Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 12:07 PM JST

PDB ID	:	6KZP
EMDB ID	:	EMD-0792
Title	:	calcium channel-ligand
Authors	:	Yan, N.
Deposited on	:	2019-09-25
Resolution	:	3.10 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:

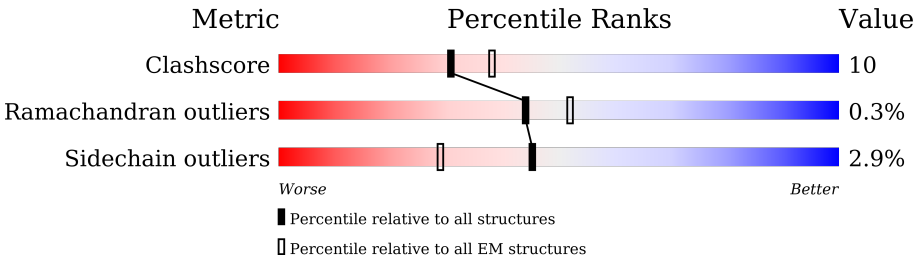
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.10 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	2146	40% 7% 53%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	Y01	A	2317	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8557 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 Voltage-dependent T-type calcium channel subunit alpha-1G, Voltage-dependent T-type calcium channel subunit alpha-1G.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1014	Total	C	N	O	S	0	0
			8159	5391	1324	1379	65		

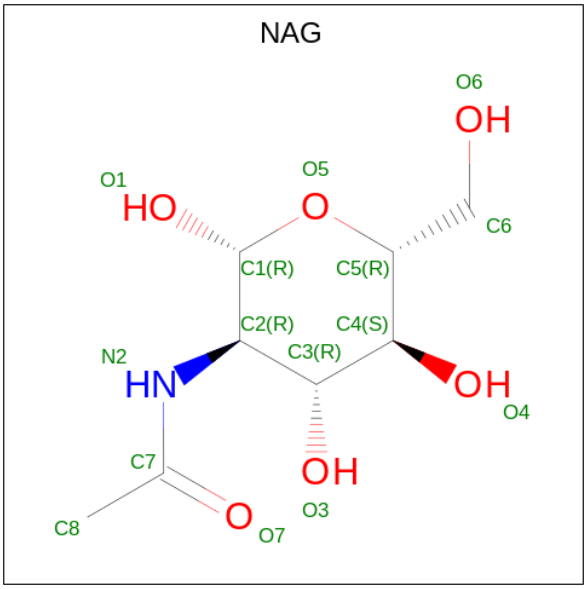
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP O43497
A	-17	HIS	-	expression tag	UNP O43497
A	-16	HIS	-	expression tag	UNP O43497
A	-15	HIS	-	expression tag	UNP O43497
A	-14	HIS	-	expression tag	UNP O43497
A	-13	HIS	-	expression tag	UNP O43497
A	-12	HIS	-	expression tag	UNP O43497
A	-11	HIS	-	expression tag	UNP O43497
A	-10	HIS	-	expression tag	UNP O43497
A	-9	GLY	-	expression tag	UNP O43497
A	-8	ASP	-	expression tag	UNP O43497
A	-7	TYR	-	expression tag	UNP O43497
A	-6	LYS	-	expression tag	UNP O43497
A	-5	ASP	-	expression tag	UNP O43497
A	-4	ASP	-	expression tag	UNP O43497
A	-3	ASP	-	expression tag	UNP O43497
A	-2	ASP	-	expression tag	UNP O43497
A	-1	LYS	-	expression tag	UNP O43497
A	0	GLY	-	expression tag	UNP O43497
A	1	THR	-	expression tag	UNP O43497

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

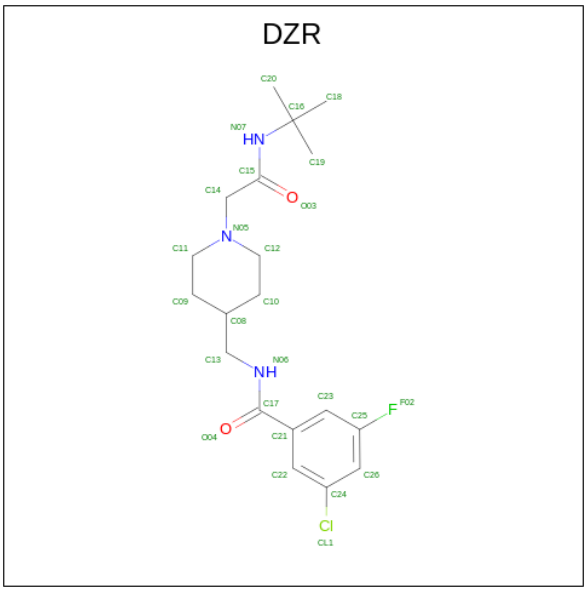
Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Ca	0
			2	2	

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



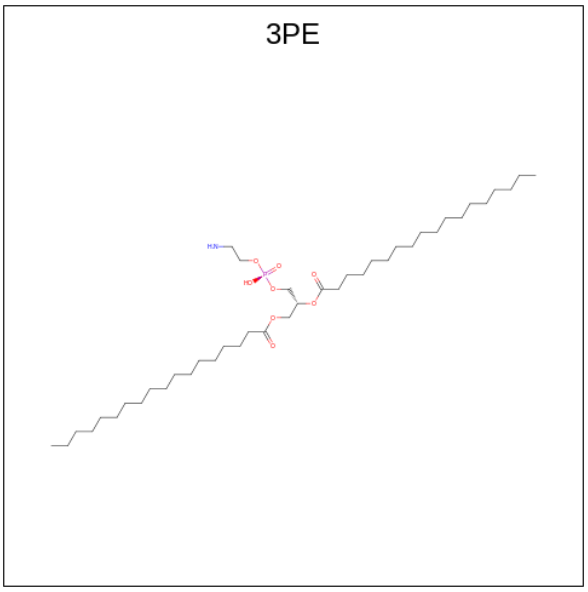
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is {N}-[[1-[2-({tert}-butylamino)-2-oxidanylidene-ethyl]piperidin-4-yl]methyl]-3-chloranyl-5-fluoranyl-benzamide (three-letter code: DZR) (formula: $C_{19}H_{27}ClFN_3O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	Cl	F	N	O	0
			26	19	1	1	3	2	

- Molecule 5 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			209	159	5	40	5	
5	A	1	Total	C	N	O	P	0
			209	159	5	40	5	

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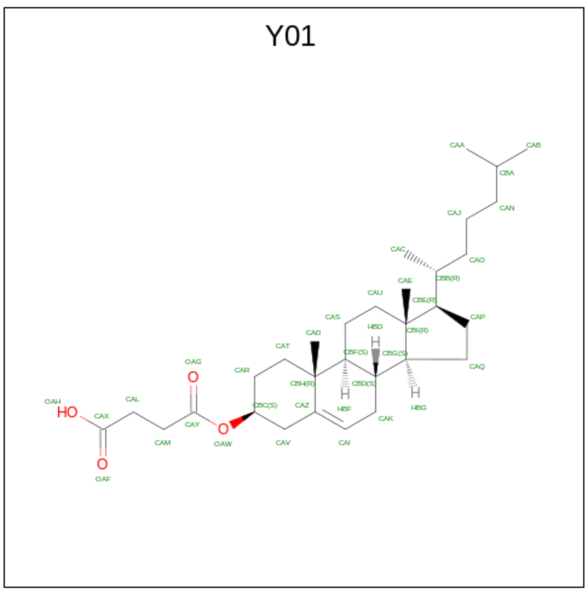
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 209	C 159	N 5	O 40	P 5	0
5	A	1	Total 209	C 159	N 5	O 40	P 5	0
5	A	1	Total 209	C 159	N 5	O 40	P 5	0
5	A	1	Total 209	C 159	N 5	O 40	P 5	0
5	A	1	Total 209	C 159	N 5	O 40	P 5	0
5	A	1	Total 209	C 159	N 5	O 40	P 5	0

- Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



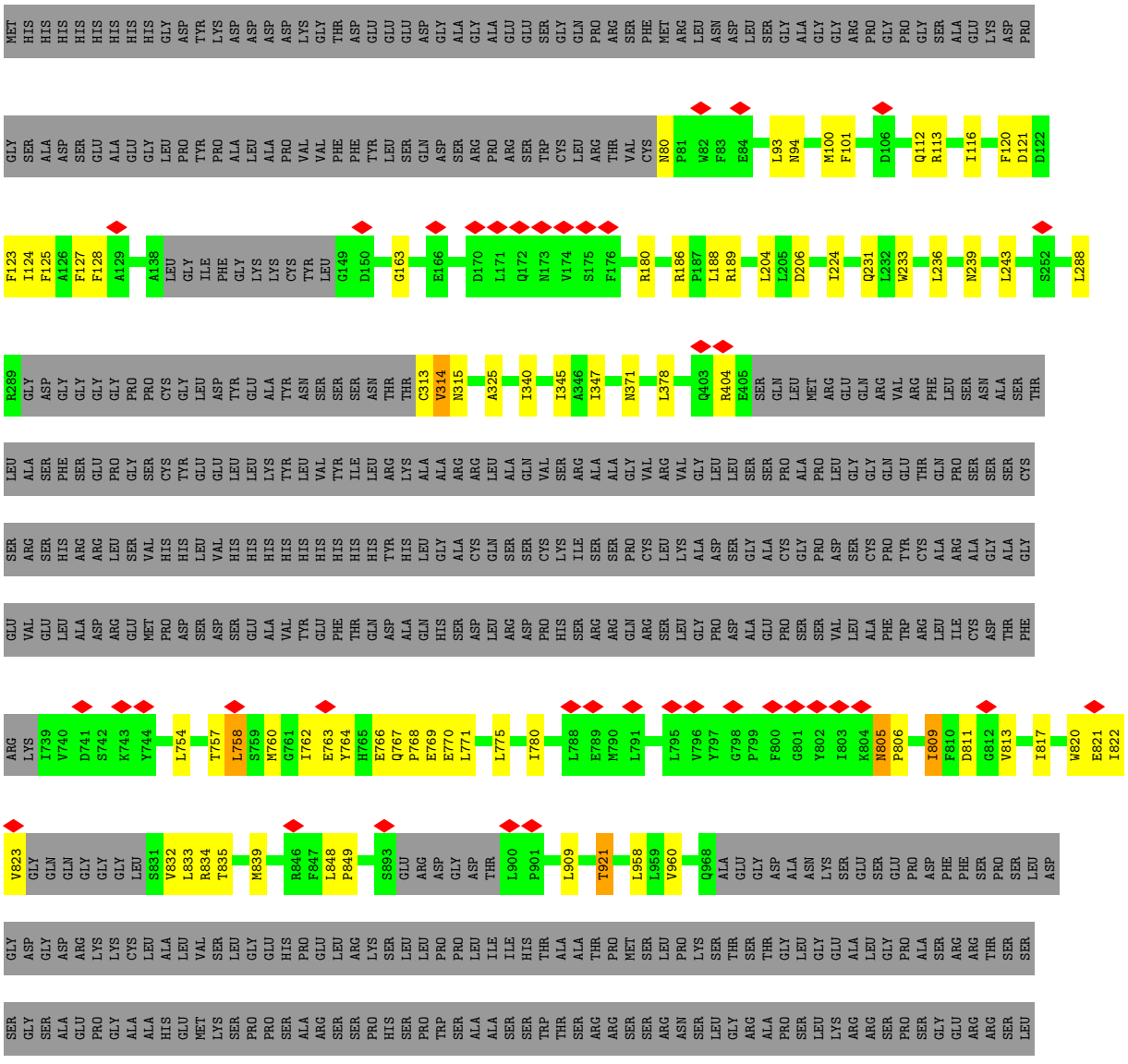
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 105	C 93	O 12	0
6	A	1	Total 105	C 93	O 12	0
6	A	1	Total 105	C 93	O 12	0

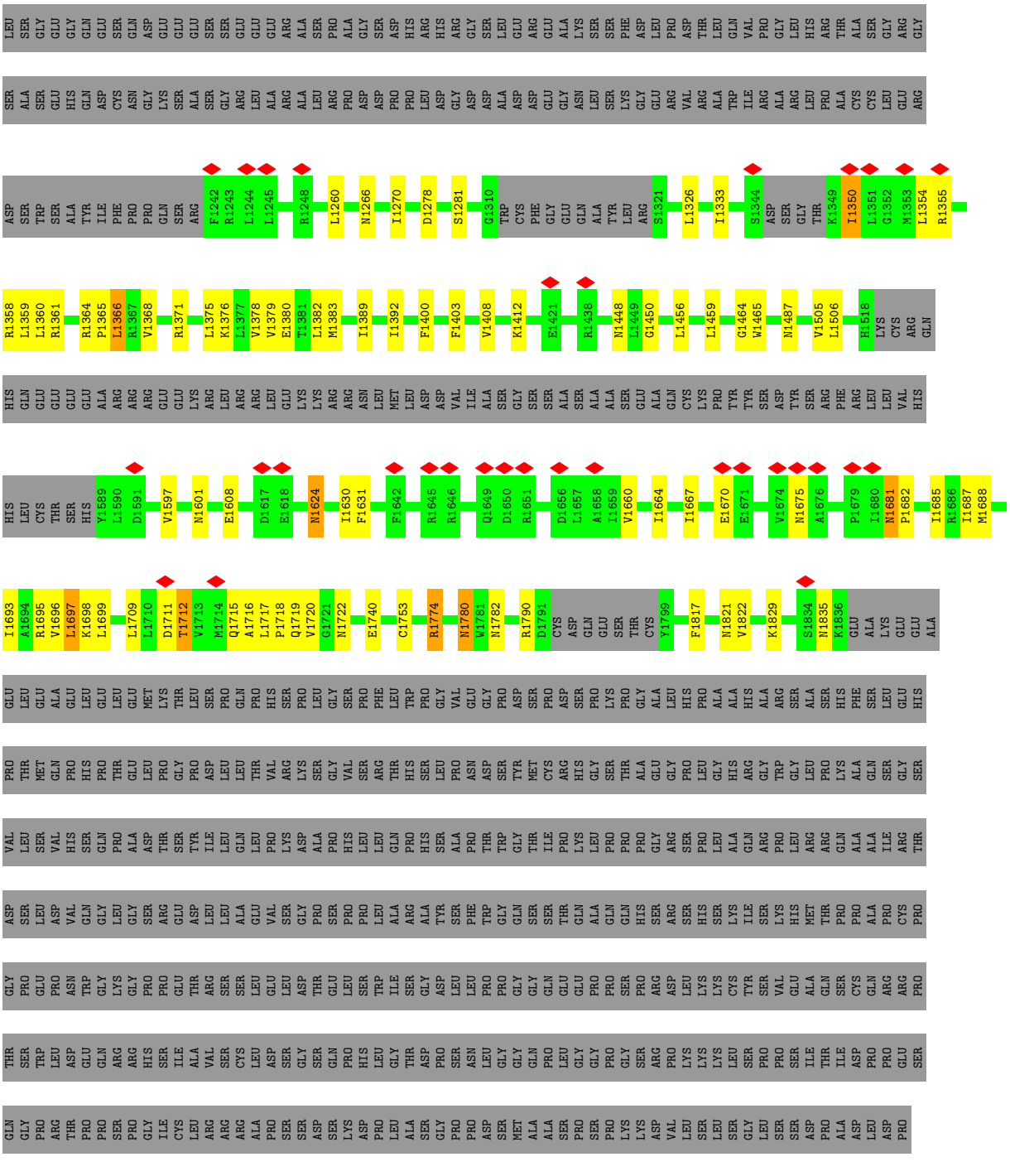
3 Residue-property plots (i)

