Full wwPDB EM Validation Report (i)

May 23, 2023 – 10:13 AM EDT

PDB ID	:	8HAF
EMDB ID	:	EMD-34587
Title	:	PTHrP-PTH1R-Gs complex
Authors	:	Zhao, L.; Xu, H.E.; Yuan, Q.
Deposited on	:	2022-10-26
Resolution	:	3.25 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:

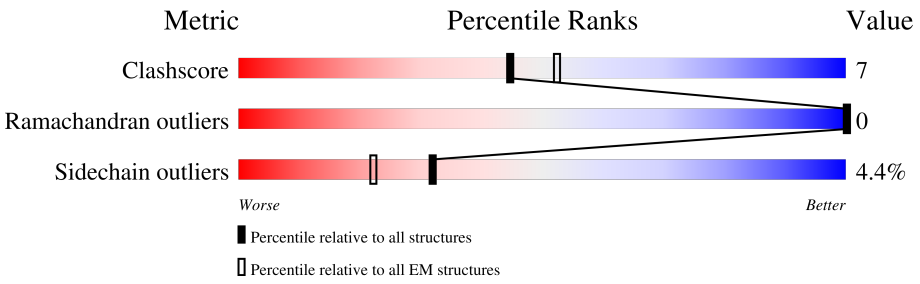
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.25 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	A	361	15% 56% 8% • 35%
2	B	400	16% 68% 16% • 15%
3	G	71	38% 72% 8% 20%
4	N	140	19% 82% 10% 8%
5	P	37	35% 70% 27% •
6	R	476	33% 59% 18% • 22%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9681 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-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	235	1950	1232	350	360	8	0	0

- 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	341	2616	1612	470	513	21	0	0

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	expression tag	UNP P54311
B	-32	HIS	-	expression tag	UNP P54311
B	-31	HIS	-	expression tag	UNP P54311
B	-30	HIS	-	expression tag	UNP P54311
B	-29	HIS	-	expression tag	UNP P54311
B	-28	HIS	-	expression tag	UNP P54311
B	-27	HIS	-	expression tag	UNP P54311
B	-26	SER	-	expression tag	UNP P54311
B	-25	SER	-	expression tag	UNP P54311
B	-24	GLY	-	expression tag	UNP P54311
B	-23	LEU	-	expression tag	UNP P54311
B	-22	VAL	-	expression tag	UNP P54311
B	-21	PRO	-	expression tag	UNP P54311
B	-20	ARG	-	expression tag	UNP P54311
B	-19	GLY	-	expression tag	UNP P54311
B	-18	SER	-	expression tag	UNP P54311
B	-17	HIS	-	expression tag	UNP P54311
B	-16	MET	-	expression tag	UNP P54311
B	-15	ALA	-	expression tag	UNP P54311
B	-14	SER	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	HIS	-	expression tag	UNP P54311
B	-12	HIS	-	expression tag	UNP P54311
B	-11	HIS	-	expression tag	UNP P54311
B	-10	HIS	-	expression tag	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 3 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		
3	G	57	436	273	77	83	3	0	0

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	N	129	983	611	173	193	6	0	0

- Molecule 5 is a protein called PTHrP[1-36].

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	P	36	301	191	59	51	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	37	NH2	-	amidation	UNP P12272

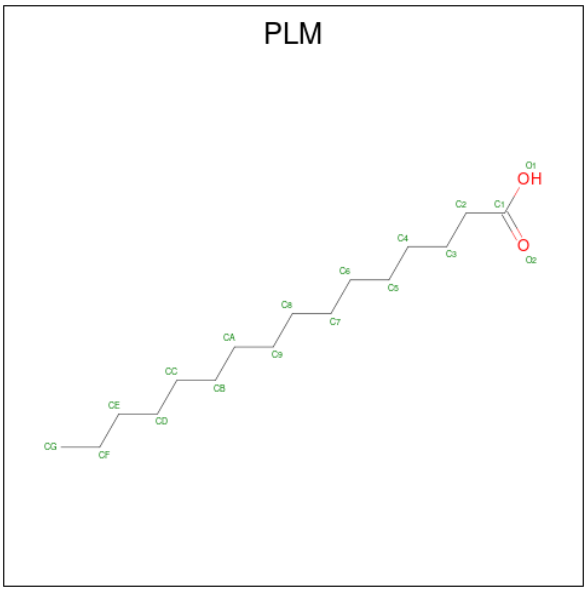
- Molecule 6 is a protein called Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	369	3029	2001	506	502	20	0	0

There are 2 discrepancies between the modelled and reference sequences:

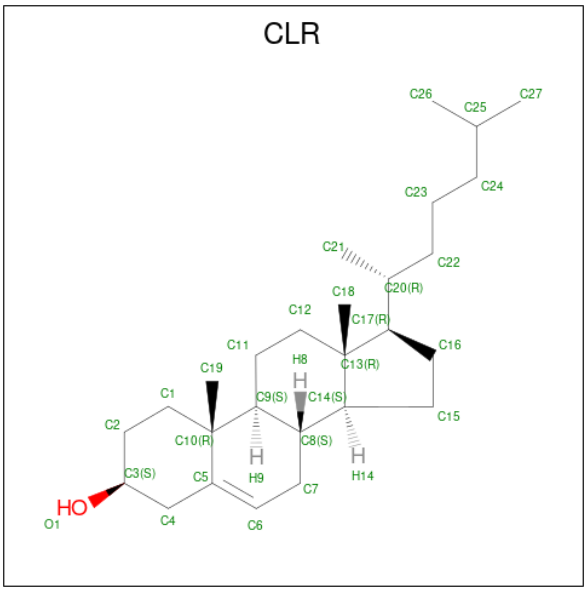
Chain	Residue	Modelled	Actual	Comment	Reference
R	188	ALA	GLY	conflict	UNP Q03431
R	484	ARG	LYS	conflict	UNP Q03431

- Molecule 7 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 8 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



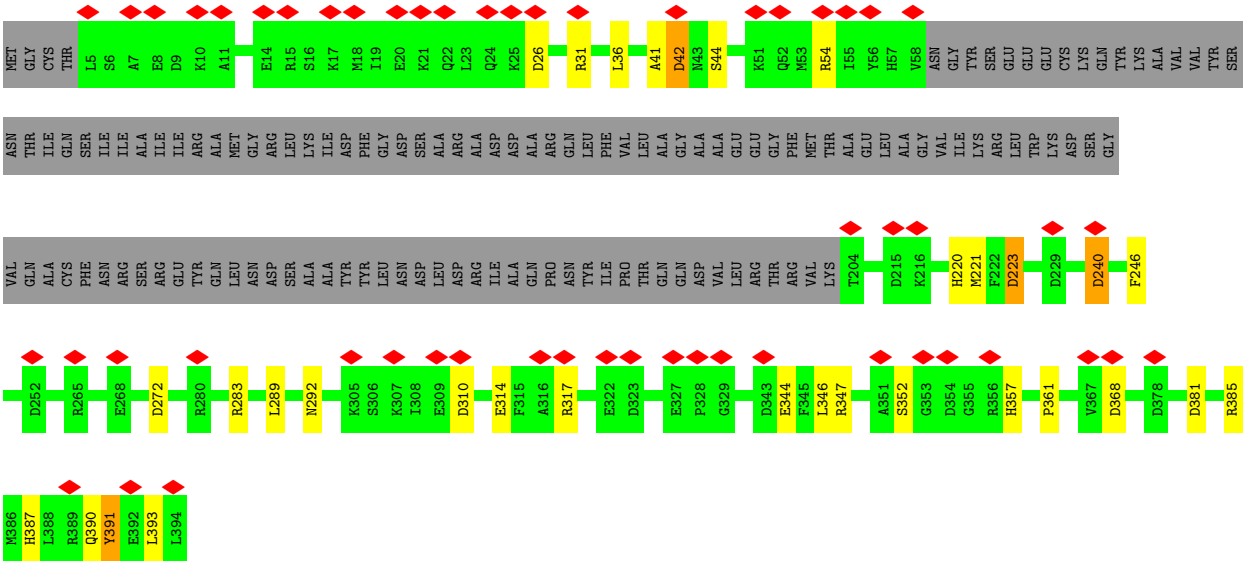
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	R	1	28	27	1	0
			Total	C	O	
8	R	1	28	27	1	0
			Total	C	O	
8	R	1	28	27	1	0
			Total	C	O	
8	R	1	28	27	1	0
			Total	C	O	
8	R	1	28	27	1	0
			Total	C	O	
8	R	1	28	27	1	0

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.

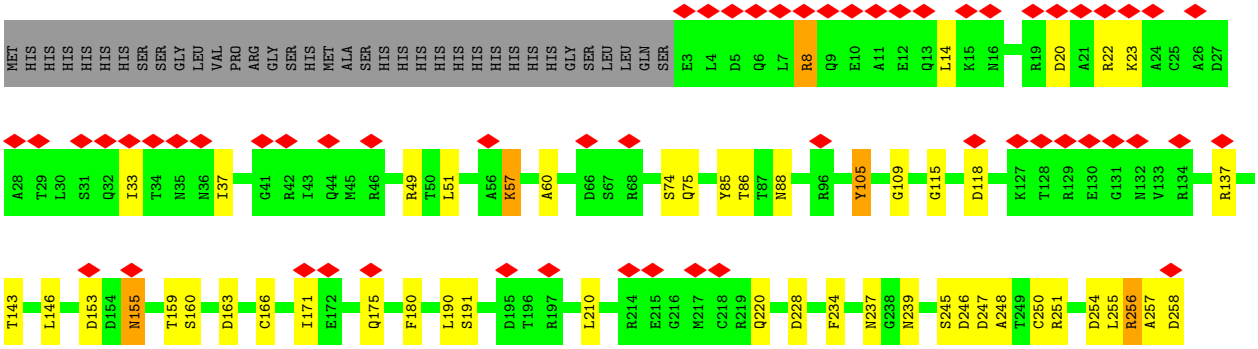
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha-1

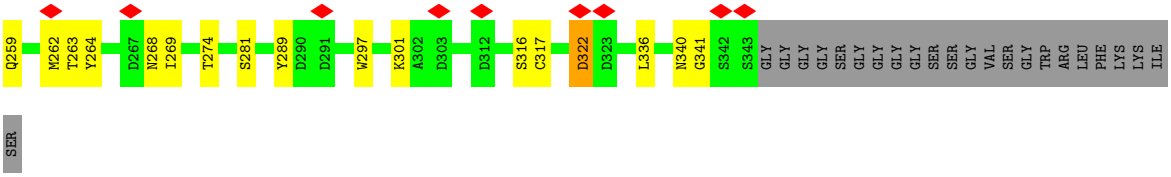
Chain A: 15% 56% 8% • 35%



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

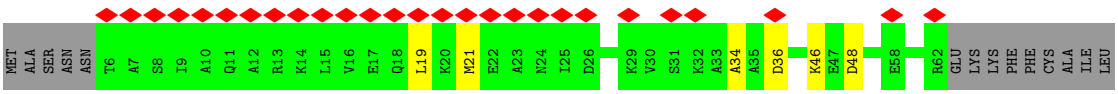
Chain B: 16% 68% 16% • 15%





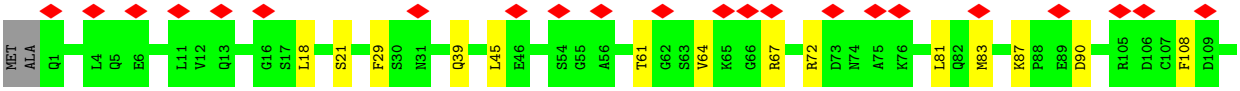
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

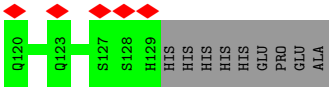
Chain G:



• Molecule 4: Nanobody 35

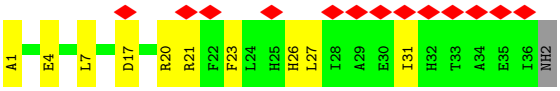
Chain N:





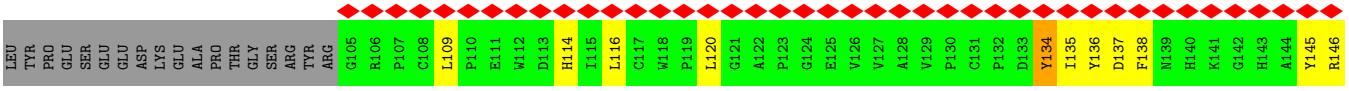
• Molecule 5: PTHrP[1-36]

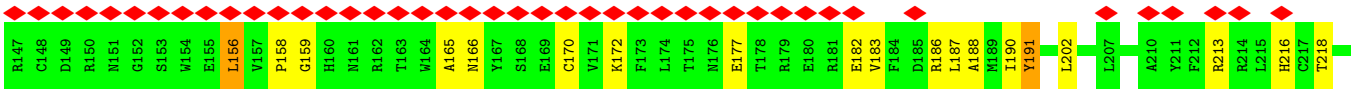
Chain P:

