Full wwPDB EM Validation Report ⓘ

Mar 26, 2025 – 02:57 PM JST

PDB ID	:	9INF
EMDB ID	:	EMD-60705
Title	:	Cryo-EM structure of human XPR1 in closed state in the presence of KIDINS220-1-432 and 10 mM KH2PO4
Authors	:	Yin, Y.; Zuo, P.; Liang, L.
Deposited on	:	2024-07-06
Resolution	:	3.36 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

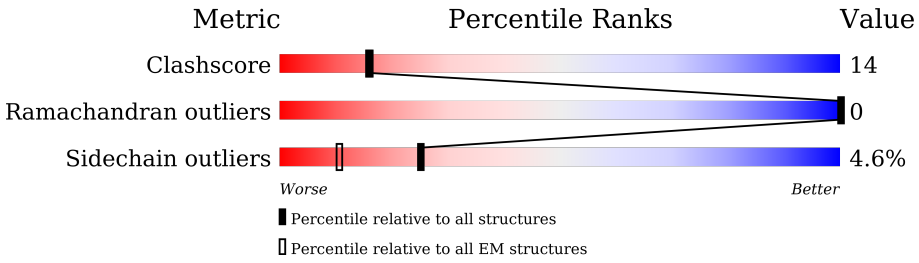
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.36 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	704	35% 21% 43%
1	B	704	5% 37% 19% 43%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7282 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.

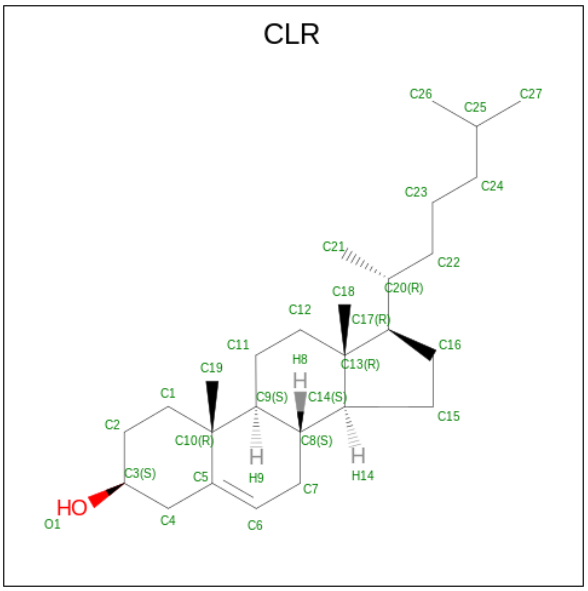
- Molecule 1 is a protein called Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	401	Total	C	N	O	S	0	0
			3333	2233	535	549	16		
1	B	401	Total	C	N	O	S	0	0
			3333	2233	535	549	16		

There are 16 discrepancies between the modelled and reference sequences:

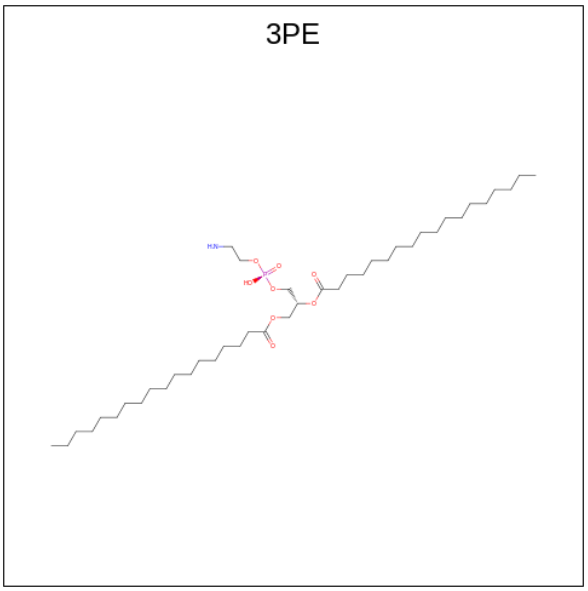
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	SER	-	expression tag	UNP Q9UBH6
A	698	ARG	-	expression tag	UNP Q9UBH6
A	699	GLU	-	expression tag	UNP Q9UBH6
A	700	ASN	-	expression tag	UNP Q9UBH6
A	701	LEU	-	expression tag	UNP Q9UBH6
A	702	TYR	-	expression tag	UNP Q9UBH6
A	703	PHE	-	expression tag	UNP Q9UBH6
A	704	GLN	-	expression tag	UNP Q9UBH6
B	697	SER	-	expression tag	UNP Q9UBH6
B	698	ARG	-	expression tag	UNP Q9UBH6
B	699	GLU	-	expression tag	UNP Q9UBH6
B	700	ASN	-	expression tag	UNP Q9UBH6
B	701	LEU	-	expression tag	UNP Q9UBH6
B	702	TYR	-	expression tag	UNP Q9UBH6
B	703	PHE	-	expression tag	UNP Q9UBH6
B	704	GLN	-	expression tag	UNP Q9UBH6

- Molecule 2 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).



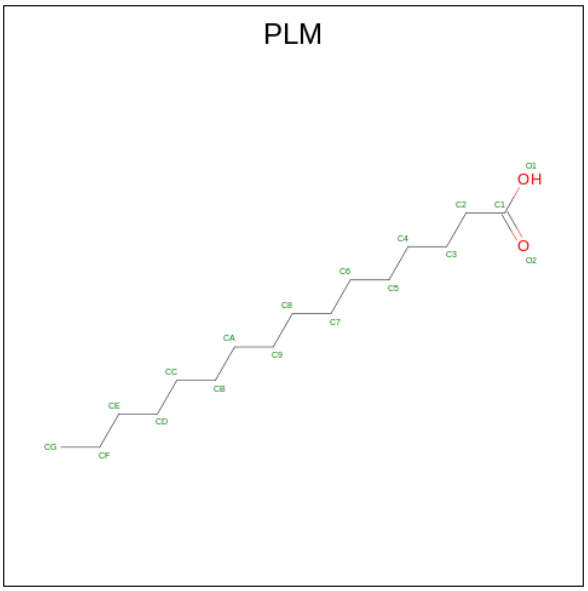
Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	A	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0
2	B	1	Total C O 28 27 1	0

- Molecule 3 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



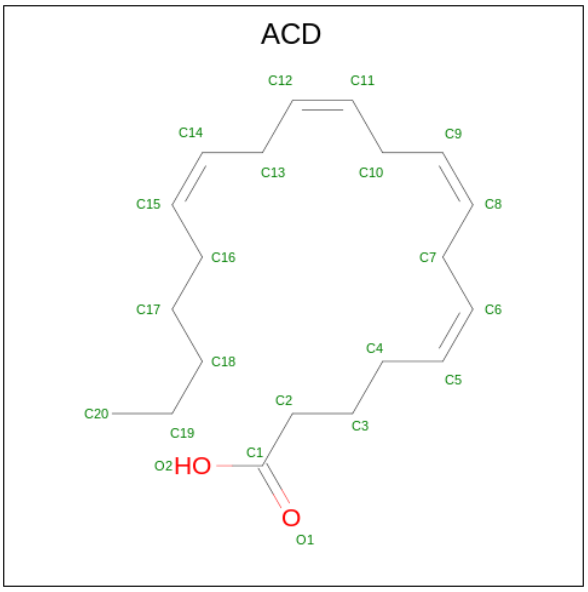
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C O 18 16 2	0
4	B	1	Total C O 18 16 2	0

- Molecule 5 is ARACHIDONIC ACID (three-letter code: ACD) (formula: $C_{20}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 22 20 2	0

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total	C	O	0
			22	20	2	

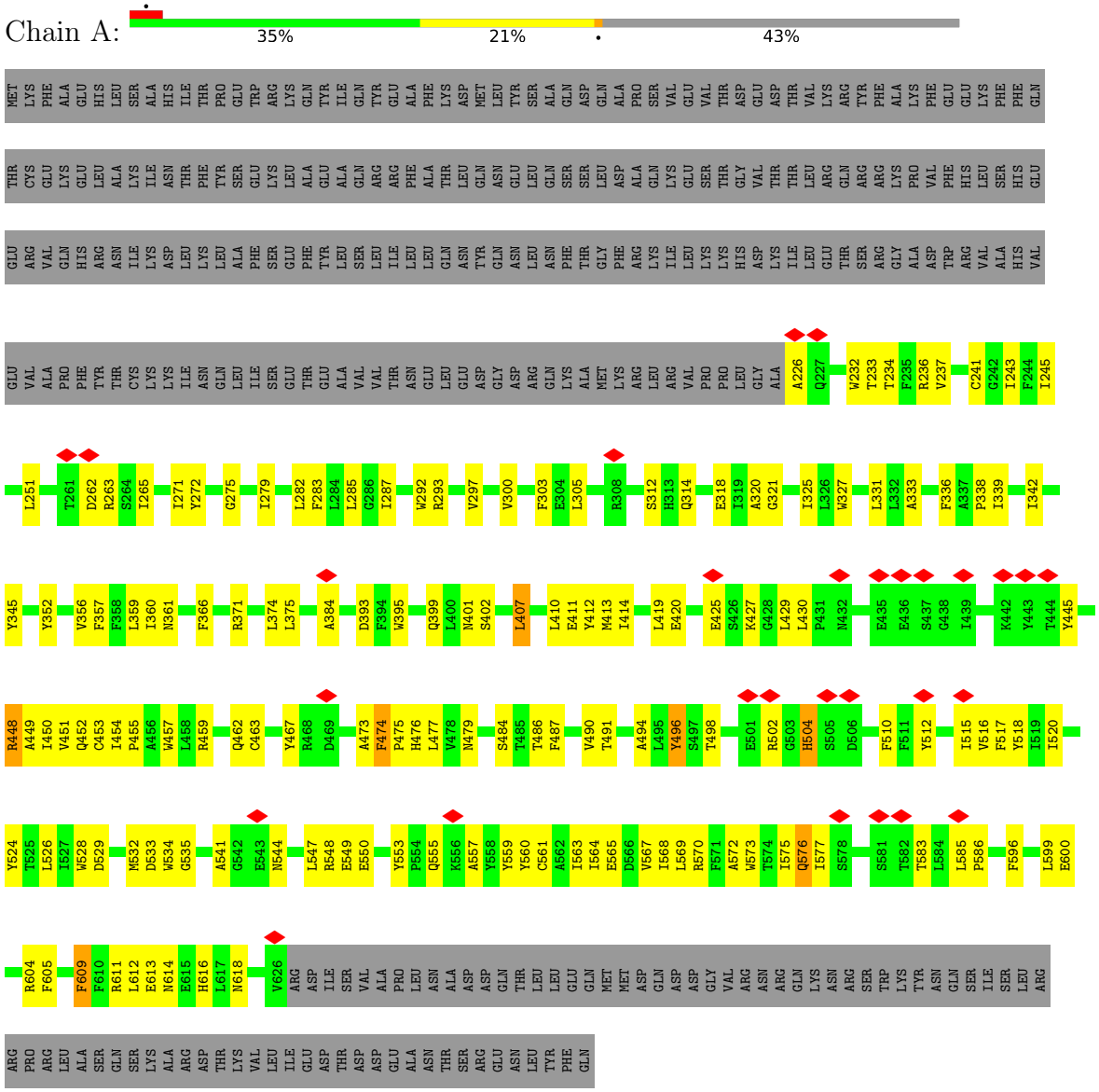
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		AltConf
6	A	3	Total	O	0
			3	3	
6	B	3	Total	O	0
			3	3	

3 Residue-property plots (i)

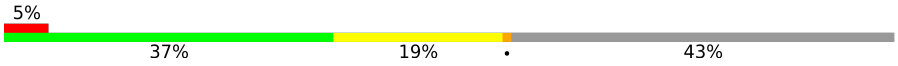
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

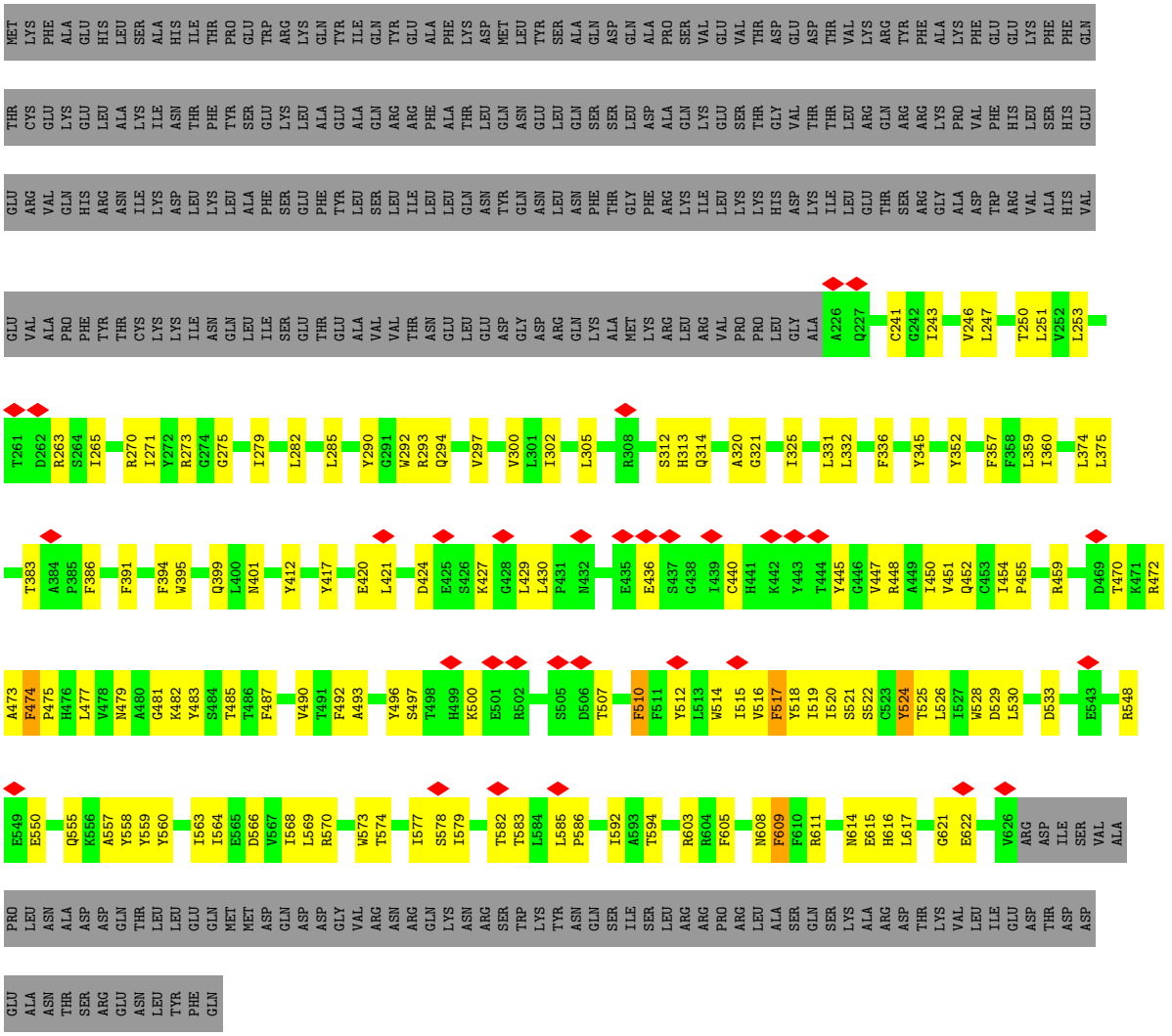
• Molecule 1: Solute carrier family 53 member 1



• Molecule 1: Solute carrier family 53 member 1

Chain B:


