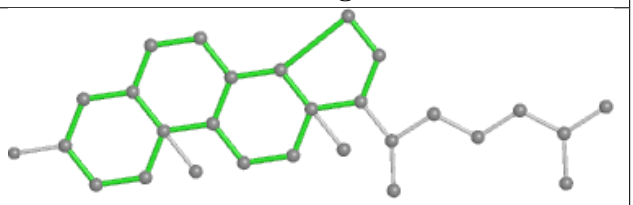
Bond lengths



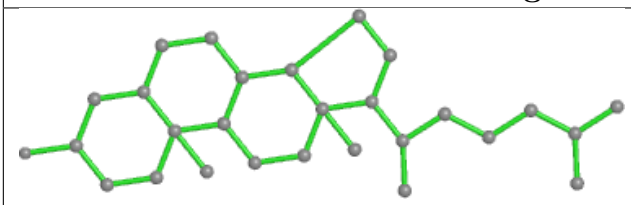
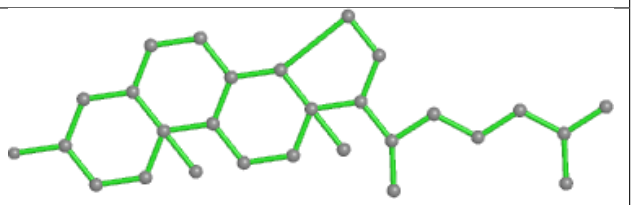
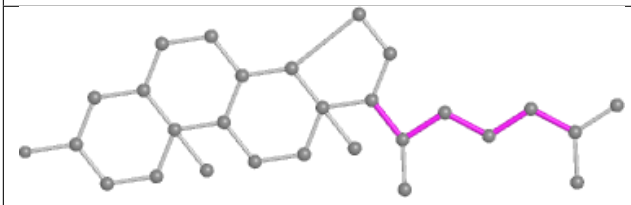
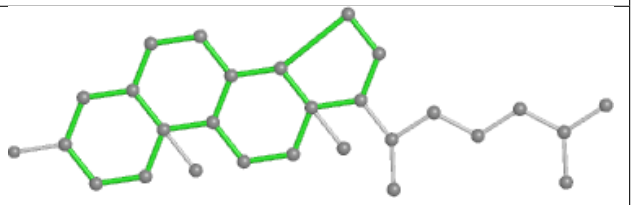
Bond angles



Torsions



Rings

Ligand CLR A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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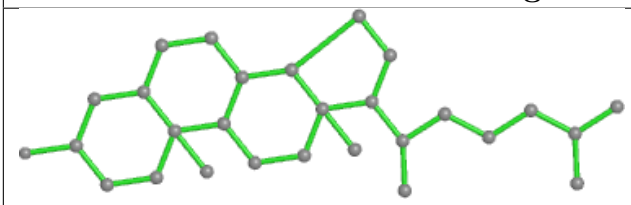
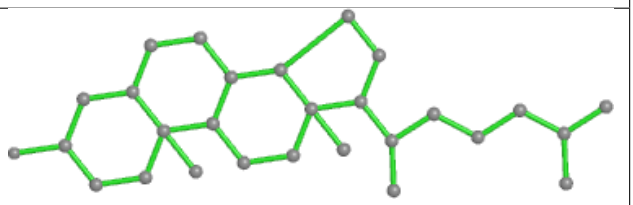
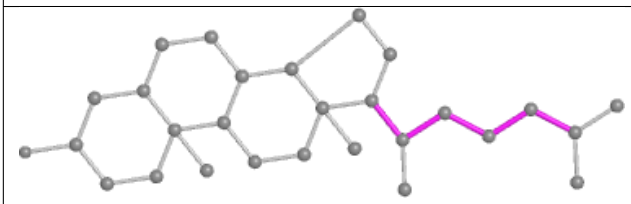
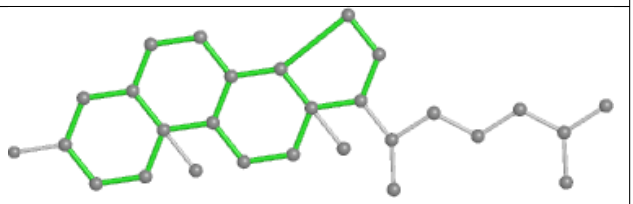
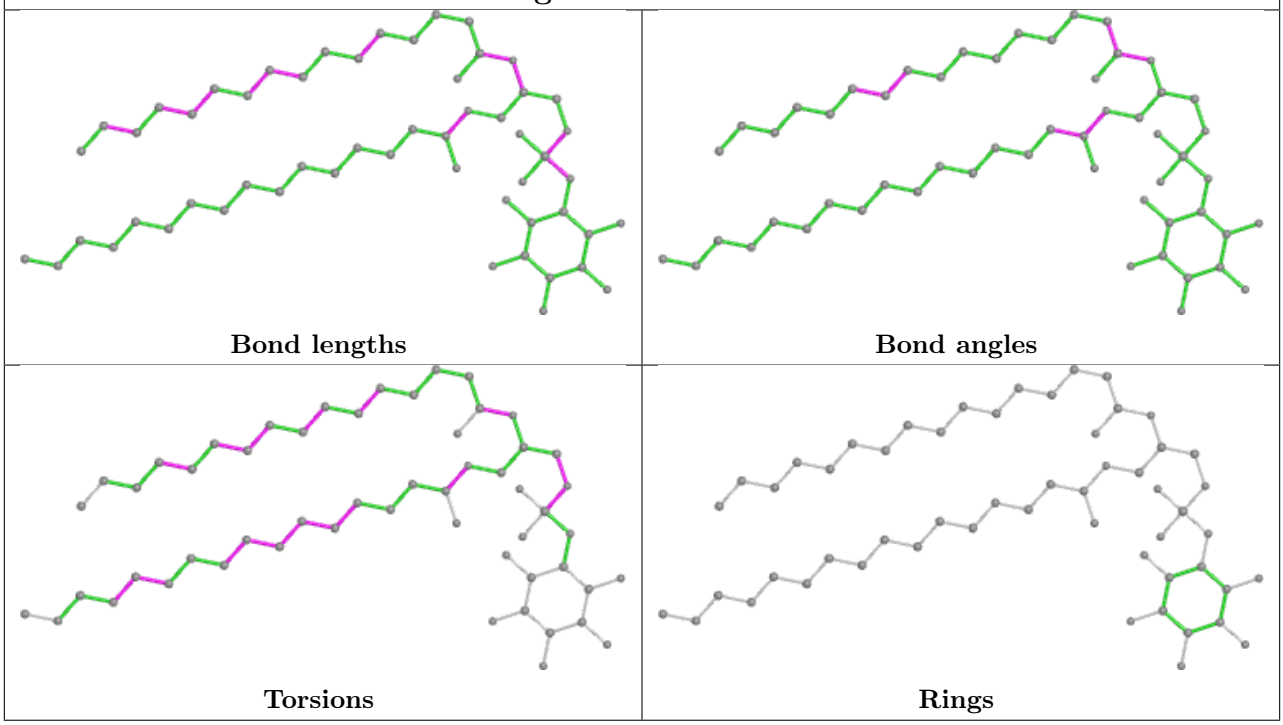
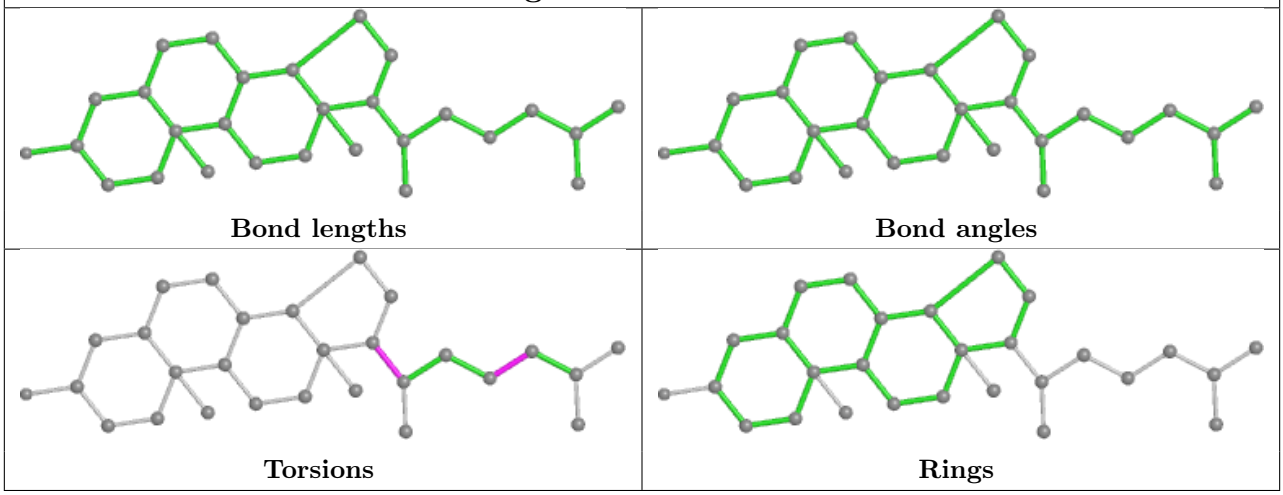
 Bond lengths	 Bond angles
 Torsions	 Rings