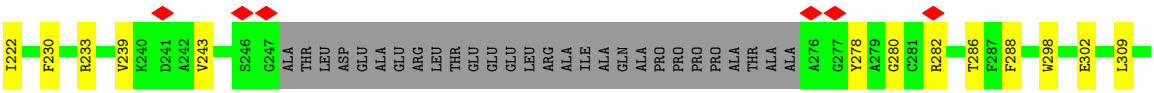


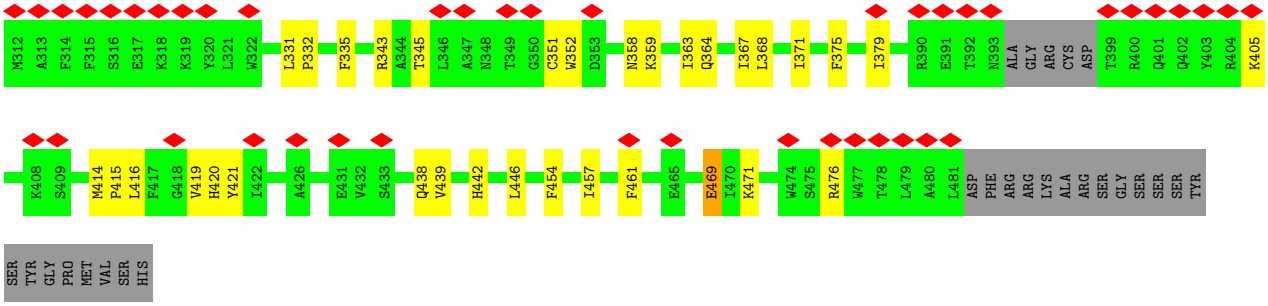
• Molecule 6: Parathyroid hormone/parathyroid hormone-related peptide receptor

Chain R:








M312
A313
F314
F315
S316
E317
K318
K319
Y320
L321
W322
L331
P332
F335
R343
A344
T345
L346
A347
N348
T349
G350
C351
W352
D353
N358
K359
I363
Q364
I367
L368
I371
F375
I379
R390
E391
T392
N393
ALA
GLY
ARG
CYS
ASP
T399
R400
Q401
Q402
Y403
R404
K405
K408
S409
M414
P415
L416
F417
G418
V419
H420
Y421
I422
A426
E431
V432
S433
Q438
V439
H442
L446
F454
I457
F461
E465
E469
I470
K471
W474
S475
R476
W477
T478
L479
A480
L481
ASP
PHE
ARG
ARG
LYS
ALA
ARG
SER
GLY
SER
SER
SER
TYR
SER
TYR
GLY
PRO
MET
VAL
SER
HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	436359	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.753	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.332	Depositor
Map size (Å)	247.2, 247.2, 247.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.824, 0.824, 0.824	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: PLM, CLR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.24	0/1989	0.51	1/2677 (0.0%)
2	B	0.25	0/2663	0.54	0/3610
3	G	0.24	0/442	0.48	0/597
4	N	0.25	0/1004	0.50	0/1360
5	P	0.23	0/307	0.45	0/411
6	R	0.26	0/3119	0.51	0/4237
All	All	0.25	0/9524	0.52	1/12892 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	ASP	CB-CG-OD1	5.32	123.09	118.30

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	1950	0	1925	14	0
2	B	2616	0	2518	37	0
3	G	436	0	448	5	0
4	N	983	0	947	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	P	301	0	305	8	0
6	R	3029	0	3018	61	0
7	R	198	0	341	5	0
8	R	168	0	271	15	0
All	All	9681	0	9773	132	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 7.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:GLY:HA3	2:B:146:LEU:HD23	1.64	0.80
6:R:278:TYR:HB2	6:R:282:ARG:HH21	1.48	0.78
2:B:86:THR:OG1	2:B:88:ASN:OD1	2.04	0.75
6:R:280:GLY:HA3	8:R:1514:CLR:H9	1.74	0.70
2:B:160:SER:HB2	2:B:190:LEU:HD23	1.75	0.69
5:P:7:LEU:HD11	6:R:187:LEU:HD13	1.75	0.69
6:R:415:PRO:HG3	8:R:1512:CLR:H17	1.78	0.66
6:R:345:THR:HG21	7:R:1503:PLM:H91	1.77	0.64
4:N:29:PHE:O	4:N:72:ARG:NH2	2.31	0.64
5:P:1:ALA:HB3	6:R:364:GLN:HE21	1.63	0.62
8:R:1512:CLR:H192	8:R:1515:CLR:H12	1.81	0.62
1:A:314:GLU:OE1	1:A:314:GLU:N	2.32	0.61
5:P:23:PHE:O	5:P:26:HIS:ND1	2.34	0.61
6:R:188:ALA:HA	6:R:191:TYR:CE2	2.35	0.61
2:B:118:ASP:N	2:B:118:ASP:OD1	2.34	0.60
2:B:245:SER:OG	2:B:247:ASP:OD1	2.17	0.59
6:R:439:VAL:HG23	7:R:1506:PLM:H91	1.84	0.59
2:B:220:GLN:NE2	2:B:258:ASP:OD1	2.33	0.59
6:R:358:ASN:HB3	7:R:1504:PLM:H41	1.84	0.58
2:B:256:ARG:NH2	3:G:36:ASP:OD2	2.37	0.58
8:R:1513:CLR:H122	8:R:1514:CLR:H152	1.85	0.58
1:A:387:HIS:HB3	6:R:309:LEU:HD21	1.86	0.57
6:R:243:VAL:HG13	8:R:1514:CLR:H71	1.86	0.57
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.87	0.57
1:A:42:ASP:N	1:A:42:ASP:OD1	2.37	0.56
8:R:1512:CLR:H211	8:R:1512:CLR:H263	1.87	0.56
6:R:213:ARG:NH1	6:R:213:ARG:HB3	2.22	0.55
6:R:302:GLU:HG2	6:R:416:LEU:HD11	1.87	0.55
6:R:41:LEU:HD22	6:R:114:HIS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:438:GLN:O	6:R:442:HIS:ND1	2.38	0.53
6:R:186:ARG:O	6:R:190:ILE:HG22	2.08	0.53
4:N:67:ARG:NH2	4:N:90:ASP:OD2	2.42	0.53
6:R:50:LYS:O	6:R:53:LYS:NZ	2.41	0.53
1:A:41:ALA:O	1:A:44:SER:OG	2.27	0.52
6:R:471:LYS:HE3	7:R:1501:PLM:H42	1.90	0.52
6:R:375:PHE:O	6:R:379:ILE:HG12	2.10	0.52
6:R:51:ARG:HH22	6:R:120:LEU:HD11	1.74	0.52
1:A:381:ASP:OD2	1:A:385:ARG:NH1	2.43	0.51
2:B:228:ASP:OD2	2:B:228:ASP:N	2.43	0.51
2:B:22:ARG:HD2	2:B:259:GLN:HB3	1.92	0.51
6:R:419:VAL:O	6:R:420:HIS:ND1	2.43	0.51
1:A:283:ARG:O	1:A:357:HIS:ND1	2.43	0.51
6:R:457:ILE:HD13	6:R:461:PHE:HD2	1.74	0.51
2:B:105:TYR:HE2	2:B:109:GLY:HA2	1.74	0.51
6:R:190:ILE:HD11	6:R:446:LEU:HD13	1.91	0.51
6:R:278:TYR:HB2	6:R:282:ARG:NH2	2.24	0.50
6:R:183:VAL:HG22	6:R:186:ARG:HH22	1.76	0.50
4:N:64:VAL:HA	4:N:67:ARG:HD3	1.93	0.50
6:R:177:GLU:OE1	6:R:177:GLU:N	2.32	0.49
6:R:286:THR:HB	6:R:352:TRP:HZ3	1.77	0.49
6:R:454:PHE:CG	8:R:1512:CLR:H151	2.47	0.49
5:P:27:LEU:O	5:P:31:ILE:HG13	2.13	0.49
2:B:137:ARG:HD3	2:B:171:ILE:O	2.14	0.48
6:R:37:GLN:HE22	6:R:136:TYR:H	1.63	0.47
2:B:340:ASN:OD1	2:B:341:GLY:N	2.46	0.47
2:B:143:THR:N	2:B:163:ASP:OD1	2.47	0.47
2:B:254:ASP:OD2	2:B:256:ARG:N	2.46	0.47
2:B:237:ASN:HD21	2:B:239:ASN:HB2	1.80	0.47
6:R:213:ARG:HB3	6:R:213:ARG:HH11	1.78	0.47
1:A:391:TYR:HB3	1:A:393:LEU:HG	1.97	0.47
5:P:17:ASP:O	5:P:21:ARG:HG2	2.15	0.47
6:R:170:CYS:O	6:R:172:LYS:HG2	2.15	0.47
8:R:1515:CLR:H162	8:R:1515:CLR:H221	1.50	0.47
1:A:246:PHE:HB3	1:A:289:LEU:HD12	1.97	0.47
6:R:476:ARG:HH21	8:R:1516:CLR:H242	1.79	0.47
6:R:363:ILE:O	6:R:367:ILE:HG22	2.15	0.46
6:R:156:LEU:HD13	6:R:159:GLY:HA2	1.96	0.46
4:N:39:GLN:HB2	4:N:45:LEU:HD23	1.96	0.46
1:A:344:GLU:OE1	1:A:347:ARG:NH1	2.49	0.46
2:B:322:ASP:N	2:B:322:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:ASP:OD2	2:B:255:LEU:N	2.49	0.46
2:B:8:ARG:NE	2:B:8:ARG:HA	2.30	0.46
2:B:251:ARG:HG2	2:B:263:THR:HG22	1.97	0.46
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.98	0.46
2:B:57:LYS:HE2	2:B:75:GLN:HG3	1.98	0.45
6:R:368:LEU:HD12	6:R:371:ILE:HD12	1.97	0.45
2:B:248:ALA:HB1	2:B:269:ILE:HG22	1.97	0.45
2:B:14:LEU:HD13	3:G:19:LEU:HB3	1.99	0.45
2:B:289:TYR:HH	2:B:297:TRP:HE1	1.63	0.45
6:R:135:ILE:HD11	6:R:138:PHE:CG	2.52	0.45
8:R:1517:CLR:H222	8:R:1517:CLR:H25	1.41	0.45
2:B:33:ILE:HG21	3:G:34:ALA:HB1	2.00	0.44
1:A:346:LEU:HD21	1:A:361:PRO:HG3	2.00	0.44
4:N:61:THR:HB	4:N:64:VAL:HG22	2.00	0.44
6:R:40:LEU:HD12	6:R:134:TYR:HD2	1.82	0.44
6:R:218:THR:O	6:R:222:ILE:HG13	2.17	0.44
6:R:146:ARG:HH21	6:R:165:ALA:HB2	1.83	0.44
2:B:49:ARG:NH2	2:B:85:TYR:O	2.36	0.44
6:R:109:LEU:HD23	6:R:109:LEU:HA	1.66	0.43
1:A:54:ARG:HG2	1:A:54:ARG:O	2.18	0.43
6:R:351:CYS:SG	6:R:352:TRP:N	2.91	0.43
2:B:250:CYS:HB3	2:B:264:TYR:HB2	2.01	0.43
6:R:145:TYR:O	6:R:166:ASN:ND2	2.44	0.43
6:R:239:VAL:O	6:R:243:VAL:HG23	2.19	0.43
2:B:210:LEU:HD23	2:B:220:GLN:HG3	2.01	0.43
6:R:405:LYS:HD3	6:R:405:LYS:HA	1.84	0.43
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.90	0.43
6:R:50:LYS:HE3	6:R:50:LYS:HB3	1.82	0.43
6:R:116:LEU:HD12	6:R:116:LEU:HA	1.85	0.43
1:A:223:ASP:OD2	1:A:223:ASP:N	2.52	0.42
5:P:21:ARG:HA	5:P:21:ARG:HD3	1.83	0.42
2:B:175:GLN:HA	2:B:175:GLN:OE1	2.19	0.42
8:R:1517:CLR:H162	8:R:1517:CLR:H221	1.62	0.42
2:B:60:ALA:HA	2:B:317:CYS:HB3	2.01	0.42
5:P:20:ARG:NH1	6:R:32:MET:O	2.44	0.42
6:R:34:LYS:O	6:R:38:ILE:HG23	2.20	0.42
5:P:4:GLU:OE2	6:R:233:ARG:NH2	2.53	0.42
6:R:52:LEU:HD12	6:R:109:LEU:HD13	2.02	0.42
2:B:37:ILE:HD11	2:B:301:LYS:HG2	2.02	0.42
6:R:33:THR:OG1	6:R:34:LYS:N	2.52	0.42
6:R:343:ARG:HG2	6:R:352:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:R:1517:CLR:H213	8:R:1517:CLR:H231	1.77	0.42
1:A:36:LEU:N	1:A:220:HIS:O	2.50	0.41
4:N:18:LEU:N	4:N:83:MET:O	2.44	0.41
6:R:371:ILE:HD13	6:R:421:TYR:HB3	2.03	0.41
3:G:46:LYS:HE3	3:G:46:LYS:HB2	1.91	0.41
8:R:1516:CLR:H162	8:R:1516:CLR:H222	1.73	0.41
2:B:257:ALA:O	2:B:259:GLN:HG2	2.20	0.41
2:B:281:SER:HB2	3:G:48:ASP:HB2	2.03	0.41
6:R:48:CYS:O	6:R:52:LEU:HB2	2.20	0.41
7:R:1504:PLM:H21	7:R:1511:PLM:H41	2.03	0.41
6:R:469:GLU:HA	6:R:469:GLU:OE1	2.20	0.41
2:B:146:LEU:HD11	2:B:159:THR:HG23	2.03	0.41
2:B:155:ASN:HA	2:B:171:ILE:HB	2.03	0.41
6:R:454:PHE:HB3	8:R:1512:CLR:H151	2.03	0.41
6:R:222:ILE:HG23	6:R:298:TRP:HZ3	1.86	0.41
2:B:274:THR:HG21	2:B:316:SER:HA	2.03	0.40
6:R:335:PHE:HD1	6:R:335:PHE:HA	1.76	0.40
8:R:1512:CLR:H191	8:R:1512:CLR:H8	1.68	0.40
6:R:182:GLU:OE1	6:R:186:ARG:NH1	2.53	0.40
6:R:202:LEU:HD13	6:R:230:PHE:HB3	2.03	0.40
6:R:331:LEU:HB3	6:R:332:PRO:HD3	2.04	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	231/361 (64%)	229 (99%)	2 (1%)	0	100	100
2	B	339/400 (85%)	335 (99%)	4 (1%)	0	100	100
3	G	55/71 (78%)	55 (100%)	0	0	100	100
4	N	127/140 (91%)	123 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
6	R	361/476 (76%)	340 (94%)	21 (6%)	0	100	100
All	All	1147/1485 (77%)	1115 (97%)	32 (3%)	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	212/315 (67%)	198 (93%)	14 (7%)	16	45
2	B	283/328 (86%)	268 (95%)	15 (5%)	22	53
3	G	46/58 (79%)	45 (98%)	1 (2%)	52	74
4	N	107/116 (92%)	103 (96%)	4 (4%)	34	62
5	P	32/32 (100%)	32 (100%)	0	100	100
6	R	322/407 (79%)	312 (97%)	10 (3%)	40	67
All	All	1002/1256 (80%)	958 (96%)	44 (4%)	32	58