5%
37%
19%
43%


MET LYS PHE ALA GLU HIS LEU SER ALA HIS ILE THR PRO GLU TRP ARG LYS GLN TYR ILE GLN TYR GLU ALA PHE LYS ASP MET LEU TYR SER ALA GLN ASP GLN ALA PRO SER VAL GLU VAL THR ASP GLU ASP THR VAL LYS ARG TYR PHE ALA LYS PHE GLU GLU LYS PHE PHE GLN
THR CYS GLU LYS GLU LEU ALA LYS ILE ASN THR PHE TYR SER GLU LYS LEU ALA GLU ALA GLN ARG ARG PHE ALA THR LEU GLN ASN GLU LEU GLN SER SER LEU ASP ALA GLN LYS GLU SER THR GLY VAL THR THR LEU ARG GLN ARG ARG LYS PRO VAL PHE HIS LEU SER HIS GLU
GLU ARG VAL GLN HIS ARG ASN ILE LYS ASP LEU LYS LEU ALA PHE SER GLU PHE TYR LEU SER LEU LEU LEU GLN ASN TYR GLN ASN LEU ASN PHE THR GLY PHE ARG LYS ILE LEU LYS LYS HIS ASP LYS ILE LEU GLU THR SER ARG GLY ALA ASP TRP ARG VAL ALA HIS VAL
GLU VAL ALA PRO PHE TYR THR CYS LYS LYS ILE ASN GLN LEU LEU GLU ASP GLY ASP ARG GLN LYS ALA MET LYS ARG LEU ARG VAL PRO PRO LEU GLY ALA A226 Q227 C241 G242 I243 V246 L247 T250 L251 V252 L253
T261 D262 R263 S264 I265 R270 I271 Y272 R273 G274 G275 I279 L282 L285 Y290 G291 W292 R293 Q294 V297 V300 L301 I302 L305 R308 S312 H313 Q314 A320 G321 I325 L331 L332 F336 Y345 Y362 F357 F358 L359 I360 L374 L375
T383 A384 P385 F386 F391 F394 W395 Q399 L400 N401 Y412 Y417 E420 L421 D424 E425 S426 K427 G428 L429 L430 P431 N432 E435 E436 S437 G438 I439 C440 H441 K442 Y443 T444 Y445 G446 V447 R448 A449 I450 V451 Q452 C453 I454 P455 R459 D469 T470 K471 R472
A473 F474 P475 H476 L477 V478 N479 A480 G481 K482 Y483 S484 T485 T486 F487 V490 T491 F492 A493 Y496 S497 T498 H499 K500 E501 R502 S505 D506 T507 F510 F511 Y512 L513 W514 I515 V516 F517 Y518 I519 I520 S521 S522 C523 Y524 T525 L526 I527 W528 D529 L530 D533 E543 R548
E549 E550 Q555 K556 A557 Y558 Y559 Y560 I563 I564 E565 D566 V567 I568 L569 R570 W573 T574 I577 S578 I579 T582 T583 L584 L585 P586 I592 A593 T594 R603 R604 F605 N608 F609 F610 R611 N614 E615 H616 L617 G621 E622 V626 ARG ASP ILE SER VAL ALA
PRO LEU ASN ALA ASP ASP GLN THR LEU LEU GLU GLN MET MET ASP GLN ASP ASP GLY VAL ARG ASN ARG GLN LYS ASN ARG SER TRP LYS TYR ASN GLN SER ILE SER LEU ARG ARG PRO ARG LEU ALA SER GLN SER LYS ALA ARG ASP THR LYS VAL LEU ILE GLU ASP THR ASP ASP
GLU ALA ASN THR SER ARG GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	230260	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)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.095	Depositor
Minimum map value	-0.718	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	394.08, 394.08, 394.08	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.821, 0.821, 0.821	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLR, PLM, ACD, 3PE

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	0.26	0/3444	0.49	0/4688
1	B	0.27	0/3444	0.49	0/4688
All	All	0.26	0/6888	0.49	0/9376

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3333	0	3317	100	0
1	B	3333	0	3317	99	0
2	A	140	0	229	7	0
2	B	84	0	138	6	0
3	A	153	0	246	11	0
3	B	153	0	246	11	0
4	A	18	0	31	1	0
4	B	18	0	31	0	0
5	A	22	0	31	0	0
5	B	22	0	31	0	0
6	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	3	0	0	0	0
All	All	7282	0	7617	212	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 14.

All (212) 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)
1:A:419:LEU:HG	1:A:420:GLU:HG3	1.61	0.81
1:B:560:TYR:HA	1:B:563:ILE:HD12	1.61	0.80
1:A:374:LEU:HD22	3:A:802:3PE:H241	1.68	0.75
1:B:293:ARG:HH12	1:B:312:SER:HA	1.55	0.72
1:B:374:LEU:HD22	3:B:802:3PE:H241	1.73	0.71
1:A:529:ASP:OD2	1:A:570:ARG:NH2	2.22	0.71
1:A:459:ARG:NH2	1:A:463:CYS:SG	2.65	0.70
1:A:560:TYR:HA	1:A:563:ILE:HD12	1.76	0.67
1:B:560:TYR:O	1:B:564:ILE:HD12	1.94	0.67
1:B:300:VAL:HG23	1:B:305:LEU:HB2	1.77	0.66
1:B:514:TRP:HZ2	1:B:578:SER:HB2	1.60	0.65
1:B:579:ILE:HD12	1:B:592:ILE:HG23	1.78	0.65
1:A:263:ARG:NH2	1:A:425:GLU:OE2	2.28	0.64
1:A:534:TRP:O	1:A:548:ARG:NH1	2.31	0.63
2:A:807:CLR:H231	2:A:807:CLR:H162	1.81	0.62
1:A:411:GLU:HA	1:A:414:ILE:HD12	1.81	0.62
1:A:454:ILE:HG23	1:A:455:PRO:HD3	1.82	0.61
1:B:395:TRP:O	1:B:399:GLN:HG2	2.01	0.61
1:A:548:ARG:NH2	1:A:613:GLU:OE1	2.34	0.60
1:B:401:ASN:HA	1:B:455:PRO:HB2	1.83	0.60
1:A:565:GLU:HB2	2:A:801:CLR:H25	1.84	0.59
1:B:481:GLY:O	1:B:485:THR:HG23	2.02	0.59
1:B:359:LEU:HD13	3:B:802:3PE:H2A2	1.84	0.59
1:A:533:ASP:OD1	1:A:611:ARG:NH1	2.37	0.58
1:B:550:GLU:N	1:B:550:GLU:OE1	2.37	0.58
1:B:579:ILE:HA	1:B:583:THR:HB	1.85	0.58
1:A:297:VAL:HG23	1:A:616:HIS:HB2	1.84	0.58
1:B:564:ILE:O	1:B:568:ILE:HG13	2.03	0.57
1:B:585:LEU:HG	1:B:586:PRO:HD3	1.86	0.57
1:A:559:TYR:O	1:A:563:ILE:HG13	2.04	0.57
1:A:559:TYR:OH	1:A:613:GLU:OE2	2.21	0.57
1:B:452:GLN:NE2	1:B:577:ILE:HG23	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:VAL:HA	1:B:305:LEU:HD12	1.87	0.56
1:A:475:PRO:HB2	1:A:528:TRP:CH2	2.39	0.56
1:A:502:ARG:HB2	1:A:504:HIS:CE1	2.40	0.56
1:A:484:SER:HA	1:A:487:PHE:CD2	2.40	0.56
1:B:314:GLN:HE22	3:B:805:3PE:H31	1.71	0.56
1:A:533:ASP:HA	1:A:611:ARG:HH11	1.69	0.56
1:A:526:LEU:HD21	1:A:567:VAL:HG22	1.87	0.55
1:B:522:SER:HB2	1:B:574:THR:HG21	1.88	0.55
1:A:300:VAL:HG23	1:A:305:LEU:HB2	1.88	0.55
3:A:806:3PE:H322	3:A:806:3PE:H241	1.89	0.55
1:A:233:THR:O	1:A:237:VAL:HG13	2.07	0.55
1:A:512:TYR:O	1:A:516:VAL:HG12	2.07	0.55
1:A:573:TRP:O	1:A:577:ILE:HD12	2.07	0.54
1:B:521:SER:O	1:B:525:THR:HG23	2.07	0.54
1:B:530:LEU:HD11	1:B:563:ILE:HG23	1.89	0.54
1:A:395:TRP:O	1:A:399:GLN:HG2	2.07	0.54
1:B:533:ASP:HA	1:B:611:ARG:HH11	1.73	0.54
1:A:236:ARG:NH2	4:A:809:PLM:O2	2.41	0.54
1:A:550:GLU:N	1:A:550:GLU:OE1	2.41	0.54
1:A:359:LEU:HD22	3:A:802:3PE:H2C2	1.90	0.54
1:B:482:LYS:HD2	1:B:525:THR:HA	1.90	0.54
1:B:417:TYR:HA	1:B:421:LEU:HD13	1.90	0.53
1:A:573:TRP:CZ3	1:A:577:ILE:HD11	2.43	0.53
1:B:451:VAL:HA	1:B:454:ILE:HG12	1.88	0.53
1:A:561:CYS:HA	1:A:564:ILE:HD12	1.90	0.53
1:B:285:LEU:HD21	1:B:395:TRP:HH2	1.73	0.52
2:A:805:CLR:H152	1:B:253:LEU:HD21	1.91	0.52
1:A:564:ILE:O	1:A:568:ILE:HG13	2.09	0.52
1:A:555:GLN:HG3	1:A:557:ALA:H	1.75	0.52
1:B:573:TRP:CE2	1:B:577:ILE:HD11	2.44	0.52
1:A:293:ARG:HH22	1:A:312:SER:HA	1.75	0.52
1:A:463:CYS:SG	1:A:479:ASN:ND2	2.83	0.52
1:A:384:ALA:HB1	1:A:462:GLN:HG3	1.92	0.52
1:B:473:ALA:HA	1:B:477:LEU:HD23	1.90	0.51
1:B:282:LEU:HB3	1:B:320:ALA:HB2	1.92	0.51
1:A:467:TYR:HB2	1:A:476:HIS:HB3	1.92	0.51
1:A:475:PRO:HG3	1:A:532:MET:HE1	1.93	0.51
1:B:493:ALA:HA	1:B:496:TYR:CE1	2.45	0.51
1:A:275:GLY:O	1:A:279:ILE:HG12	2.11	0.51
1:B:500:LYS:HD3	1:B:507:THR:HG21	1.93	0.50
1:B:412:TYR:HB2	1:B:448:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:GLN:OE1	1:B:608:ASN:ND2	2.44	0.50
1:B:359:LEU:HG	1:B:375:LEU:HD21	1.93	0.50
1:B:275:GLY:O	1:B:279:ILE:HG12	2.12	0.50
1:B:297:VAL:HG23	1:B:616:HIS:HB2	1.94	0.50
1:A:333:ALA:HB2	3:A:803:3PE:H282	1.94	0.50
1:A:412:TYR:HB2	1:A:448:ARG:HH22	1.76	0.49
1:B:293:ARG:HH22	1:B:312:SER:HB3	1.77	0.49
1:B:297:VAL:HG23	1:B:616:HIS:CB	2.43	0.49
1:B:533:ASP:OD1	1:B:611:ARG:NH1	2.45	0.49
1:B:391:PHE:CE1	1:B:615:GLU:HG3	2.47	0.49
1:A:285:LEU:HD21	1:A:395:TRP:HH2	1.77	0.49
1:A:449:ALA:HB1	2:A:804:CLR:H152	1.94	0.49
1:B:383:THR:HB	1:B:386:PHE:HD2	1.77	0.49
1:A:448:ARG:HA	1:A:451:VAL:HG22	1.95	0.49
1:A:576:GLN:NE2	1:A:600:GLU:OE1	2.46	0.49
1:B:559:TYR:O	1:B:563:ILE:HG13	2.13	0.49
1:A:241:CYS:SG	3:A:806:3PE:H381	2.53	0.49
1:A:494:ALA:O	1:A:498:THR:HG23	2.13	0.49
1:A:303:PHE:HE1	1:A:612:LEU:HD11	1.78	0.49
1:A:535:GLY:HA3	1:A:614:ASN:ND2	2.28	0.49
1:B:447:VAL:O	1:B:451:VAL:HG22	2.13	0.48
1:B:420:GLU:OE2	1:B:440:CYS:HB2	2.12	0.48
1:A:339:ILE:HG22	1:A:342:ILE:H	1.77	0.48
1:A:237:VAL:HG12	1:A:318:GLU:HB2	1.96	0.48
1:A:245:ILE:HG13	3:A:806:3PE:H3F1	1.96	0.48
1:A:361:ASN:O	1:A:371:ARG:NH1	2.47	0.48
1:A:410:LEU:O	1:A:414:ILE:HG13	2.13	0.48
1:A:366:PHE:O	1:A:371:ARG:NH2	2.47	0.48
1:A:263:ARG:NH2	1:A:427:LYS:HB2	2.29	0.47
1:B:270:ARG:NH2	1:B:436:GLU:OE2	2.47	0.47
1:A:321:GLY:O	1:A:325:ILE:HG12	2.14	0.47
1:B:517:PHE:HA	1:B:520:ILE:HG12	1.97	0.47
1:A:282:LEU:HB3	1:A:320:ALA:HB2	1.95	0.47
1:B:263:ARG:NH2	1:B:427:LYS:HB2	2.29	0.47
1:B:512:TYR:O	1:B:516:VAL:HG12	2.14	0.47
1:A:517:PHE:HA	1:A:520:ILE:HG12	1.96	0.47
2:A:807:CLR:H25	2:A:807:CLR:H222	1.68	0.47
1:A:560:TYR:O	1:A:564:ILE:HG13	2.15	0.46
1:B:447:VAL:HA	1:B:450:ILE:HD12	1.97	0.46
1:B:514:TRP:CZ2	1:B:578:SER:HB2	2.47	0.46
1:A:338:PRO:HB2	1:A:339:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:ARG:HD2	1:B:459:ARG:HA	1.64	0.46
1:B:529:ASP:HA	1:B:533:ASP:HB2	1.96	0.46
1:A:283:PHE:HZ	3:A:806:3PE:H2C1	1.80	0.46
3:A:806:3PE:H352	3:A:806:3PE:H382	1.73	0.46
1:B:548:ARG:HE	1:B:548:ARG:HB2	1.59	0.46
1:B:292:TRP:HE1	1:B:609:PHE:HA	1.81	0.46
1:A:407:LEU:HD12	1:A:407:LEU:H	1.80	0.46
1:B:555:GLN:HG3	1:B:557:ALA:H	1.81	0.46
1:B:569:LEU:HD13	1:B:603:ARG:HB2	1.98	0.46
1:A:272:TYR:HB3	1:A:327:TRP:HE1	1.81	0.46
2:A:801:CLR:H211	2:A:801:CLR:H232	1.81	0.45
1:B:321:GLY:O	1:B:325:ILE:HG12	2.16	0.45
1:B:512:TYR:O	1:B:515:ILE:HG22	2.16	0.45
1:A:475:PRO:HB2	1:A:528:TRP:HH2	1.82	0.45
1:B:578:SER:O	1:B:583:THR:OG1	2.22	0.45
3:B:803:3PE:H3F1	2:B:804:CLR:H25	1.98	0.45
1:A:251:LEU:HD11	1:A:331:LEU:HB3	1.97	0.45
1:A:271:ILE:O	1:A:352:TYR:OH	2.26	0.45
3:B:805:3PE:H3E1	3:B:805:3PE:H2H1	1.99	0.45
1:A:457:TRP:HA	1:A:487:PHE:HZ	1.82	0.45
1:A:360:ILE:HA	1:A:375:LEU:HD11	1.99	0.45
1:B:485:THR:HG21	1:B:524:TYR:HD2	1.82	0.45
1:A:359:LEU:HD13	3:A:802:3PE:H2A2	1.99	0.44
3:B:802:3PE:H362	3:B:802:3PE:H232	1.98	0.44
1:B:357:PHE:HA	1:B:360:ILE:HG22	1.98	0.44
1:B:558:TYR:CE2	2:B:801:CLR:H12	2.53	0.44
1:A:345:TYR:HB3	1:A:429:LEU:HB2	2.00	0.44
2:B:806:CLR:H221	2:B:806:CLR:H162	1.49	0.44
1:B:243:ILE:HG22	1:B:325:ILE:HD12	2.00	0.44
1:B:285:LEU:HD21	3:B:802:3PE:H342	2.00	0.44
3:A:803:3PE:H3E1	1:B:246:VAL:HG22	2.00	0.44
1:B:247:LEU:HD21	3:B:803:3PE:H3C1	1.98	0.44
1:B:265:ILE:HA	1:B:430:LEU:HD22	1.99	0.44
1:B:251:LEU:HD21	1:B:331:LEU:HD23	2.00	0.43
1:B:497:SER:OG	1:B:582:THR:O	2.33	0.43
1:A:265:ILE:HA	1:A:430:LEU:HD22	2.00	0.43
1:B:290:TYR:CE1	1:B:294:GLN:HG3	2.53	0.43
1:B:302:ILE:HD11	1:B:616:HIS:HB2	1.99	0.43
1:B:566:ASP:O	1:B:570:ARG:HG2	2.17	0.43
1:A:357:PHE:HA	1:A:360:ILE:HG22	1.99	0.43
1:A:585:LEU:HG	1:A:586:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:ARG:HD3	1:B:594:THR:HG23	2.00	0.43
1:B:533:ASP:HA	1:B:611:ARG:NH1	2.33	0.43
1:A:243:ILE:HG22	1:A:325:ILE:HD12	2.00	0.43
1:B:470:THR:HG23	1:B:472:ARG:H	1.82	0.43
1:B:621:GLY:O	1:B:622:GLU:HG2	2.18	0.43
1:B:271:ILE:O	1:B:352:TYR:OH	2.25	0.43
1:A:585:LEU:N	1:A:586:PRO:HD2	2.34	0.43
1:A:553:TYR:HB2	1:A:559:TYR:CE1	2.54	0.43
1:B:493:ALA:HA	1:B:496:TYR:CD1	2.54	0.43
1:A:226:ALA:HA	1:A:293:ARG:HH11	1.84	0.43
1:B:526:LEU:HB2	1:B:570:ARG:HG3	2.00	0.43
1:A:515:ILE:O	1:A:518:TYR:HB3	2.18	0.42
3:B:803:3PE:H2A1	2:B:804:CLR:H232	2.01	0.42
2:B:806:CLR:H25	2:B:806:CLR:H222	1.93	0.42
1:A:512:TYR:O	1:A:515:ILE:HG22	2.19	0.42
1:B:548:ARG:NH1	1:B:614:ASN:HB2	2.34	0.42
1:A:402:SER:OG	1:A:604:ARG:NE	2.51	0.42
1:A:474:PHE:HA	1:A:475:PRO:HA	1.93	0.42
1:A:491:THR:HA	2:A:804:CLR:H151	2.01	0.42
1:A:292:TRP:HE1	1:A:609:PHE:HA	1.85	0.42
1:A:356:VAL:O	1:A:360:ILE:HG22	2.18	0.42
1:A:453:CYS:HB3	1:A:487:PHE:CD1	2.54	0.42
1:B:250:THR:HG21	3:B:803:3PE:H381	2.01	0.42
1:B:492:PHE:HE1	1:B:510:PHE:HE1	1.67	0.42
2:B:804:CLR:H162	2:B:804:CLR:H221	1.83	0.42
1:B:520:ILE:HG13	1:B:521:SER:N	2.35	0.42
1:A:572:ALA:HA	1:A:575:ILE:HD12	2.01	0.42
1:B:412:TYR:HB2	1:B:448:ARG:HH22	1.84	0.42
1:A:410:LEU:HD23	1:A:414:ILE:HD11	2.00	0.42
1:A:541:ALA:HA	1:A:549:GLU:HA	2.02	0.42
1:A:283:PHE:CZ	1:A:287:ILE:HD11	2.55	0.42
1:A:450:ILE:H	1:A:450:ILE:HG13	1.62	0.41
1:A:473:ALA:HA	1:A:477:LEU:HD23	2.01	0.41
1:A:448:ARG:HE	1:A:448:ARG:HB2	1.78	0.41
1:A:569:LEU:HD21	1:A:599:LEU:HD12	2.02	0.41
3:A:806:3PE:H222	3:A:806:3PE:H251	1.85	0.41
1:B:251:LEU:HD13	1:B:332:LEU:HG	2.02	0.41
1:A:271:ILE:HG12	1:A:413:MET:HG3	2.03	0.41
1:B:417:TYR:HA	1:B:421:LEU:CD1	2.49	0.41
1:B:474:PHE:HA	1:B:475:PRO:HA	1.92	0.41
1:A:234:THR:O	1:A:237:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:OD1	1:A:262:ASP:N	2.54	0.41
1:B:263:ARG:HH21	1:B:427:LYS:HB2	1.86	0.41
1:B:331:LEU:HD12	1:B:331:LEU:HA	1.88	0.41
1:B:424:ASP:OD1	1:B:424:ASP:N	2.54	0.41
1:B:452:GLN:HG2	1:B:490:VAL:HG21	2.03	0.41
1:A:486:THR:O	1:A:490:VAL:HG12	2.21	0.41
1:A:496:TYR:HE2	1:A:583:THR:HG23	1.86	0.41
1:B:459:ARG:HB3	1:B:483:TYR:CE2	2.56	0.40
1:B:519:ILE:HD13	1:B:519:ILE:HA	1.98	0.40
1:A:232:TRP:HZ3	3:B:805:3PE:H231	1.86	0.40
1:A:544:ASN:HB3	1:A:547:LEU:HB2	2.03	0.40
1:B:475:PRO:HB2	1:B:528:TRP:CH2	2.57	0.40
1:B:617:LEU:HD23	1:B:617:LEU:HA	1.87	0.40
1:B:290:TYR:HB2	1:B:313:HIS:CD2	2.56	0.40
1:B:332:LEU:HD23	1:B:332:LEU:HA	1.91	0.40
1:B:450:ILE:H	1:B:450:ILE:HG13	1.62	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	399/704 (57%)	382 (96%)	17 (4%)	0	100	100
1	B	399/704 (57%)	388 (97%)	11 (3%)	0	100	100
All	All	798/1408 (57%)	770 (96%)	28 (4%)	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	355/629 (56%)	337 (95%)	18 (5%)	20 46
1	B	355/629 (56%)	340 (96%)	15 (4%)	25 51
All	All	710/1258 (56%)	677 (95%)	33 (5%)	25 50