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: Voltage-dependent T-type calcium channel subunit alpha-1G,Voltage-dependent T-type calcium channel subunit alpha-1G

Chain A:




LEU SER GLY GLU GLY GLN GLU SER GLN ASP GLU GLU GLU SER SER GLU GLU GLU ARG ALA SER PRO ALA GLY SER ASP HIS ARG HIS ARG GLY SER LEU GLU ARG GLU ALA LYS SER SER PHE ASP LEU PRO ASP THR LEU GLN VAL PRO GLY LEU HIS ARG THR ALA SER GLY ARG GLY
SER ALA SER GLU HIS GLN ASP CYS ASN GLY LYS SER ALA SER GLY ARG LEU ALA ARG ALA LEU ARG PRO ASP PRO ALA GLY GLU ARG VAL ARG ALA TRP ILE ARG ALA ARG LEU PRO ALA CYS CYS LEU GLU ARG
ASP SER TRP SER ALA TYR ILE PHE PRO PRO GLN SER ARG F1242 R1243 L1244 L1245 R1248 L1260 N1266 I1270 D1278 S1281 G1310 TRP CYS PHE GLY GLU GLN ALA TYR LEU ARG S1321 L1326 I1333 S1344 ASP SER GLY THR K1349 I1350 L1351 G1352 M1353 L1354 R1355
R1358 L1359 L1360 R1361 R1364 P1365 L1366 R1367 V1368 R1371 L1375 K1376 L1377 V1378 V1379 E1380 T1381 L1382 M1383 I1389 I1392 F1400 F1403 V1408 K1412 E1421 R1438 N1448 L1449 G1450 L1456 L1459 G1464 W1465 N1487 V1505 L1506 H1518 LYS CYS ARG GLN
HIS GLN GLU GLU GLU ALA ARG ARG ARG GLU GLU LYS ARG LEU ARG ARG LEU GLU LYS LYS ARG ARG ASN LEU MET LEU ASP ASP VAL ILE ALA SER GLY SER SER ALA SER ALA ALA SER GLU ALA GLN CYS LYS PRO TYR TYR SER ASP TYR SER ARG PHE ARG LEU LEU VAL HIS
HIS LEU CYS THR SER HIS Y1589 L1590 D1591 V1597 N1601 E1608 D1617 E1618 N1624 I1630 F1631 F1642 R1645 R1646 Q1649 D1650 R1651 D1656 L1657 A1658 I1659 V1660 I1664 I1667 E1670 E1671 V1674 N1675 A1676 P1679 I1680 N1681 P1682 I1685 R1686 I1687 M1688
I1693 A1694 R1695 V1696 L1697 K1698 L1699 L1709 L1710 D1711 T1712 V1713 M1714 Q1715 A1716 L1717 P1718 Q1719 V1720 G1721 N1722 E1740 C1753 R1774 N1780 W1781 N1782 R1790 D1791 CYS ASP GLN GLU SER THR CYS Y1799 F1817 N1821 V1822 K1829 S1834 N1835 K1836 GLU ALA LYS GLU GLU ALA
GLU LEU GLU ALA GLU LEU GLU LEU GLU MET LYS THR LEU SER PRO GLN PRO HIS SER PRO LEU PRO GLY VAL GLU GLY PRO ASP SER PRO ASP SER PRO LYS PRO GLY ALA LEU HIS PRO ALA ALA HIS ALA ARG SER ALA SER HIS PHE SER LEU GLU HIS
PRO THR MET GLN PRO HIS PRO THR GLU LEU PRO GLY PRO ASP LEU LEU THR VAL ARG LYS SER GLY VAL SER ARG THR HIS SER LEU PRO ASN ASP SER TYR MET CYS ARG HIS GLY SER THR ALA GLU GLY PRO LEU GLY HIS ARG GLY TRP GLY LEU LEU PRO LYS ALA GLN SER GLY SER
VAL LEU SER VAL HIS SER GLN PRO ALA ASP THR SER TYR ILE LEU GLN LEU PRO LYS ASP ALA PRO HIS LEU LEU GLN PRO HIS SER SER ALA PRO THR TRP GLY THR ILE PRO LYS LEU PRO PRO GLY ARG SER PRO LEU GLU ALA GLN ARG PRO LEU ARG ARG GLN ALA ALA ILE ARG THR
ASP SER LEU ASP VAL GLN GLY LEU GLY SER ARG GLU ASP LEU THR GLU VAL SER GLY PRO SER PRO PRO LEU ALA ARG ALA TYR SER PHE TRP GLY GLN SER SER THR GLN ALA GLN GLN HIS SER ARG SER HIS SER LYS ILE SER LYS HIS MET THR PRO PRO ALA PRO ALA ARG CYS PRO
GLY PRO GLU PRO ASN TRP GLY LYS GLY PRO PRO GLU THR ARG SER SER GLU LEU GLU LEU ASP SER THR GLU GLU SER LEU PRO ILE SER GLY ASP LEU LEU PRO PRO GLY GLY GLN GLU GLU GLY PRO PRO SER PRO ARG ASP LEU LYS LYS CYS TYR SER VAL GLU ALA GLN SER CYS GLN ARG PRO
THR SER TRP LEU ASP GLU GLN ARG HIS SER ILE ALA VAL SER CYS LEU ASP SER ARG ASP PRO HIS LEU GLY THR ASP PRO SER ASN LEU GLY GLY GLN PRO LEU GLY GLY PRO GLY SER ARG PRO LYS LYS LYS LEU SER PRO SER ILE THR ILE ASP PRO ARG PRO GLU SER
GLN GLY PRO LEU ASP ARG THR PRO ILE CYS LEU ARG ARG ALA PRO SER SER ASP SER LYS ASP PRO LEU ALA SER GLY PRO PRO ASP SER MET ALA ALA SER PRO SER PRO LYS LYS ASP VAL LEU SER LEU SER GLY LEU PRO SER ASP LEU ALA ASP PRO GLU SER

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.147	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	349.12, 349.12, 349.12	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, Y01, NAG, CA, DZR

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	0.38	0/8337	0.60	0/11298

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	8159	0	8358	152	0
2	A	2	0	0	0	0
3	A	56	0	52	0	0
4	A	26	0	0	1	0
5	A	209	0	282	15	0
6	A	105	0	147	33	0
All	All	8557	0	8839	170	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 10.