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	31	ARG
1	A	42	ASP
1	A	221	MET
1	A	223	ASP
1	A	240	ASP
1	A	272	ASP
1	A	292	ASN
1	A	310	ASP
1	A	317	ARG
1	A	352	SER
1	A	368	ASP

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Mol	Chain	Res	Type
1	A	390	GLN
1	A	391	TYR
2	B	8	ARG
2	B	20	ASP
2	B	23	LYS
2	B	57	LYS
2	B	74	SER
2	B	105	TYR
2	B	153	ASP
2	B	155	ASN
2	B	191	SER
2	B	234	PHE
2	B	246	ASP
2	B	256	ARG
2	B	262	MET
2	B	268	ASN
2	B	322	ASP
3	G	21	MET
4	N	21	SER
4	N	81	LEU
4	N	87	LYS
4	N	108	PHE
6	R	134	TYR
6	R	137	ASP
6	R	156	LEU
6	R	158	PRO
6	R	191	TYR
6	R	216	HIS
6	R	288	PHE
6	R	359	LYS
6	R	414	MET
6	R	469	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
6	R	364	GLN

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)

17 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	$\#\|Z\| > 2$
7	PLM	R	1504	-	17,17,17	0.93	1 (5%)	17,17,17	0.74	1 (5%)
7	PLM	R	1501	-	17,17,17	0.93	1 (5%)	17,17,17	0.75	2 (11%)
8	CLR	R	1512	-	31,31,31	0.53	0	48,48,48	2.21	12 (25%)
8	CLR	R	1516	-	31,31,31	0.37	0	48,48,48	0.73	0
7	PLM	R	1505	-	17,17,17	0.93	1 (5%)	17,17,17	0.75	2 (11%)
8	CLR	R	1514	-	31,31,31	0.40	0	48,48,48	0.87	0
7	PLM	R	1507	-	17,17,17	0.95	1 (5%)	17,17,17	0.75	2 (11%)
7	PLM	R	1508	-	17,17,17	0.93	1 (5%)	17,17,17	0.75	2 (11%)
7	PLM	R	1503	-	17,17,17	0.93	1 (5%)	17,17,17	0.74	2 (11%)
7	PLM	R	1509	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	1 (5%)
7	PLM	R	1511	-	17,17,17	0.94	1 (5%)	17,17,17	0.74	2 (11%)
8	CLR	R	1513	-	31,31,31	0.35	0	48,48,48	0.59	0
7	PLM	R	1502	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	1 (5%)
8	CLR	R	1515	-	31,31,31	0.61	0	48,48,48	5.17	17 (35%)
7	PLM	R	1506	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	2 (11%)
8	CLR	R	1517	-	31,31,31	0.30	0	48,48,48	0.59	0
7	PLM	R	1510	-	17,17,17	0.92	1 (5%)	17,17,17	0.74	1 (5%)

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
7	PLM	R	1504	-	-	6/15/15/15	-
7	PLM	R	1501	-	-	6/15/15/15	-
8	CLR	R	1512	-	-	4/10/68/68	0/4/4/4
8	CLR	R	1516	-	-	7/10/68/68	0/4/4/4
7	PLM	R	1505	-	-	2/15/15/15	-
8	CLR	R	1514	-	-	3/10/68/68	0/4/4/4
7	PLM	R	1507	-	-	7/15/15/15	-
7	PLM	R	1508	-	-	1/15/15/15	-
7	PLM	R	1503	-	-	6/15/15/15	-
7	PLM	R	1509	-	-	2/15/15/15	-
7	PLM	R	1511	-	-	3/15/15/15	-
8	CLR	R	1513	-	-	2/10/68/68	0/4/4/4
7	PLM	R	1502	-	-	7/15/15/15	-
8	CLR	R	1515	-	-	9/10/68/68	0/4/4/4
7	PLM	R	1506	-	-	4/15/15/15	-
8	CLR	R	1517	-	-	10/10/68/68	0/4/4/4
7	PLM	R	1510	-	-	2/15/15/15	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	1507	PLM	C2-C1	3.08	1.57	1.50
7	R	1501	PLM	C2-C1	3.02	1.57	1.50
7	R	1511	PLM	C2-C1	2.99	1.57	1.50
7	R	1504	PLM	C2-C1	2.99	1.57	1.50
7	R	1503	PLM	C2-C1	2.98	1.57	1.50
7	R	1508	PLM	C2-C1	2.98	1.57	1.50
7	R	1509	PLM	C2-C1	2.97	1.57	1.50
7	R	1505	PLM	C2-C1	2.96	1.57	1.50
7	R	1502	PLM	C2-C1	2.93	1.57	1.50
7	R	1506	PLM	C2-C1	2.93	1.57	1.50
7	R	1510	PLM	C2-C1	2.90	1.57	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	R	1515	CLR	C18-C13-C12	-20.03	78.96	110.59
8	R	1515	CLR	C18-C13-C17	-18.19	77.79	111.71
8	R	1515	CLR	C12-C13-C17	11.60	133.93	116.57
8	R	1515	CLR	C2-C3-C4	-10.13	96.41	110.31
8	R	1512	CLR	O1-C3-C4	9.66	130.39	109.68
8	R	1515	CLR	C18-C13-C14	-8.91	95.10	111.71
8	R	1515	CLR	C1-C2-C3	6.53	118.85	110.47
8	R	1515	CLR	O1-C3-C4	-6.31	96.16	109.68
8	R	1512	CLR	C10-C9-C8	-5.72	104.15	112.73
8	R	1515	CLR	C17-C13-C14	5.57	106.67	100.07
8	R	1515	CLR	C12-C13-C14	4.70	114.57	107.27
8	R	1512	CLR	C1-C10-C9	3.91	114.18	108.73
8	R	1515	CLR	C7-C8-C9	3.88	114.42	109.71
8	R	1515	CLR	C3-C4-C5	3.52	118.00	112.03
8	R	1512	CLR	C14-C8-C9	3.51	113.78	109.09
8	R	1515	CLR	C2-C1-C10	3.44	120.18	112.74
8	R	1512	CLR	C3-C4-C5	3.43	117.85	112.03
8	R	1512	CLR	C19-C10-C9	-3.40	107.62	111.68
8	R	1515	CLR	C10-C9-C8	3.09	117.37	112.73
8	R	1515	CLR	C11-C9-C8	-3.02	107.40	111.75
8	R	1515	CLR	C11-C9-C10	2.78	116.74	113.08
8	R	1512	CLR	C17-C13-C14	2.64	103.20	100.07
8	R	1512	CLR	C12-C13-C14	-2.28	103.73	107.27
7	R	1508	PLM	O1-C1-O2	2.23	128.85	123.30
7	R	1505	PLM	O1-C1-O2	2.22	128.82	123.30
7	R	1506	PLM	O1-C1-O2	2.22	128.82	123.30
7	R	1507	PLM	O1-C1-O2	2.22	128.82	123.30
7	R	1503	PLM	O1-C1-O2	2.21	128.81	123.30
7	R	1511	PLM	O1-C1-O2	2.21	128.80	123.30
7	R	1502	PLM	O1-C1-O2	2.20	128.78	123.30
7	R	1509	PLM	O1-C1-O2	2.20	128.78	123.30
7	R	1501	PLM	O1-C1-O2	2.19	128.77	123.30
7	R	1510	PLM	O1-C1-O2	2.19	128.75	123.30
7	R	1504	PLM	O1-C1-O2	2.18	128.73	123.30
8	R	1512	CLR	C12-C11-C9	2.16	116.86	113.11
8	R	1512	CLR	C2-C3-C4	2.14	113.25	110.31
8	R	1515	CLR	C15-C16-C17	2.11	109.32	105.13
8	R	1512	CLR	C7-C8-C14	2.10	113.95	110.91
8	R	1512	CLR	C2-C1-C10	-2.07	108.26	112.74
7	R	1507	PLM	O2-C1-C2	-2.04	116.53	123.08
7	R	1501	PLM	O2-C1-C2	-2.02	116.60	123.08
7	R	1505	PLM	O2-C1-C2	-2.02	116.61	123.08
7	R	1503	PLM	O2-C1-C2	-2.01	116.62	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	R	1506	PLM	O2-C1-C2	-2.01	116.62	123.08
7	R	1511	PLM	O2-C1-C2	-2.00	116.64	123.08
7	R	1508	PLM	O2-C1-C2	-2.00	116.64	123.08
8	R	1515	CLR	C13-C17-C20	2.00	122.62	119.49

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	R	1517	CLR	C22-C23-C24-C25
8	R	1517	CLR	C21-C20-C22-C23
8	R	1512	CLR	C21-C20-C22-C23
8	R	1517	CLR	C13-C17-C20-C22
8	R	1517	CLR	C16-C17-C20-C21
8	R	1517	CLR	C13-C17-C20-C21
8	R	1512	CLR	C17-C20-C22-C23
8	R	1514	CLR	C21-C20-C22-C23
8	R	1514	CLR	C17-C20-C22-C23
8	R	1517	CLR	C20-C22-C23-C24
8	R	1517	CLR	C17-C20-C22-C23
8	R	1517	CLR	C16-C17-C20-C22
8	R	1514	CLR	C20-C22-C23-C24
8	R	1512	CLR	C20-C22-C23-C24
8	R	1515	CLR	C17-C20-C22-C23
7	R	1502	PLM	C6-C7-C8-C9
7	R	1502	PLM	C8-C9-CA-CB
7	R	1506	PLM	CA-CB-CC-CD
7	R	1507	PLM	C9-CA-CB-CC
7	R	1507	PLM	C7-C8-C9-CA
7	R	1507	PLM	C3-C4-C5-C6
7	R	1504	PLM	C1-C2-C3-C4
8	R	1515	CLR	C23-C24-C25-C26
7	R	1508	PLM	C6-C7-C8-C9
7	R	1511	PLM	CC-CD-CE-CF
7	R	1504	PLM	C3-C4-C5-C6
7	R	1502	PLM	C3-C4-C5-C6
8	R	1517	CLR	C23-C24-C25-C27
8	R	1515	CLR	C16-C17-C20-C21
8	R	1515	CLR	C13-C17-C20-C22
8	R	1512	CLR	C22-C23-C24-C25
8	R	1516	CLR	C20-C22-C23-C24
8	R	1516	CLR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
8	R	1515	CLR	C23-C24-C25-C27
8	R	1517	CLR	C23-C24-C25-C26
8	R	1515	CLR	C16-C17-C20-C22
8	R	1515	CLR	C13-C17-C20-C21
7	R	1507	PLM	C5-C6-C7-C8
7	R	1503	PLM	C4-C5-C6-C7
7	R	1511	PLM	C8-C9-CA-CB
7	R	1502	PLM	CC-CD-CE-CF
8	R	1515	CLR	C22-C23-C24-C25
7	R	1503	PLM	C5-C6-C7-C8
7	R	1501	PLM	C7-C8-C9-CA
7	R	1507	PLM	C6-C7-C8-C9
7	R	1504	PLM	C6-C7-C8-C9
7	R	1503	PLM	C8-C9-CA-CB
7	R	1504	PLM	C4-C5-C6-C7
7	R	1502	PLM	C1-C2-C3-C4
8	R	1516	CLR	C23-C24-C25-C26
7	R	1501	PLM	O2-C1-C2-C3
8	R	1516	CLR	C16-C17-C20-C22
7	R	1506	PLM	O2-C1-C2-C3
7	R	1505	PLM	O2-C1-C2-C3
7	R	1506	PLM	O1-C1-C2-C3
7	R	1504	PLM	O2-C1-C2-C3
7	R	1509	PLM	O2-C1-C2-C3
7	R	1503	PLM	O1-C1-C2-C3
8	R	1516	CLR	C23-C24-C25-C27
8	R	1513	CLR	C17-C20-C22-C23
7	R	1509	PLM	O1-C1-C2-C3
7	R	1504	PLM	O1-C1-C2-C3
7	R	1510	PLM	O1-C1-C2-C3
7	R	1507	PLM	O1-C1-C2-C3
7	R	1507	PLM	O2-C1-C2-C3
7	R	1510	PLM	O2-C1-C2-C3
7	R	1503	PLM	O2-C1-C2-C3
8	R	1516	CLR	C13-C17-C20-C21
7	R	1501	PLM	O1-C1-C2-C3
7	R	1505	PLM	O1-C1-C2-C3
7	R	1506	PLM	C2-C3-C4-C5
8	R	1516	CLR	C13-C17-C20-C22
7	R	1503	PLM	C7-C8-C9-CA
7	R	1501	PLM	C1-C2-C3-C4
7	R	1501	PLM	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
7	R	1502	PLM	O1-C1-C2-C3
7	R	1502	PLM	O2-C1-C2-C3
7	R	1501	PLM	CD-CE-CF-CG
7	R	1511	PLM	C9-CA-CB-CC
8	R	1515	CLR	C21-C20-C22-C23
8	R	1513	CLR	C21-C20-C22-C23