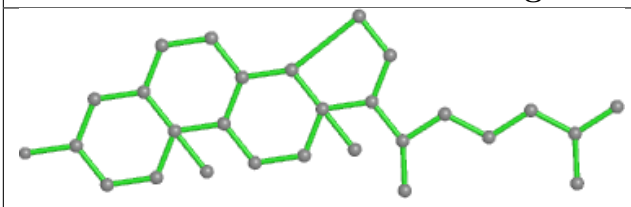
Ligand EIJ A 813



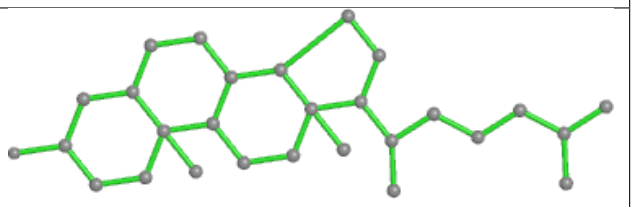
Ligand CLR A 807



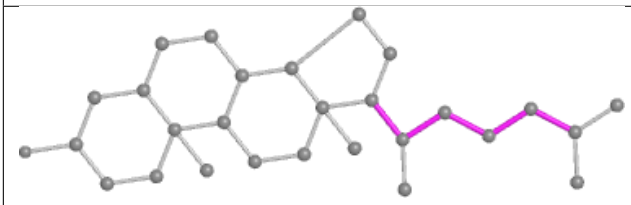
Ligand CLR B 810



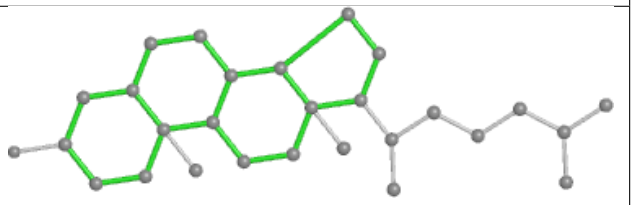
Bond lengths



Bond angles

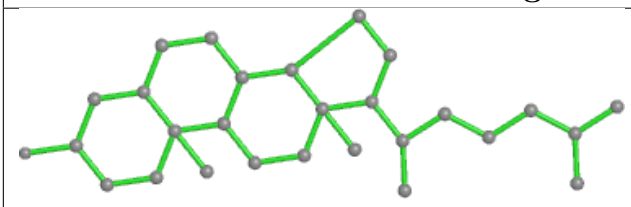


Torsions



Rings

Ligand CLR A 801



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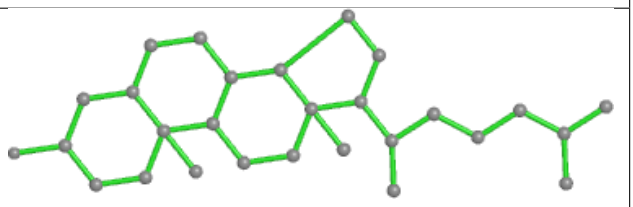
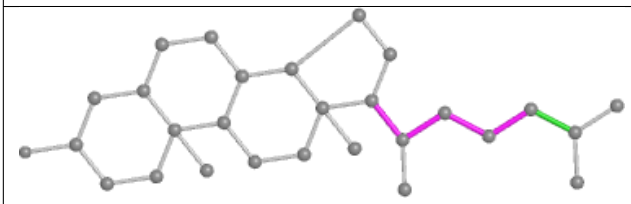


Bond angles



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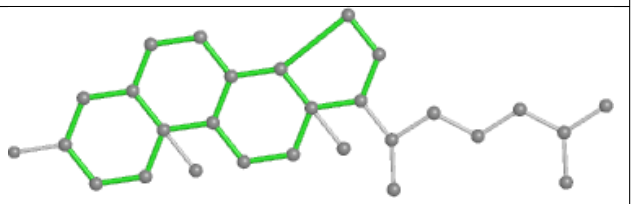
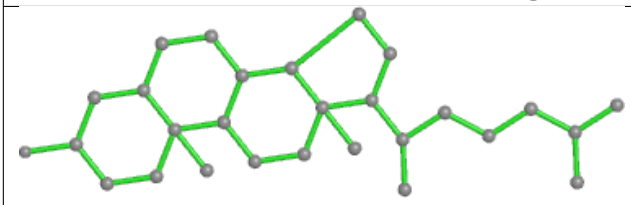


Rings

Ligand CLR B 804



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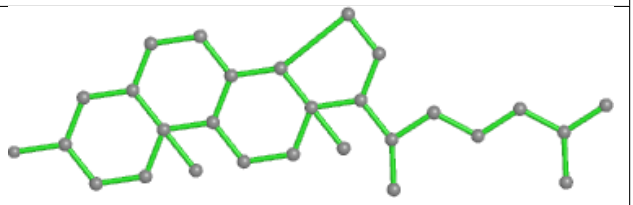
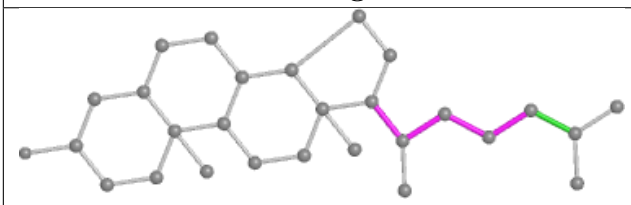


Bond angles



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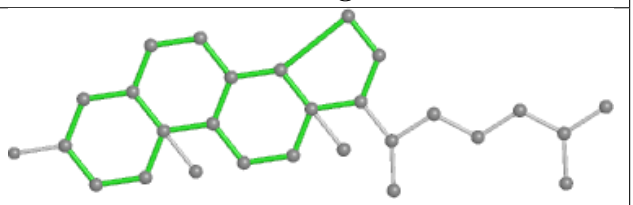
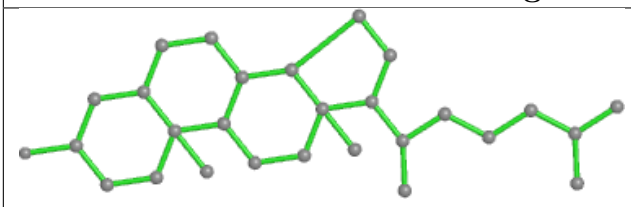


Rings

Ligand CLR A 812



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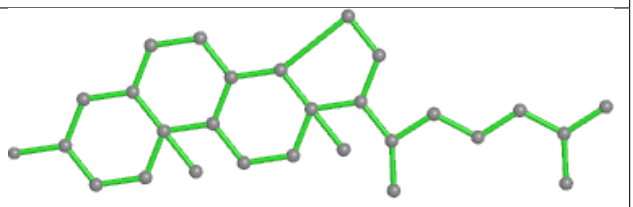
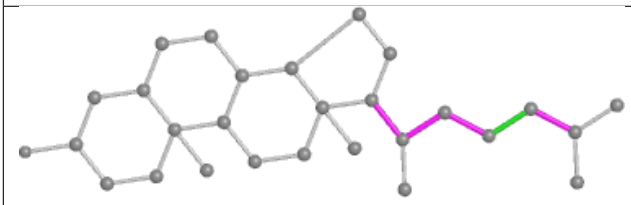


Bond angles



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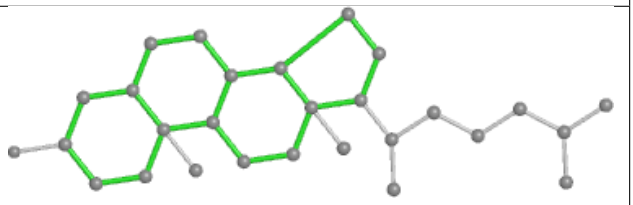
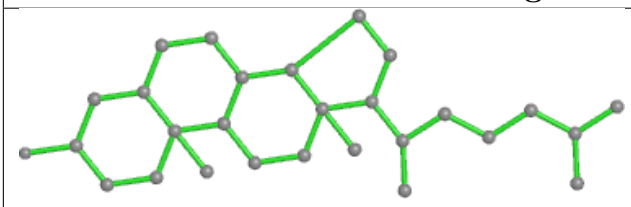