All (170) 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)
6:A:2316:Y01:HAN1	6:A:2316:Y01:HAP1	1.23	1.11
1:A:1326:LEU:HD21	1:A:1366:LEU:HD11	1.38	1.01
1:A:1400:PHE:CE2	6:A:2317:Y01:HAB1	1.97	0.99
6:A:2316:Y01:HAN1	6:A:2316:Y01:CAP	1.95	0.97
1:A:125:PHE:HE2	1:A:163:GLY:HA3	1.27	0.96
1:A:1326:LEU:HD21	1:A:1366:LEU:CD1	2.00	0.91
1:A:1624:ASN:HD21	1:A:1695:ARG:HH22	0.96	0.89
1:A:101:PHE:HE1	1:A:180:ARG:NH2	1.73	0.87
1:A:780:ILE:HG12	1:A:822:ILE:HD11	1.58	0.86
1:A:1400:PHE:HE2	6:A:2317:Y01:HAB1	1.40	0.86
5:A:2313:3PE:H31	5:A:2313:3PE:H222	1.58	0.86
6:A:2316:Y01:HAP1	6:A:2316:Y01:CAN	2.06	0.86
1:A:835:THR:HG21	5:A:2315:3PE:H352	1.58	0.85
1:A:1624:ASN:ND2	1:A:1695:ARG:HH22	1.75	0.83
1:A:128:PHE:CE2	1:A:189:ARG:NH1	2.48	0.82
5:A:2313:3PE:H31	5:A:2313:3PE:C22	2.09	0.80
1:A:1270:ILE:HG12	1:A:1364:ARG:HH11	1.45	0.80
1:A:1354:LEU:HD22	1:A:1354:LEU:O	1.83	0.79
1:A:1448:ASN:ND2	6:A:2316:Y01:HAD1	1.99	0.78
1:A:1359:LEU:HD13	1:A:1740:GLU:HG2	1.65	0.78
1:A:1717:LEU:O	1:A:1717:LEU:HD13	1.83	0.77
1:A:762:ILE:HG22	6:A:2316:Y01:CAK	2.13	0.77
1:A:288:LEU:HB3	1:A:315:ASN:HB2	1.67	0.77
1:A:762:ILE:HG22	6:A:2316:Y01:HAK1	1.67	0.76
1:A:1270:ILE:CG1	1:A:1364:ARG:HH11	1.97	0.76
1:A:1670:GLU:HG2	1:A:1685:ILE:HG23	1.68	0.76
1:A:1400:PHE:CD2	6:A:2317:Y01:HAB1	2.19	0.76
1:A:839:MET:HG3	5:A:2315:3PE:H3A1	1.68	0.74
1:A:1403:PHE:CZ	5:A:2315:3PE:H281	2.24	0.72
1:A:1450:GLY:O	6:A:2317:Y01:HAD2	1.90	0.71
1:A:1355:ARG:NE	1:A:1358:ARG:HH11	1.89	0.71
1:A:813:VAL:O	1:A:817:ILE:HG12	1.90	0.71
1:A:835:THR:CG2	5:A:2315:3PE:H352	2.21	0.70
6:A:2317:Y01:CAO	6:A:2317:Y01:HAA2	2.21	0.70
1:A:767:GLN:HB2	1:A:768:PRO:HD2	1.73	0.70
1:A:1364:ARG:N	1:A:1365:PRO:HD2	2.05	0.70
6:A:2317:Y01:HAA2	6:A:2317:Y01:HAO2	1.73	0.69
6:A:2317:Y01:HAO2	6:A:2317:Y01:CAA	2.23	0.68
1:A:771:LEU:O	1:A:775:LEU:HG	1.93	0.68
1:A:1709:LEU:O	1:A:1712:THR:HG23	1.93	0.67
1:A:101:PHE:CE1	1:A:180:ARG:NH2	2.62	0.67
1:A:1688:MET:HA	1:A:1688:MET:CE	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1624:ASN:HD21	1:A:1695:ARG:NH2	1.81	0.66
1:A:1693:ILE:O	1:A:1696:VAL:HG12	1.96	0.66
1:A:1717:LEU:HD13	1:A:1717:LEU:C	2.16	0.66
1:A:125:PHE:CE2	1:A:163:GLY:HA3	2.20	0.66
1:A:1400:PHE:CD2	6:A:2317:Y01:CAB	2.79	0.65
1:A:763:GLU:HG2	1:A:1412:LYS:HD3	1.79	0.65
1:A:1450:GLY:CA	6:A:2317:Y01:CAD	2.75	0.64
4:A:2307:DZR:C12	5:A:2313:3PE:O14	2.46	0.64
1:A:1366:LEU:C	1:A:1366:LEU:HD12	2.18	0.63
1:A:960:VAL:HG22	1:A:1506:LEU:HD11	1.78	0.63
1:A:1355:ARG:CZ	1:A:1358:ARG:HH11	2.13	0.62
1:A:112:GLN:O	1:A:116:ILE:HG22	1.99	0.60
1:A:754:LEU:O	1:A:758:LEU:HD22	2.00	0.60
1:A:921:THR:HG21	1:A:1465:TRP:HE1	1.66	0.60
1:A:823:VAL:HG23	1:A:823:VAL:O	2.02	0.59
1:A:839:MET:CG	5:A:2315:3PE:H3A1	2.32	0.59
1:A:1459:LEU:HD23	1:A:1465:TRP:HB2	1.85	0.59
1:A:921:THR:HG21	1:A:1465:TRP:NE1	2.18	0.59
1:A:347:ILE:HG23	1:A:378:LEU:HD21	1.85	0.58
1:A:204:LEU:HD12	1:A:958:LEU:HD22	1.84	0.58
1:A:766:GLU:HA	1:A:766:GLU:OE1	2.03	0.58
1:A:1688:MET:HA	1:A:1688:MET:HE3	1.83	0.58
1:A:1400:PHE:HD2	6:A:2317:Y01:CAB	2.16	0.58
1:A:125:PHE:HE2	1:A:163:GLY:CA	2.09	0.57
1:A:128:PHE:CD2	1:A:189:ARG:NH1	2.71	0.57
1:A:93:LEU:HD11	1:A:120:PHE:CD2	2.39	0.57
1:A:809:ILE:HD12	1:A:809:ILE:C	2.26	0.56
1:A:757:THR:HA	1:A:760:MET:HE2	1.88	0.56
6:A:2316:Y01:HAR1	6:A:2316:Y01:OAG	2.07	0.55
1:A:93:LEU:HD11	1:A:120:PHE:CE2	2.42	0.54
1:A:1688:MET:CE	1:A:1688:MET:CA	2.86	0.54
1:A:1716:ALA:HB2	1:A:1829:LYS:HB2	1.89	0.54
1:A:1448:ASN:HD22	6:A:2316:Y01:HAD1	1.71	0.54
1:A:1716:ALA:HB2	1:A:1829:LYS:CB	2.38	0.54
1:A:1382:LEU:CD2	1:A:1821:ASN:ND2	2.71	0.53
1:A:768:PRO:HB2	1:A:770:GLU:OE1	2.08	0.53
1:A:832:VAL:HG23	5:A:2315:3PE:H321	1.90	0.53
6:A:2317:Y01:CAO	6:A:2317:Y01:CAA	2.86	0.53
6:A:2317:Y01:HAR1	6:A:2317:Y01:OAG	2.08	0.53
1:A:1450:GLY:HA3	6:A:2317:Y01:HAD1	1.90	0.52
1:A:233:TRP:HA	1:A:236:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1709:LEU:O	1:A:1712:THR:CG2	2.58	0.52
1:A:767:GLN:CB	1:A:768:PRO:HD2	2.37	0.52
1:A:1366:LEU:HD12	1:A:1366:LEU:O	2.10	0.52
1:A:1450:GLY:CA	6:A:2317:Y01:HAD1	2.41	0.52
1:A:1403:PHE:CE1	5:A:2315:3PE:H281	2.45	0.51
1:A:1753:CYS:SG	1:A:1790:ARG:NH2	2.84	0.51
1:A:805:ASN:HD22	1:A:806:PRO:HD2	1.76	0.51
1:A:93:LEU:HD12	1:A:124:ILE:HD11	1.93	0.51
1:A:313:CYS:SG	1:A:314:VAL:N	2.85	0.50
1:A:766:GLU:O	1:A:766:GLU:HG3	2.12	0.50
1:A:1260:LEU:HD12	1:A:1371:ARG:HB3	1.93	0.50
1:A:127:PHE:CD1	1:A:127:PHE:C	2.85	0.49
1:A:1270:ILE:CG1	1:A:1364:ARG:NH1	2.73	0.49
1:A:1355:ARG:CZ	1:A:1358:ARG:NH1	2.76	0.49
1:A:1364:ARG:N	1:A:1365:PRO:CD	2.74	0.49
1:A:371:ASN:ND2	6:A:2318:Y01:HAR2	2.28	0.49
1:A:1717:LEU:N	1:A:1718:PRO:HD2	2.28	0.49
1:A:1719:GLN:HA	1:A:1719:GLN:OE1	2.13	0.49
1:A:921:THR:CG2	1:A:1465:TRP:HE1	2.25	0.49
1:A:1378:VAL:HG21	1:A:1722:ASN:HB3	1.94	0.48
1:A:1403:PHE:HZ	5:A:2315:3PE:H281	1.76	0.48
1:A:1681:ASN:HD22	1:A:1682:PRO:HD2	1.78	0.48
1:A:1333:ILE:HD13	1:A:1360:LEU:HB3	1.95	0.48
1:A:1375:LEU:O	1:A:1379:VAL:HG23	2.14	0.48
1:A:123:PHE:C	1:A:123:PHE:CD1	2.87	0.48
1:A:100:MET:HB2	1:A:113:ARG:HH12	1.79	0.47
1:A:1382:LEU:HD22	1:A:1821:ASN:ND2	2.28	0.47
1:A:1505:VAL:HG11	5:A:2313:3PE:H32	1.97	0.47
1:A:1359:LEU:HD13	1:A:1740:GLU:CG	2.41	0.47
1:A:1774:ARG:HH21	1:A:1780:ASN:HB3	1.80	0.46
1:A:1368:VAL:O	1:A:1368:VAL:HG22	2.16	0.46
1:A:206:ASP:OD2	1:A:404:ARG:NH1	2.48	0.46
1:A:1389:ILE:HG22	1:A:1392:ILE:HD12	1.98	0.46
5:A:2313:3PE:C22	5:A:2313:3PE:C3	2.88	0.45
1:A:1450:GLY:HA2	6:A:2317:Y01:CAD	2.46	0.45
1:A:231:GLN:NE2	1:A:1608:GLU:OE1	2.50	0.45
1:A:1664:ILE:HA	1:A:1667:ILE:HG22	1.99	0.45
1:A:1350:ILE:HD12	1:A:1350:ILE:O	2.15	0.45
1:A:1720:VAL:HG22	1:A:1822:VAL:HG13	1.97	0.45
1:A:1382:LEU:HD21	1:A:1821:ASN:ND2	2.32	0.45
1:A:1696:VAL:O	1:A:1696:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:MET:HG3	5:A:2315:3PE:C3A	2.44	0.44
1:A:1597:VAL:HG11	1:A:1630:ILE:HD11	1.99	0.44
1:A:1355:ARG:O	1:A:1359:LEU:HD23	2.17	0.44
1:A:1400:PHE:HD2	6:A:2317:Y01:HAB3	1.81	0.44
1:A:1697:LEU:O	1:A:1699:LEU:N	2.51	0.44
1:A:224:ILE:HA	1:A:1693:ILE:HD11	2.00	0.44
1:A:921:THR:HG23	1:A:921:THR:O	2.18	0.44
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.78	0.43
1:A:1379:VAL:O	1:A:1383:MET:HG2	2.19	0.43
1:A:345:ILE:HD11	5:A:2310:3PE:H2C2	2.00	0.43
1:A:821:GLU:HB3	1:A:833:LEU:HD13	1.99	0.43
1:A:1817:PHE:O	1:A:1821:ASN:ND2	2.51	0.43
1:A:820:TRP:CD1	1:A:820:TRP:C	2.91	0.43
1:A:1450:GLY:C	6:A:2317:Y01:HAD2	2.39	0.43
6:A:2317:Y01:HAC3	6:A:2317:Y01:HAJ1	1.75	0.43
1:A:1354:LEU:HD22	1:A:1354:LEU:C	2.33	0.42
1:A:1722:ASN:HD22	1:A:1722:ASN:HA	1.71	0.42
6:A:2318:Y01:HAE2	6:A:2318:Y01:HBB	1.79	0.42
1:A:1450:GLY:C	6:A:2317:Y01:CAD	2.88	0.42
1:A:101:PHE:CE1	1:A:180:ARG:CZ	3.02	0.42
6:A:2317:Y01:HAS2	6:A:2317:Y01:HAE1	1.85	0.42
1:A:1717:LEU:HB3	1:A:1718:PRO:HD3	2.02	0.42
1:A:1408:VAL:O	1:A:1412:LYS:HB2	2.20	0.42
1:A:1464:GLY:HA3	1:A:1782:ASN:HD21	1.83	0.42
1:A:848:LEU:HA	1:A:849:PRO:HD3	1.82	0.42
1:A:1456:LEU:HD23	1:A:1459:LEU:HD12	2.01	0.42
1:A:288:LEU:C	1:A:288:LEU:HD13	2.40	0.41
1:A:1631:PHE:HB3	1:A:1660:VAL:HG22	2.02	0.41
1:A:121:ASP:OD2	1:A:186:ARG:NH1	2.51	0.41
6:A:2317:Y01:HAB3	6:A:2317:Y01:HAJ2	1.84	0.41
1:A:757:THR:HA	1:A:760:MET:CE	2.51	0.41
1:A:1697:LEU:C	1:A:1699:LEU:N	2.73	0.41
1:A:371:ASN:HD22	1:A:371:ASN:HA	1.61	0.41
1:A:1270:ILE:HG12	1:A:1364:ARG:NH1	2.24	0.41
1:A:1350:ILE:HD13	1:A:1350:ILE:HA	1.75	0.41
1:A:1697:LEU:C	1:A:1699:LEU:H	2.24	0.41
1:A:1278:ASP:HB2	1:A:1281:SER:HB2	2.03	0.41
1:A:239:ASN:HA	1:A:325:ALA:HA	2.02	0.40
1:A:340:ILE:HD12	1:A:340:ILE:HA	1.93	0.40
1:A:1376:LYS:O	1:A:1380:GLU:HG3	2.21	0.40
1:A:767:GLN:HB2	1:A:768:PRO:CD	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:LEU:CD1	1:A:1366:LEU:C	2.89	0.40
1:A:1450:GLY:HA2	6:A:2317:Y01:HAD3	2.02	0.40
1:A:1711:ASP:O	1:A:1715:GLN:HG3	2.20	0.40
6:A:2318:Y01:HAP1	6:A:2318:Y01:HAO2	1.82	0.40
1:A:1506:LEU:HD12	1:A:1506:LEU:HA	1.91	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	992/2146 (46%)	956 (96%)	33 (3%)	3 (0%)	41 73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	909	LEU
1	A	764	TYR
1	A	1698	LYS

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	902/1852 (49%)	876 (97%)	26 (3%)	42 72

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	94	ASN
1	A	243	LEU
1	A	314	VAL
1	A	758	LEU
1	A	769	GLU
1	A	805	ASN
1	A	809	ILE
1	A	811	ASP
1	A	834	ARG
1	A	921	THR
1	A	1266	ASN
1	A	1350	ILE
1	A	1361	ARG
1	A	1366	LEU
1	A	1487	ASN
1	A	1601	ASN
1	A	1624	ASN
1	A	1675	ASN
1	A	1681	ASN
1	A	1687	ILE
1	A	1697	LEU
1	A	1712	THR
1	A	1774	ARG
1	A	1780	ASN
1	A	1835	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	371	ASN
1	A	805	ASN
1	A	918	GLN
1	A	957	ASN
1	A	1266	ASN
1	A	1442	HIS
1	A	1451	GLN
1	A	1624	ASN
1	A	1649	GLN
1	A	1675	ASN

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Mol	Chain	Res	Type
1	A	1681	ASN
1	A	1722	ASN
1	A	1780	ASN
1	A	1821	ASN
1	A	1835	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
6	Y01	A	2317	-	38,38,38	4.02	11 (28%)	57,57,57	2.41	19 (33%)
5	3PE	A	2310	-	13,13,50	0.20	0	12,12,55	1.01	0
5	3PE	A	2315	-	34,34,50	1.18	3 (8%)	37,39,55	1.45	6 (16%)
3	NAG	A	2303	1	14,14,15	1.56	2 (14%)	17,19,21	1.31	1 (5%)
6	Y01	A	2316	-	38,38,38	3.99	12 (31%)	57,57,57	2.16	16 (28%)
5	3PE	A	2314	-	15,15,50	0.25	0	14,14,55	0.87	0
5	3PE	A	2313	-	35,35,50	1.07	4 (11%)	38,40,55	1.27	4 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	3PE	A	2309	-	30,30,50	1.18	4 (13%)	33,35,55	1.26	3 (9%)
4	DZR	A	2307	-	27,27,27	2.74	7 (25%)	38,38,38	1.74	10 (26%)
3	NAG	A	2304	1	14,14,15	0.31	0	17,19,21	0.65	1 (5%)
5	3PE	A	2311	-	32,32,50	1.14	4 (12%)	35,37,55	1.29	3 (8%)
5	3PE	A	2308	-	30,30,50	1.17	3 (10%)	33,35,55	1.34	4 (12%)
3	NAG	A	2306	1	14,14,15	0.67	0	17,19,21	2.31	4 (23%)
6	Y01	A	2318	-	38,38,38	4.03	12 (31%)	57,57,57	2.09	15 (26%)
3	NAG	A	2305	1	14,14,15	0.37	0	17,19,21	0.79	1 (5%)
5	3PE	A	2312	-	12,12,50	0.28	0	11,11,55	0.89	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
6	Y01	A	2317	-	-	11/19/77/77	0/4/4/4
5	3PE	A	2310	-	-	4/11/11/54	-
5	3PE	A	2315	-	-	12/38/38/54	-
3	NAG	A	2303	1	-	0/6/23/26	0/1/1/1
6	Y01	A	2316	-	-	15/19/77/77	0/4/4/4
5	3PE	A	2314	-	-	6/13/13/54	-
5	3PE	A	2313	-	-	24/39/39/54	-
5	3PE	A	2309	-	-	19/34/34/54	-
4	DZR	A	2307	-	-	2/18/28/28	0/2/2/2
3	NAG	A	2304	1	-	2/6/23/26	0/1/1/1
5	3PE	A	2311	-	-	16/36/36/54	-
5	3PE	A	2308	-	-	16/34/34/54	-
3	NAG	A	2306	1	-	5/6/23/26	0/1/1/1
6	Y01	A	2318	-	-	14/19/77/77	0/4/4/4
3	NAG	A	2305	1	-	0/6/23/26	0/1/1/1
5	3PE	A	2312	-	-	2/10/10/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2317	Y01	CAI-CAZ	16.49	1.69	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2318	Y01	CAI-CAZ	16.45	1.69	1.33
6	A	2316	Y01	CAI-CAZ	16.21	1.68	1.33
6	A	2318	Y01	CBH-CBF	7.06	1.67	1.56
4	A	2307	DZR	C14-N05	-7.05	1.31	1.47
6	A	2317	Y01	CAQ-CAP	7.01	1.73	1.54
6	A	2316	Y01	CBH-CBF	6.96	1.67	1.56
6	A	2318	Y01	CAQ-CAP	6.95	1.73	1.54
6	A	2317	Y01	CAU-CBI	-6.88	1.41	1.54
6	A	2316	Y01	CAU-CBI	-6.77	1.42	1.54
6	A	2316	Y01	CAQ-CAP	6.74	1.72	1.54
6	A	2318	Y01	CAU-CBI	-6.73	1.42	1.54
6	A	2317	Y01	CBH-CBF	6.69	1.67	1.56
4	A	2307	DZR	C15-N07	6.59	1.45	1.34
6	A	2317	Y01	CBB-CBE	-6.34	1.43	1.54
6	A	2318	Y01	CAK-CBD	6.32	1.63	1.53
6	A	2318	Y01	CAU-CAS	6.01	1.66	1.53
6	A	2316	Y01	CAU-CAS	5.99	1.66	1.53
6	A	2316	Y01	CAK-CBD	5.96	1.63	1.53
6	A	2316	Y01	CBB-CBE	-5.92	1.44	1.54
6	A	2317	Y01	CAU-CAS	5.88	1.65	1.53
6	A	2316	Y01	CBI-CBE	5.81	1.66	1.55
6	A	2317	Y01	CAK-CBD	5.78	1.62	1.53
4	A	2307	DZR	C11-N05	-5.60	1.31	1.46
6	A	2318	Y01	CBI-CBE	5.46	1.65	1.55
4	A	2307	DZR	C12-N05	-5.34	1.32	1.46
6	A	2317	Y01	CBI-CBE	5.28	1.65	1.55
4	A	2307	DZR	C17-N06	5.28	1.45	1.33
6	A	2318	Y01	CAQ-CBG	5.12	1.65	1.54
6	A	2318	Y01	CBB-CBE	-5.03	1.45	1.54
6	A	2317	Y01	CAQ-CBG	5.01	1.64	1.54
3	A	2303	NAG	O5-C1	4.86	1.51	1.43
6	A	2316	Y01	CAQ-CBG	4.84	1.64	1.54
5	A	2315	3PE	O31-C31	3.36	1.43	1.33
6	A	2318	Y01	OAW-CAY	3.06	1.42	1.34
6	A	2317	Y01	OAW-CAY	2.99	1.42	1.34
3	A	2303	NAG	C1-C2	2.91	1.56	1.52
6	A	2316	Y01	OAW-CAY	2.81	1.42	1.34
6	A	2318	Y01	CAO-CBB	2.76	1.61	1.54
5	A	2309	3PE	O21-C2	-2.76	1.39	1.46
5	A	2308	3PE	O21-C21	2.58	1.41	1.34
5	A	2311	3PE	O21-C2	-2.58	1.40	1.46
5	A	2315	3PE	C3-C2	2.55	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2317	Y01	CBH-CAZ	-2.50	1.47	1.52
5	A	2311	3PE	O31-C31	2.46	1.40	1.33
6	A	2316	Y01	CBH-CAZ	-2.44	1.48	1.52
4	A	2307	DZR	O04-C17	-2.42	1.18	1.23
5	A	2309	3PE	O31-C31	2.42	1.40	1.33
5	A	2313	3PE	O21-C2	-2.37	1.40	1.46
5	A	2313	3PE	O31-C31	2.32	1.40	1.33
6	A	2318	Y01	CBH-CAZ	-2.29	1.48	1.52
6	A	2316	Y01	CAO-CBB	2.28	1.60	1.54
5	A	2308	3PE	O31-C3	-2.26	1.40	1.45
5	A	2308	3PE	O31-C31	2.21	1.39	1.33
5	A	2309	3PE	O21-C21	2.16	1.40	1.34
5	A	2309	3PE	O31-C3	-2.15	1.40	1.45
5	A	2311	3PE	O31-C3	-2.13	1.40	1.45
5	A	2311	3PE	O21-C21	2.12	1.40	1.34
5	A	2315	3PE	C32-C31	2.11	1.56	1.50
5	A	2313	3PE	O21-C21	2.11	1.40	1.34
4	A	2307	DZR	O03-C15	-2.07	1.19	1.23
5	A	2313	3PE	P-O12	-2.04	1.45	1.55