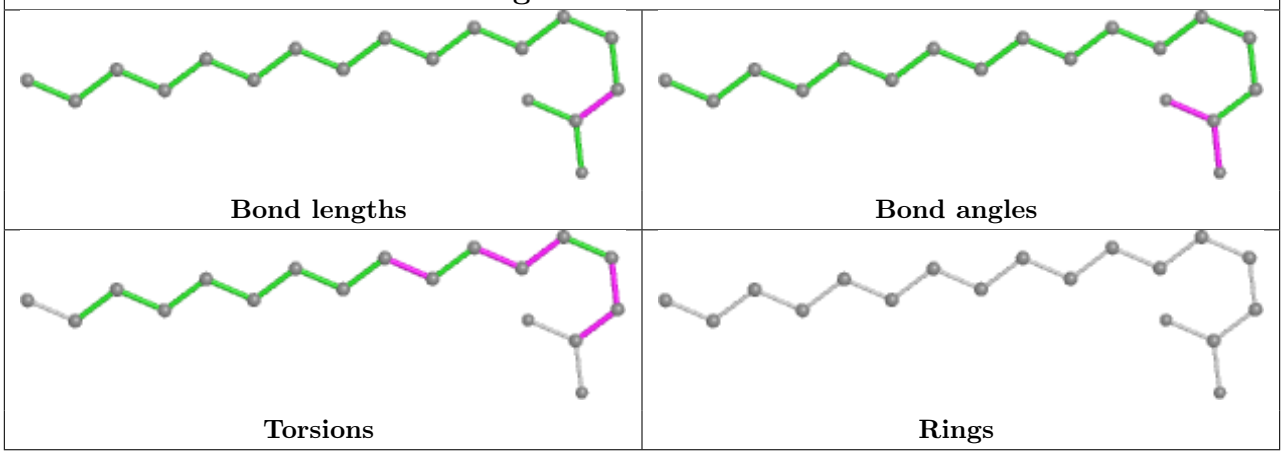
There are no ring outliers.

11 monomers are involved in 20 short contacts:

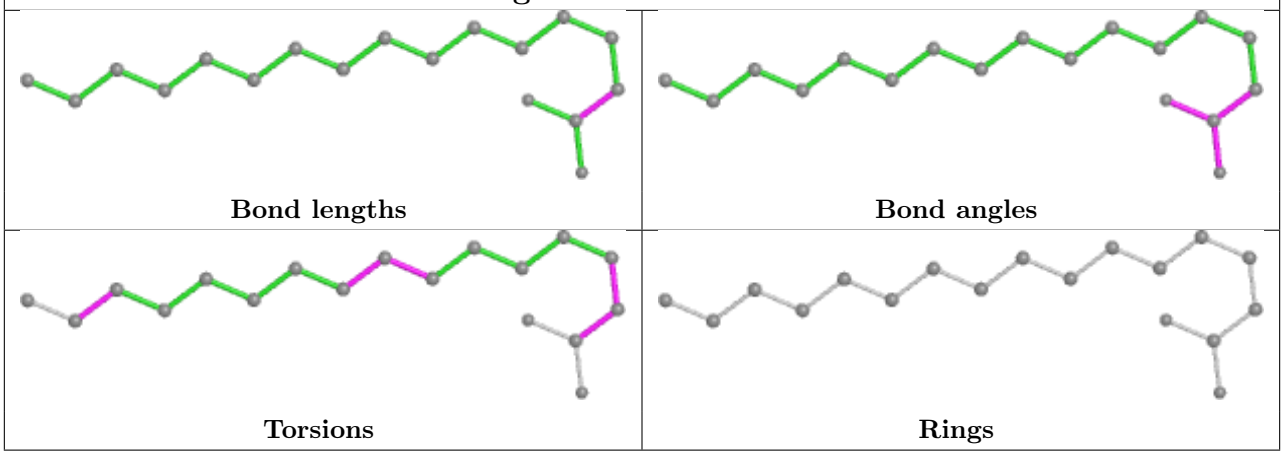
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1504	PLM	2	0
7	R	1501	PLM	1	0
8	R	1512	CLR	6	0
8	R	1516	CLR	2	0
8	R	1514	CLR	3	0
7	R	1503	PLM	1	0
7	R	1511	PLM	1	0
8	R	1513	CLR	1	0
8	R	1515	CLR	2	0
7	R	1506	PLM	1	0
8	R	1517	CLR	3	0

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.

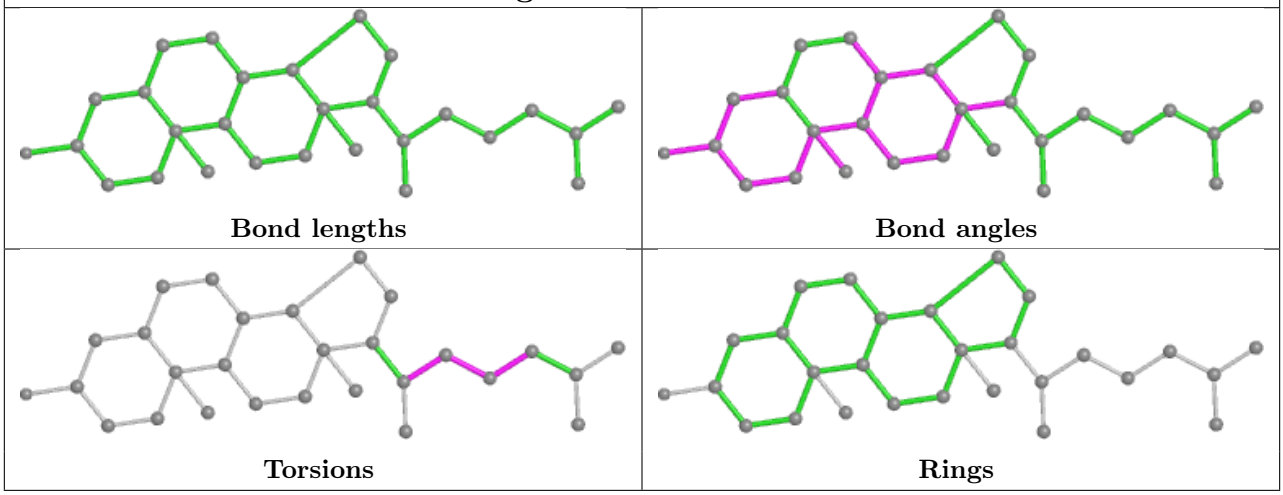
Ligand PLM R 1504



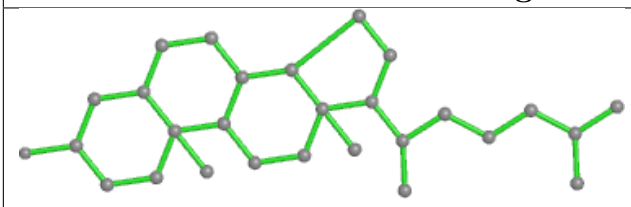
Ligand PLM R 1501



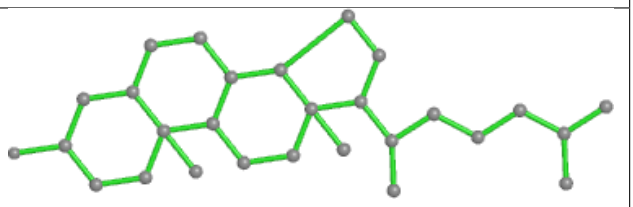
Ligand CLR R 1512



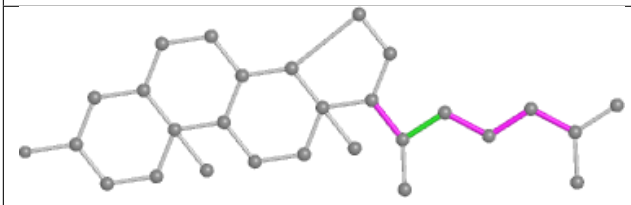
Ligand CLR R 1516



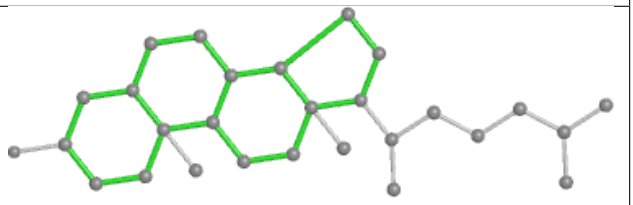
Bond lengths



Bond angles

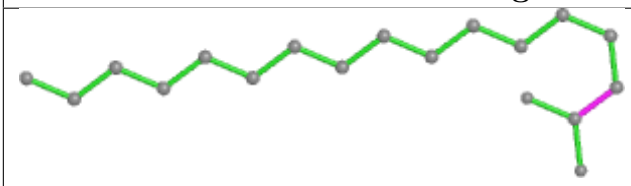


Torsions

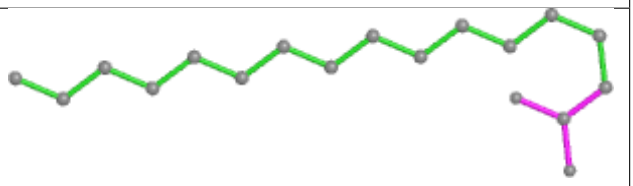


Rings

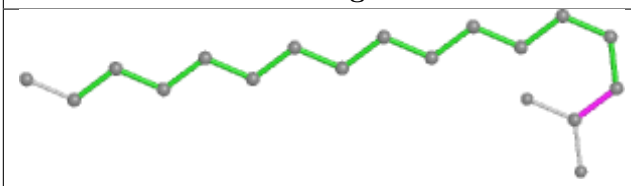
Ligand PLM R 1505



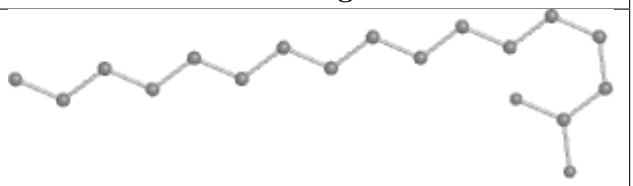
Bond lengths



Bond angles

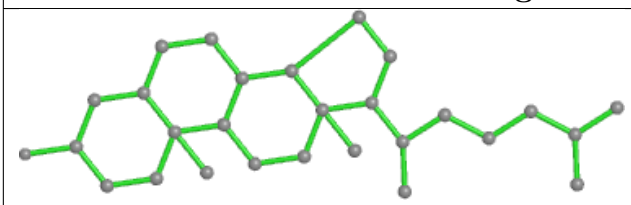


Torsions

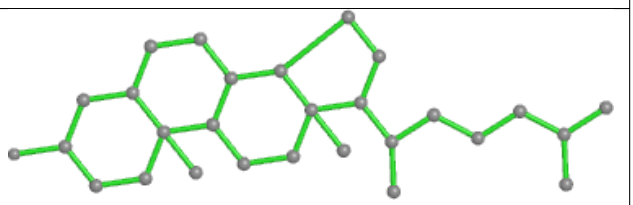


Rings

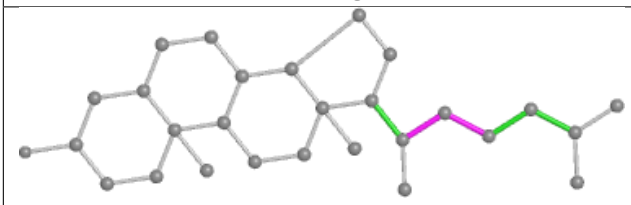
Ligand CLR R 1514



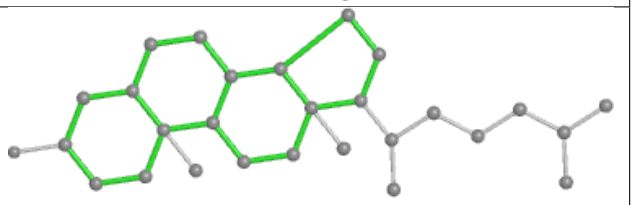
Bond lengths



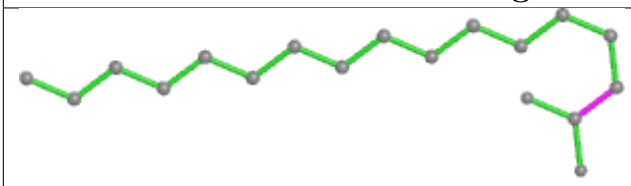
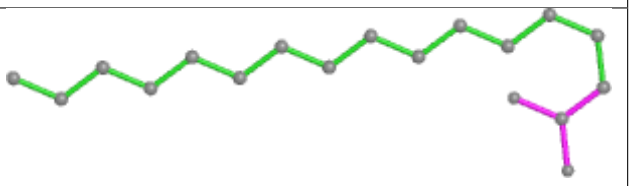
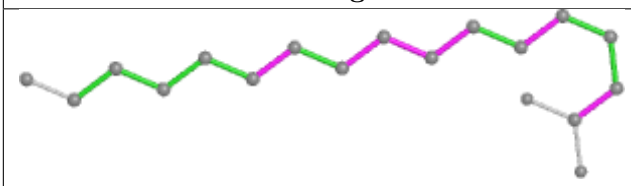
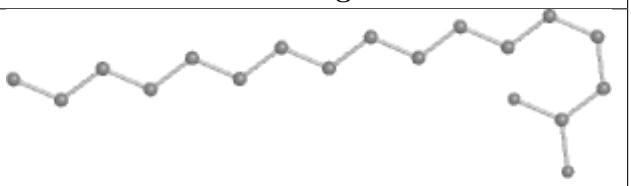
Bond angles