Rings

Ligand CLR B 802



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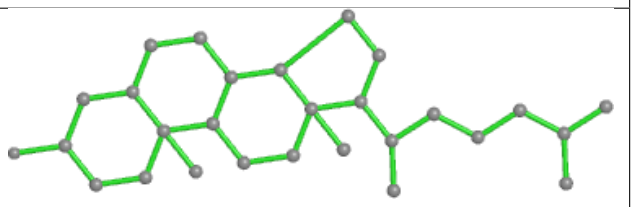
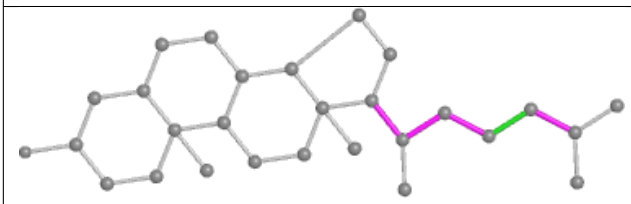
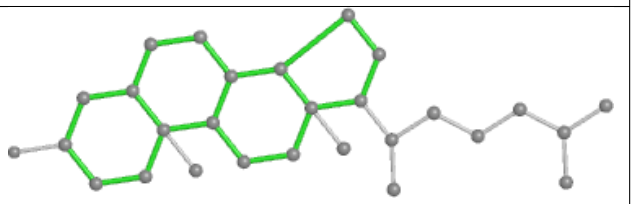


Bond angles

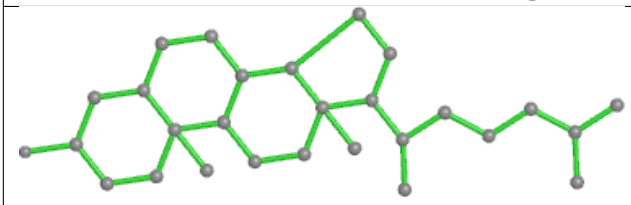


Torsions



Rings

Ligand CLR A 810



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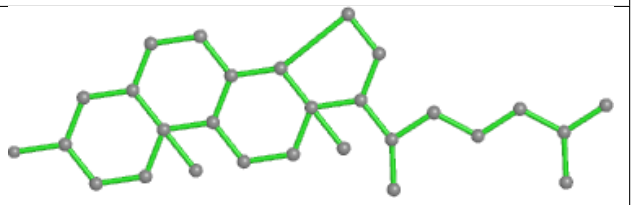
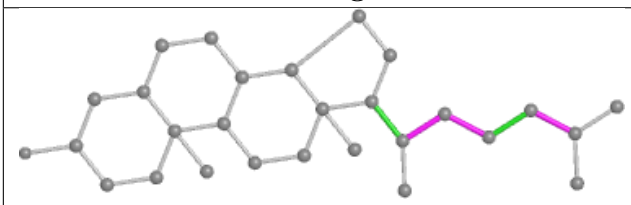
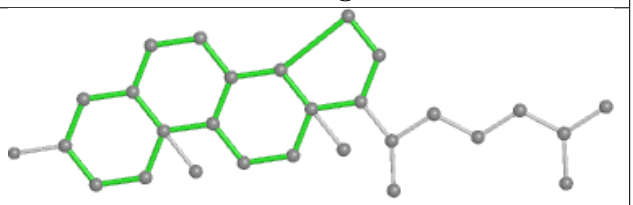