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	336	PHE
1	A	393	ASP
1	A	401	ASN
1	A	407	LEU
1	A	445	TYR
1	A	448	ARG
1	A	452	GLN
1	A	474	PHE
1	A	496	TYR
1	A	504	HIS
1	A	510	PHE
1	A	524	TYR
1	A	576	GLN
1	A	596	PHE
1	A	605	PHE
1	A	609	PHE
1	A	618	ASN
1	B	241	CYS
1	B	336	PHE
1	B	345	TYR
1	B	394	PHE
1	B	429	LEU
1	B	445	TYR
1	B	474	PHE
1	B	479	ASN
1	B	487	PHE

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Mol	Chain	Res	Type
1	B	510	PHE
1	B	517	PHE
1	B	518	TYR
1	B	524	TYR
1	B	605	PHE
1	B	609	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	ASN
1	B	314	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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	$\#\|Z\| > 2$
2	CLR	B	801	-	31,31,31	0.36	0	48,48,48	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CLR	A	804	-	31,31,31	0.35	0	48,48,48	0.53	0
2	CLR	B	804	-	31,31,31	0.36	0	48,48,48	0.50	0
3	3PE	B	803	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
3	3PE	B	805	-	50,50,50	0.51	0	53,55,55	0.54	1 (1%)
4	PLM	A	809	-	17,17,17	0.90	1 (5%)	17,17,17	0.75	2 (11%)
2	CLR	A	807	-	31,31,31	0.42	0	48,48,48	1.12	5 (10%)
5	ACD	A	810	-	21,21,21	0.57	0	21,21,21	0.58	0
2	CLR	A	808	-	31,31,31	0.36	0	48,48,48	0.53	0
2	CLR	B	806	-	31,31,31	0.35	0	48,48,48	0.57	0
5	ACD	B	808	-	21,21,21	0.57	0	21,21,21	0.59	0
3	3PE	A	803	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
3	3PE	A	802	-	50,50,50	0.51	0	53,55,55	0.58	2 (3%)
3	3PE	B	802	-	50,50,50	0.51	0	53,55,55	0.57	2 (3%)
2	CLR	A	805	-	31,31,31	0.35	0	48,48,48	0.49	0
4	PLM	B	807	-	17,17,17	0.91	1 (5%)	17,17,17	0.75	2 (11%)
3	3PE	A	806	-	50,50,50	0.51	0	53,55,55	0.53	1 (1%)
2	CLR	A	801	-	31,31,31	0.36	0	48,48,48	0.51	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
2	CLR	B	801	-	-	2/10/68/68	0/4/4/4
2	CLR	A	804	-	-	5/10/68/68	0/4/4/4
2	CLR	B	804	-	-	7/10/68/68	0/4/4/4
3	3PE	B	803	-	-	17/54/54/54	-
3	3PE	B	805	-	-	17/54/54/54	-
4	PLM	A	809	-	-	4/15/15/15	-
2	CLR	A	807	-	-	6/10/68/68	0/4/4/4
5	ACD	A	810	-	-	3/19/19/19	-
2	CLR	A	808	-	-	6/10/68/68	0/4/4/4
2	CLR	B	806	-	-	8/10/68/68	0/4/4/4
5	ACD	B	808	-	-	4/19/19/19	-
3	3PE	A	803	-	-	15/54/54/54	-
3	3PE	A	802	-	-	22/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3PE	B	802	-	-	24/54/54/54	-
2	CLR	A	805	-	-	7/10/68/68	0/4/4/4
4	PLM	B	807	-	-	3/15/15/15	-
3	3PE	A	806	-	-	27/54/54/54	-
2	CLR	A	801	-	-	3/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	807	PLM	C2-C1	2.92	1.57	1.50
4	A	809	PLM	C2-C1	2.86	1.57	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	807	CLR	C13-C17-C20	3.54	125.03	119.49
2	A	807	CLR	C22-C20-C17	3.40	117.30	110.28
2	A	807	CLR	C17-C13-C14	-3.08	96.42	100.07
2	A	807	CLR	C16-C17-C20	2.48	115.98	112.15
3	A	802	3PE	C2-O21-C21	2.38	123.64	117.79
3	B	803	3PE	O12-P-O14	2.34	123.81	112.24
3	A	803	3PE	O12-P-O14	2.34	123.80	112.24
3	B	805	3PE	O12-P-O14	2.34	123.79	112.24
3	B	802	3PE	O12-P-O14	2.33	123.78	112.24
3	A	806	3PE	O12-P-O14	2.33	123.77	112.24
3	A	802	3PE	O12-P-O14	2.32	123.71	112.24
3	B	802	3PE	C2-O21-C21	2.30	123.46	117.79
4	B	807	PLM	O1-C1-O2	2.23	128.87	123.30
4	A	809	PLM	O1-C1-O2	2.23	128.85	123.30
2	A	807	CLR	C23-C22-C20	2.11	121.11	115.03
4	A	809	PLM	O2-C1-C2	-2.01	116.61	123.08
4	B	807	PLM	O2-C1-C2	-2.00	116.65	123.08

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	806	CLR	C13-C17-C20-C21
2	B	806	CLR	C13-C17-C20-C22
2	B	806	CLR	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
3	A	802	3PE	C1-O11-P-O12
3	A	802	3PE	C1-O11-P-O13
3	A	802	3PE	C1-O11-P-O14
3	A	802	3PE	C11-O13-P-O12
3	A	802	3PE	C12-C11-O13-P
3	A	802	3PE	O13-C11-C12-N
3	A	802	3PE	O22-C21-O21-C2
3	A	803	3PE	C11-O13-P-O12
3	A	803	3PE	O13-C11-C12-N
3	A	803	3PE	O22-C21-O21-C2
3	A	806	3PE	O13-C11-C12-N
3	A	806	3PE	C22-C21-O21-C2
3	B	802	3PE	C11-O13-P-O12
3	B	802	3PE	C12-C11-O13-P
3	B	802	3PE	O13-C11-C12-N
3	B	802	3PE	C22-C21-O21-C2
3	B	803	3PE	C11-O13-P-O12
3	B	803	3PE	C11-O13-P-O14
3	B	803	3PE	O13-C11-C12-N
3	B	803	3PE	O22-C21-O21-C2
3	B	805	3PE	O13-C11-C12-N
3	B	805	3PE	O22-C21-O21-C2
3	B	805	3PE	C22-C21-O21-C2
5	B	808	ACD	C12-C13-C14-C15
2	B	804	CLR	C21-C20-C22-C23
3	A	803	3PE	O32-C31-O31-C3
3	B	803	3PE	O32-C31-O31-C3
2	B	806	CLR	C16-C17-C20-C21
3	A	806	3PE	O22-C21-O21-C2
3	B	802	3PE	O22-C21-O21-C2
3	A	803	3PE	C32-C31-O31-C3
3	B	803	3PE	C32-C31-O31-C3
3	A	802	3PE	C22-C21-O21-C2
3	A	803	3PE	C22-C21-O21-C2
3	B	803	3PE	C22-C21-O21-C2
2	B	806	CLR	C21-C20-C22-C23
3	A	806	3PE	C35-C36-C37-C38
2	A	805	CLR	C21-C20-C22-C23
2	A	805	CLR	C17-C20-C22-C23
2	A	808	CLR	C21-C20-C22-C23
2	B	801	CLR	C17-C20-C22-C23
3	B	805	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
2	A	805	CLR	C22-C23-C24-C25
2	B	804	CLR	C22-C23-C24-C25
3	A	802	3PE	C34-C35-C36-C37
2	A	807	CLR	C13-C17-C20-C22
2	B	804	CLR	C17-C20-C22-C23
2	A	801	CLR	C20-C22-C23-C24
2	A	807	CLR	C22-C23-C24-C25
4	A	809	PLM	C1-C2-C3-C4
2	B	806	CLR	C17-C20-C22-C23
2	A	801	CLR	C22-C23-C24-C25
2	A	807	CLR	C16-C17-C20-C21
2	A	807	CLR	C13-C17-C20-C21
2	B	806	CLR	C20-C22-C23-C24
3	A	802	3PE	C11-O13-P-O11
3	A	803	3PE	C11-O13-P-O11
3	B	802	3PE	C11-O13-P-O11
3	B	803	3PE	C11-O13-P-O11
3	B	802	3PE	C21-C22-C23-C24
2	A	805	CLR	C13-C17-C20-C22
3	A	803	3PE	C27-C28-C29-C2A
3	B	802	3PE	C37-C38-C39-C3A
3	A	806	3PE	C23-C24-C25-C26
4	B	807	PLM	C4-C5-C6-C7
3	A	802	3PE	C37-C38-C39-C3A
3	A	803	3PE	C28-C29-C2A-C2B
3	A	803	3PE	C3C-C3D-C3E-C3F
3	B	803	3PE	C28-C29-C2A-C2B
2	A	808	CLR	C13-C17-C20-C22
3	A	806	3PE	C27-C28-C29-C2A
3	B	805	3PE	C23-C24-C25-C26
4	B	807	PLM	C3-C4-C5-C6
2	A	804	CLR	C22-C23-C24-C25
3	A	802	3PE	C22-C23-C24-C25
3	A	806	3PE	C38-C39-C3A-C3B
3	A	802	3PE	C36-C37-C38-C39
3	B	802	3PE	C22-C23-C24-C25
3	B	803	3PE	C36-C37-C38-C39
2	B	804	CLR	C13-C17-C20-C22
3	B	802	3PE	C36-C37-C38-C39
3	A	806	3PE	O11-C1-C2-O21
2	A	805	CLR	C13-C17-C20-C21
2	A	808	CLR	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
2	A	801	CLR	C21-C20-C22-C23
2	B	801	CLR	C21-C20-C22-C23
3	A	802	3PE	C1-C2-C3-O31
2	A	805	CLR	C16-C17-C20-C22
2	A	805	CLR	C16-C17-C20-C21
4	B	807	PLM	CA-CB-CC-CD
2	A	808	CLR	C16-C17-C20-C22
4	A	809	PLM	CA-CB-CC-CD
2	A	808	CLR	C16-C17-C20-C21
2	B	804	CLR	C16-C17-C20-C21
2	B	804	CLR	C13-C17-C20-C21
2	A	807	CLR	C20-C22-C23-C24
3	B	805	3PE	C27-C28-C29-C2A
2	B	804	CLR	C16-C17-C20-C22
3	B	805	3PE	O11-C1-C2-C3
3	A	806	3PE	C1-C2-C3-O31
3	B	802	3PE	C1-C2-C3-O31
5	A	810	ACD	C6-C7-C8-C9
3	A	806	3PE	C32-C33-C34-C35
3	A	806	3PE	C39-C3A-C3B-C3C
3	B	802	3PE	O11-C1-C2-O21
3	B	802	3PE	C26-C27-C28-C29
3	B	802	3PE	C34-C35-C36-C37
2	A	804	CLR	C20-C22-C23-C24
3	A	802	3PE	C26-C27-C28-C29
3	B	803	3PE	C27-C28-C29-C2A
3	A	806	3PE	O11-C1-C2-C3
3	B	802	3PE	O11-C1-C2-C3
3	B	803	3PE	C2D-C2E-C2F-C2G
3	A	806	3PE	C22-C23-C24-C25
3	A	802	3PE	C35-C36-C37-C38
3	A	806	3PE	C32-C31-O31-C3
3	B	805	3PE	C2-C1-O11-P
3	A	802	3PE	C21-C22-C23-C24
3	B	805	3PE	C25-C26-C27-C28
3	B	802	3PE	C3B-C3C-C3D-C3E
3	A	802	3PE	O21-C2-C3-O31
3	A	806	3PE	O21-C2-C3-O31
3	A	802	3PE	C24-C25-C26-C27
3	A	806	3PE	O32-C31-O31-C3
3	A	806	3PE	C2-C1-O11-P
3	A	802	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
2	A	804	CLR	C13-C17-C20-C21
3	A	806	3PE	C1-O11-P-O13
3	B	802	3PE	C1-O11-P-O13
3	B	805	3PE	C1-O11-P-O13
3	B	803	3PE	C32-C33-C34-C35
3	B	805	3PE	C1-C2-C3-O31
3	A	806	3PE	C36-C37-C38-C39
3	A	803	3PE	C36-C37-C38-C39
3	B	802	3PE	C24-C25-C26-C27
3	A	806	3PE	C2D-C2E-C2F-C2G
3	B	805	3PE	C26-C27-C28-C29
2	A	804	CLR	C13-C17-C20-C22
4	A	809	PLM	O2-C1-C2-C3
5	B	808	ACD	C11-C12-C13-C14
3	A	806	3PE	C37-C38-C39-C3A
3	A	803	3PE	C38-C39-C3A-C3B
2	A	808	CLR	C20-C22-C23-C24
3	B	802	3PE	O21-C2-C3-O31
3	A	802	3PE	C2B-C2C-C2D-C2E
3	B	802	3PE	C2B-C2C-C2D-C2E
3	A	802	3PE	C32-C33-C34-C35
3	B	802	3PE	C32-C33-C34-C35
3	B	803	3PE	C1-O11-P-O13
4	A	809	PLM	O1-C1-C2-C3
3	A	803	3PE	C2B-C2C-C2D-C2E
3	B	802	3PE	C2E-C2F-C2G-C2H
3	B	805	3PE	C2F-C2G-C2H-C2I
3	B	803	3PE	O21-C21-C22-C23
2	A	804	CLR	C16-C17-C20-C22
3	A	803	3PE	O21-C21-C22-C23
3	B	805	3PE	O21-C21-C22-C23
3	A	806	3PE	O21-C21-C22-C23
2	A	807	CLR	C23-C24-C25-C27
3	B	803	3PE	O22-C21-C22-C23
3	A	806	3PE	C34-C35-C36-C37
3	A	806	3PE	C3D-C3E-C3F-C3G
3	A	803	3PE	O22-C21-C22-C23
3	B	805	3PE	O22-C21-C22-C23
3	B	802	3PE	C35-C36-C37-C38
3	B	805	3PE	C21-C22-C23-C24
3	A	806	3PE	C1-O11-P-O14
3	A	806	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
3	B	802	3PE	C1-O11-P-O14
3	B	803	3PE	C1-O11-P-O14
5	A	810	ACD	O2-C1-C2-C3
5	B	808	ACD	O2-C1-C2-C3
5	A	810	ACD	O1-C1-C2-C3
2	B	806	CLR	C22-C23-C24-C25
5	B	808	ACD	O1-C1-C2-C3
3	A	806	3PE	O22-C21-C22-C23
3	B	805	3PE	C35-C36-C37-C38