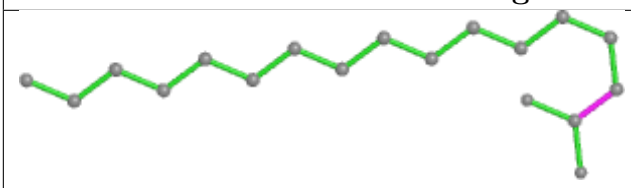
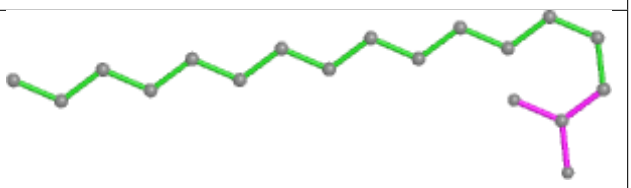
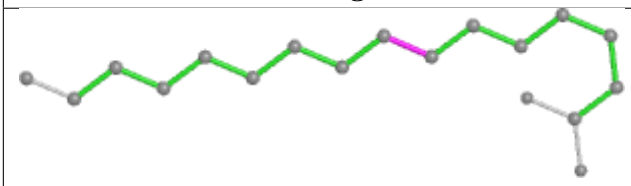


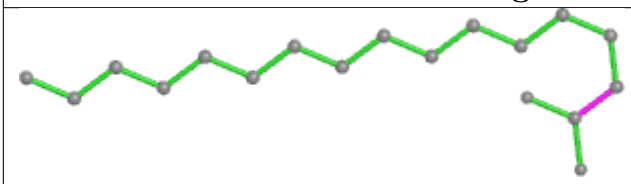
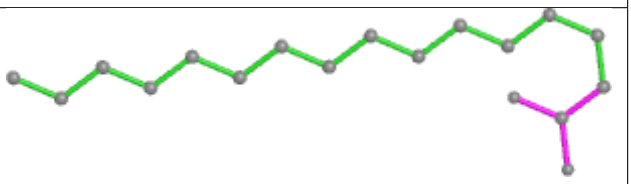
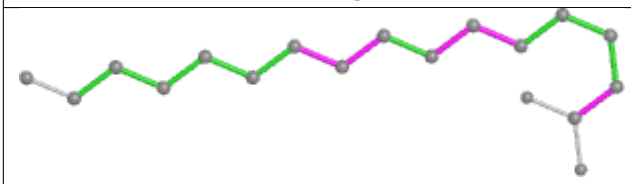
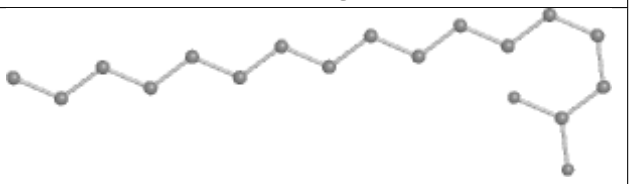
Torsions



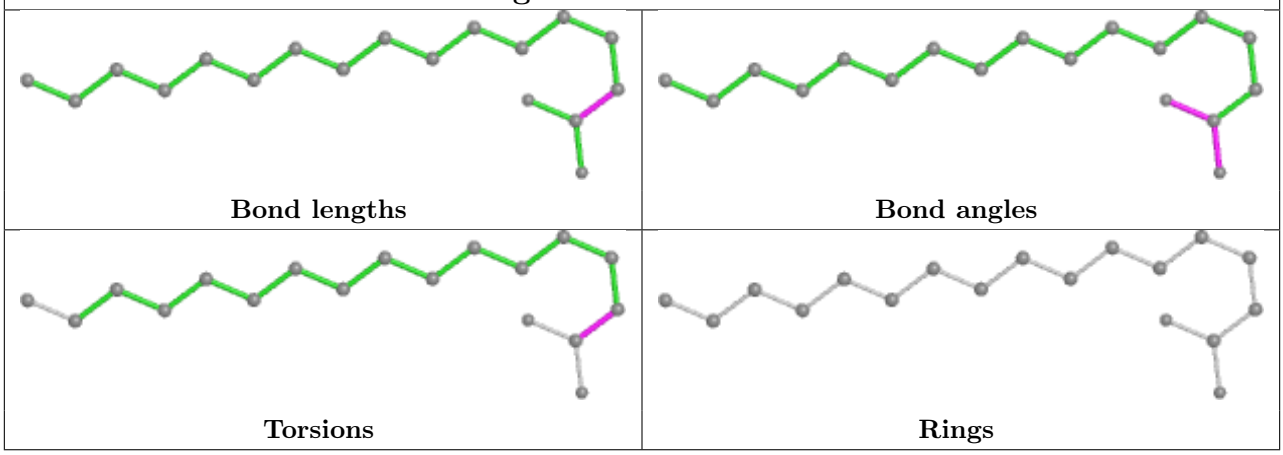
Rings

Ligand PLM R 1507	
 Bond lengths	 Bond angles
 Torsions	 Rings

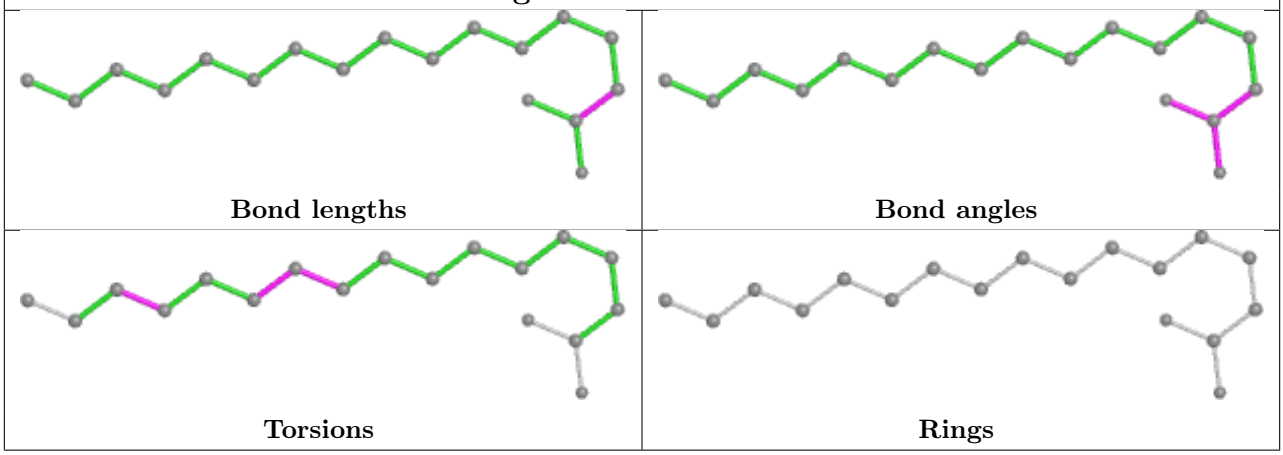
Ligand PLM R 1508	
 Bond lengths	 Bond angles
 Torsions	Rings