Bond angles

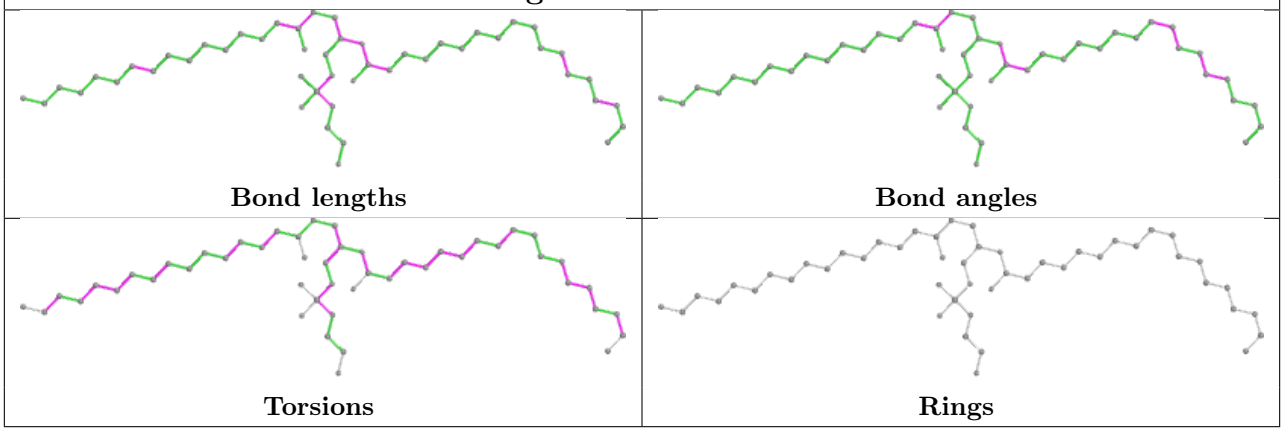


Torsions

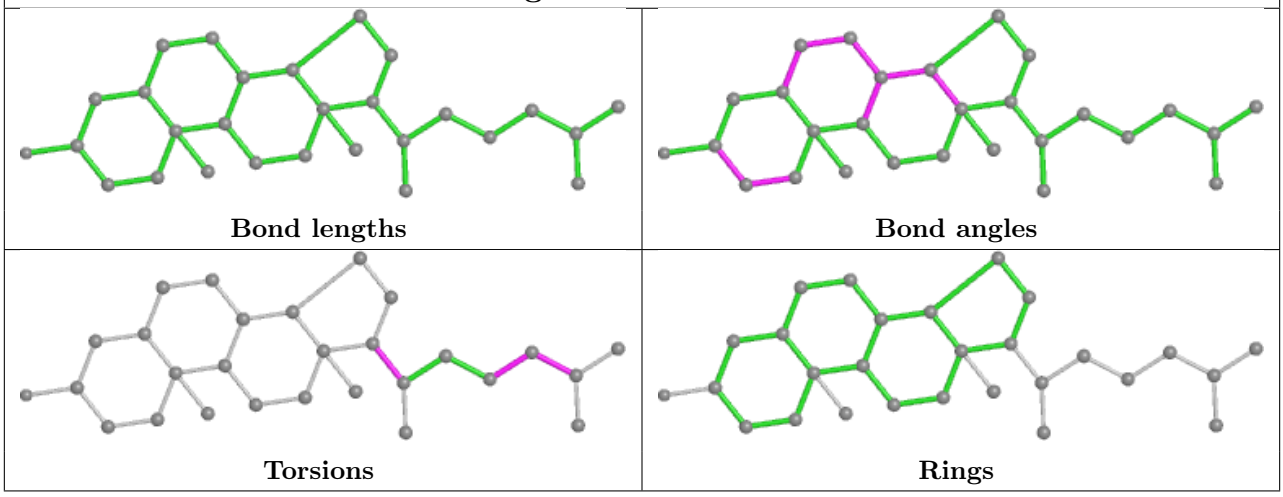


Rings

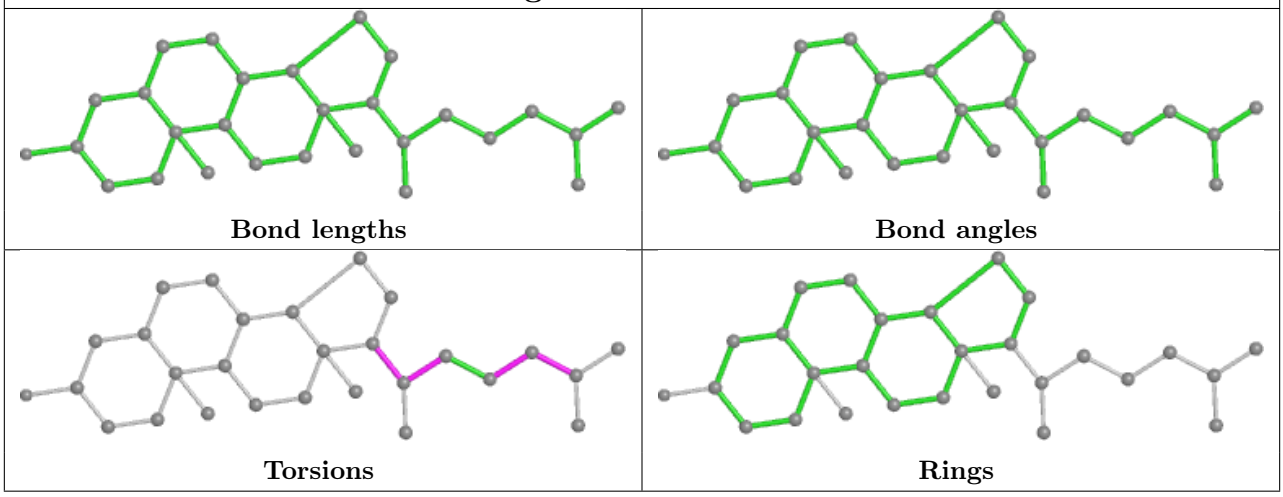
Ligand PEE A 814



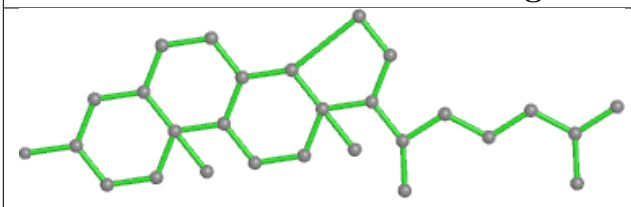
Ligand CLR A 803



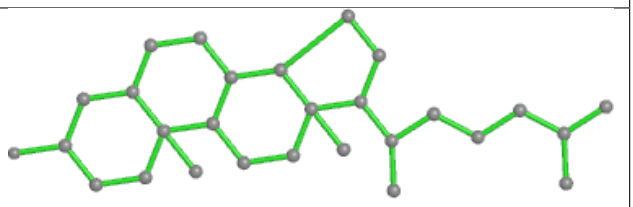
Ligand CLR A 805



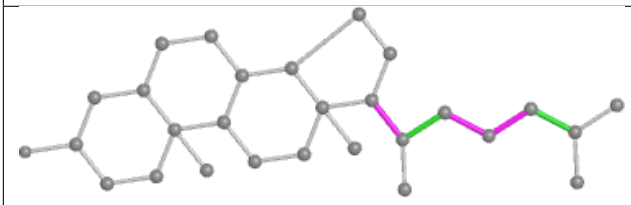
Ligand CLR B 806



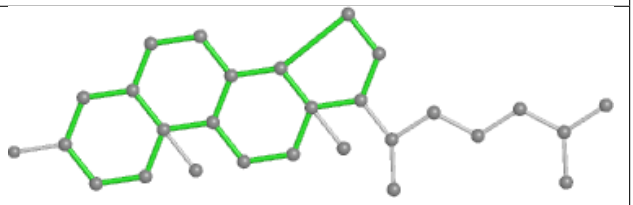
Bond lengths



Bond angles

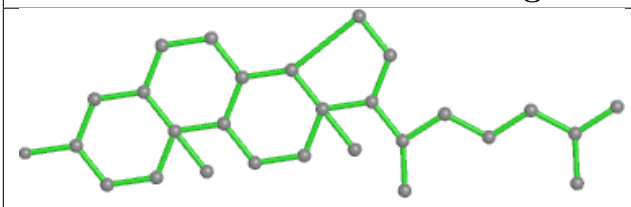


Torsions

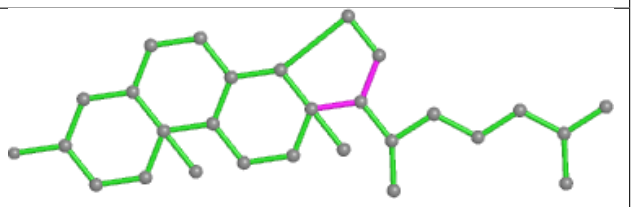


Rings

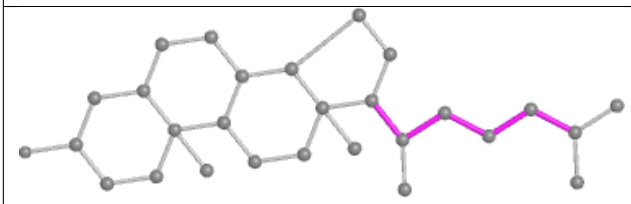
Ligand CLR A 811



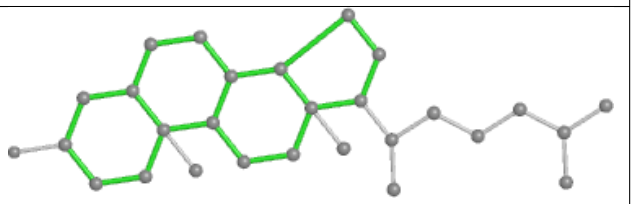
Bond lengths



Bond angles

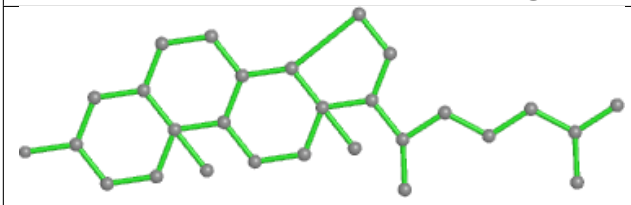


Torsions

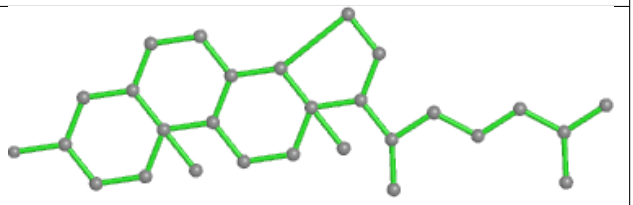


Rings

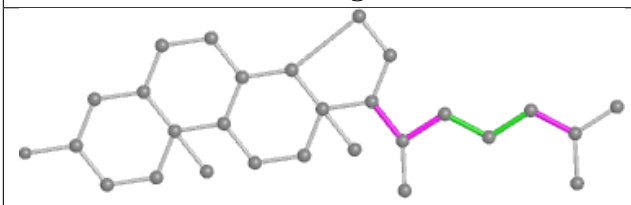
Ligand CLR B 805



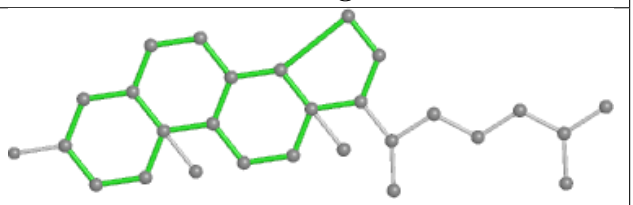
Bond lengths



Bond angles

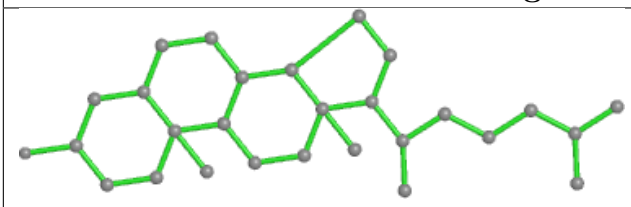


Torsions

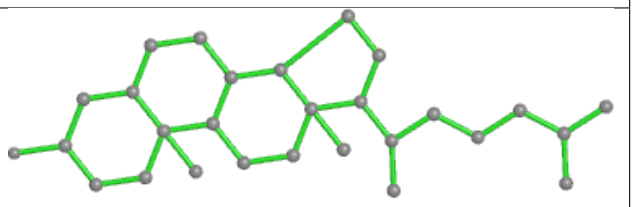