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2306	NAG	C2-N2-C7	7.88	134.13	122.90
6	A	2317	Y01	CBI-CBE-CBB	-6.70	108.99	119.49
6	A	2317	Y01	CBG-CBI-CBE	6.17	107.38	100.07
5	A	2315	3PE	O21-C21-C22	5.84	124.09	111.50
6	A	2317	Y01	CAV-CAZ-CBH	-5.63	108.94	116.42
6	A	2316	Y01	CAK-CAI-CAZ	-5.45	115.01	125.06
6	A	2316	Y01	CBI-CBE-CBB	-5.34	111.13	119.49
6	A	2316	Y01	CBG-CBI-CBE	5.18	106.21	100.07
6	A	2318	Y01	CAK-CAI-CAZ	-5.10	115.65	125.06
3	A	2303	NAG	C1-O5-C5	5.03	119.01	112.19
6	A	2318	Y01	CBH-CAZ-CAI	-4.63	115.81	122.90
6	A	2317	Y01	CAK-CAI-CAZ	-4.50	116.76	125.06
6	A	2318	Y01	CAD-CBH-CBF	-4.46	106.36	111.68
5	A	2308	3PE	O21-C21-C22	4.40	120.99	111.50
6	A	2318	Y01	OAW-CAY-CAM	4.27	120.69	111.50
4	A	2307	DZR	C16-N07-C15	-4.25	121.49	126.32
6	A	2316	Y01	CAE-CBI-CAU	-4.19	103.97	110.59
6	A	2318	Y01	CAU-CBI-CBE	4.18	122.83	116.57
5	A	2309	3PE	O21-C21-C22	4.17	120.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2313	3PE	O21-C21-C22	4.11	120.36	111.50
5	A	2311	3PE	O21-C21-C22	4.08	120.30	111.50
6	A	2317	Y01	CAU-CBI-CBE	4.03	122.60	116.57
6	A	2317	Y01	CBH-CAZ-CAI	-3.99	116.79	122.90
6	A	2317	Y01	CBI-CBG-CBD	-3.98	108.48	114.38
6	A	2316	Y01	CBH-CAZ-CAI	-3.85	117.01	122.90
6	A	2317	Y01	CAE-CBI-CAU	-3.81	104.58	110.59
6	A	2317	Y01	CAE-CBI-CBG	-3.79	104.64	111.71
6	A	2316	Y01	OAW-CAY-CAM	3.79	119.66	111.50
6	A	2317	Y01	OAW-CAY-CAM	3.73	119.55	111.50
6	A	2317	Y01	CAE-CBI-CBE	-3.66	104.89	111.71
6	A	2318	Y01	CAE-CBI-CBG	-3.59	105.01	111.71
4	A	2307	DZR	C12-N05-C11	3.58	116.89	108.83
6	A	2316	Y01	CAU-CBI-CBE	3.58	121.93	116.57
6	A	2318	Y01	CAE-CBI-CBE	-3.55	105.08	111.71
3	A	2306	NAG	C1-C2-N2	3.55	116.55	110.49
6	A	2318	Y01	CBI-CBE-CBB	-3.53	113.96	119.49
6	A	2318	Y01	CBG-CBI-CBE	3.47	104.18	100.07
6	A	2318	Y01	CAU-CBI-CBG	3.44	112.61	107.27
6	A	2316	Y01	CAP-CBE-CBI	3.41	107.95	103.84
6	A	2316	Y01	CAE-CBI-CBG	-3.40	105.37	111.71
6	A	2316	Y01	CAD-CBH-CBF	-3.38	107.65	111.68
6	A	2318	Y01	CAK-CBD-CBF	3.38	113.81	109.71
4	A	2307	DZR	C10-C12-N05	3.37	116.34	111.11
5	A	2311	3PE	O31-C31-C32	3.26	119.92	111.38
6	A	2317	Y01	CAS-CBF-CBH	-3.17	108.91	113.08
6	A	2318	Y01	CAE-CBI-CAU	-3.13	105.64	110.59
4	A	2307	DZR	O03-C15-N07	-3.04	118.15	123.05
4	A	2307	DZR	C09-C11-N05	2.96	115.71	111.11
6	A	2316	Y01	CAU-CBI-CBG	2.93	111.83	107.27
6	A	2316	Y01	CAE-CBI-CBE	-2.93	106.26	111.71
4	A	2307	DZR	C24-C26-C25	2.91	119.90	117.42
3	A	2305	NAG	C1-O5-C5	2.87	116.08	112.19
6	A	2317	Y01	CAD-CBH-CBF	-2.84	108.30	111.68
5	A	2315	3PE	O31-C31-O32	-2.81	116.51	123.59
6	A	2317	Y01	CAK-CBD-CBF	2.73	113.02	109.71
6	A	2317	Y01	CBF-CBH-CAZ	2.71	113.91	109.65
3	A	2306	NAG	C1-O5-C5	2.67	115.81	112.19
6	A	2316	Y01	CAC-CBB-CBE	-2.66	108.84	112.92
5	A	2315	3PE	O21-C21-O22	-2.65	117.30	123.70
5	A	2308	3PE	O31-C31-C32	2.59	120.03	111.91
5	A	2313	3PE	O31-C31-C32	2.58	120.00	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2309	3PE	O31-C31-C32	2.56	119.95	111.91
6	A	2316	Y01	CAV-CAZ-CBH	-2.56	113.02	116.42
4	A	2307	DZR	C14-C15-N07	2.55	119.44	114.85
4	A	2307	DZR	C26-C25-C23	-2.52	120.34	123.52
5	A	2308	3PE	O12-P-O14	-2.50	99.86	112.24
6	A	2317	Y01	CAU-CBI-CBG	2.49	111.13	107.27
6	A	2317	Y01	CAQ-CBG-CBD	2.43	123.08	119.08
6	A	2316	Y01	CAK-CBD-CBF	2.41	112.64	109.71
6	A	2317	Y01	CAQ-CBG-CBI	2.41	106.75	103.84
6	A	2318	Y01	CAC-CBB-CBE	-2.32	109.37	112.92
5	A	2315	3PE	O12-P-O14	-2.32	100.79	112.24
6	A	2316	Y01	CAM-CAL-CAX	-2.30	108.66	113.60
5	A	2315	3PE	O31-C31-C32	2.30	119.11	111.91
5	A	2311	3PE	O12-P-O14	-2.27	101.04	112.24
5	A	2313	3PE	O12-P-O14	-2.26	101.05	112.24
6	A	2318	Y01	CAO-CBB-CBE	2.26	114.95	110.28
3	A	2304	NAG	C1-O5-C5	2.24	115.22	112.19
4	A	2307	DZR	C14-N05-C11	2.23	114.55	111.09
6	A	2318	Y01	CAQ-CBG-CBD	2.22	122.74	119.08
6	A	2317	Y01	CAC-CBB-CBE	-2.16	109.61	112.92
5	A	2315	3PE	C3-C2-C1	2.16	116.89	111.79
5	A	2308	3PE	C2-O21-C21	2.14	123.07	117.79
3	A	2306	NAG	C8-C7-N2	2.13	119.70	116.10
5	A	2313	3PE	O31-C3-C2	2.11	114.57	108.43
4	A	2307	DZR	C14-N05-C12	2.08	114.32	111.09
5	A	2309	3PE	O12-P-O14	-2.07	101.99	112.24

There are no chirality outliers.

All (148) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2309	3PE	C1-O11-P-O12
5	A	2309	3PE	C1-O11-P-O14
5	A	2309	3PE	C11-O13-P-O11
5	A	2309	3PE	C11-O13-P-O12
5	A	2309	3PE	C11-O13-P-O14
5	A	2309	3PE	O13-C11-C12-N
5	A	2309	3PE	O22-C21-O21-C2
5	A	2311	3PE	C1-O11-P-O14
5	A	2311	3PE	O13-C11-C12-N
5	A	2311	3PE	O21-C2-C3-O31
5	A	2313	3PE	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
5	A	2313	3PE	C1-O11-P-O14
5	A	2313	3PE	O13-C11-C12-N
5	A	2313	3PE	O22-C21-O21-C2
5	A	2313	3PE	C22-C21-O21-C2
5	A	2315	3PE	C22-C21-O21-C2
6	A	2316	Y01	CAR-CBC-OAW-CAY
6	A	2317	Y01	CAR-CBC-OAW-CAY
6	A	2318	Y01	OAG-CAY-OAW-CBC
5	A	2315	3PE	O32-C31-O31-C3
5	A	2315	3PE	C32-C31-O31-C3
6	A	2318	Y01	CAJ-CAO-CBB-CAC
5	A	2313	3PE	O32-C31-O31-C3
6	A	2318	Y01	CAC-CBB-CBE-CAP
6	A	2318	Y01	CAC-CBB-CBE-CBI
5	A	2308	3PE	O22-C21-O21-C2
5	A	2315	3PE	O22-C21-O21-C2
5	A	2308	3PE	C32-C31-O31-C3
5	A	2313	3PE	C32-C31-O31-C3
5	A	2309	3PE	C22-C21-O21-C2
6	A	2318	Y01	CAM-CAY-OAW-CBC
6	A	2316	Y01	CAJ-CAO-CBB-CAC
6	A	2316	Y01	CAC-CBB-CBE-CAP
6	A	2318	Y01	CAO-CBB-CBE-CBI
3	A	2306	NAG	O5-C5-C6-O6
6	A	2316	Y01	CAO-CBB-CBE-CAP
6	A	2316	Y01	CAO-CBB-CBE-CBI
3	A	2304	NAG	O5-C5-C6-O6
5	A	2308	3PE	O32-C31-O31-C3
5	A	2308	3PE	C22-C21-O21-C2
3	A	2306	NAG	C4-C5-C6-O6
6	A	2316	Y01	CAC-CBB-CBE-CBI
6	A	2318	Y01	CAO-CBB-CBE-CAP
6	A	2317	Y01	CAC-CBB-CBE-CBI
6	A	2316	Y01	CAJ-CAO-CBB-CBE
3	A	2304	NAG	C4-C5-C6-O6
3	A	2306	NAG	C8-C7-N2-C2
3	A	2306	NAG	O7-C7-N2-C2
6	A	2317	Y01	CAN-CAJ-CAO-CBB
6	A	2318	Y01	CAJ-CAO-CBB-CBE
5	A	2313	3PE	C34-C35-C36-C37
5	A	2308	3PE	C21-C22-C23-C24
5	A	2311	3PE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
6	A	2316	Y01	CAO-CAJ-CAN-CBA
5	A	2309	3PE	C1-O11-P-O13
5	A	2311	3PE	C1-O11-P-O13
5	A	2313	3PE	C1-O11-P-O13
6	A	2318	Y01	CAJ-CAN-CBA-CAB
6	A	2317	Y01	CAO-CBB-CBE-CBI
5	A	2313	3PE	C32-C33-C34-C35
5	A	2311	3PE	C29-C2A-C2B-C2C
5	A	2314	3PE	C32-C33-C34-C35
5	A	2314	3PE	C35-C36-C37-C38
5	A	2311	3PE	C23-C24-C25-C26
5	A	2308	3PE	C23-C24-C25-C26
6	A	2316	Y01	CAJ-CAN-CBA-CAA
6	A	2316	Y01	CAJ-CAN-CBA-CAB
6	A	2318	Y01	CAJ-CAN-CBA-CAA
5	A	2310	3PE	C2E-C2F-C2G-C2H
5	A	2310	3PE	C2D-C2E-C2F-C2G
5	A	2308	3PE	C31-C32-C33-C34
6	A	2316	Y01	CAM-CAY-OAW-CBC
6	A	2316	Y01	OAG-CAY-OAW-CBC
5	A	2313	3PE	C23-C24-C25-C26
5	A	2313	3PE	C22-C23-C24-C25
5	A	2314	3PE	C3A-C3B-C3C-C3D
5	A	2311	3PE	C1-C2-C3-O31
6	A	2317	Y01	CAV-CBC-OAW-CAY
5	A	2310	3PE	C2B-C2C-C2D-C2E
5	A	2308	3PE	C3-C2-O21-C21
5	A	2309	3PE	O11-C1-C2-O21
6	A	2317	Y01	CAC-CBB-CBE-CAP
5	A	2313	3PE	O11-C1-C2-C3
5	A	2315	3PE	O11-C1-C2-C3
5	A	2313	3PE	C31-C32-C33-C34
5	A	2309	3PE	C1-C2-C3-O31
5	A	2314	3PE	C37-C38-C39-C3A
5	A	2311	3PE	C2C-C2D-C2E-C2F
5	A	2308	3PE	C1-O11-P-O13
5	A	2315	3PE	C11-O13-P-O11
5	A	2308	3PE	O11-C1-C2-O21
5	A	2314	3PE	C3C-C3D-C3E-C3F
5	A	2308	3PE	C22-C23-C24-C25
5	A	2311	3PE	C28-C29-C2A-C2B
4	A	2307	DZR	C15-C14-N05-C11