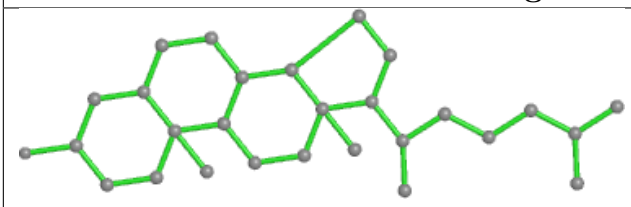
There are no ring outliers.

14 monomers are involved in 34 short contacts:

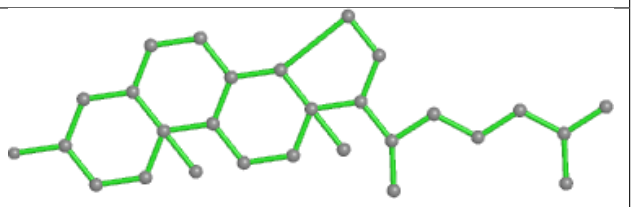
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	CLR	1	0
2	A	804	CLR	2	0
2	B	804	CLR	3	0
3	B	803	3PE	4	0
3	B	805	3PE	3	0
4	A	809	PLM	1	0
2	A	807	CLR	2	0
2	B	806	CLR	2	0
3	A	803	3PE	2	0
3	A	802	3PE	3	0
3	B	802	3PE	4	0
2	A	805	CLR	1	0
3	A	806	3PE	6	0
2	A	801	CLR	2	0

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.