Rings

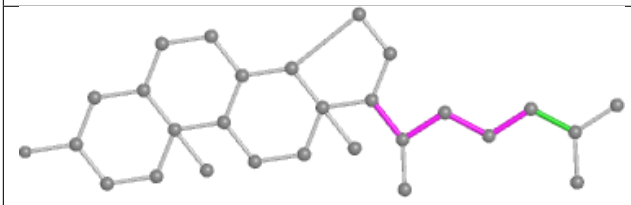
Ligand CLR A 809



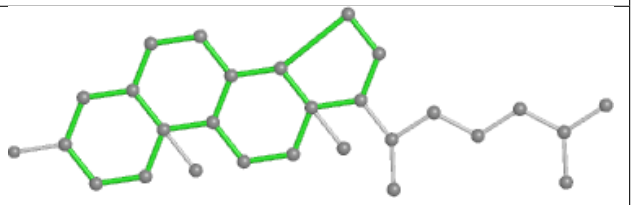
Bond lengths



Bond angles

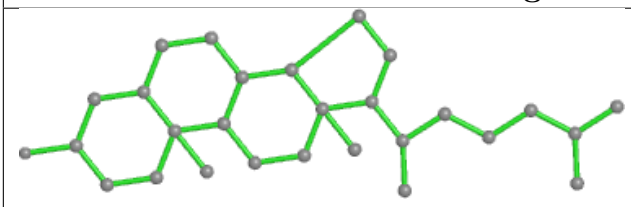


Torsions

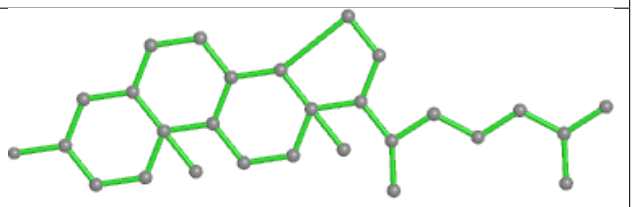


Rings

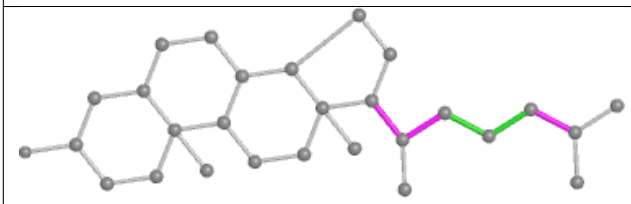
Ligand CLR A 804



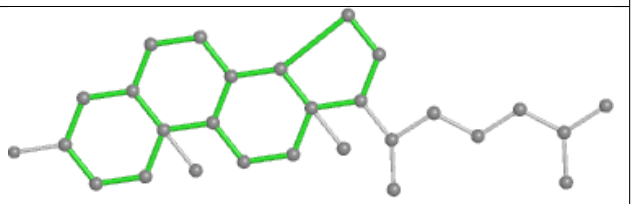
Bond lengths



Bond angles

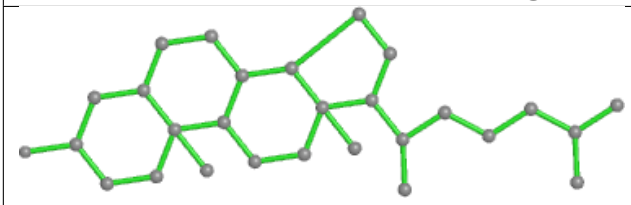


Torsions

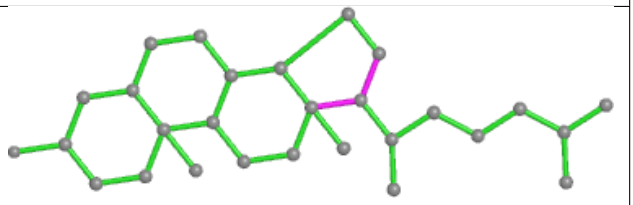


Rings

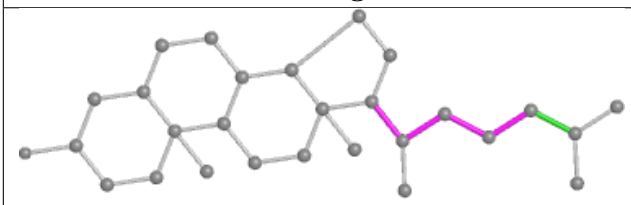
Ligand CLR B 803



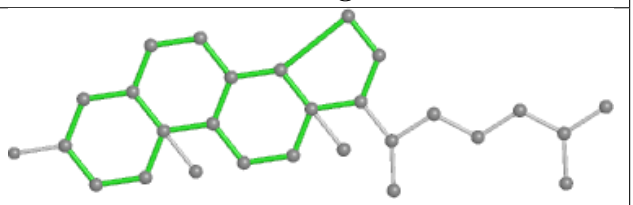
Bond lengths



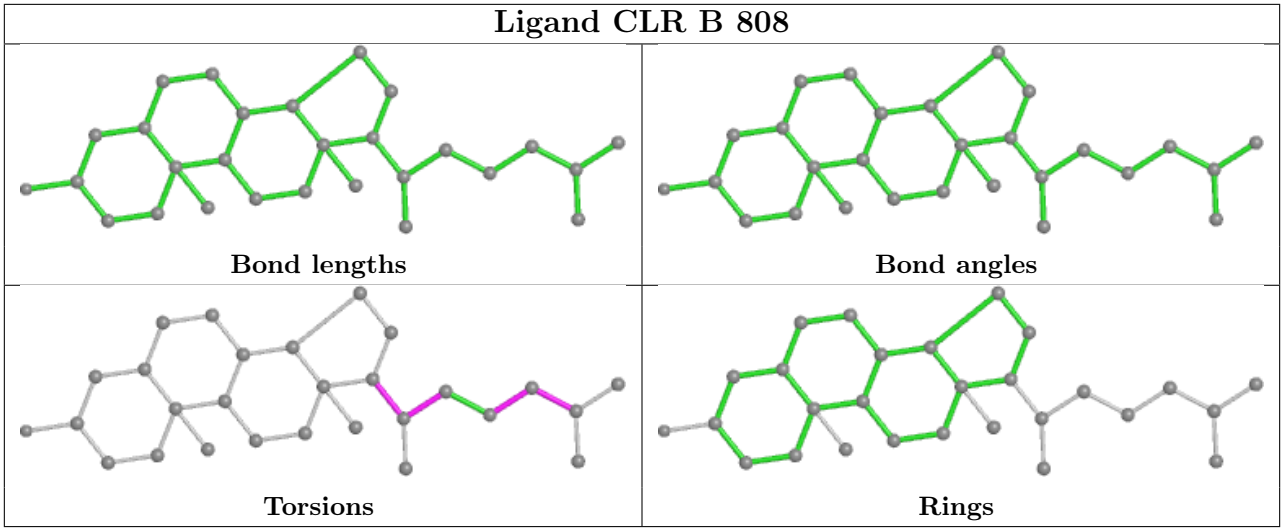
Bond angles

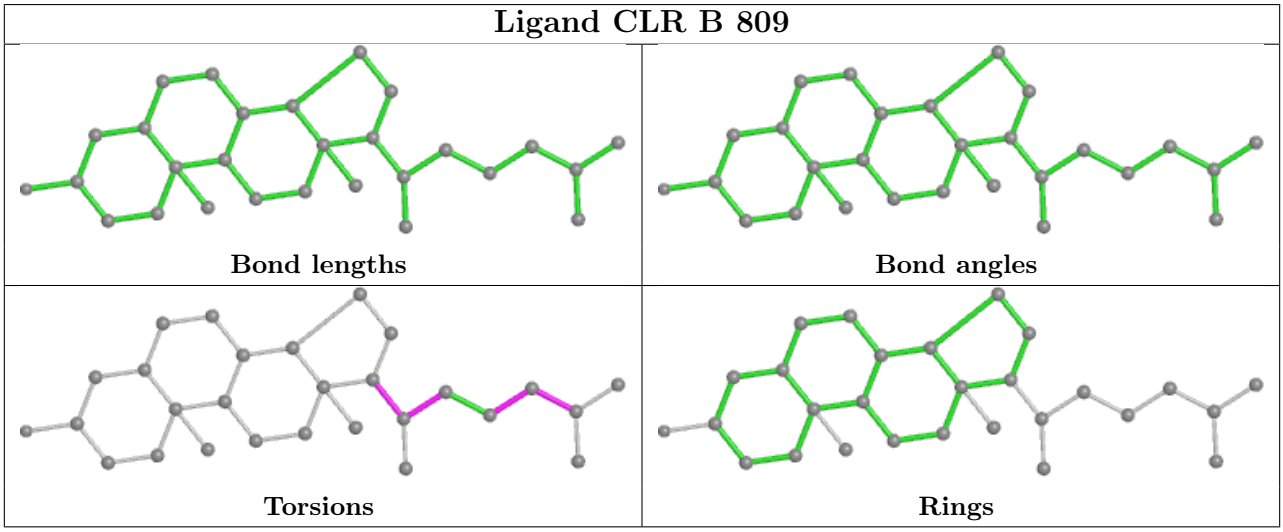


Torsions



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.

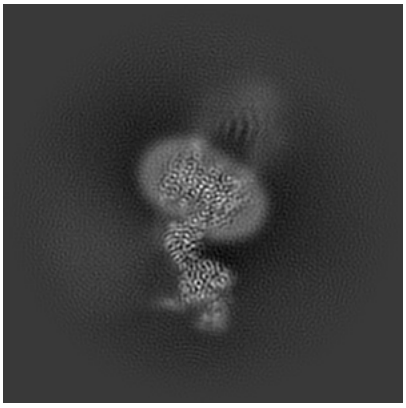
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-25126. These allow visual inspection of the internal detail of the map and identification of artifacts.