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Mol	Chain	Res	Type	Atoms
4	A	2307	DZR	C15-C14-N05-C12
5	A	2308	3PE	O11-C1-C2-C3
5	A	2311	3PE	C26-C27-C28-C29
6	A	2317	Y01	CAJ-CAO-CBB-CAC
5	A	2313	3PE	C3-C2-O21-C21
5	A	2315	3PE	C3-C2-O21-C21
5	A	2313	3PE	C2-C1-O11-P
5	A	2313	3PE	O11-C1-C2-O21
5	A	2310	3PE	C2A-C2B-C2C-C2D
5	A	2311	3PE	C27-C28-C29-C2A
5	A	2308	3PE	C1-O11-P-O12
5	A	2308	3PE	C11-O13-P-O12
5	A	2311	3PE	C1-O11-P-O12
6	A	2317	Y01	CAO-CBB-CBE-CAP
5	A	2315	3PE	C12-C11-O13-P
5	A	2315	3PE	O11-C1-C2-O21
5	A	2309	3PE	C22-C23-C24-C25
5	A	2312	3PE	C28-C29-C2A-C2B
5	A	2313	3PE	C1-C2-C3-O31
5	A	2309	3PE	O21-C2-C3-O31
5	A	2313	3PE	O21-C2-C3-O31
5	A	2313	3PE	C33-C34-C35-C36
5	A	2312	3PE	C2A-C2B-C2C-C2D
5	A	2315	3PE	C1-C2-O21-C21
5	A	2309	3PE	O11-C1-C2-C3
6	A	2316	Y01	CAN-CAJ-CAO-CBB
5	A	2313	3PE	C11-O13-P-O11
5	A	2309	3PE	C32-C31-O31-C3
5	A	2309	3PE	O32-C31-O31-C3
5	A	2309	3PE	C2-C1-O11-P
5	A	2308	3PE	C1-C2-C3-O31
6	A	2317	Y01	CAM-CAL-CAX-OAH
6	A	2318	Y01	CAM-CAL-CAX-OAH
5	A	2309	3PE	C25-C26-C27-C28
5	A	2315	3PE	O31-C31-C32-C33
5	A	2314	3PE	C3B-C3C-C3D-C3E
6	A	2317	Y01	CAM-CAL-CAX-OAF
6	A	2318	Y01	CAM-CAL-CAX-OAF
5	A	2308	3PE	O21-C21-C22-C23
5	A	2313	3PE	C21-C22-C23-C24
5	A	2313	3PE	C38-C39-C3A-C3B
5	A	2313	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
5	A	2311	3PE	O32-C31-O31-C3
6	A	2316	Y01	CAL-CAM-CAY-OAW
5	A	2311	3PE	C32-C31-O31-C3
3	A	2306	NAG	C3-C2-N2-C7
5	A	2311	3PE	C2A-C2B-C2C-C2D
6	A	2316	Y01	CAL-CAM-CAY-OAG
5	A	2315	3PE	O32-C31-C32-C33
6	A	2318	Y01	CAL-CAM-CAY-OAW
5	A	2309	3PE	C12-C11-O13-P
6	A	2317	Y01	CAO-CAJ-CAN-CBA
6	A	2318	Y01	CAL-CAM-CAY-OAG

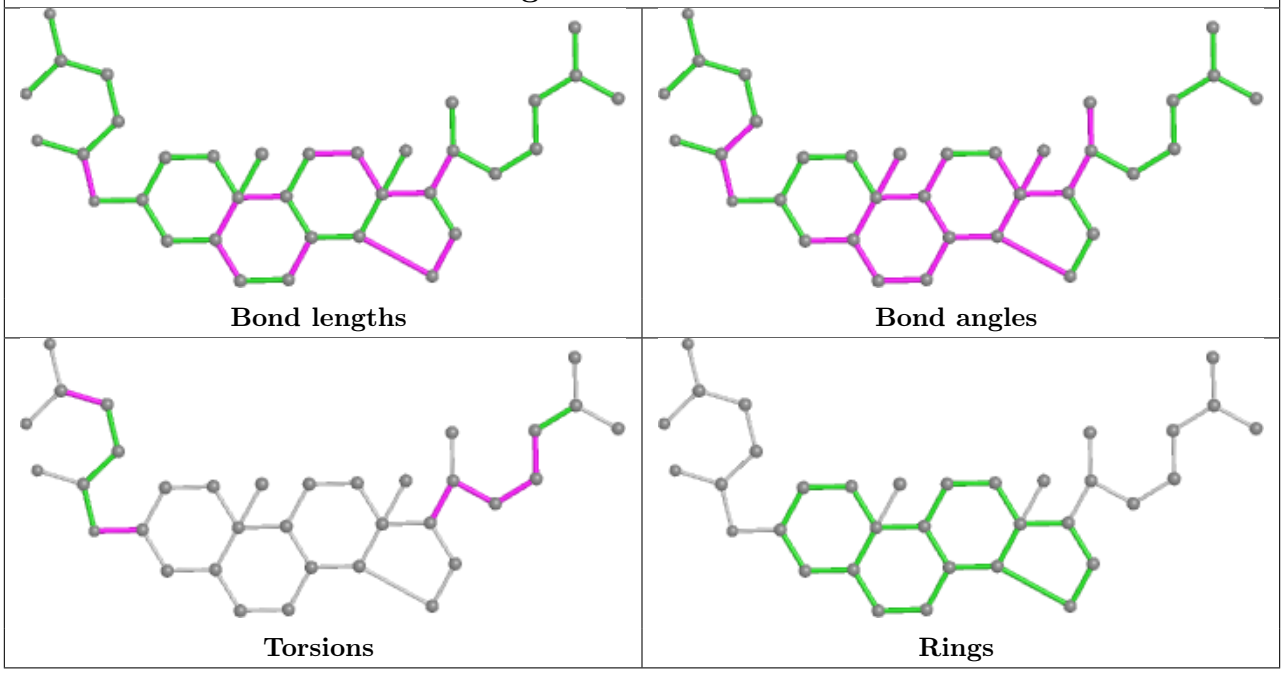
There are no ring outliers.

7 monomers are involved in 48 short contacts:

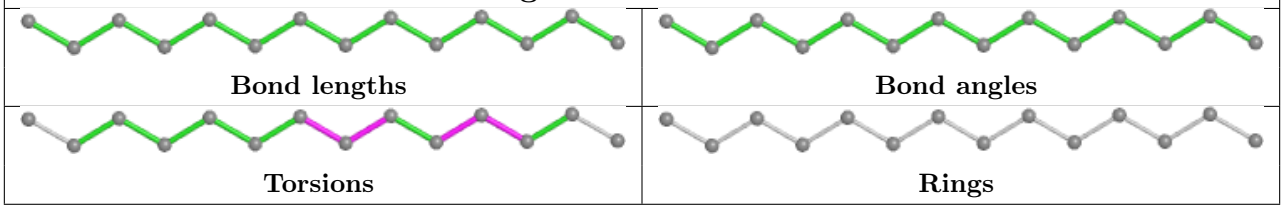
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2317	Y01	22	0
5	A	2310	3PE	1	0
5	A	2315	3PE	9	0
6	A	2316	Y01	8	0
5	A	2313	3PE	5	0
4	A	2307	DZR	1	0
6	A	2318	Y01	3	0

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.