Ligand PLM R 1503	
 Bond lengths	 Bond angles
 Torsions	 Rings

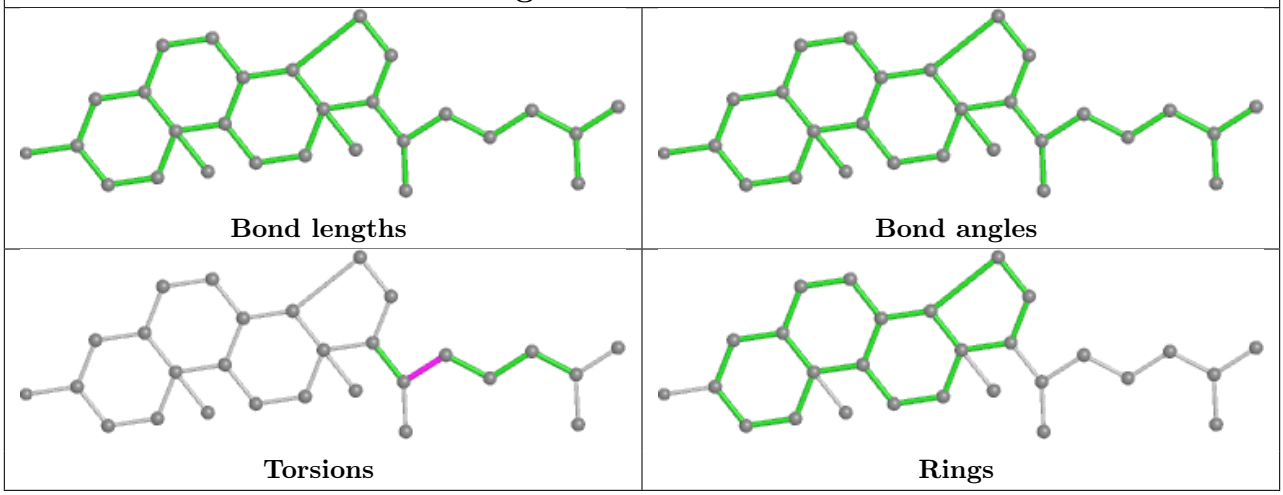
Ligand PLM R 1509



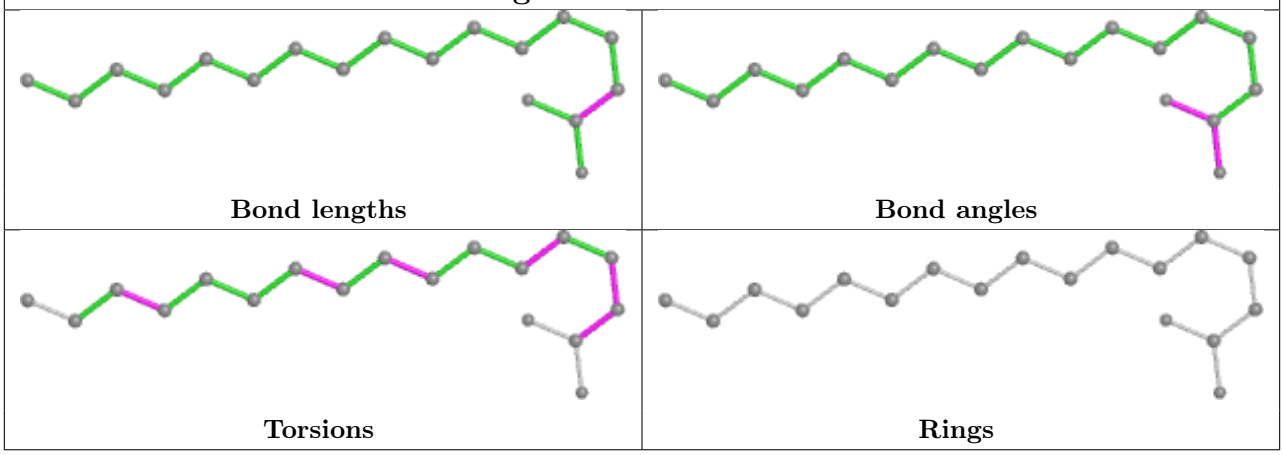
Ligand PLM R 1511



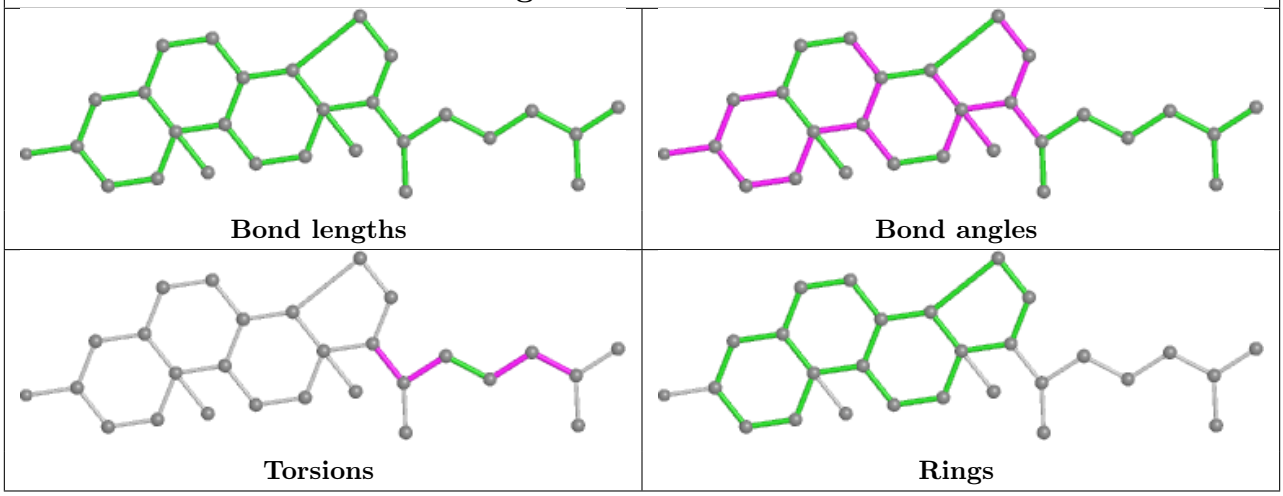
Ligand CLR R 1513



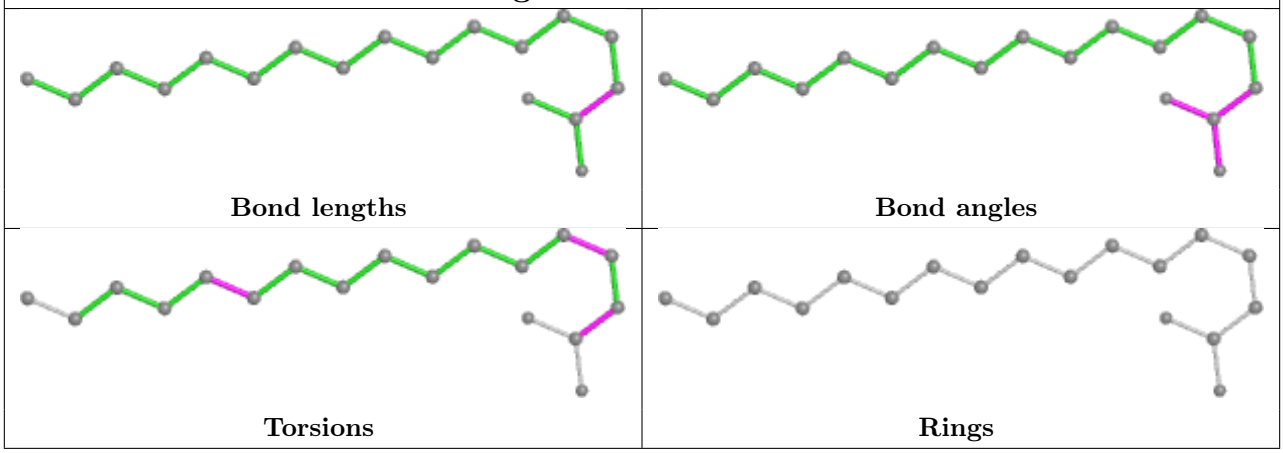
Ligand PLM R 1502

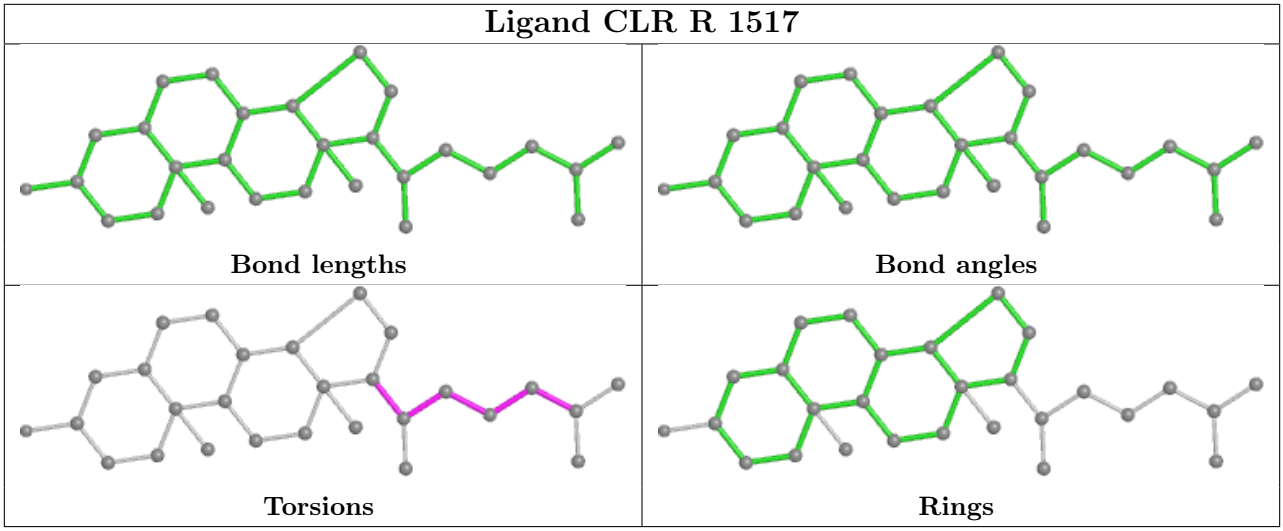


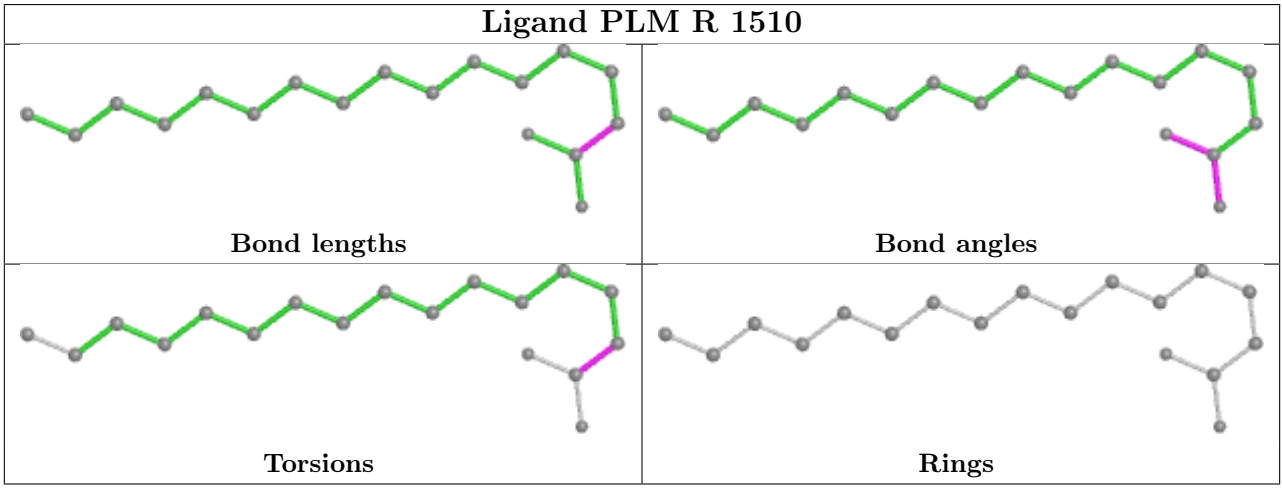
Ligand CLR R 1515



Ligand PLM R 1506







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.

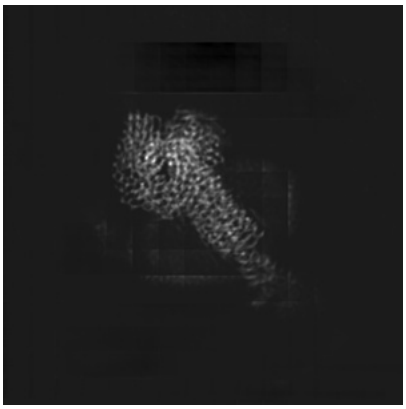
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34587. These allow visual inspection of the internal detail of the map and identification of artifacts.

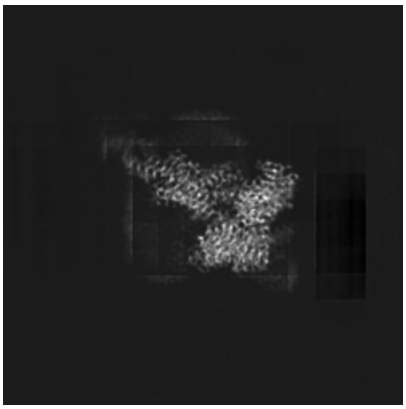
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



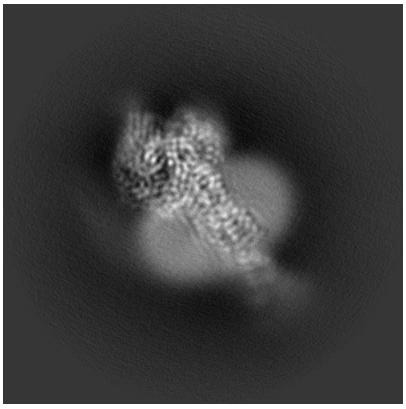
X



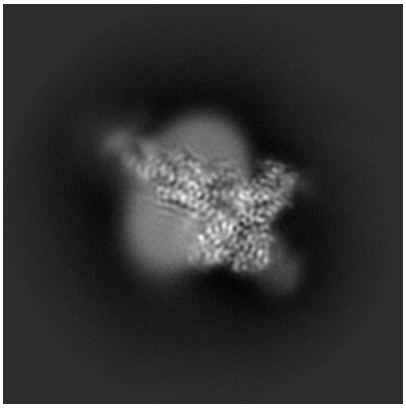
Y

Z

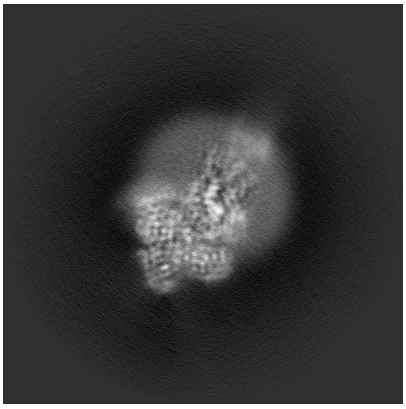
6.1.2 Raw map



X



Y



Z

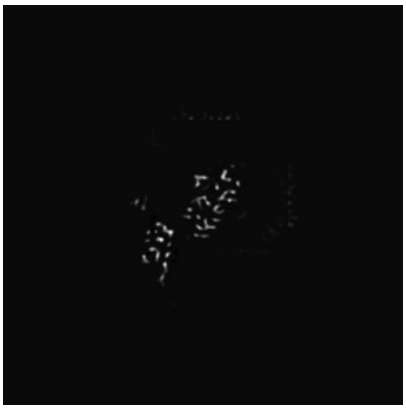
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

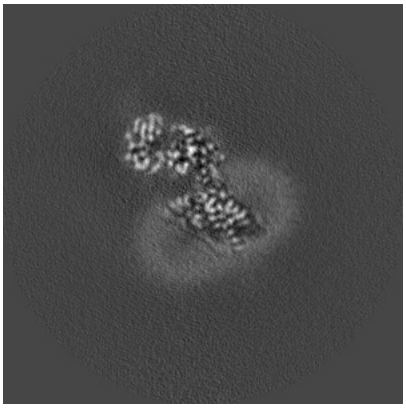
6.2.1 Primary map

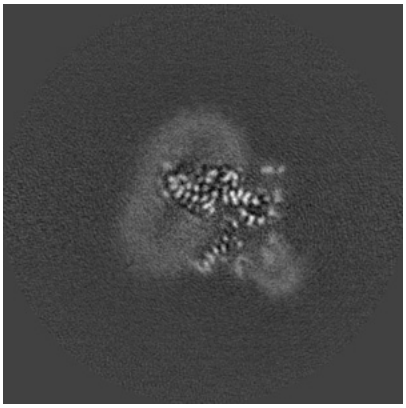
X Index: 150

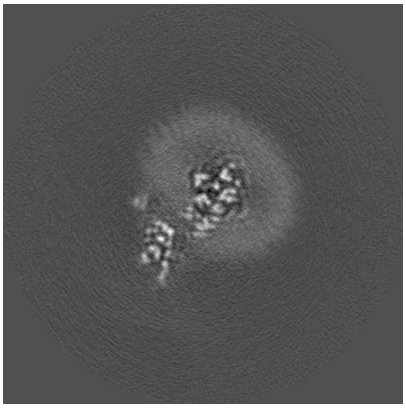
Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150


Y Index: 150

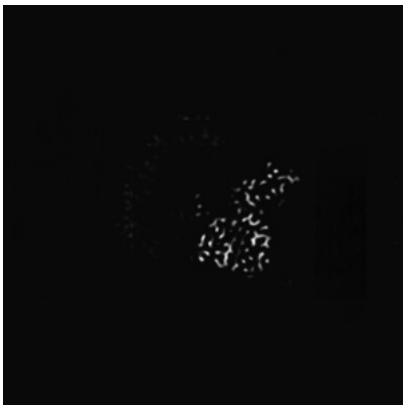

Z Index: 150

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

6.3 Largest variance slices (i)

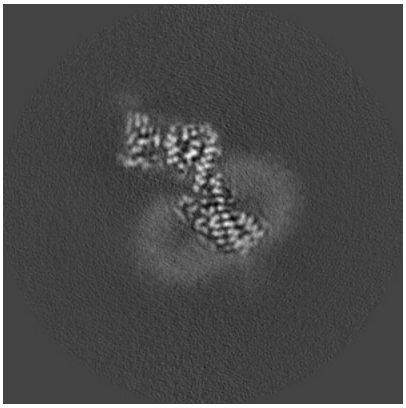
6.3.1 Primary map

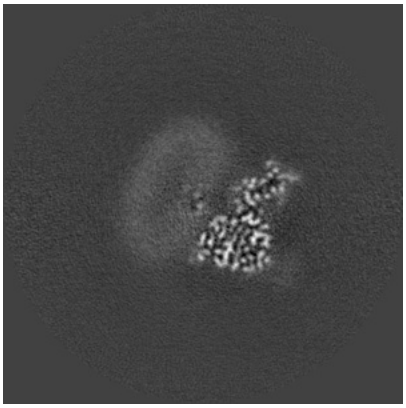
X Index: 158

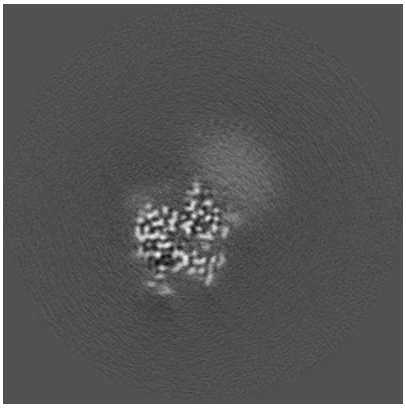

Y Index: 129

Z Index: 181

6.3.2 Raw map


X Index: 155

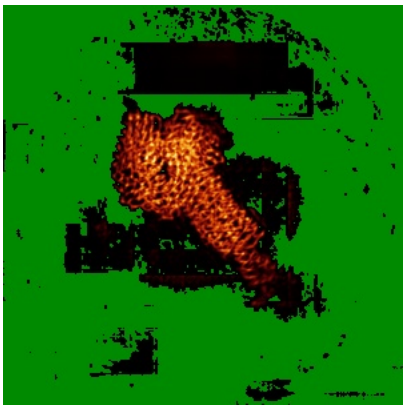

Y Index: 129

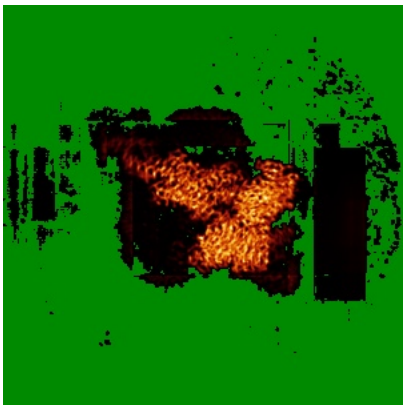

Z Index: 181

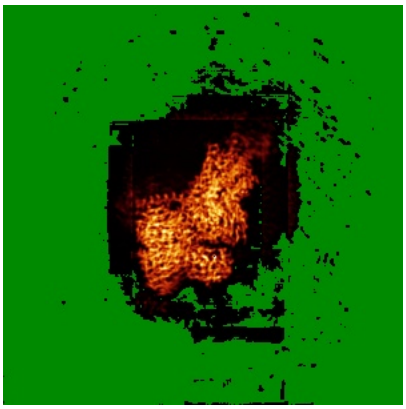
The images above show the largest variance slices of the map in three orthogonal directions.