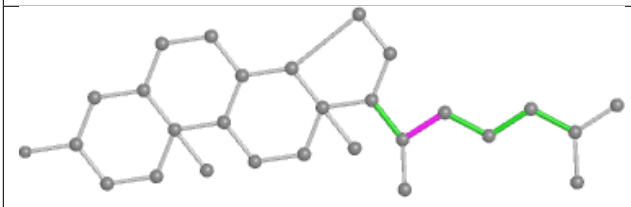
Ligand CLR B 801



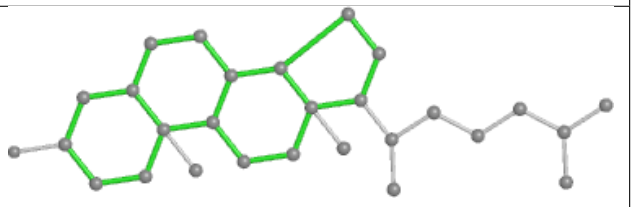
Bond lengths



Bond angles

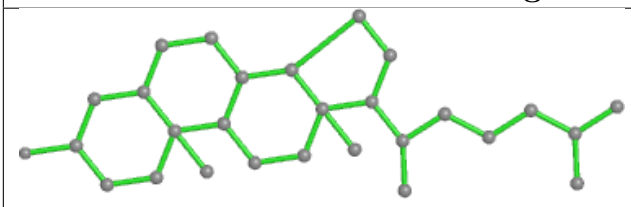


Torsions

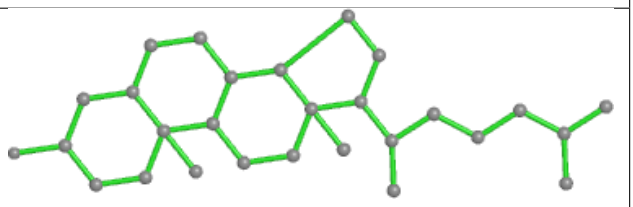


Rings

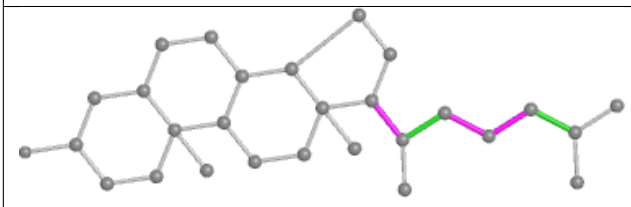
Ligand CLR A 804



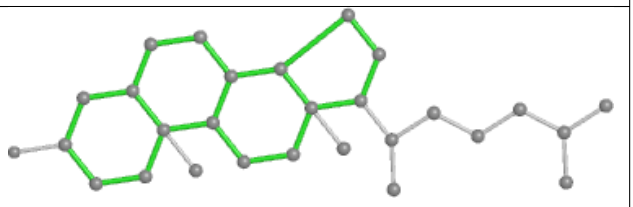
Bond lengths



Bond angles

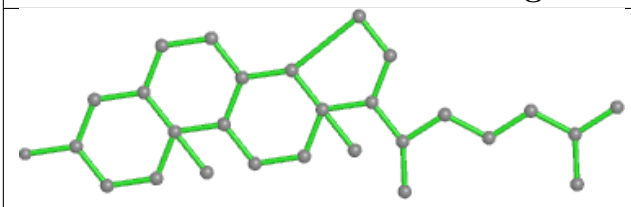


Torsions

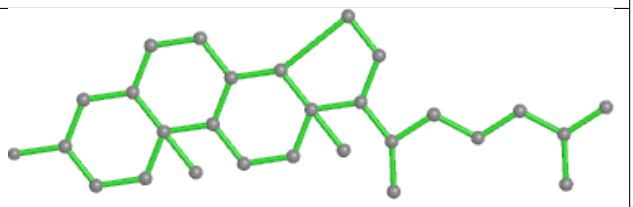


Rings

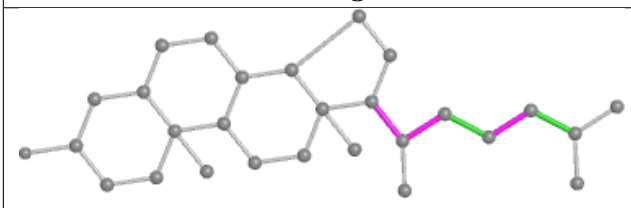
Ligand CLR B 804



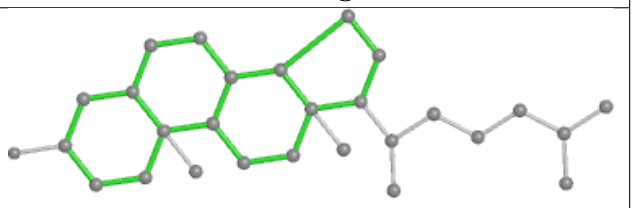
Bond lengths



Bond angles

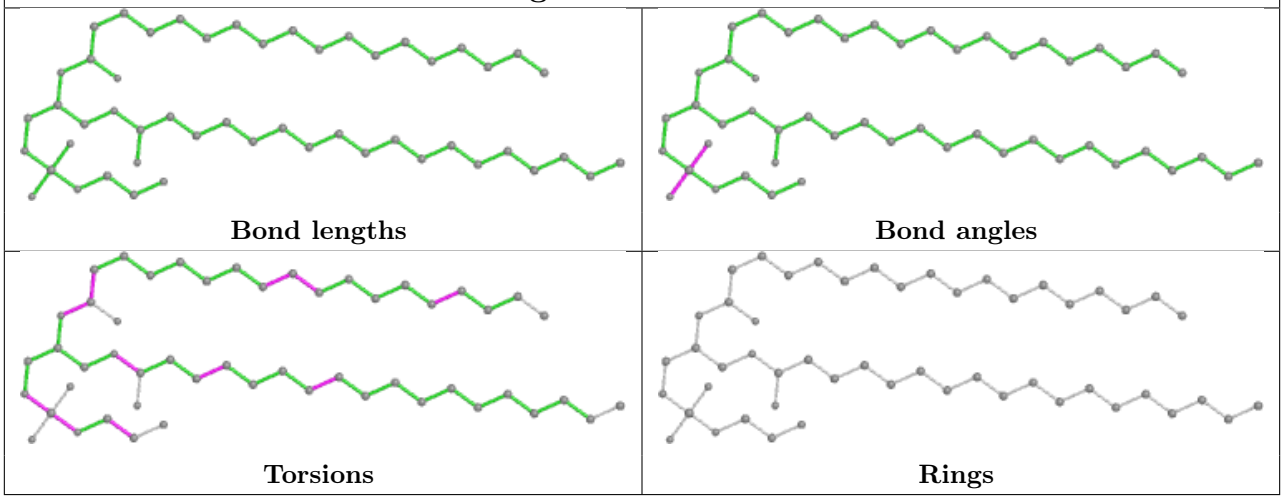


Torsions

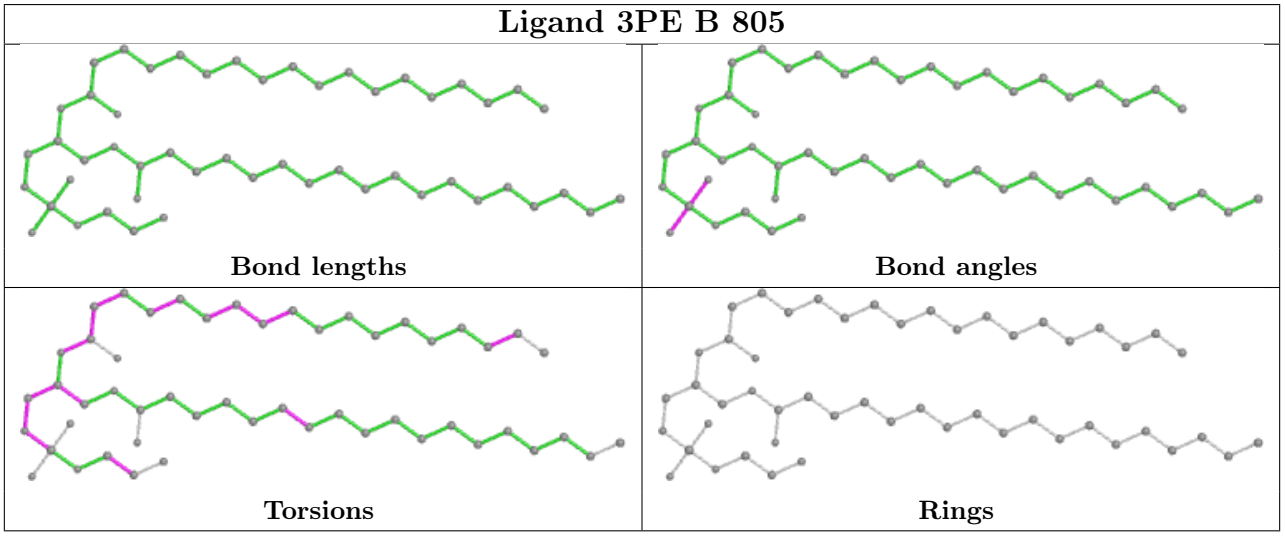


Rings

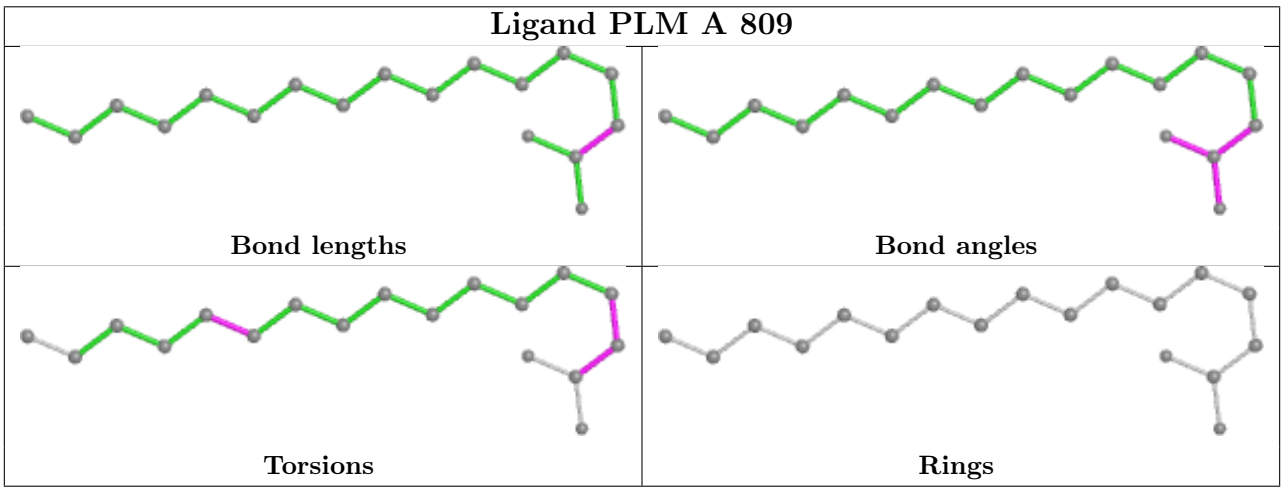
Ligand 3PE B 803



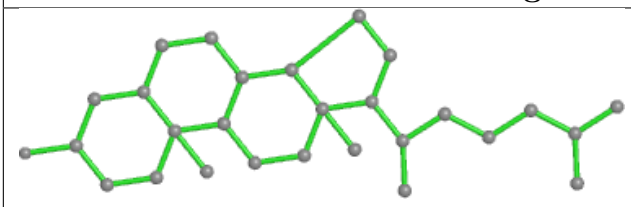
Ligand 3PE B 805



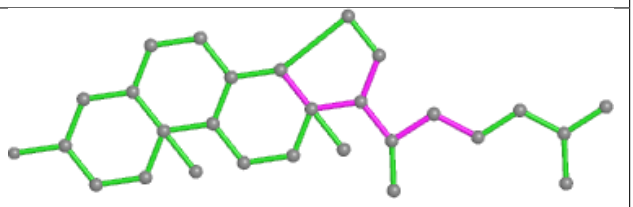
Ligand PLM A 809



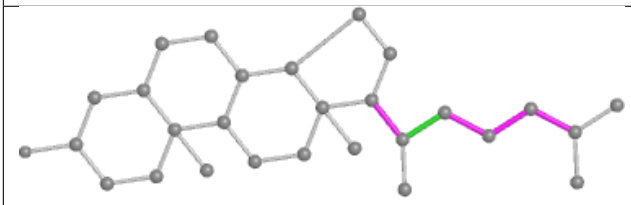
Ligand CLR A 807



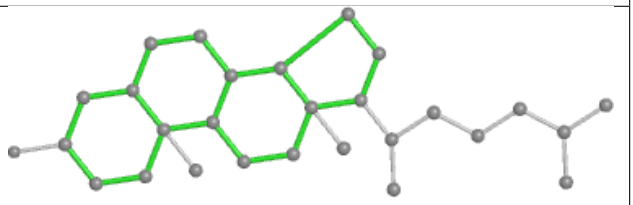
Bond lengths



Bond angles

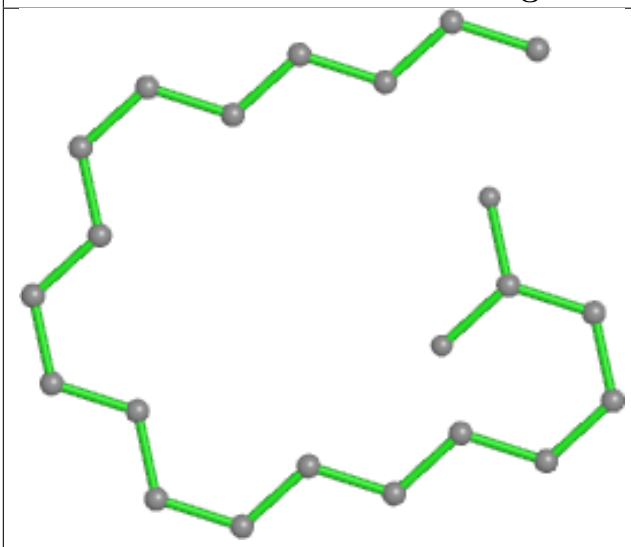


Torsions

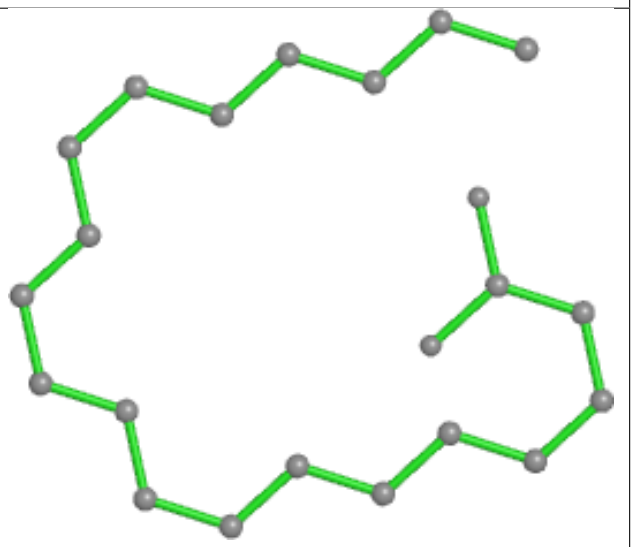


Rings

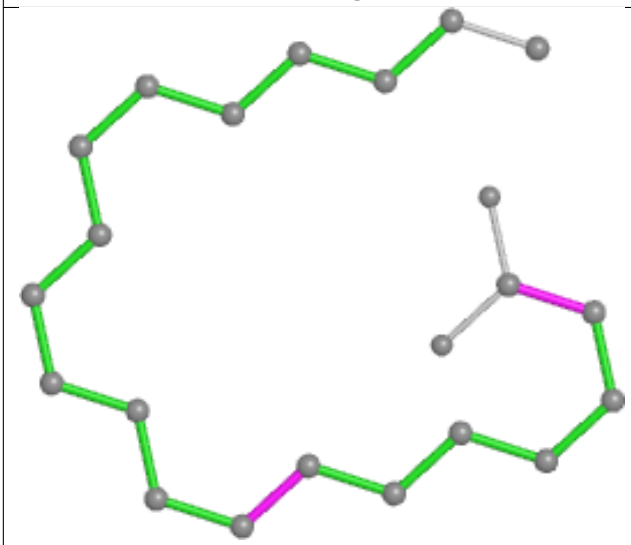
Ligand ACD A 810



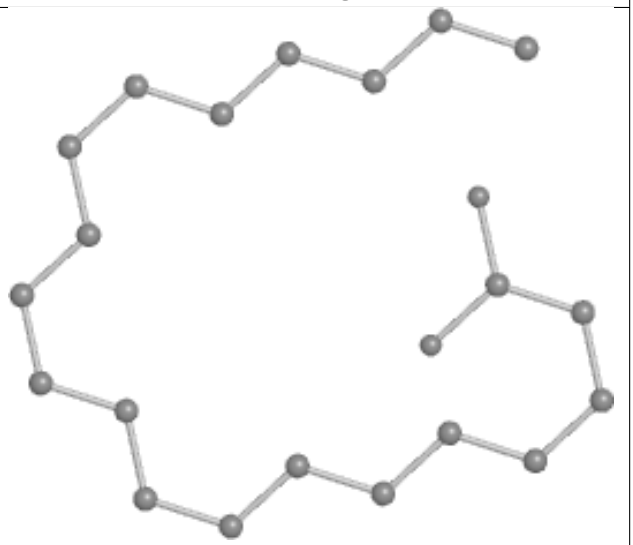
Bond lengths



Bond angles

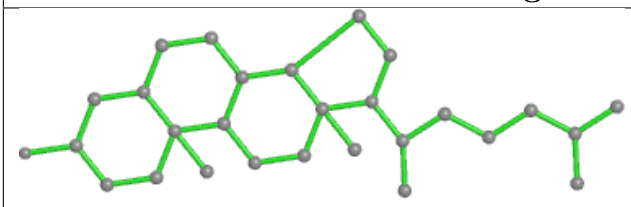


Torsions

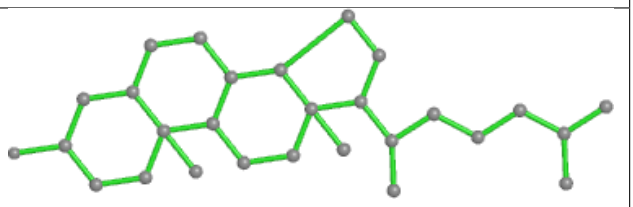


Rings

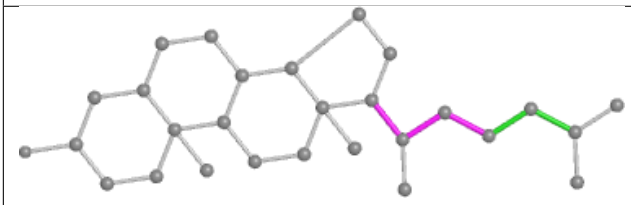
Ligand CLR A 808



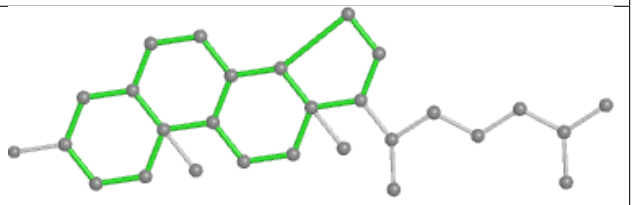
Bond lengths



Bond angles

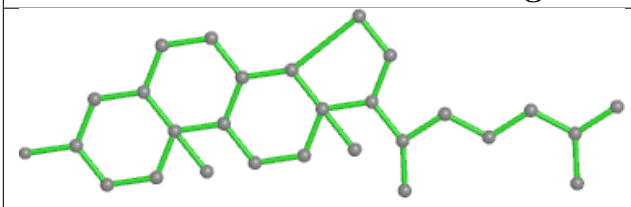


Torsions

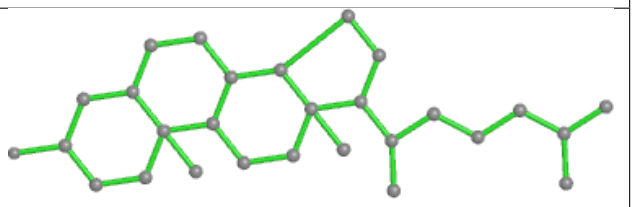


Rings

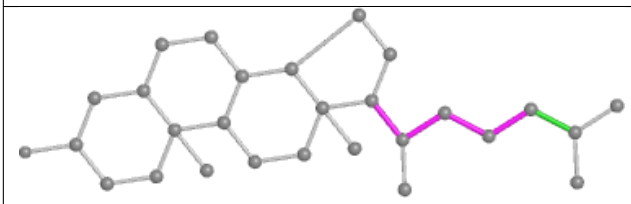
Ligand CLR B 806