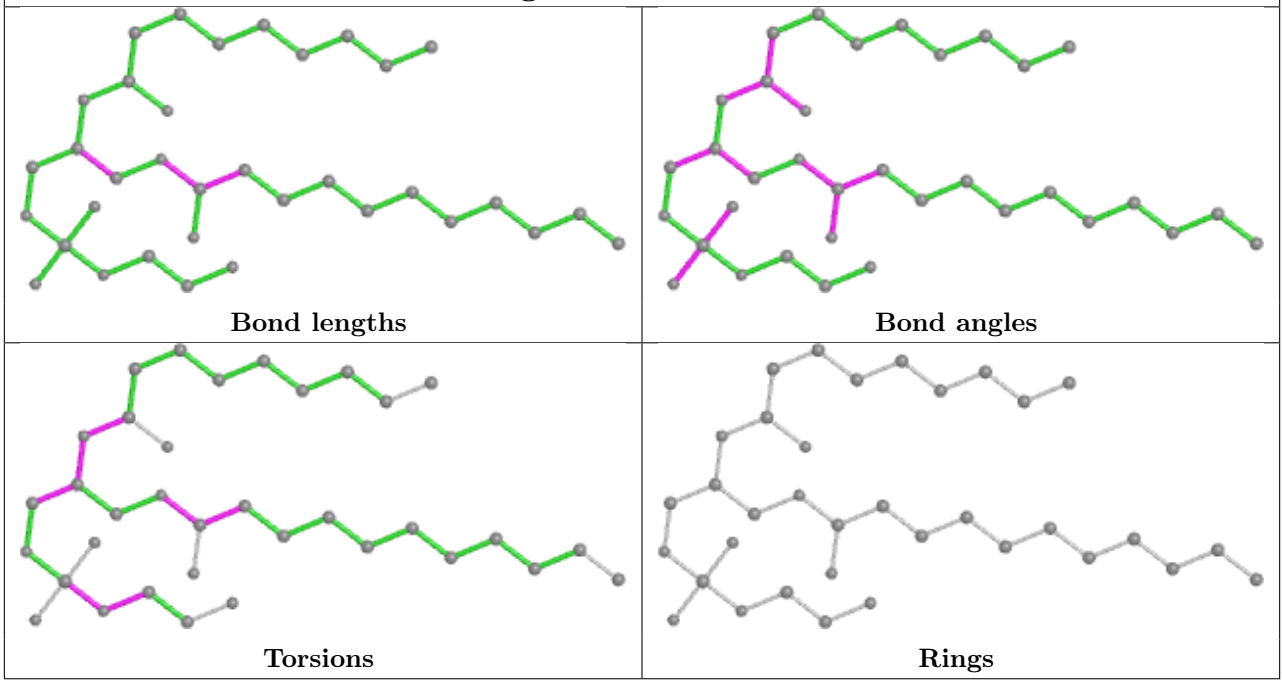
Ligand Y01 A 2317



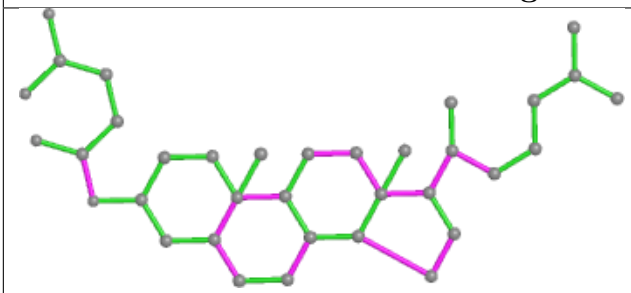
Ligand 3PE A 2310



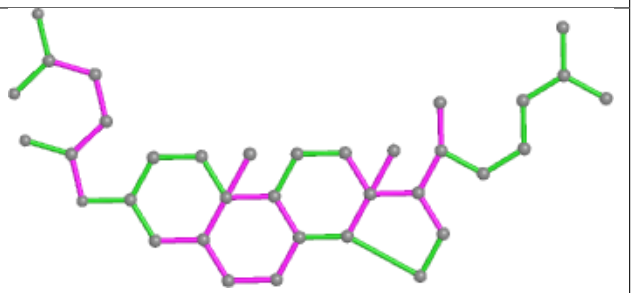
Ligand 3PE A 2315



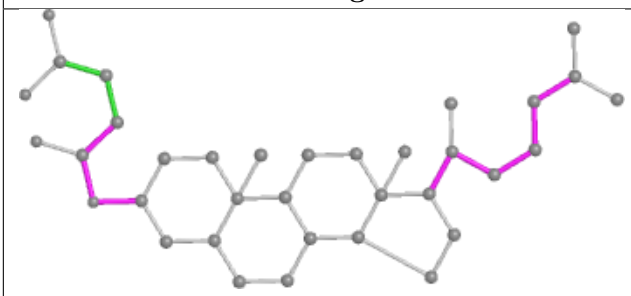
Ligand Y01 A 2316



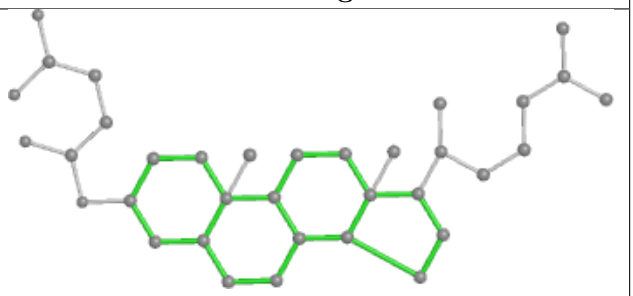
Bond lengths



Bond angles



Torsions

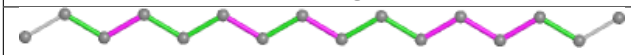


Rings

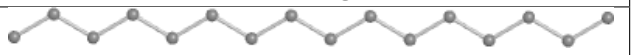
Ligand 3PE A 2314

Bond lengths

Bond angles

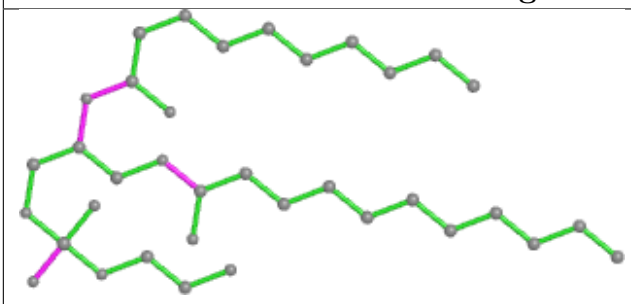


Torsions

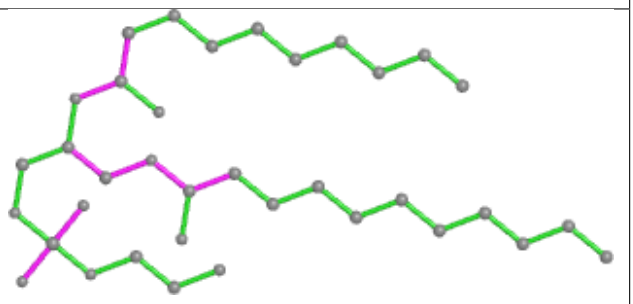


Rings

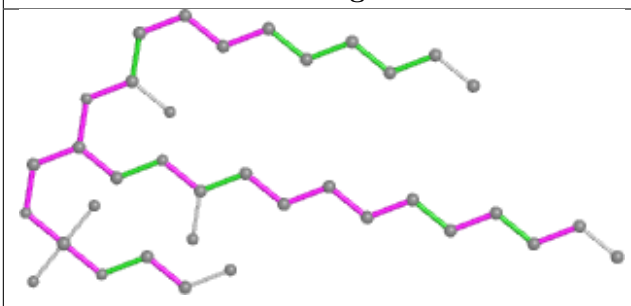
Ligand 3PE A 2313



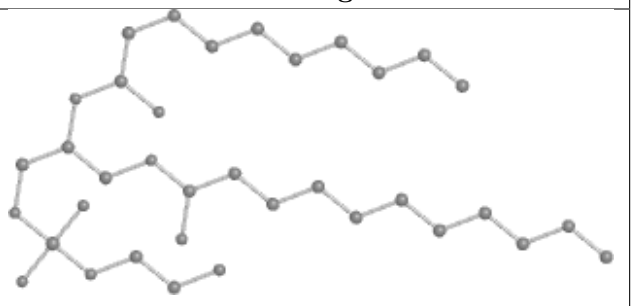
Bond lengths



Bond angles

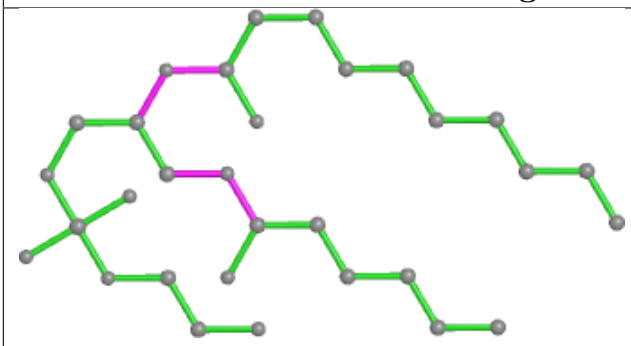


Torsions

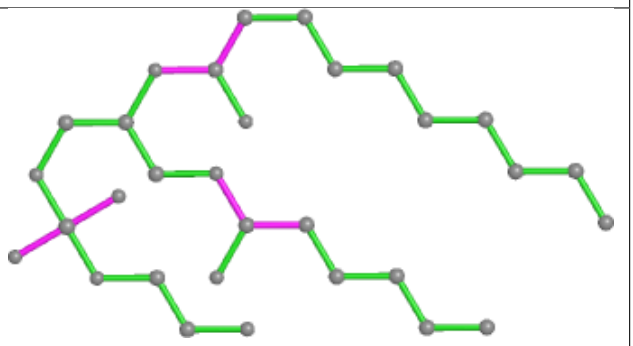


Rings

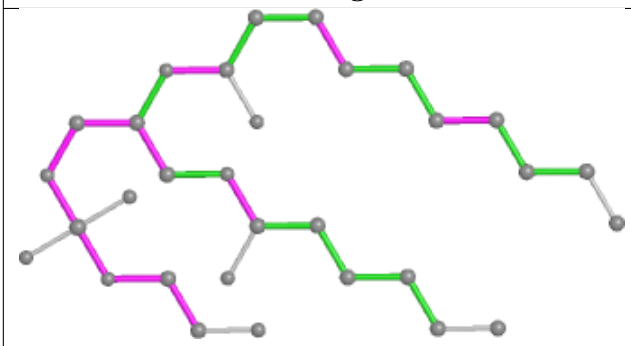
Ligand 3PE A 2309



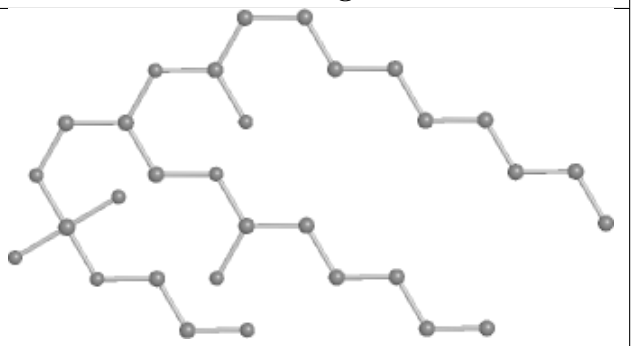
Bond lengths



Bond angles

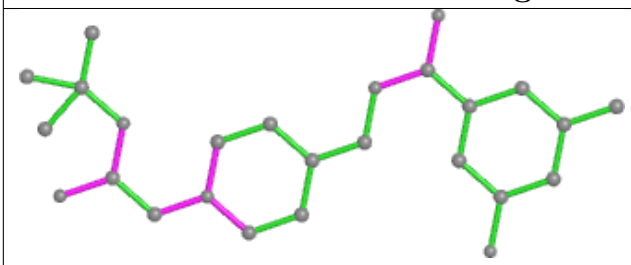


Torsions

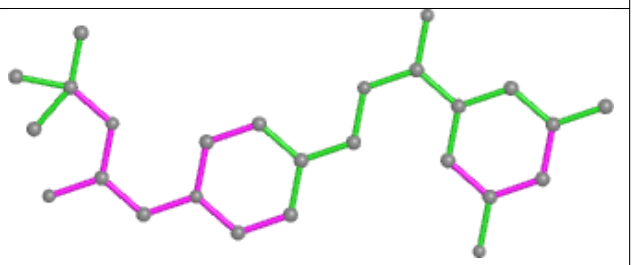


Rings

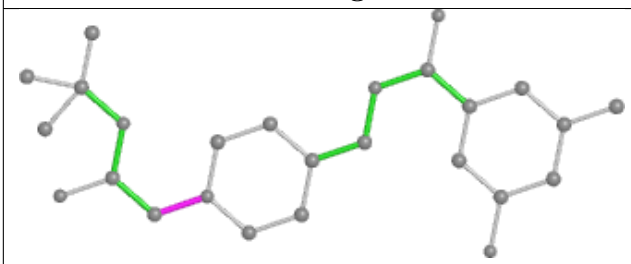
Ligand DZR A 2307



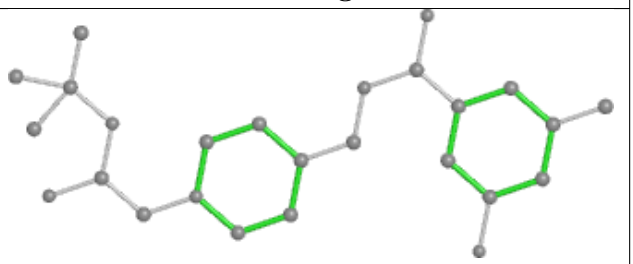
Bond lengths



Bond angles

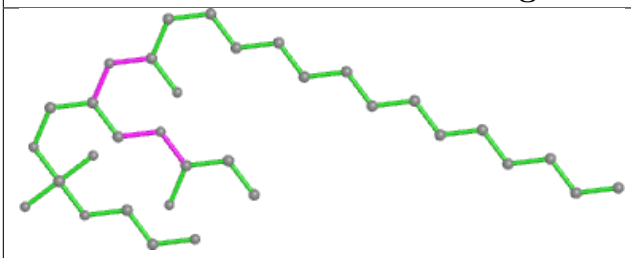


Torsions

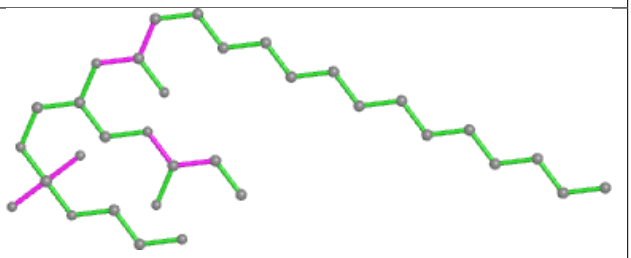


Rings

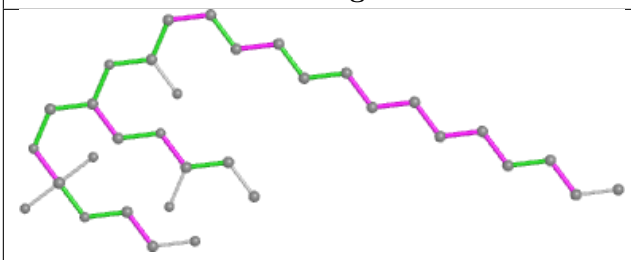
Ligand 3PE A 2311



Bond lengths



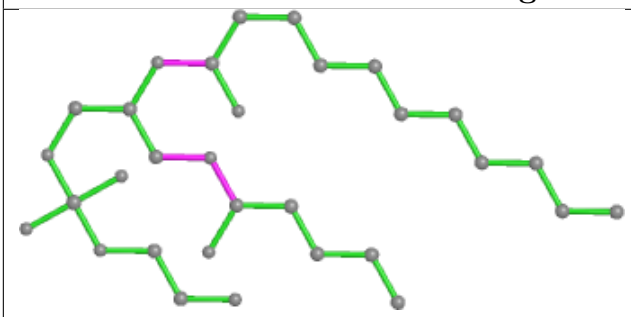
Bond angles



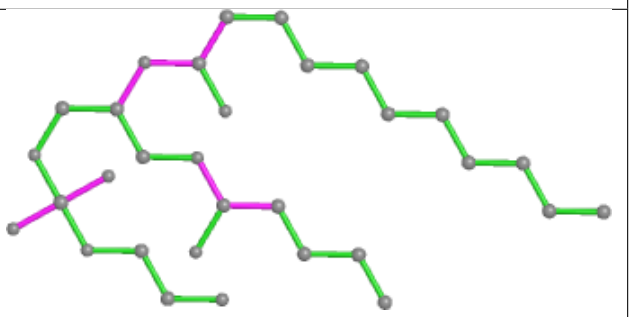
Torsions

Rings

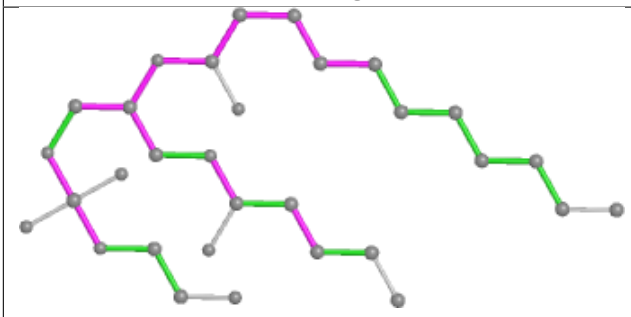
Ligand 3PE A 2308



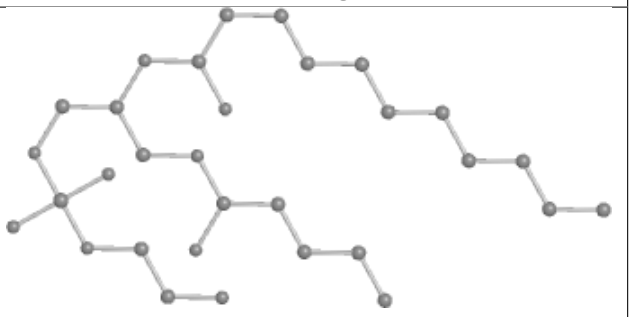
Bond lengths



Bond angles

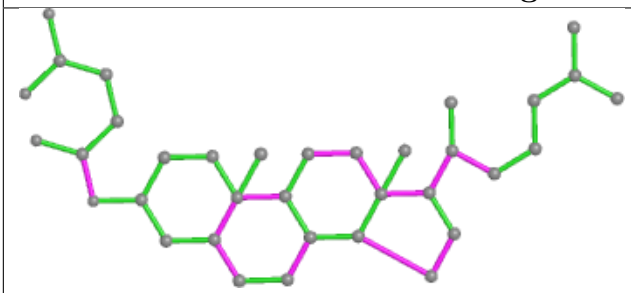


Torsions

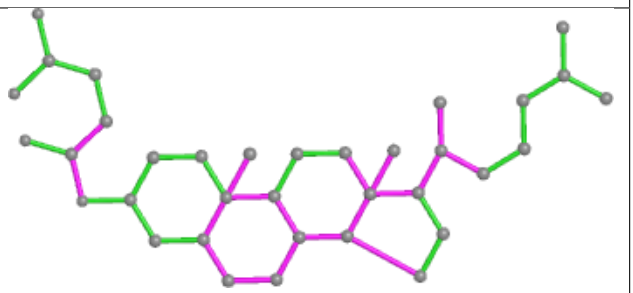


Rings

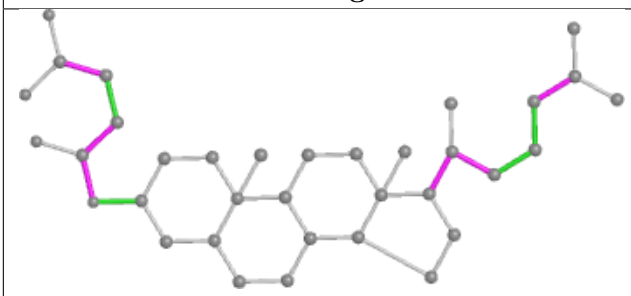
Ligand Y01 A 2318



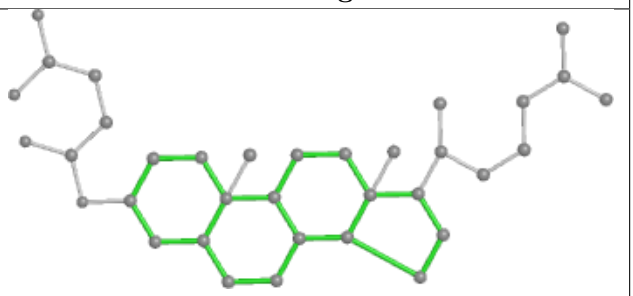
Bond lengths



Bond angles



Torsions

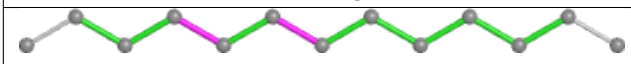


Rings

Ligand 3PE A 2312

Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

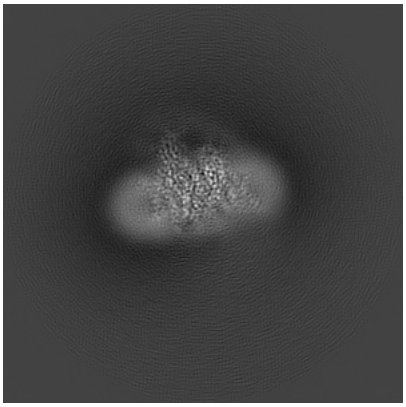
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-0792. These allow visual inspection of the internal detail of the map and identification of artifacts.