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

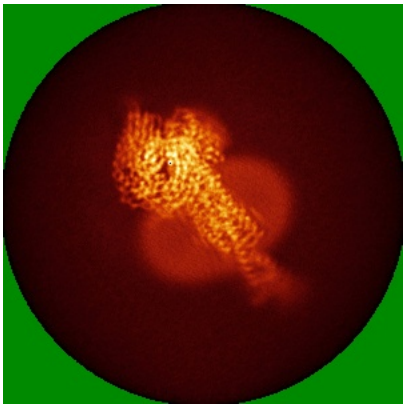
6.4.1 Primary map

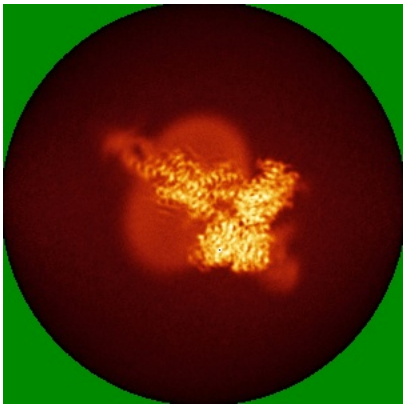

X

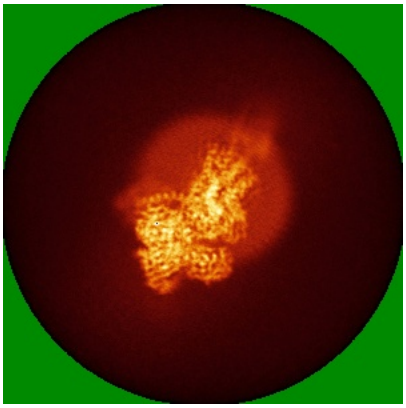

Y


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 0.332. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

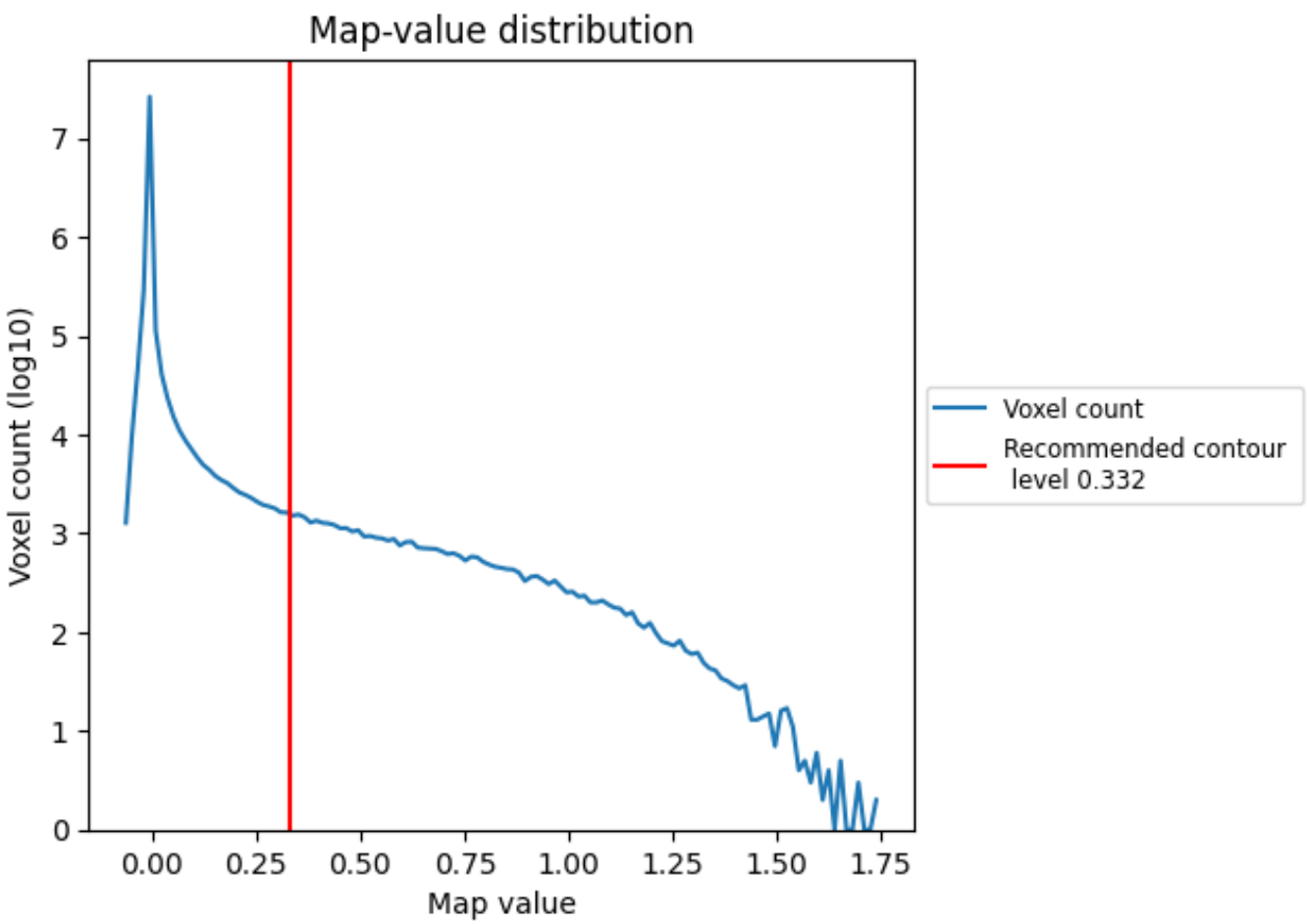
6.6 Mask visualisation (i)

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

7 Map analysis (i)

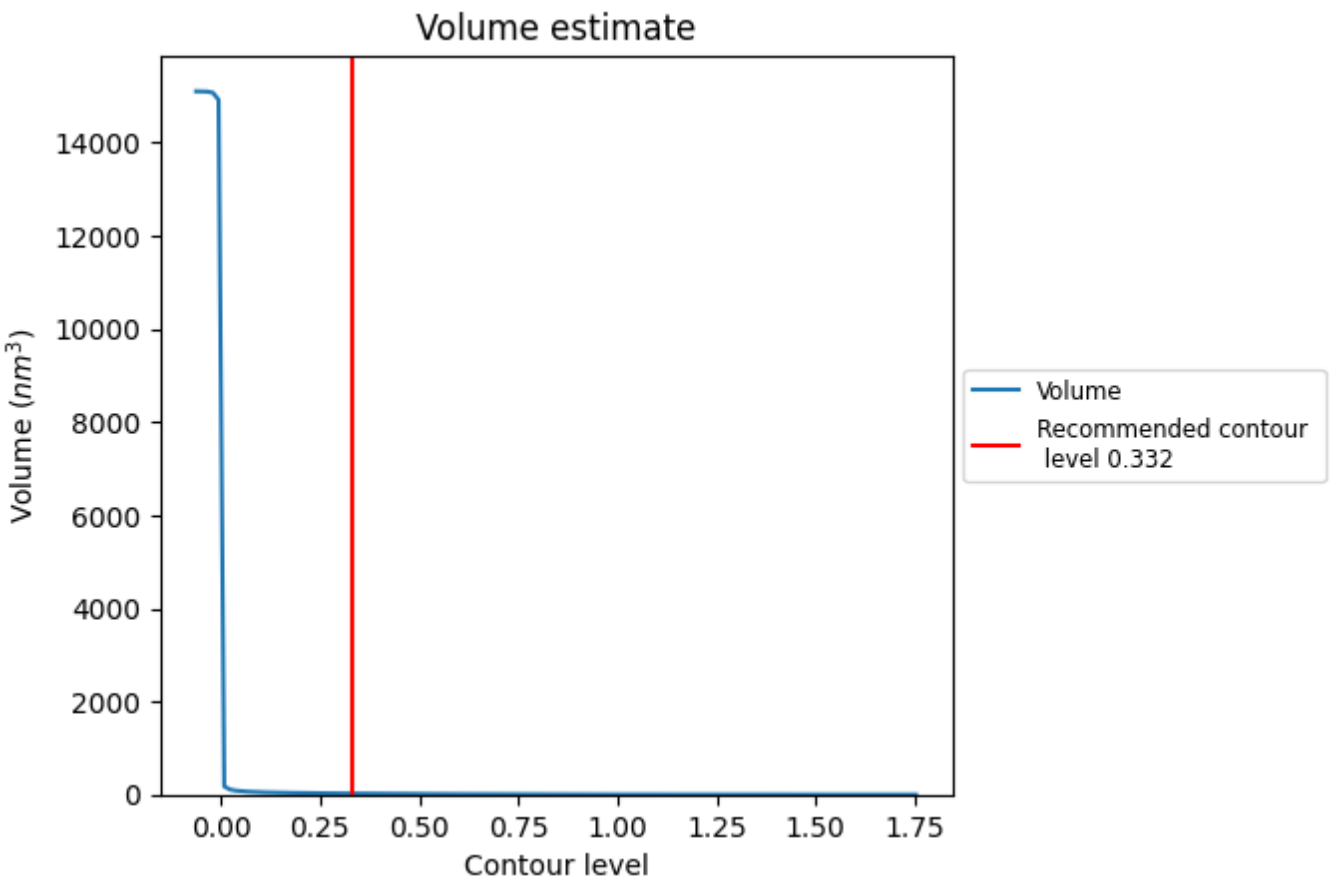
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

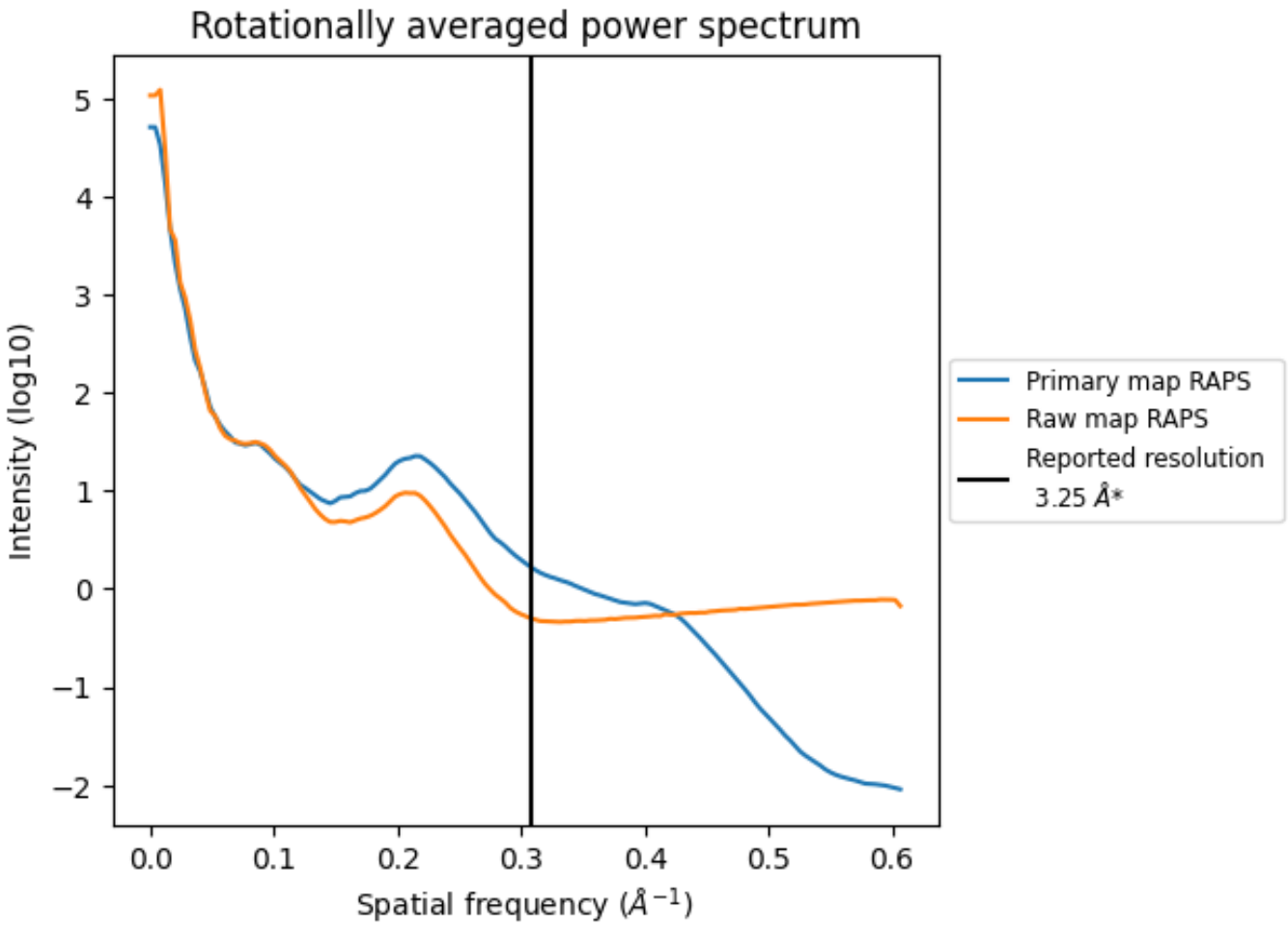
7.2 Volume estimate (i)