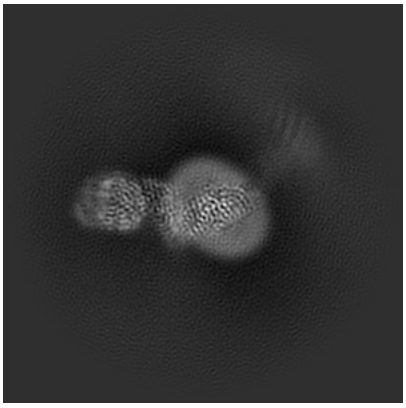
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

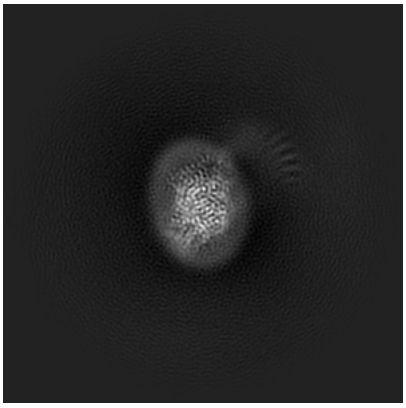
6.1.1 Primary map



X



Y

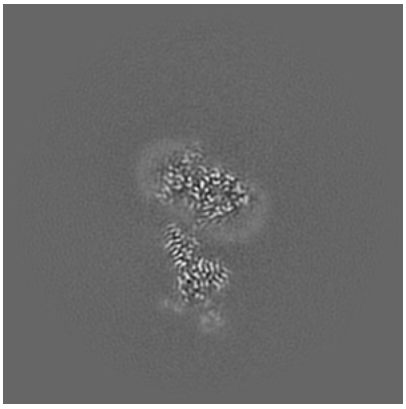


Z

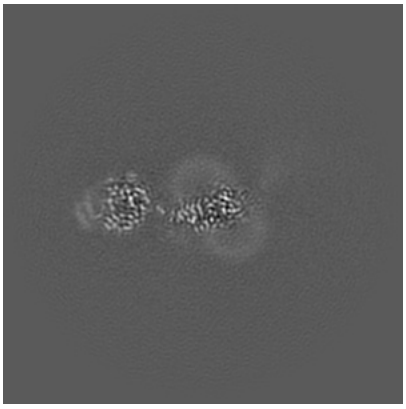
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

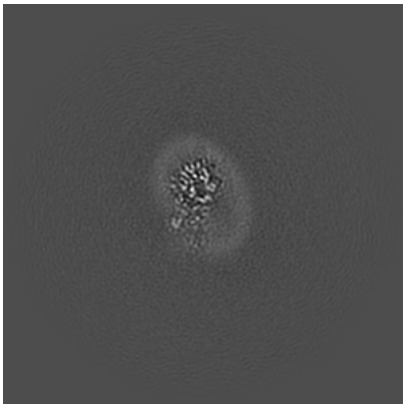
6.2.1 Primary map



X Index: 200



Y Index: 200

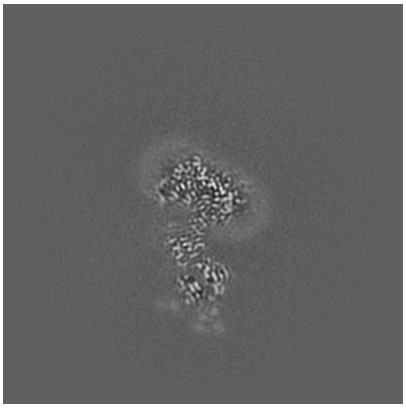


Z Index: 200

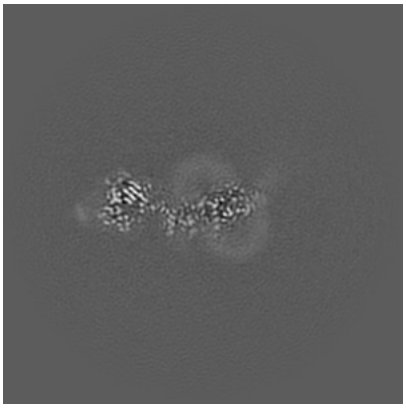
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

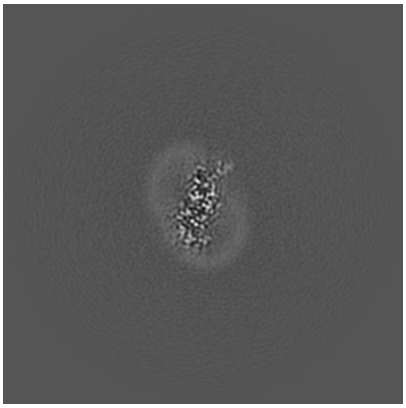
6.3.1 Primary map



X Index: 193



Y Index: 195



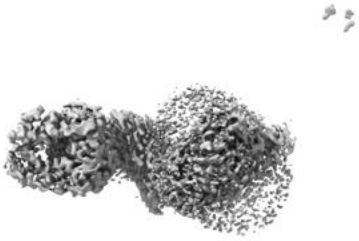
Z Index: 218

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

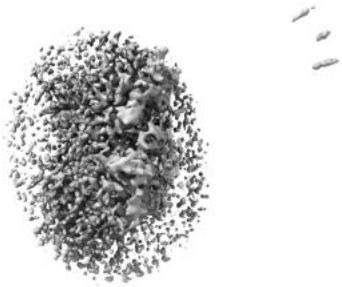
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

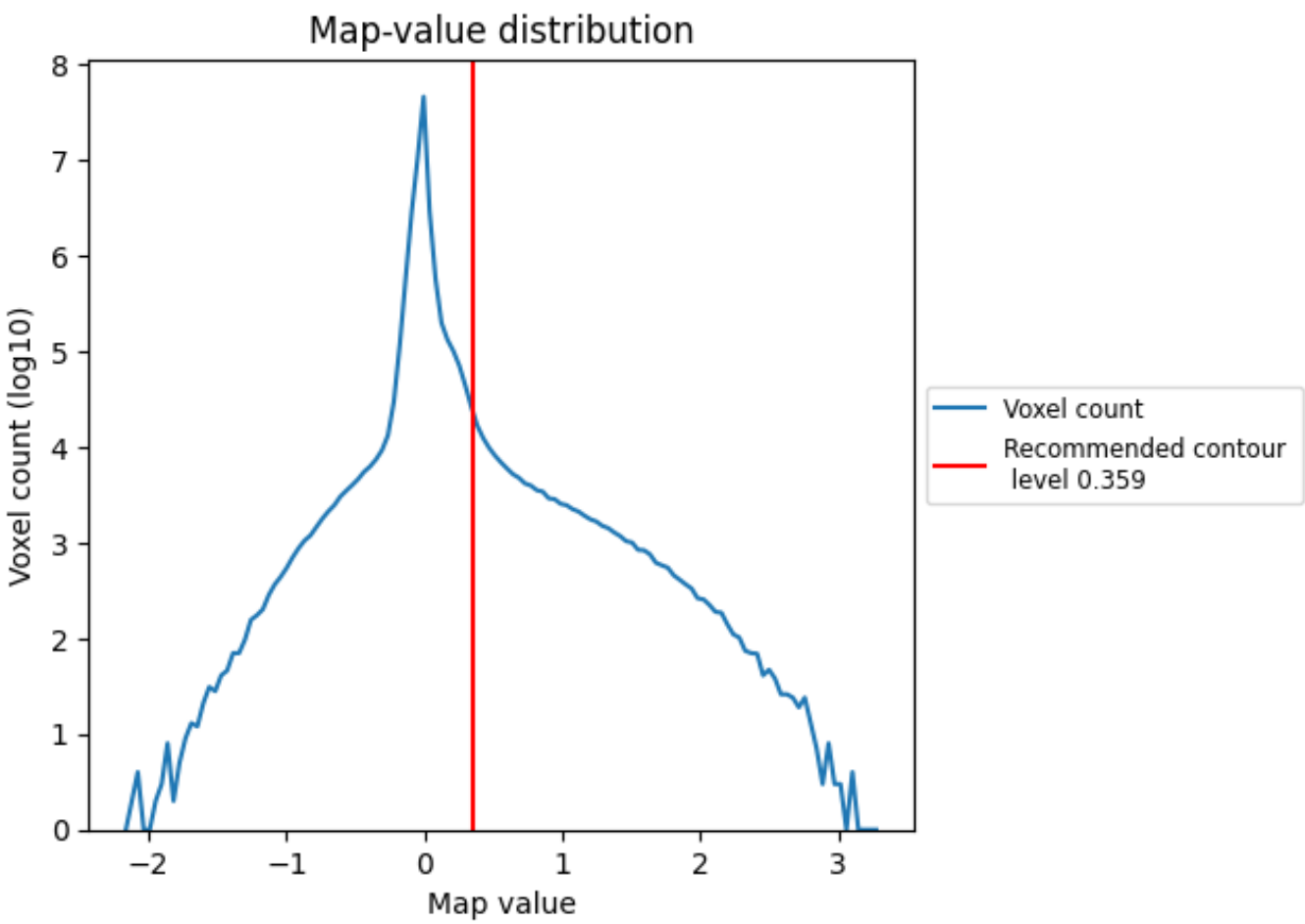
6.5 Mask visualisation (i)