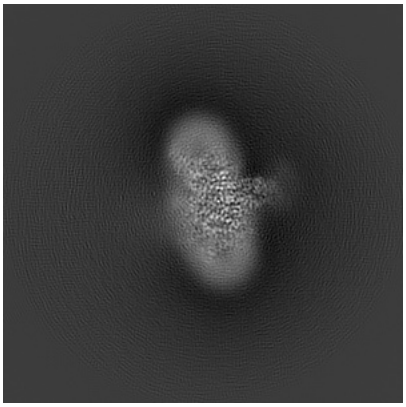
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

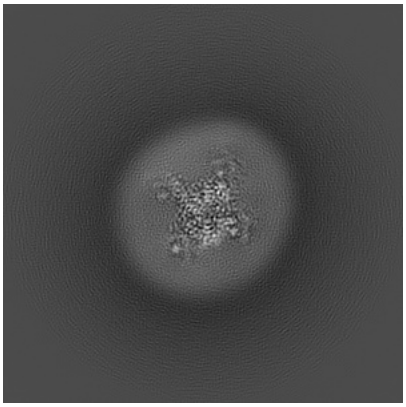
6.1.1 Primary map



X



Y

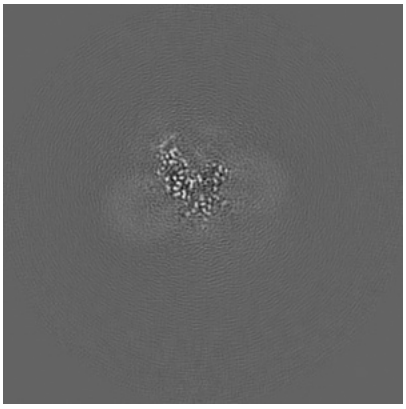


Z

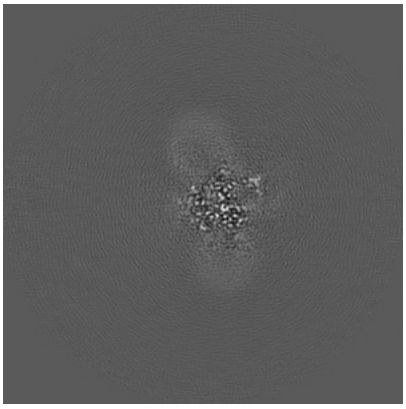
The images above show the map projected in three orthogonal directions.

6.2 Central slices

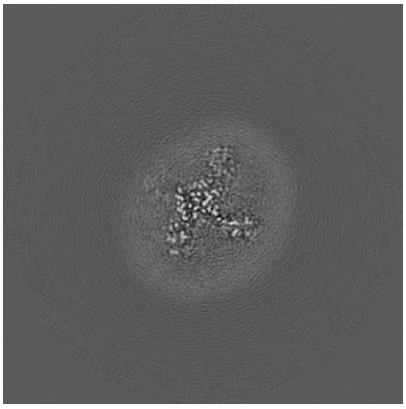
6.2.1 Primary map



X Index: 160



Y Index: 160

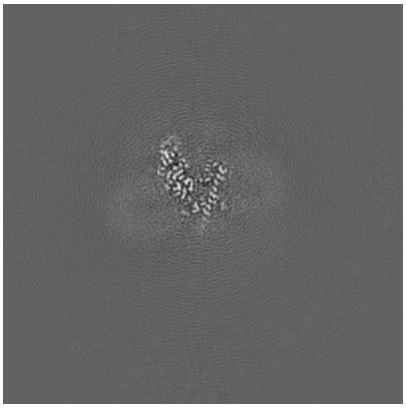


Z Index: 160

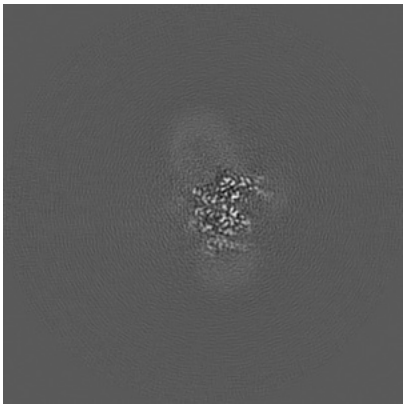
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

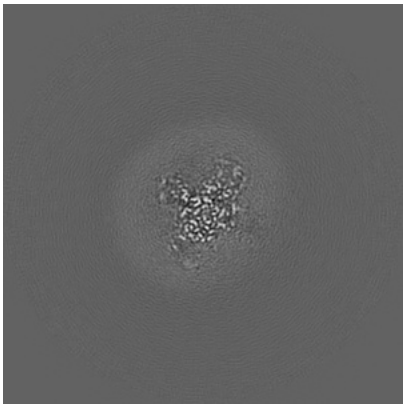
6.3.1 Primary map



X Index: 161



Y Index: 166



Z Index: 179

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

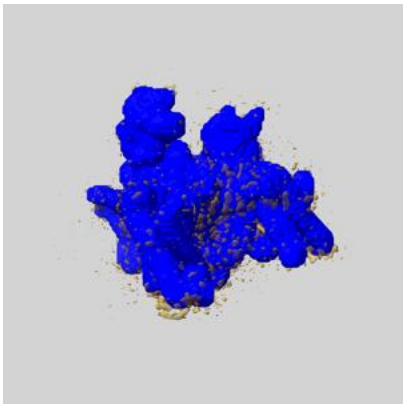
6.5 Mask visualisation (i)

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

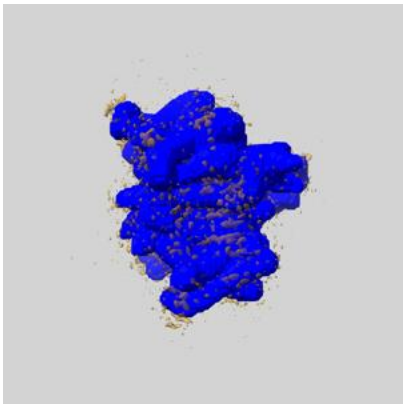
A mask typically either:

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

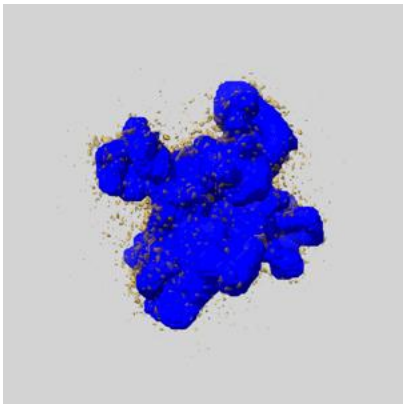
6.5.1 emd_0792_msk_1.map (i)



X



Y

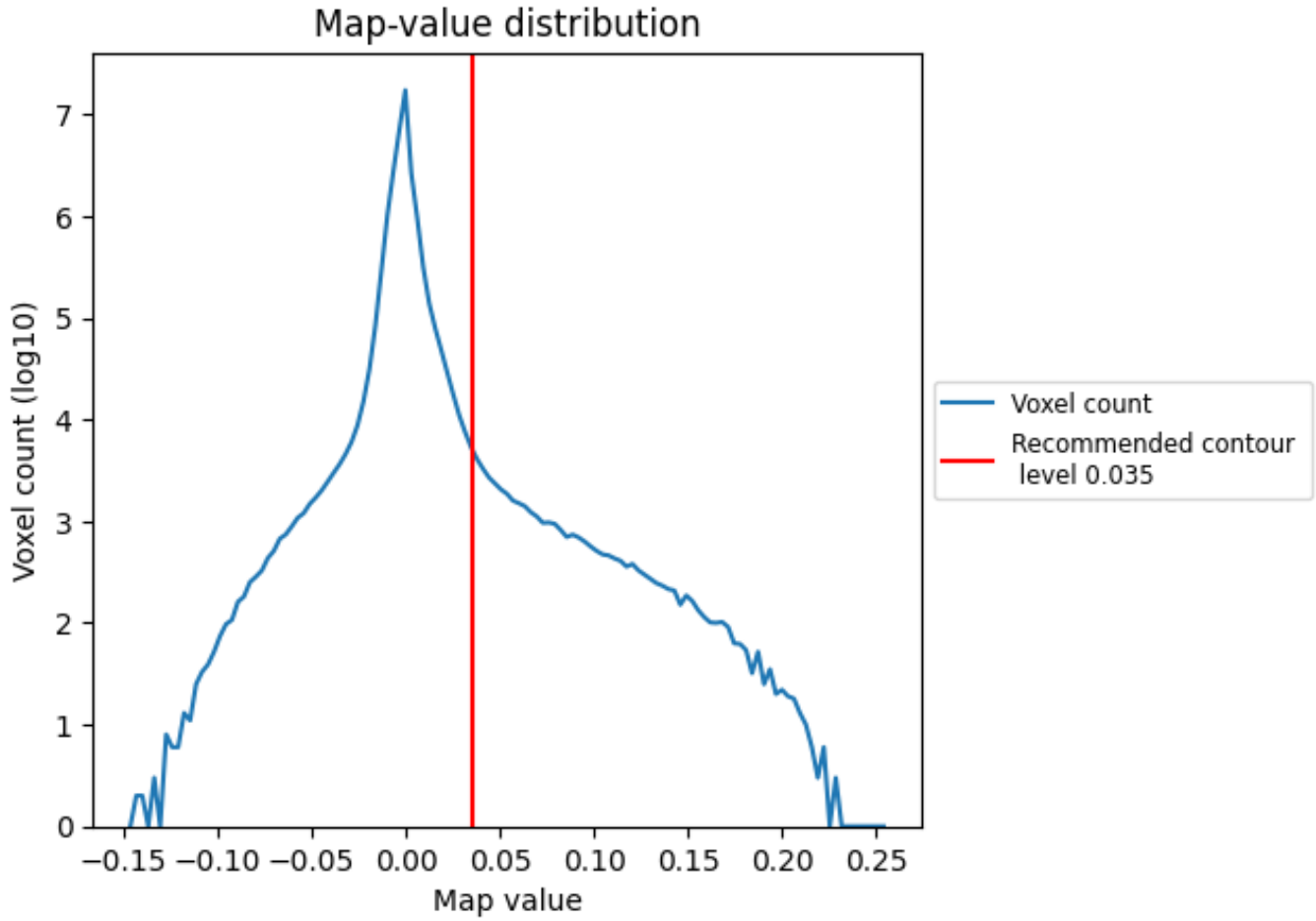


Z

7 Map analysis

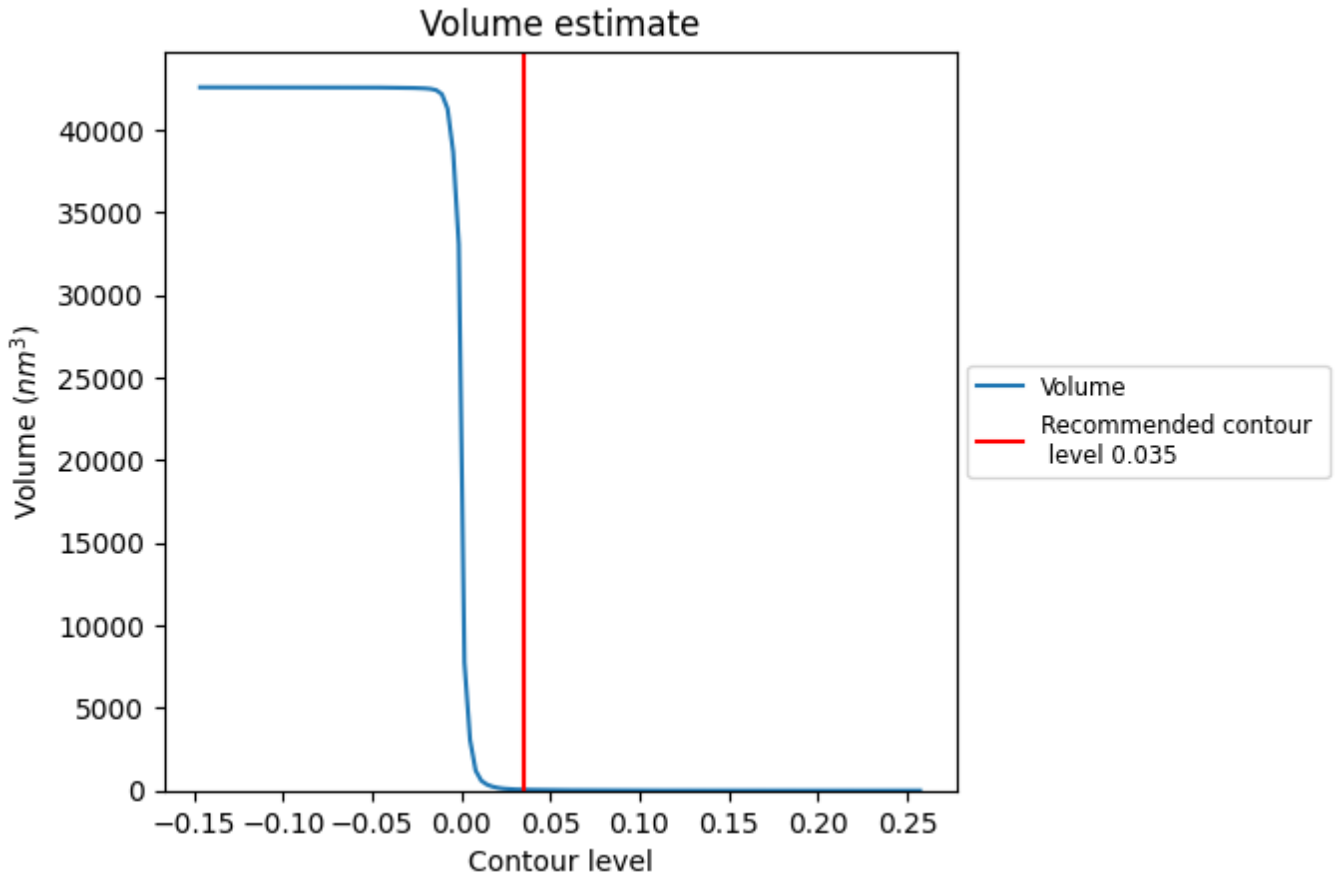
This section contains the results of statistical analysis of the map.