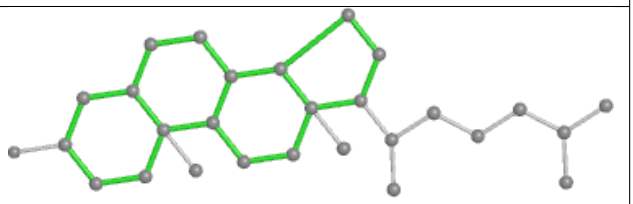
Bond lengths



Bond angles

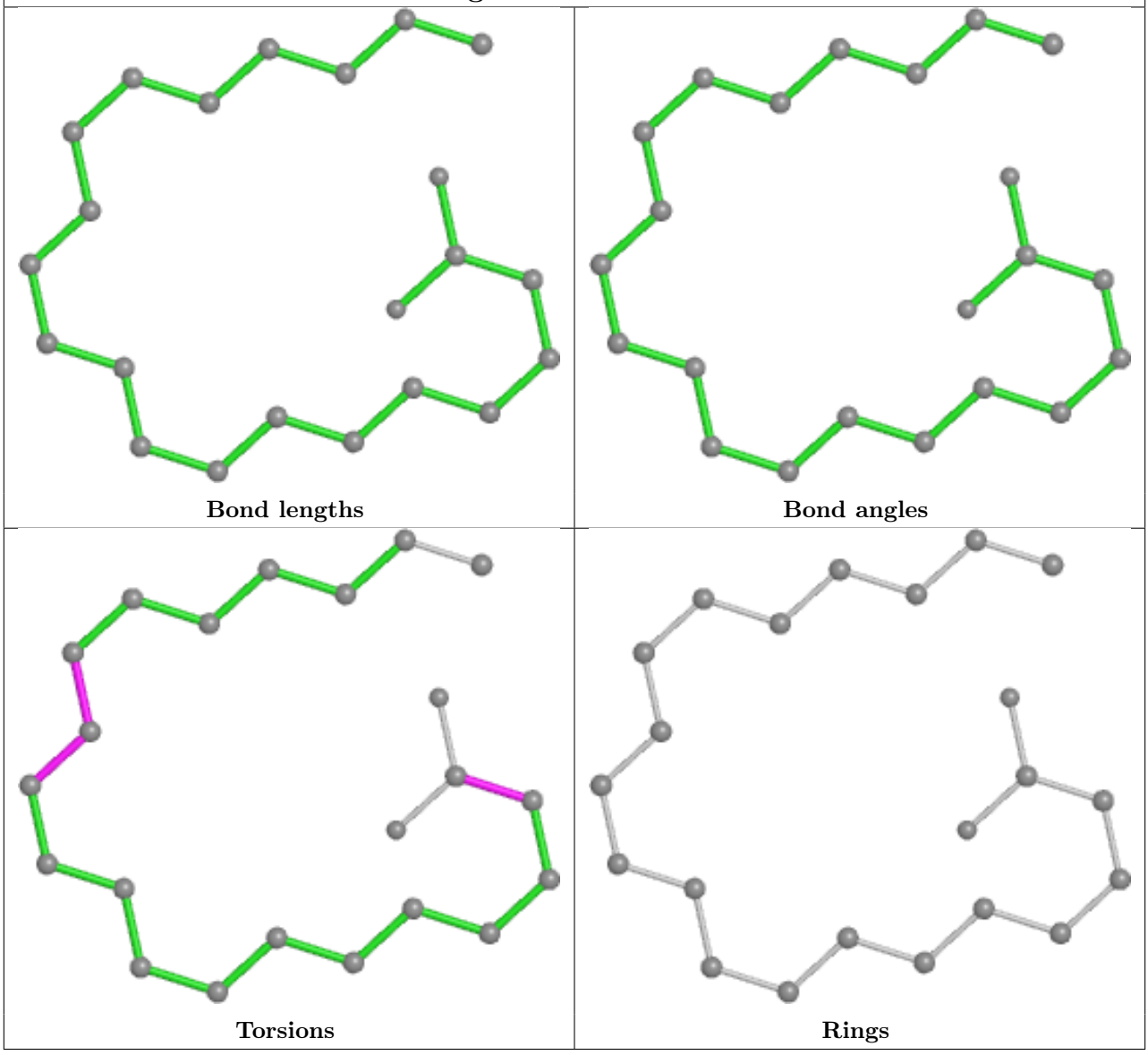


Torsions

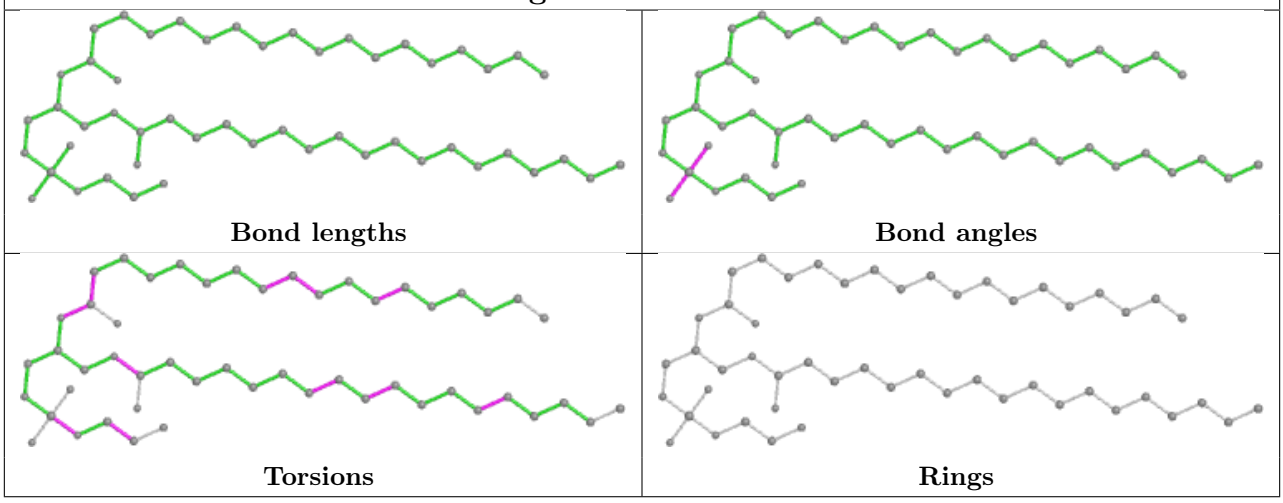


Rings

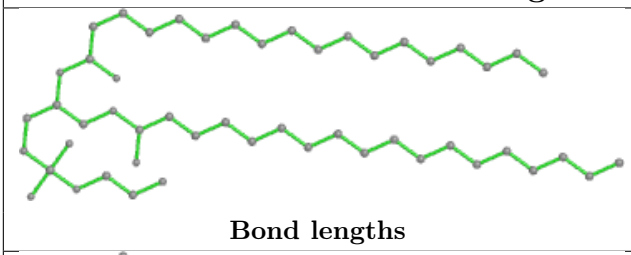
Ligand ACD B 808



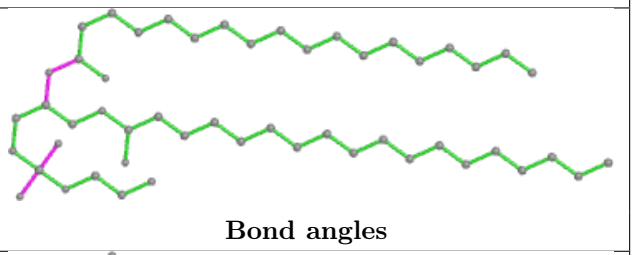
Ligand 3PE A 803



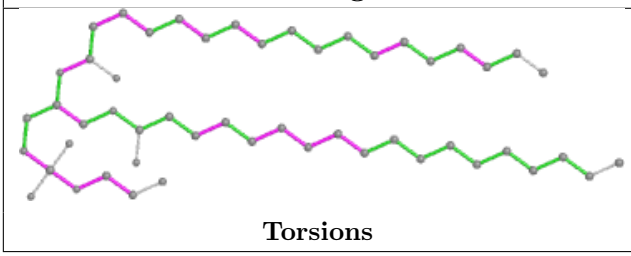
Ligand 3PE A 802



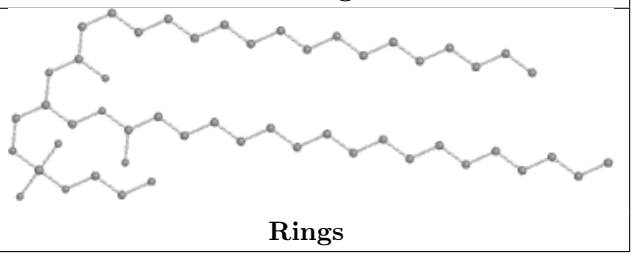
Bond lengths



Bond angles

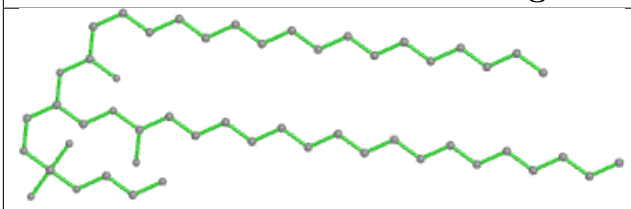


Torsions

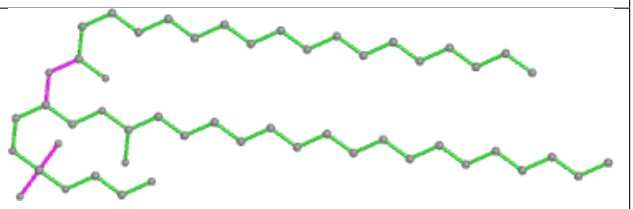


Rings

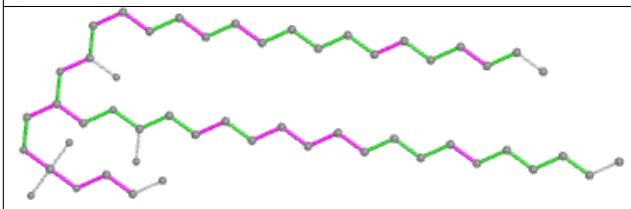
Ligand 3PE B 802



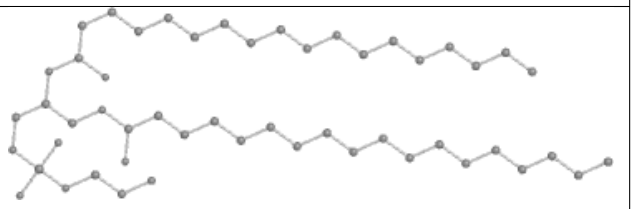
Bond lengths



Bond angles

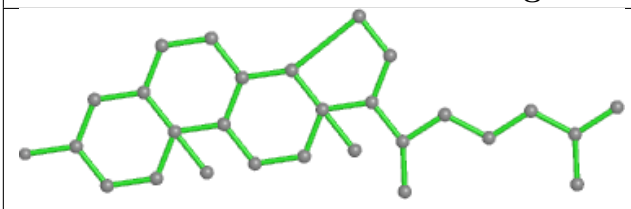


Torsions

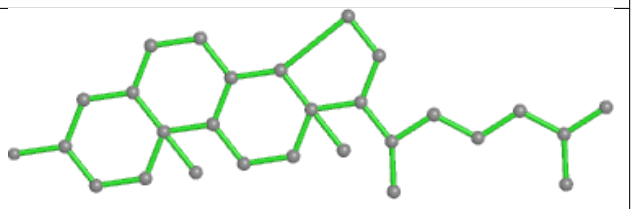


Rings

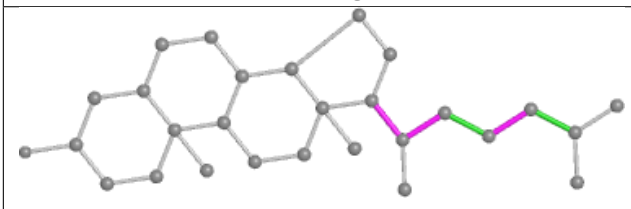
Ligand CLR A 805



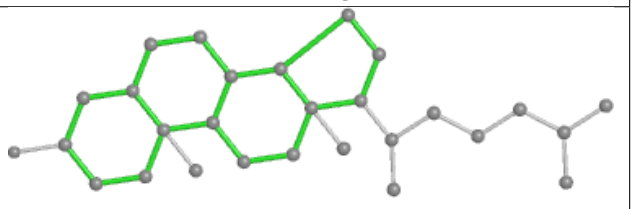
Bond lengths



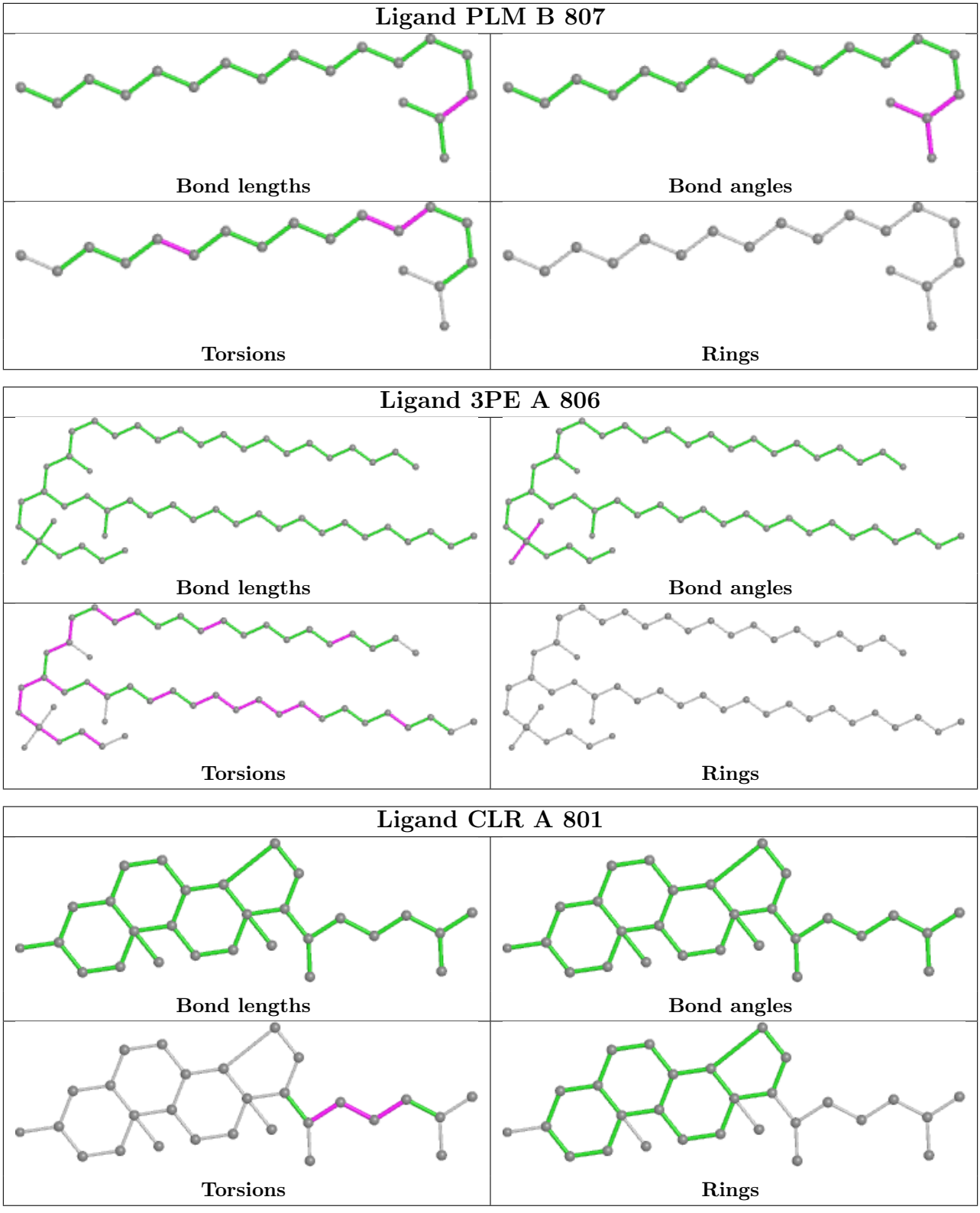
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

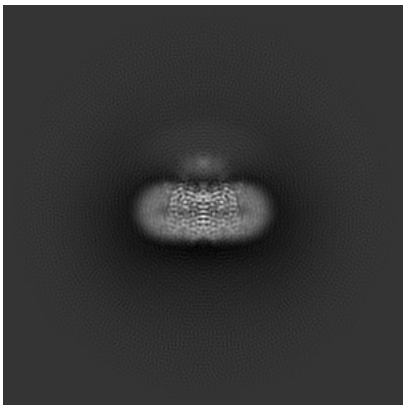
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60705. These allow visual inspection of the internal detail of the map and identification of artifacts.

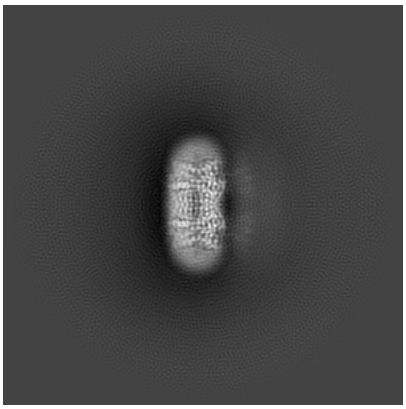
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

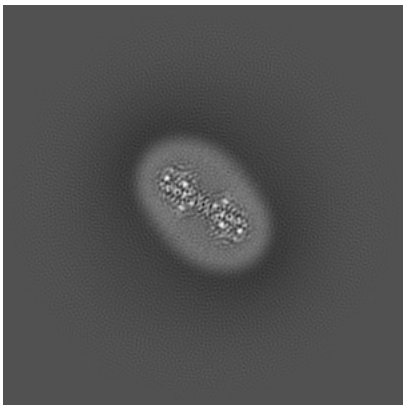
6.1.1 Primary map



X

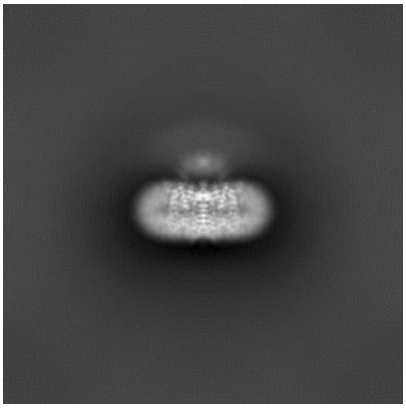


Y

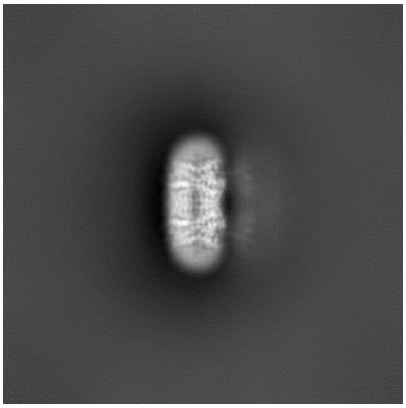


Z

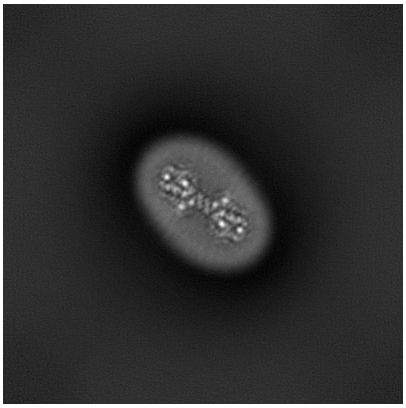
6.1.2 Raw map



X



Y

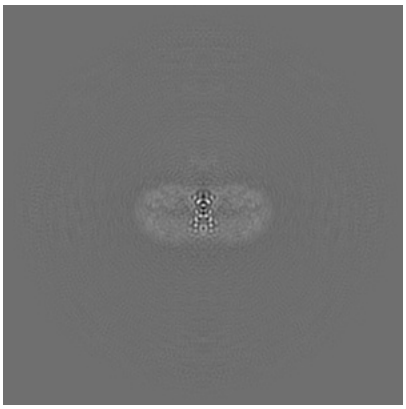


Z

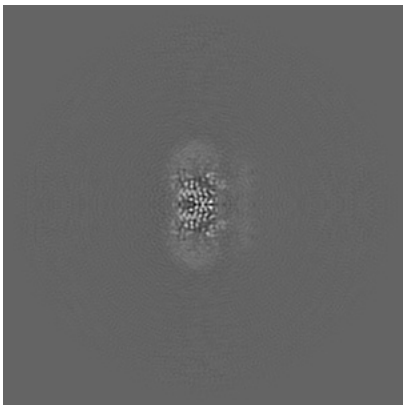
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