The volume at the recommended contour level is 22 nm^3; this corresponds to an approximate mass of 20 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)

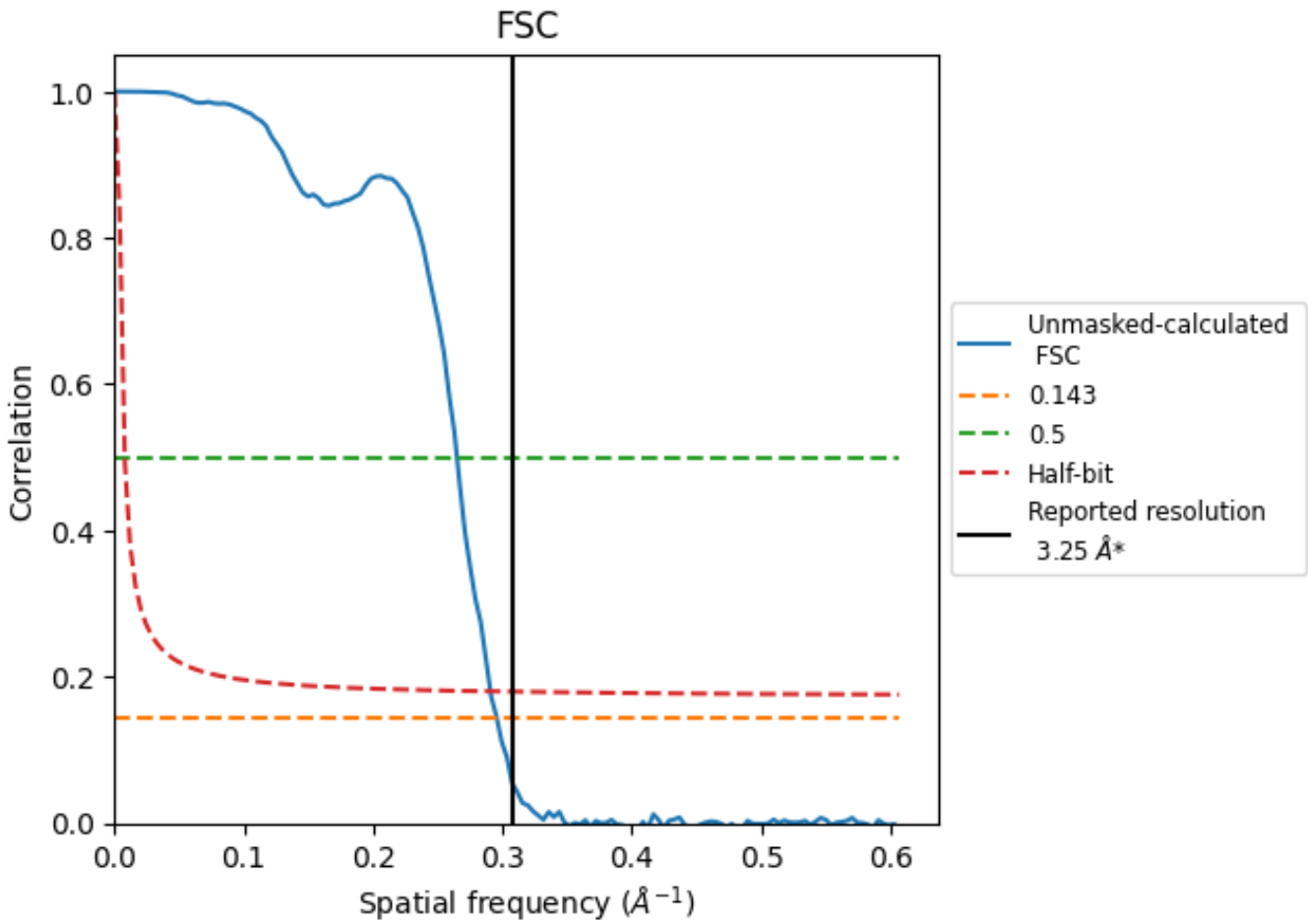


*Reported resolution corresponds to spatial frequency of 0.308 Å^{-1}

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 0.308 Å^{-1}

8.2 Resolution estimates (i)

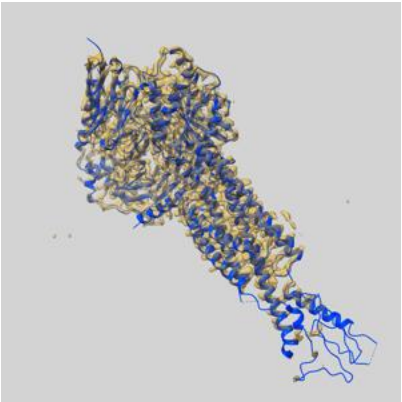
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	3.78	3.44

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

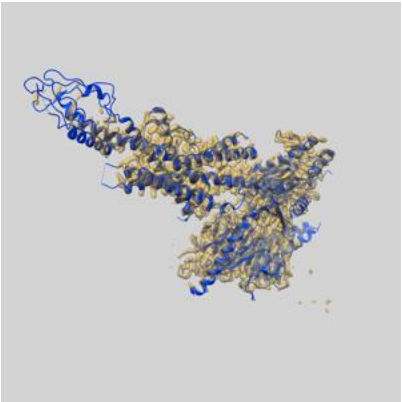
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34587 and PDB model 8HAF. Per-residue inclusion information can be found in section 3 on page 8.

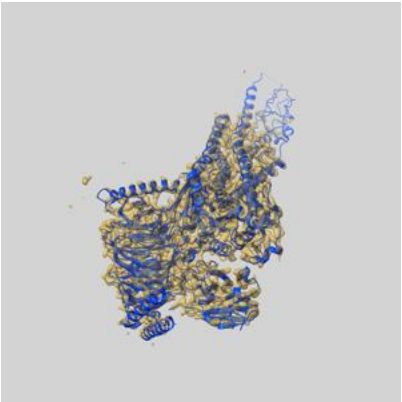
9.1 Map-model overlay (i)



X



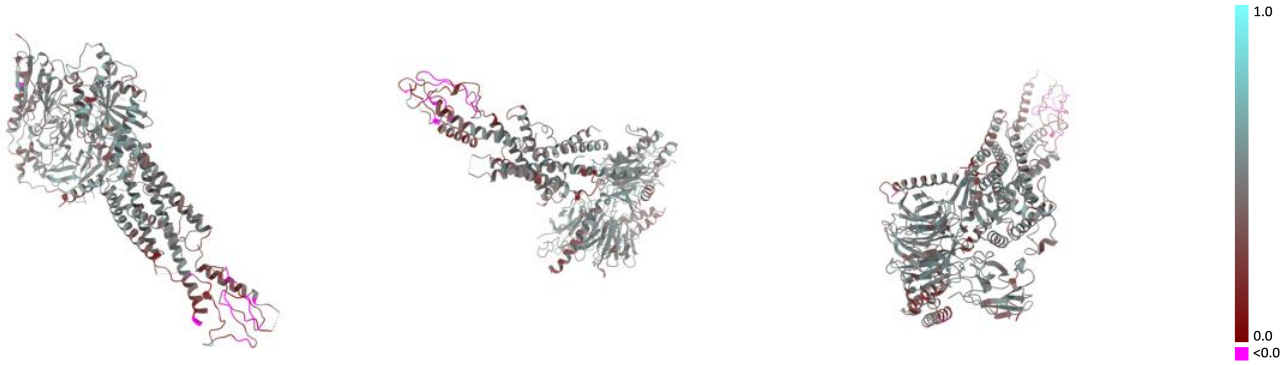
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.332 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.

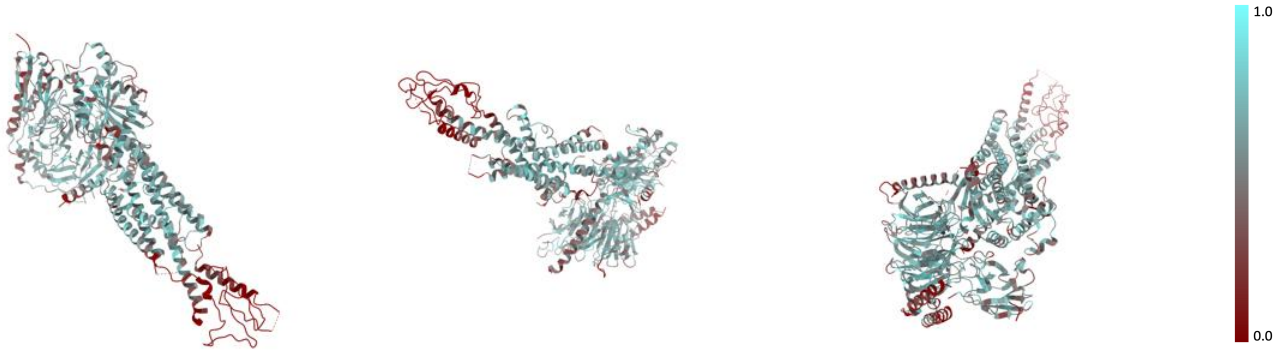
9.2 Q-score mapped to coordinate model (i)



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.

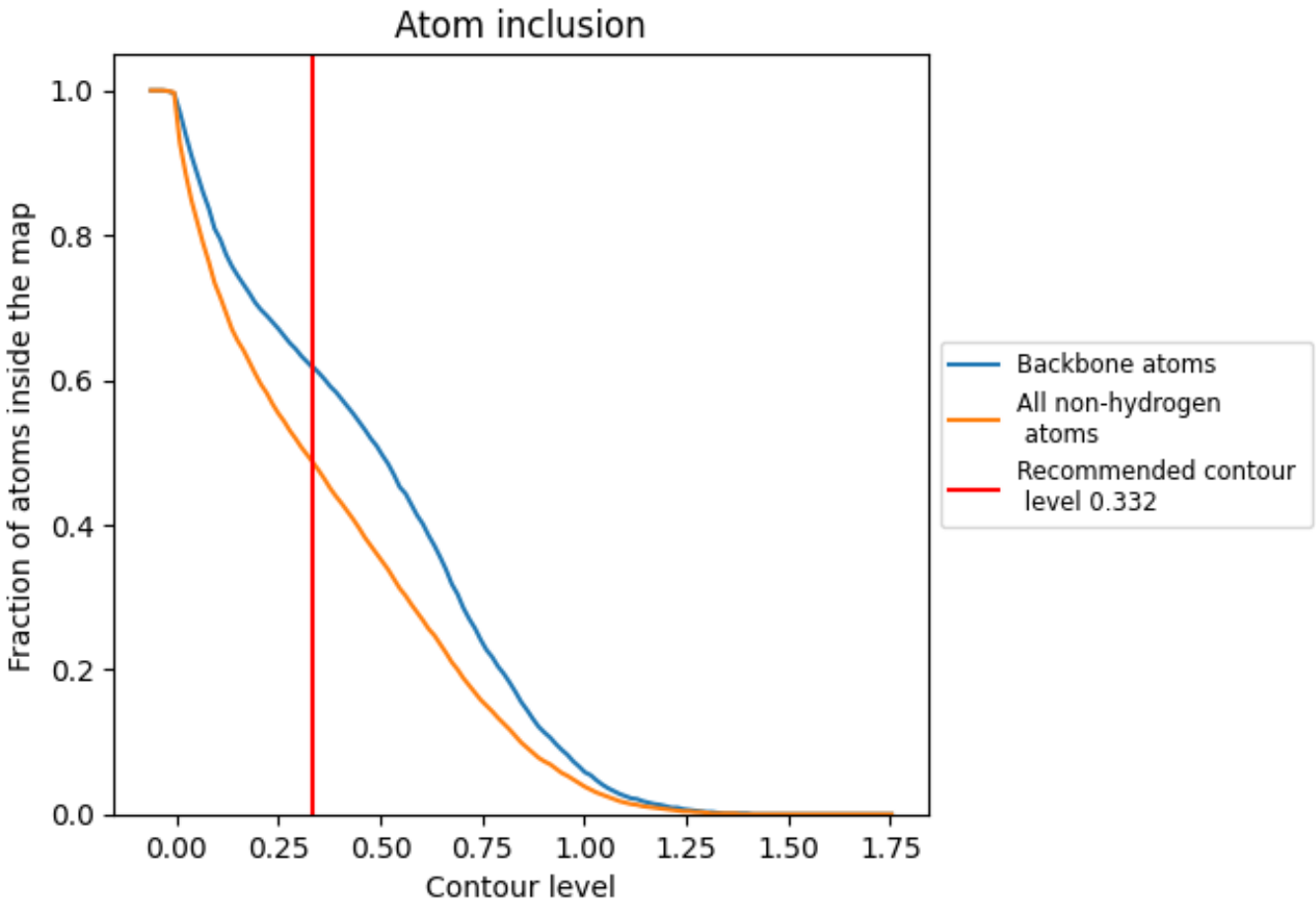
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.332).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 49% 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 (0.332) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4880	0.4300
A	0.5730	0.4730
B	0.5680	0.4840
G	0.4150	0.4070
N	0.5500	0.4630
P	0.4680	0.4020
R	0.3710	0.3600