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.

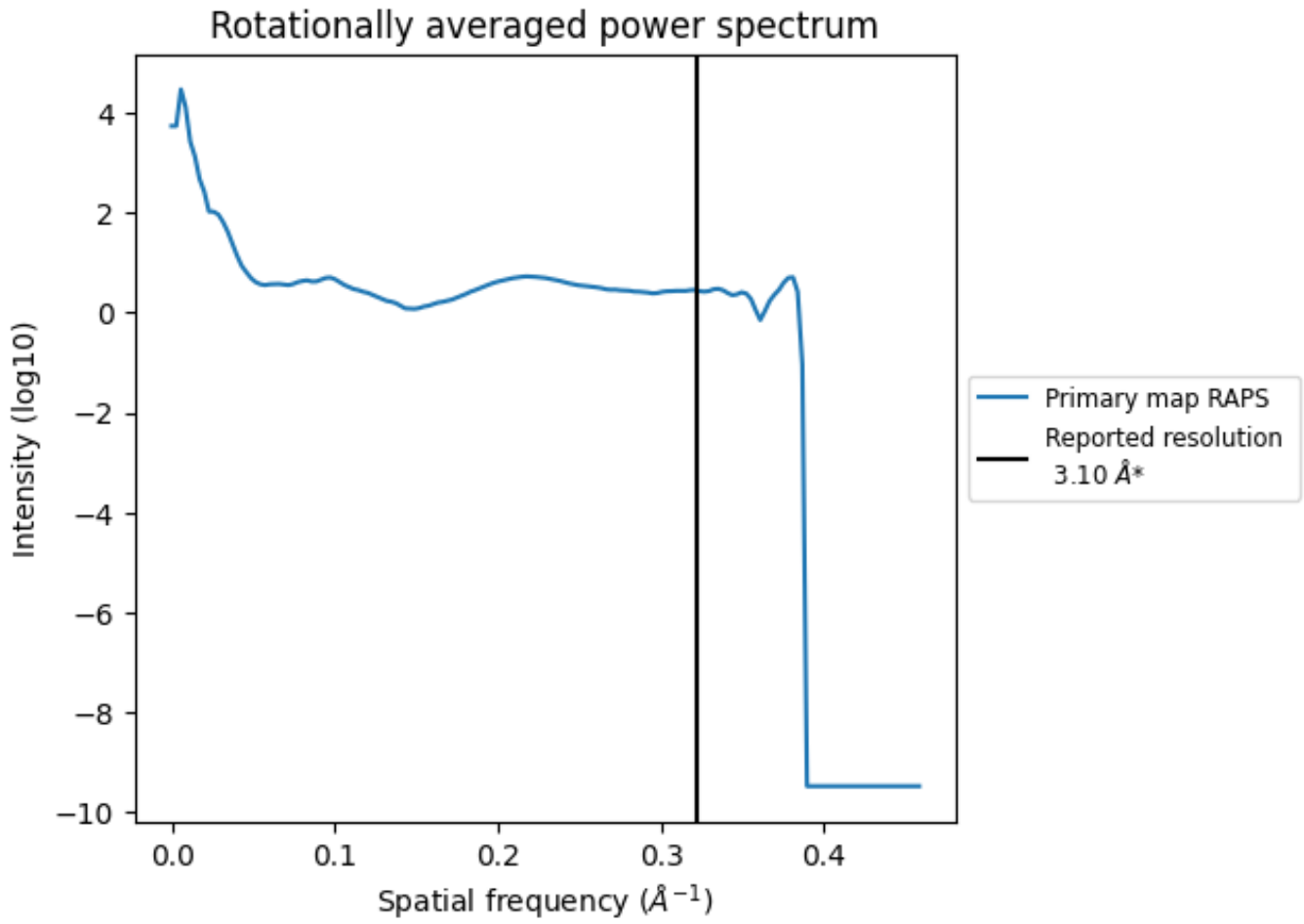
7.2 Volume estimate



The volume at the recommended contour level is 54 nm^3; this corresponds to an approximate mass of 49 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 0.323 Å^{-1}

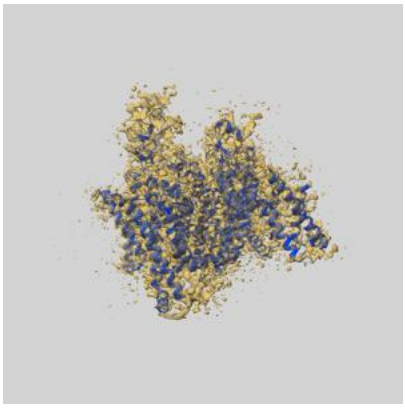
8 Fourier-Shell correlation (i)

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

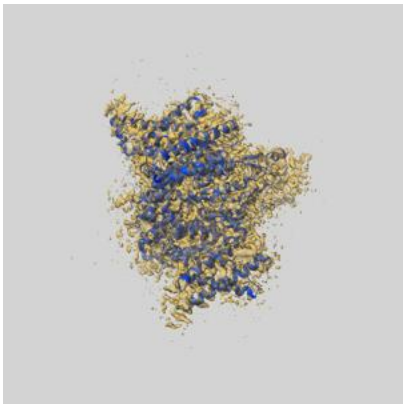
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0792 and PDB model 6KZP. Per-residue inclusion information can be found in section 3 on page 7.

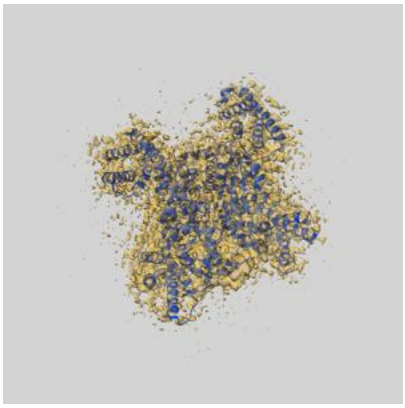
9.1 Map-model overlay



X



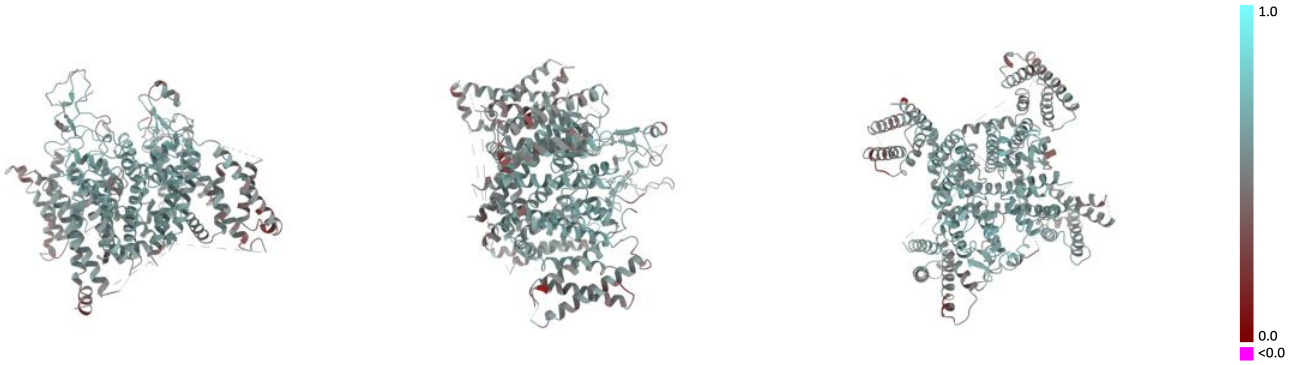
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

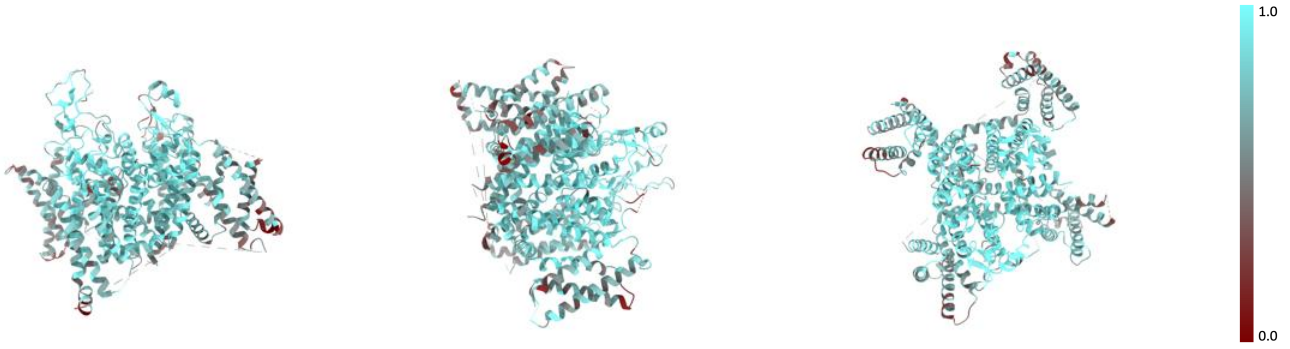
9.2 Q-score mapped to coordinate model (i)



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.

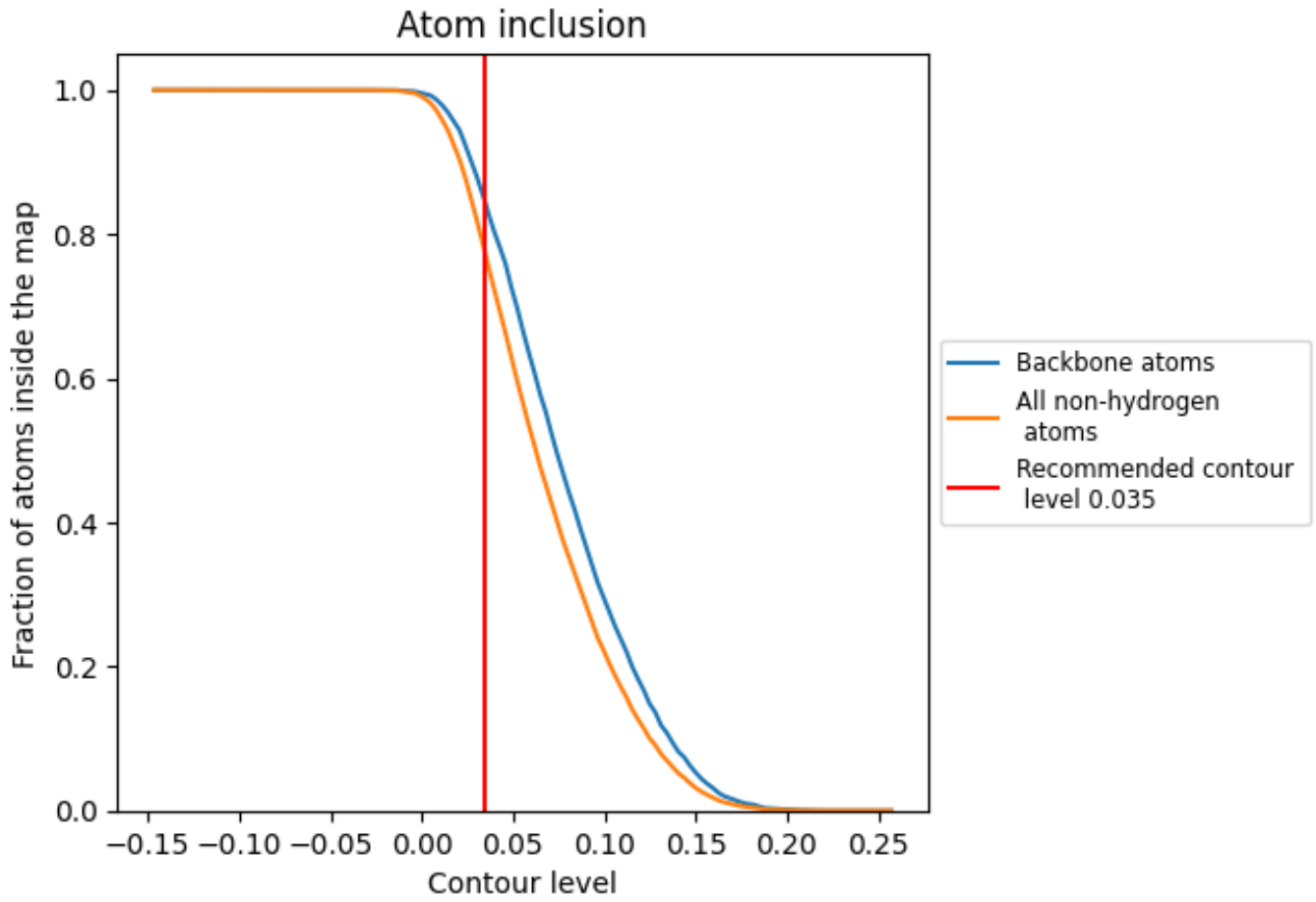
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7717	0.5480
A	0.7717	0.5480