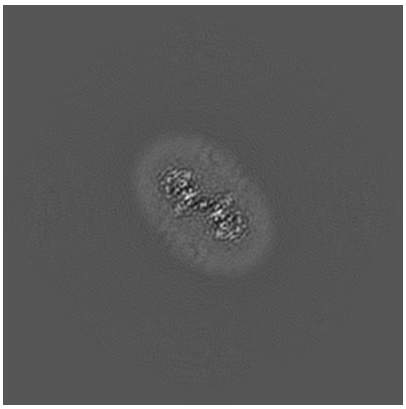
6.2.1 Primary map



X Index: 240

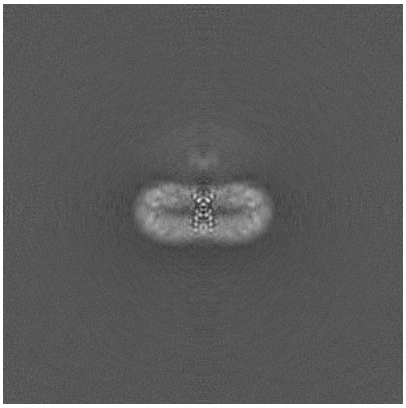


Y Index: 240

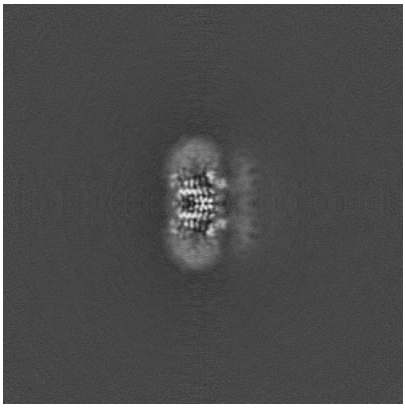


Z Index: 240

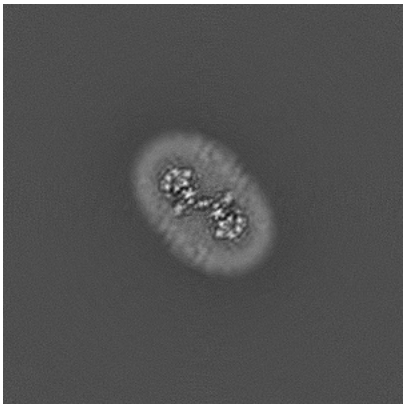
6.2.2 Raw map



X Index: 240



Y Index: 240

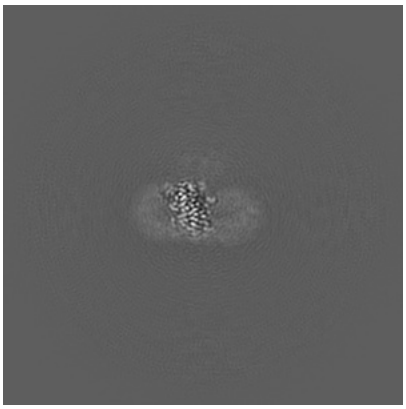


Z Index: 240

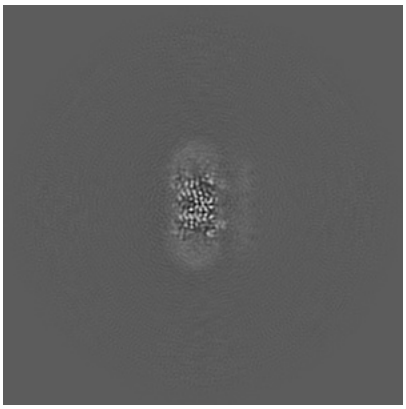
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

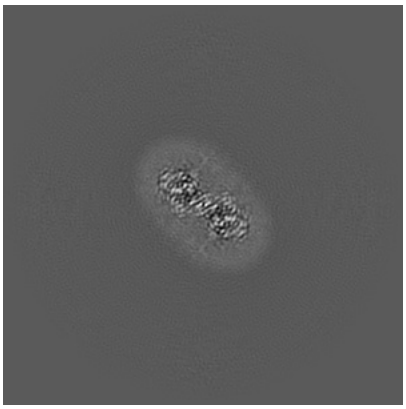
6.3.1 Primary map



X Index: 262

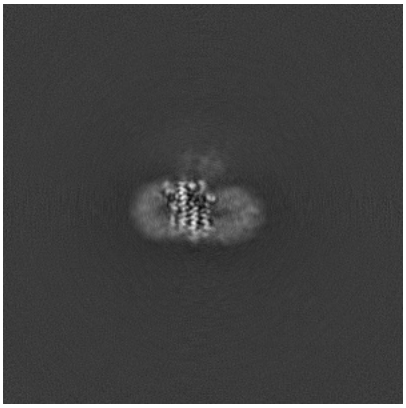


Y Index: 241

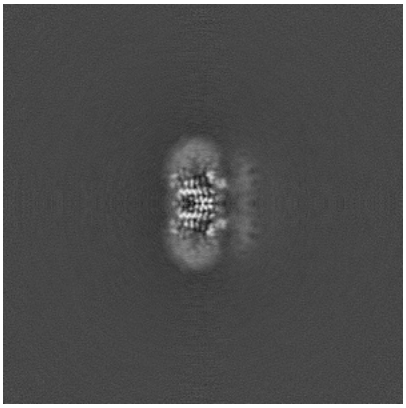


Z Index: 249

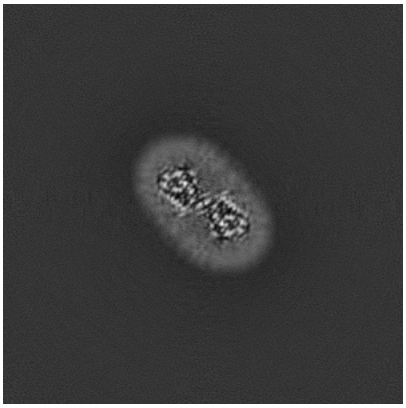
6.3.2 Raw map



X Index: 263



Y Index: 240

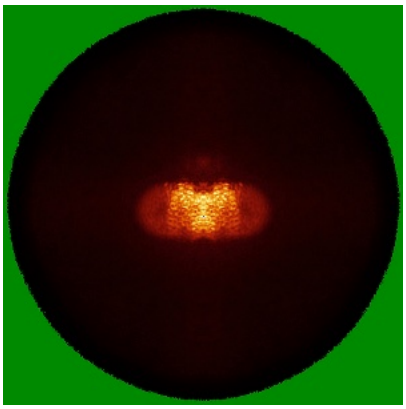


Z Index: 248

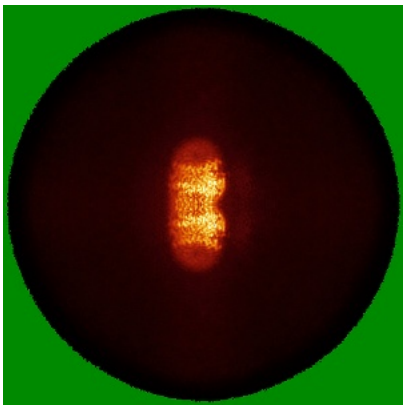
The images above show the largest variance slices of the map in three orthogonal directions.

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

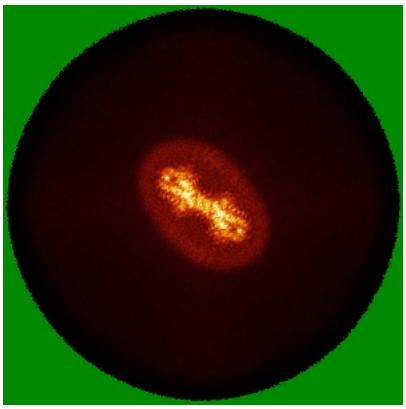
6.4.1 Primary map



X

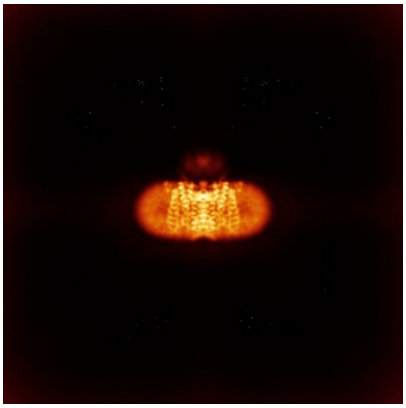


Y

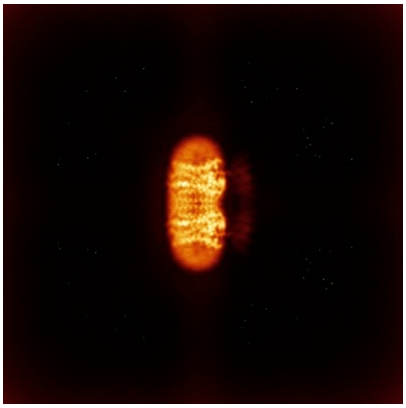


Z

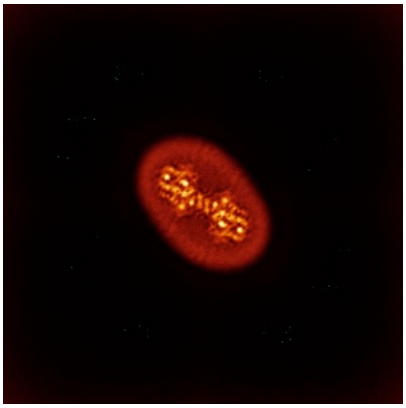
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

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

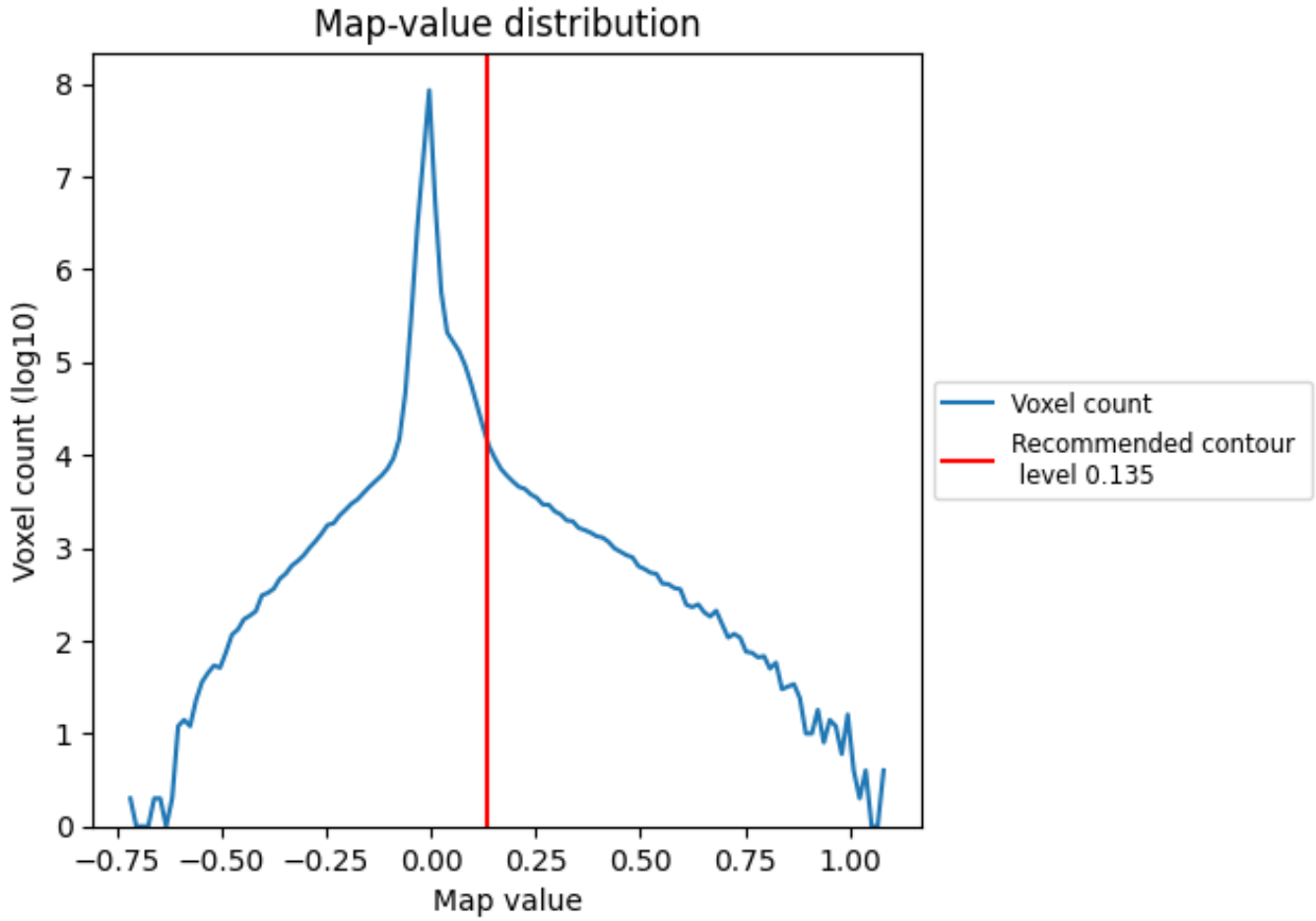
6.6 Mask visualisation (i)

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

7 Map analysis

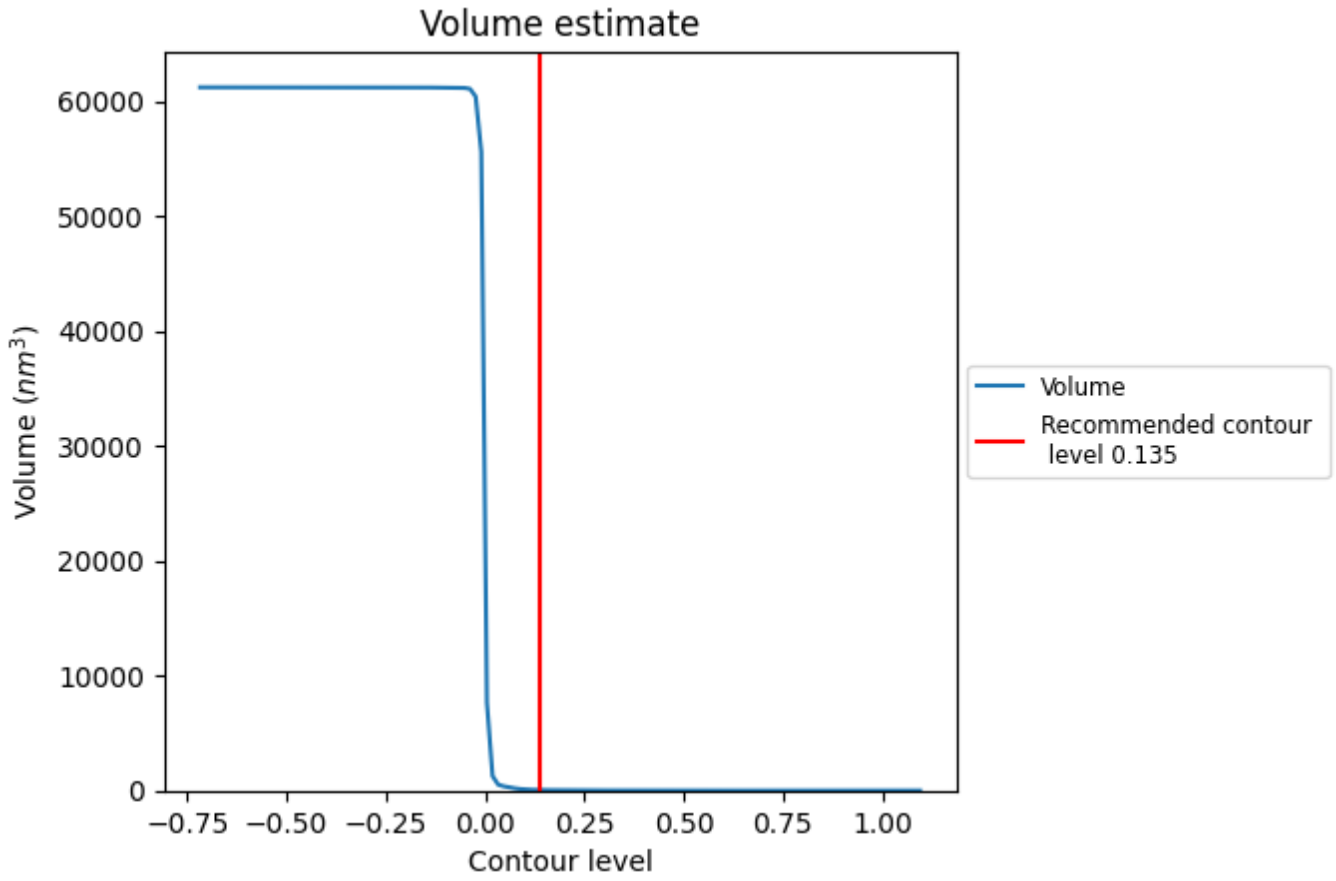
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