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

7 Map analysis (i)

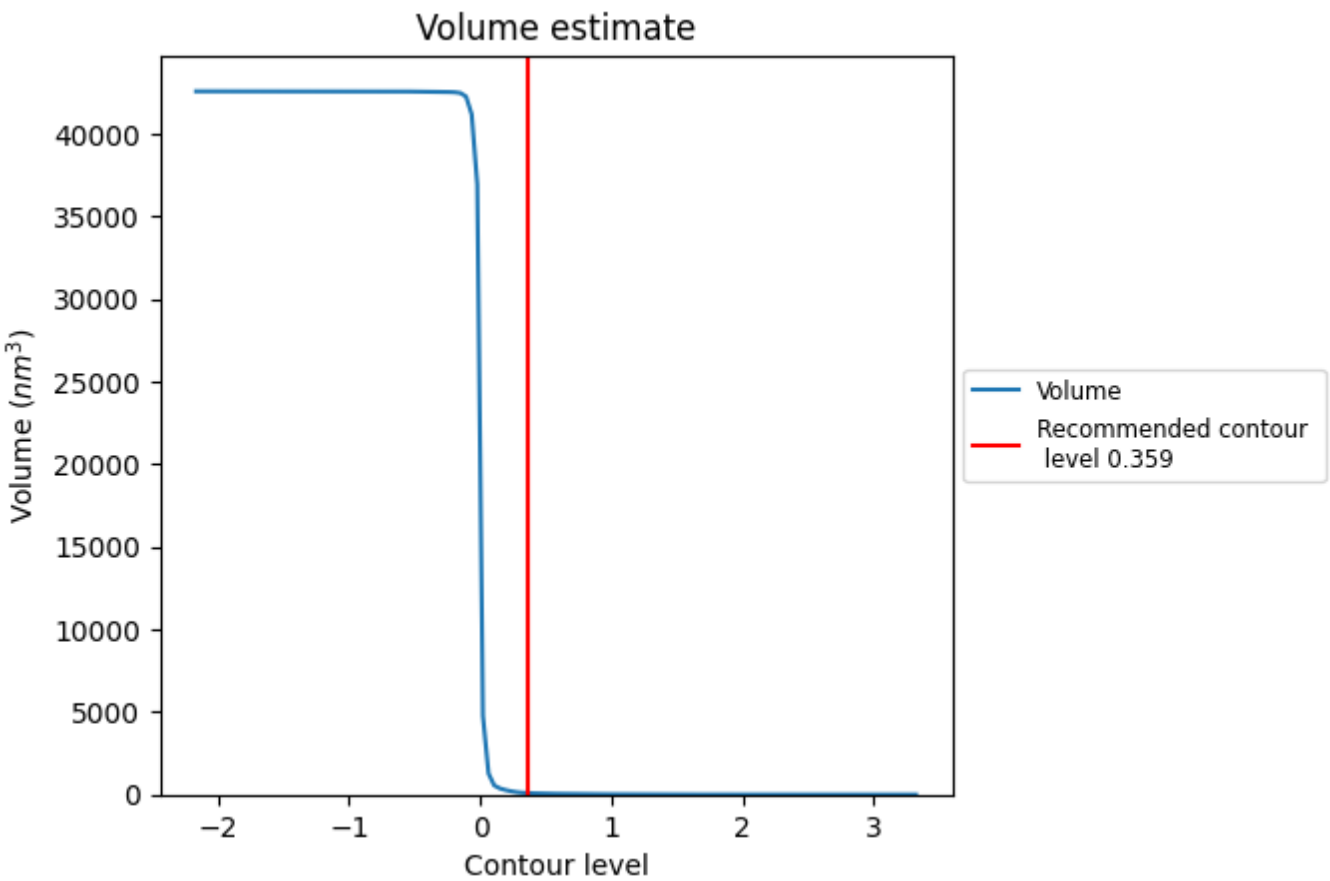
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

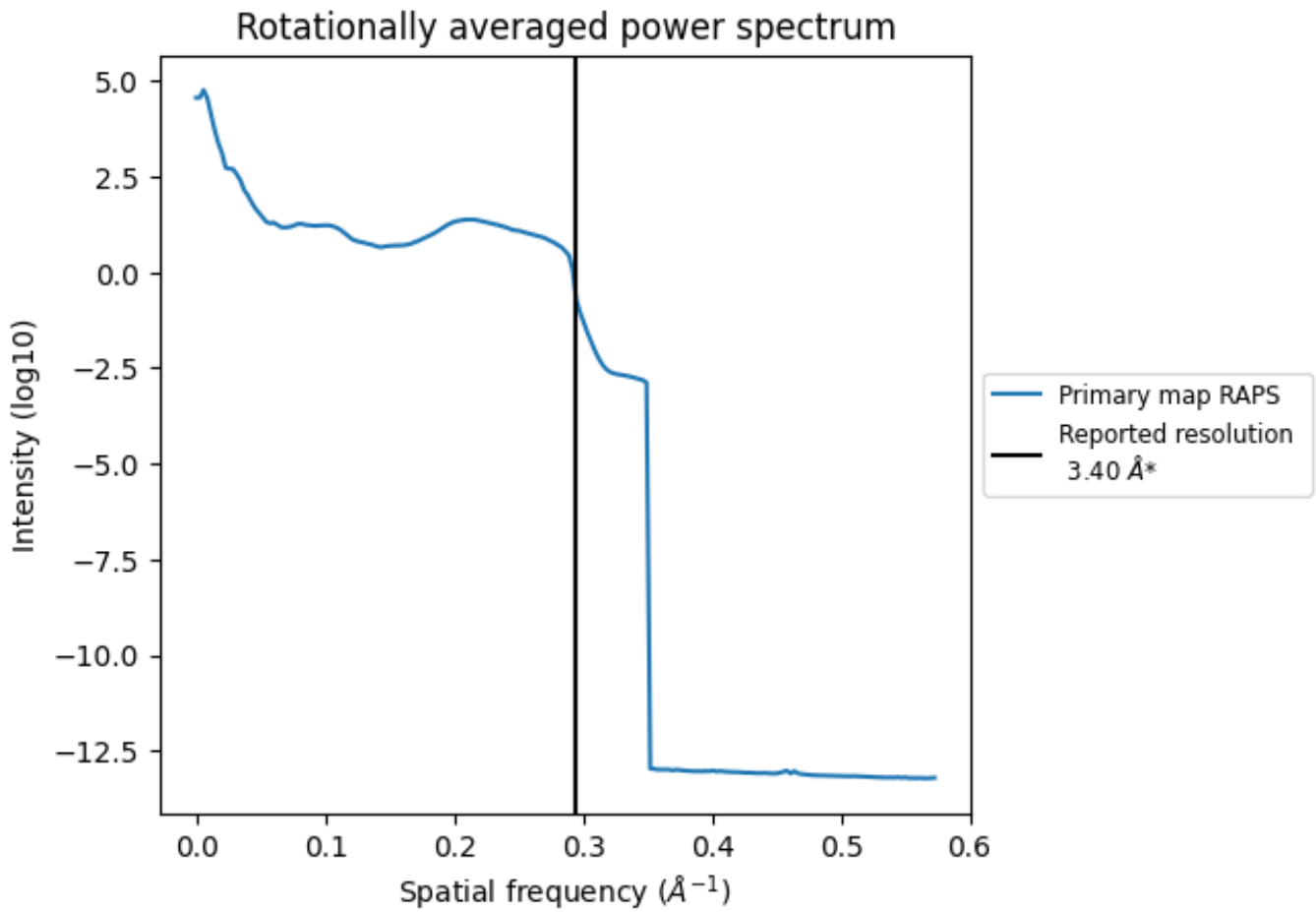
7.2 Volume estimate (i)



The volume at the recommended contour level is 90 nm^3; this corresponds to an approximate mass of 81 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 0.294 Å^{-1}

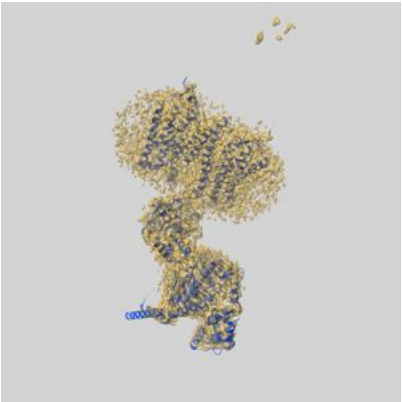
8 Fourier-Shell correlation (i)

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

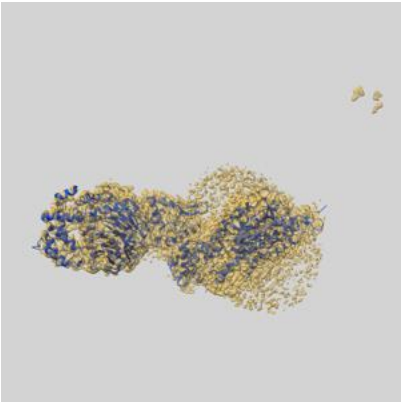
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-25126 and PDB model 7SHF. Per-residue inclusion information can be found in section 3 on page 8.