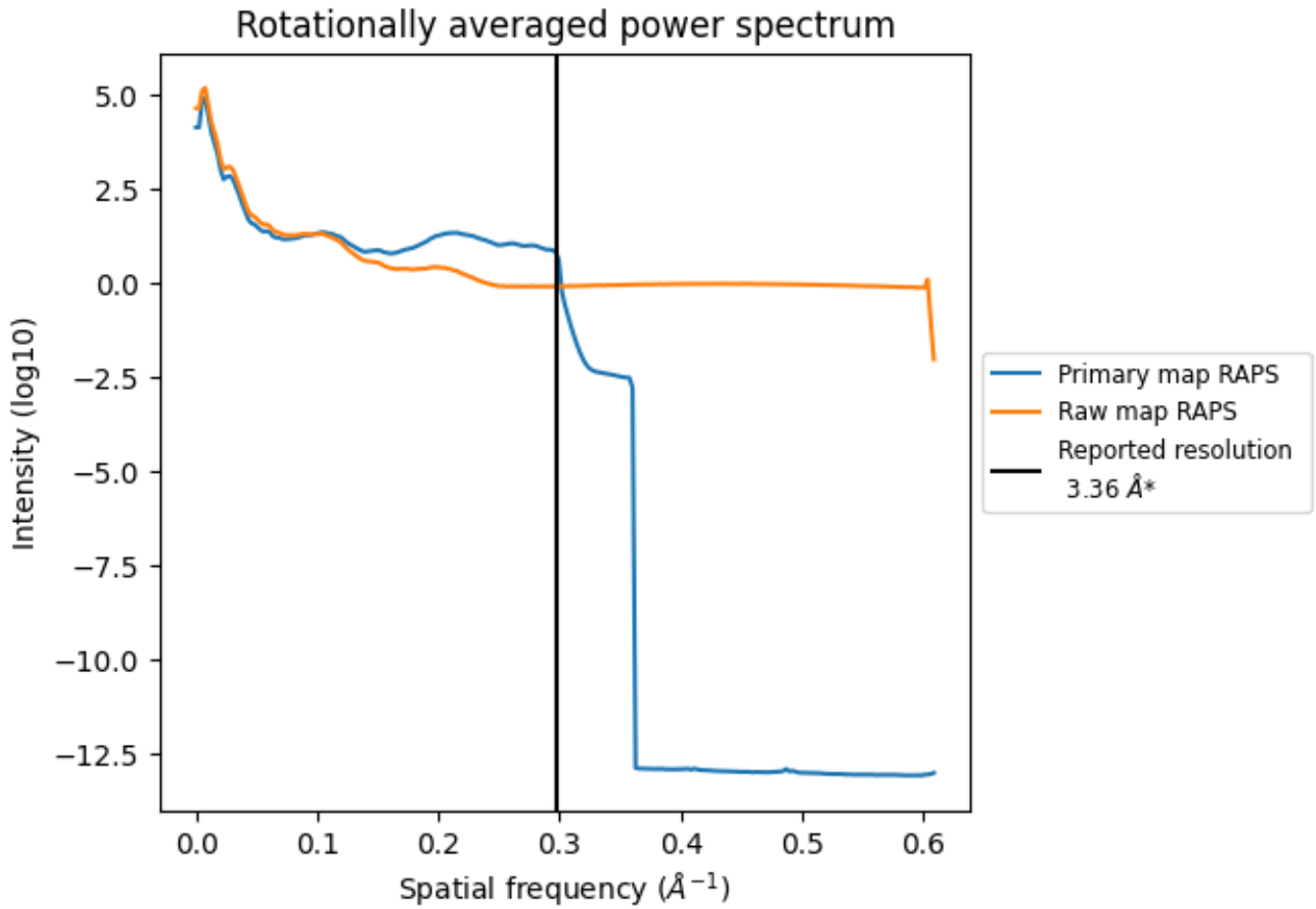
7.2 Volume estimate (i)



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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)

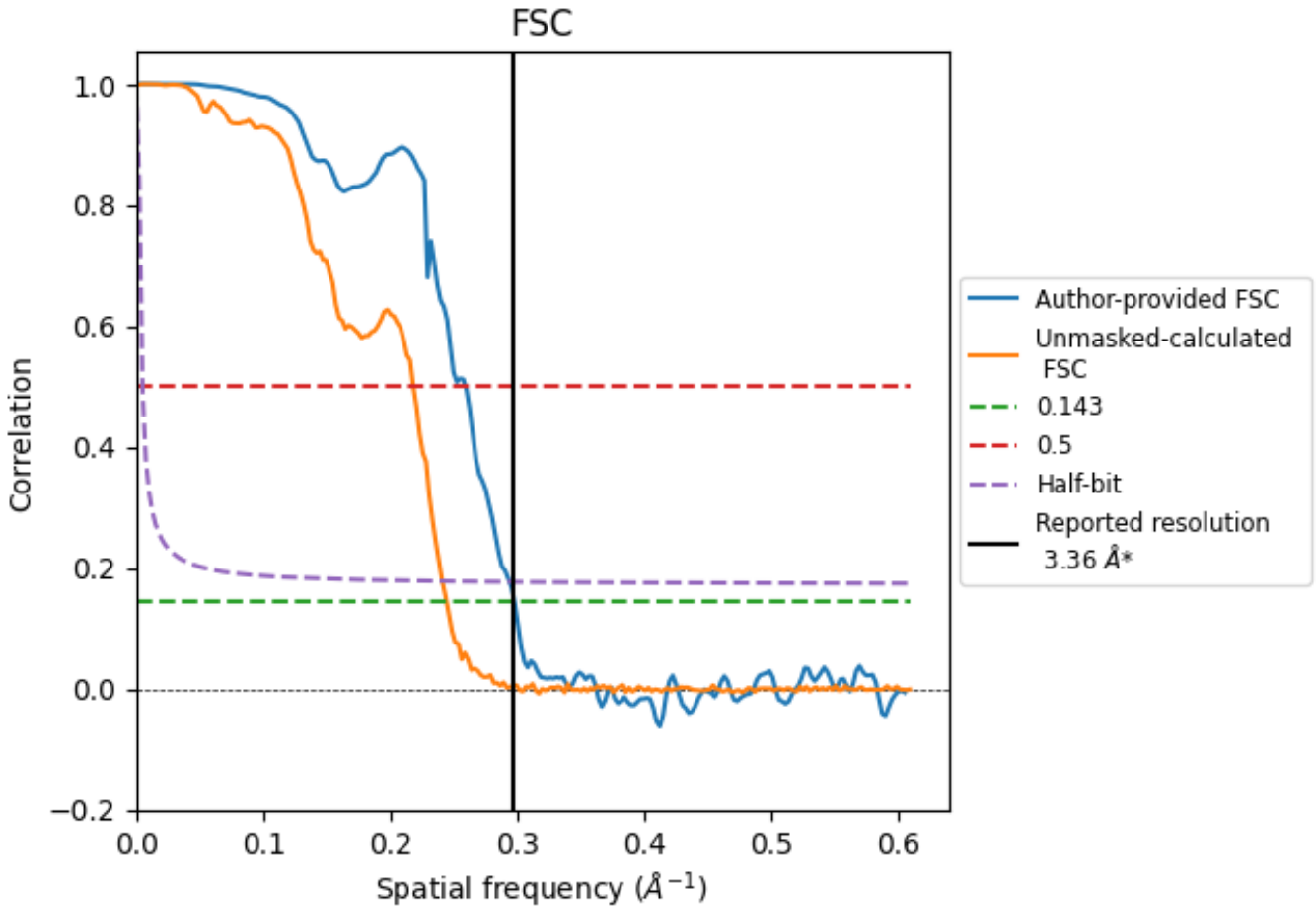


*Reported resolution corresponds to spatial frequency of 0.298 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.298 Å^{-1}

8.2 Resolution estimates (i)

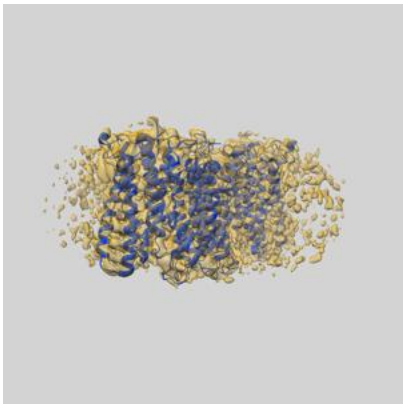
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.36	-	-
Author-provided FSC curve	3.36	3.86	3.40
Unmasked-calculated*	4.09	4.58	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.09 differs from the reported value 3.36 by more than 10 %

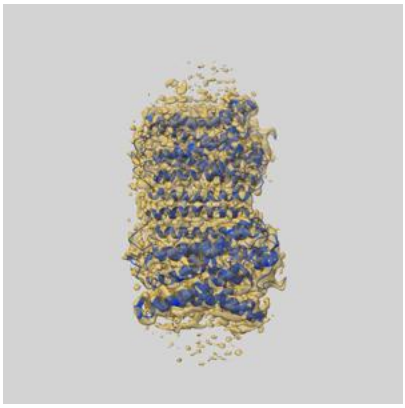
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60705 and PDB model 9INF. Per-residue inclusion information can be found in section 3 on page 8.

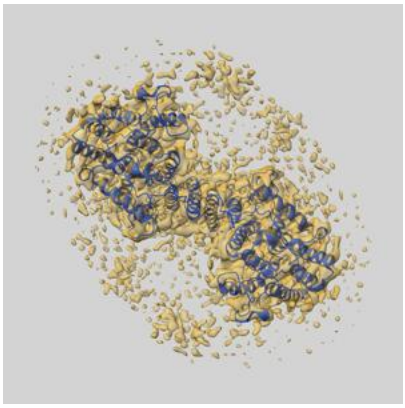
9.1 Map-model overlay



X



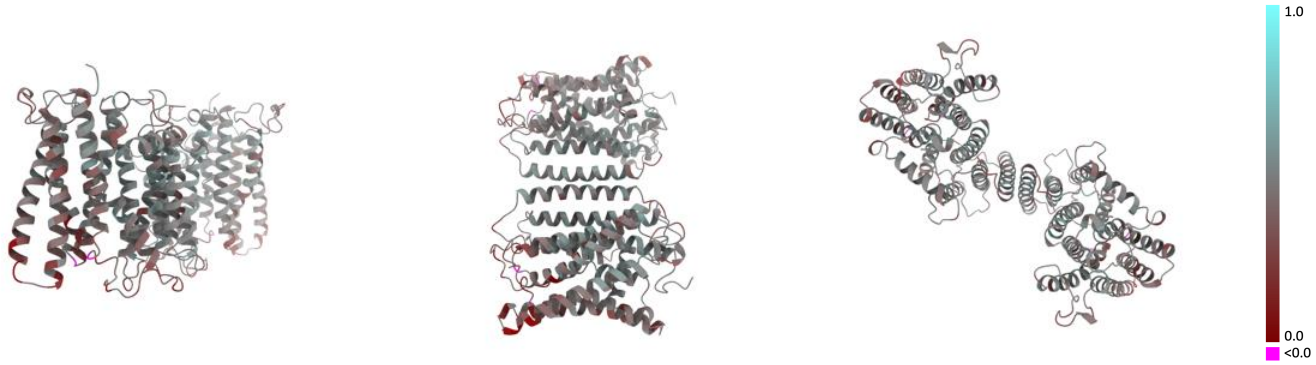
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.135 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.

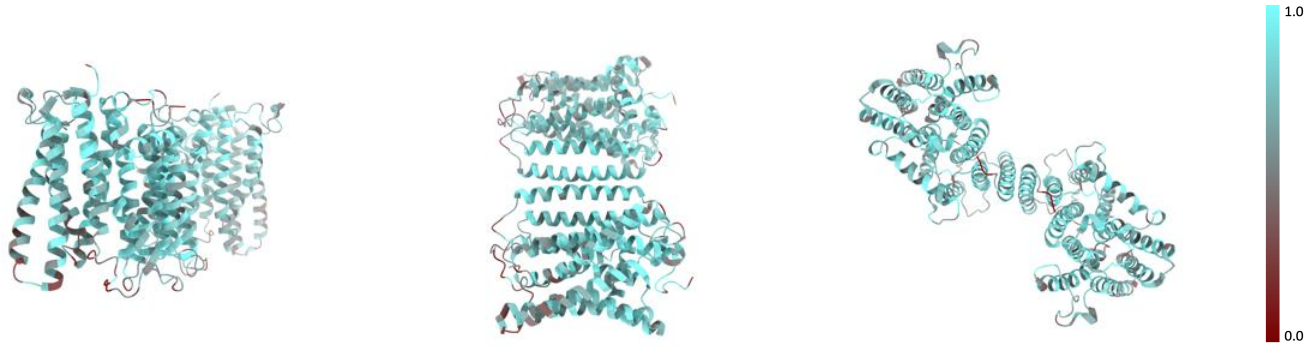
9.2 Q-score mapped to coordinate model (i)



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.

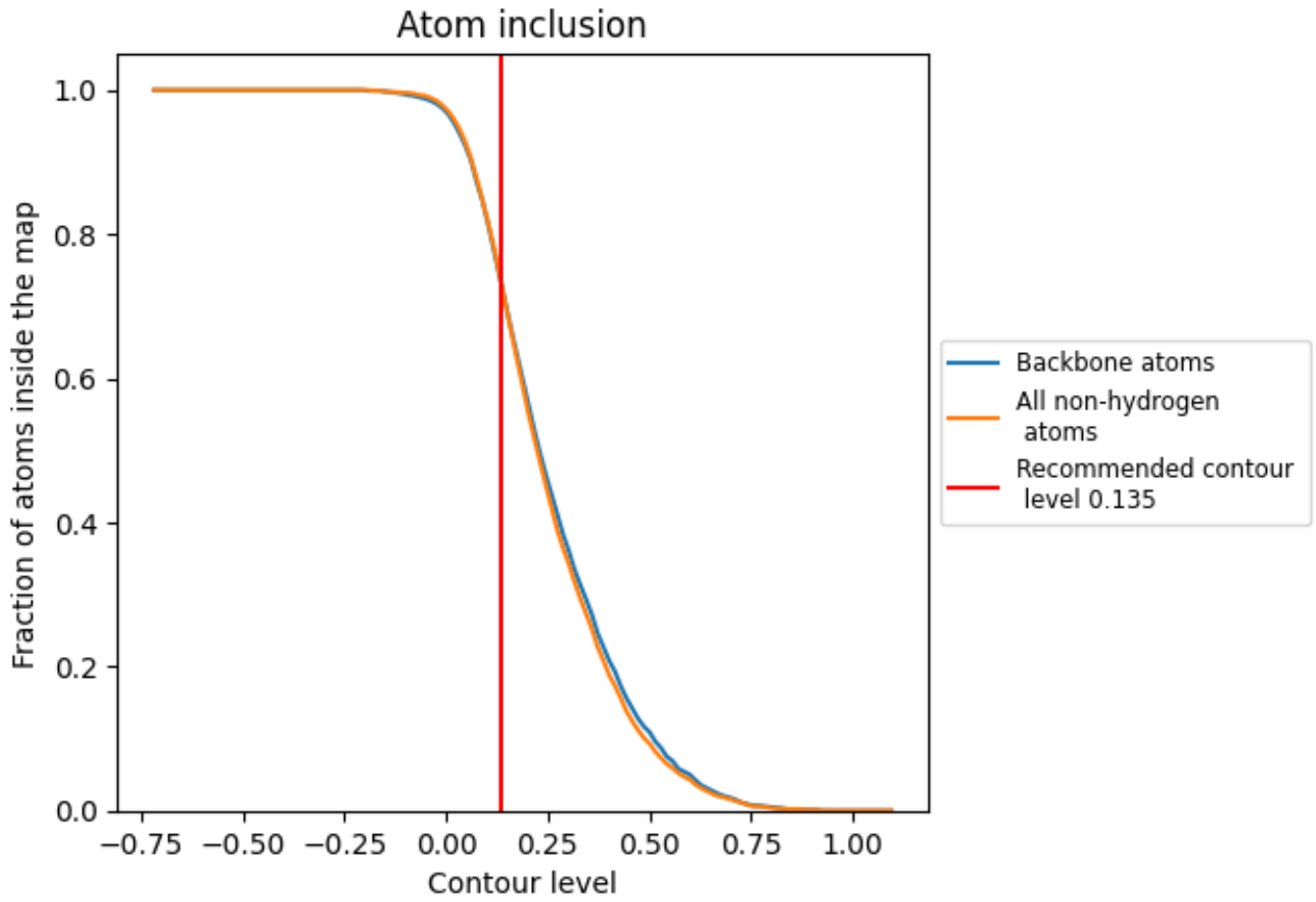
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.135).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 73% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.4410
A	0.7370	0.4420
B	0.7400	0.4400