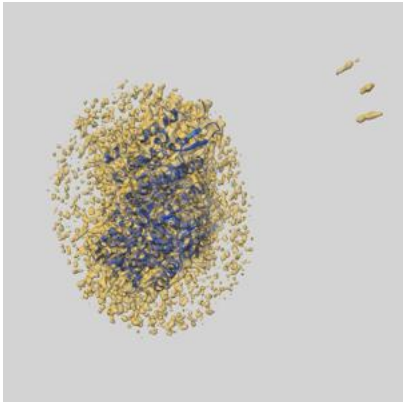
9.1 Map-model overlay (i)



X



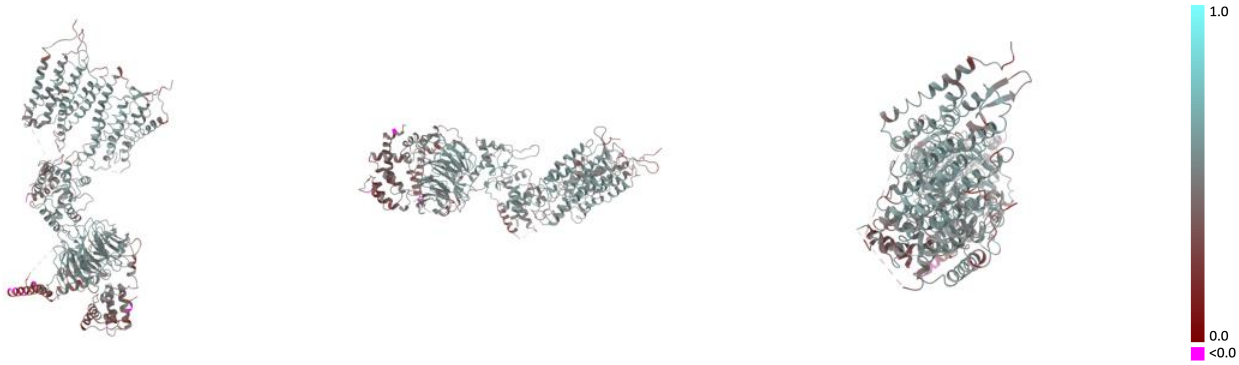
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.359 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.

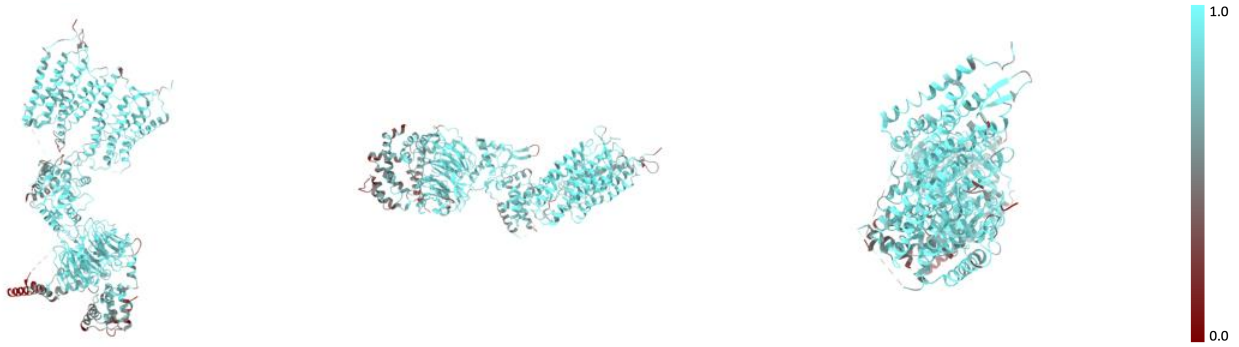
9.2 Q-score mapped to coordinate model (i)



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.

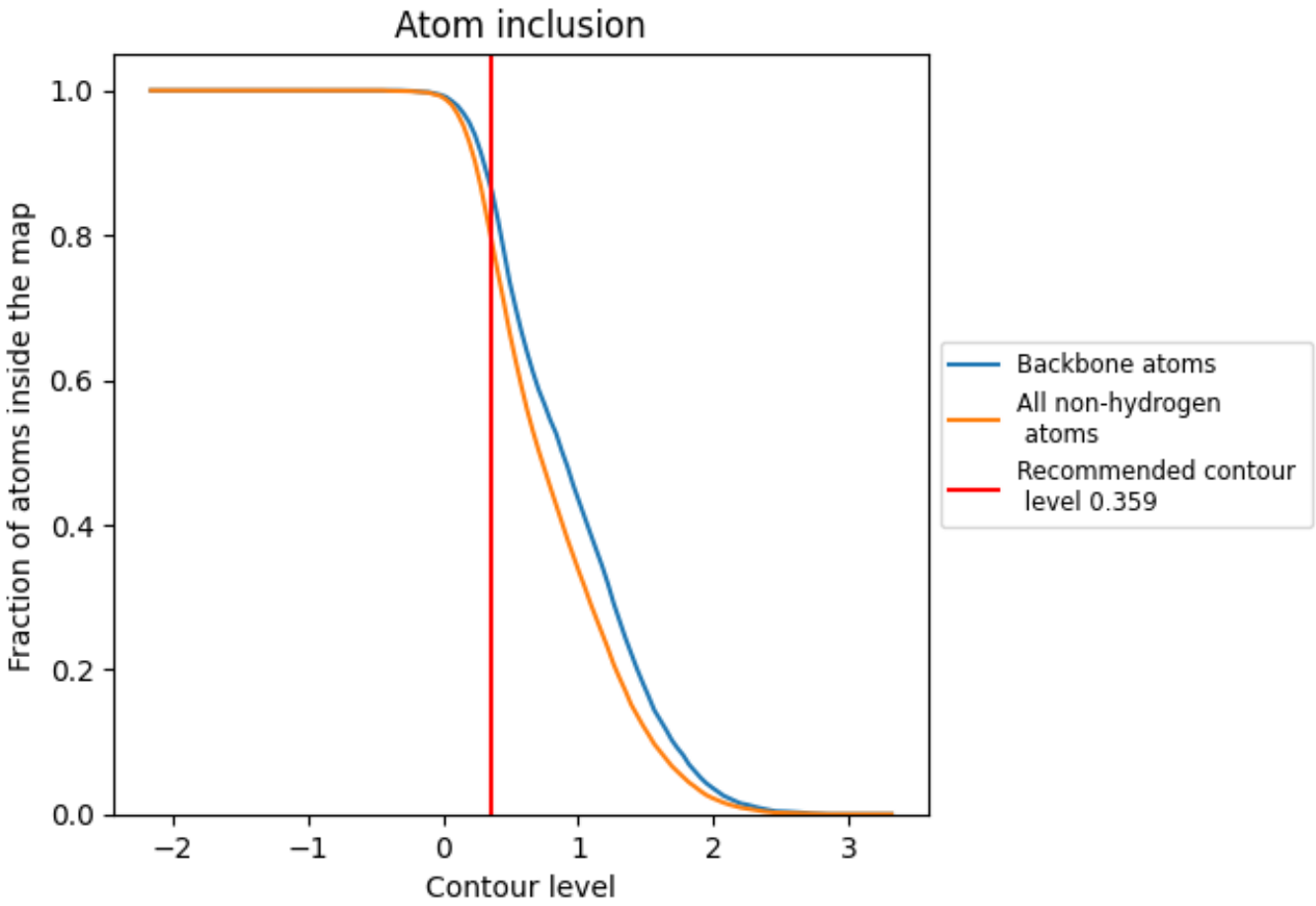
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.359).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7928	0.4780
A	0.8409	0.4970
B	0.7841	0.4680
C	0.7259	0.4540
D	0.8330	0.4980