



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:28 AM UTC

PDB ID : 6O74 / pdb_00006o74
Title : Crystal structure of Csm1-Csm4 cassette in complex with AMPPNP
Authors : Jia, N.; Patel, D.J.
Deposited on : 2019-03-07
Resolution : 2.71 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

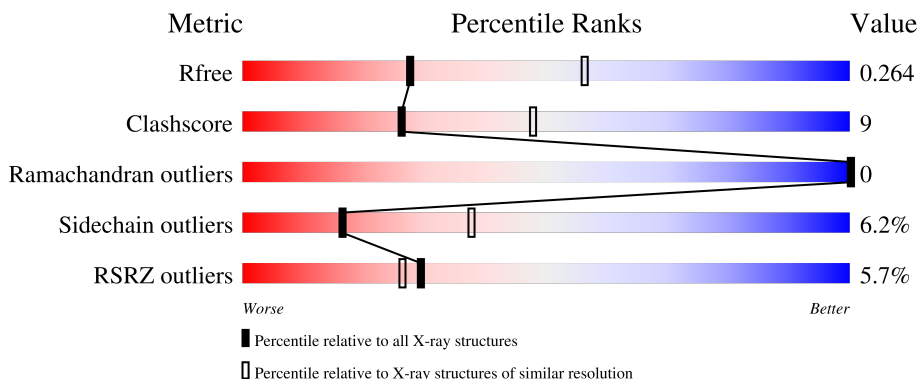
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	289	 4% 71% 13% • 13%
2	A	791	 5% 68% 20% • 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7728 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Csm4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	250	1995	1301	328	362	4	0	0	0

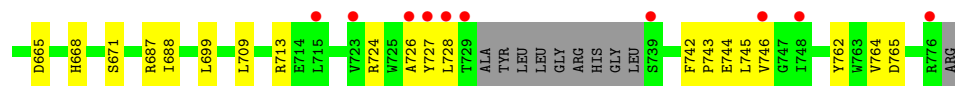
- Molecule 2 is a protein called Csm1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	704	5668	3649	975	1028	16	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP B6YWB8
A	-12	GLY	-	expression tag	UNP B6YWB8
A	-11	SER	-	expression tag	UNP B6YWB8
A	-10	SER	-	expression tag	UNP B6YWB8
A	-9	HIS	-	expression tag	UNP B6YWB8
A	-8	HIS	-	expression tag	UNP B6YWB8
A	-7	HIS	-	expression tag	UNP B6YWB8
A	-6	HIS	-	expression tag	UNP B6YWB8
A	-5	HIS	-	expression tag	UNP B6YWB8
A	-4	HIS	-	expression tag	UNP B6YWB8
A	-3	SER	-	expression tag	UNP B6YWB8
A	-2	GLN	-	expression tag	UNP B6YWB8
A	-1	ASP	-	expression tag	UNP B6YWB8
A	0	PRO	-	expression tag	UNP B6YWB8

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.43Å 156.43Å 185.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.41 – 2.71 49.41 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.41-2.71) 100.0 (49.41-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.215 , 0.259 0.218 , 0.264	Depositor DCC
R_{free} test set	1876 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtrriage
Anisotropy	0.202	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ANP

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	B	0.98	0/2044	1.37	0/2763
2	A	0.97	0/5791	1.45	6/7804 (0.1%)
All	All	0.97	0/7835	1.43	6/10567 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	614	THR	N-CA-C	-6.25	102.44	110.19
2	A	533	ASP	CB-CA-C	-5.76	101.06	110.85
2	A	195	ILE	N-CA-CB	-5.76	105.88	112.21
2	A	614	THR	CA-C-O	-5.28	116.46	122.01
2	A	726	ALA	CA-C-N	5.25	128.09	120.79
2	A	726	ALA	C-N-CA	5.25	128.09	120.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1995	0	1997	29	0
2	A	5668	0	5666	115	0
3	A	62	0	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
All	All	7728	0	7689	145	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:26:TYR:H	2:A:33:GLN:NE2	1.48	1.11
1:B:224:PRO:HG3	1:B:247:ILE:HD11	1.47	0.94
2:A:24:GLY:C	2:A:25:LEU:HD23	1.90	0.94
2:A:522:VAL:HG21	2:A:545:MET:CE	1.98	0.94
2:A:522:VAL:HG21	2:A:545:MET:HE1	1.54	0.88
1:B:263:LEU:HD12	1:B:265:LEU:HD21	1.56	0.87
2:A:619:THR:CG2	2:A:653:ASN:HA	2.06	0.85
1:B:263:LEU:CD1	1:B:265:LEU:HD21	2.07	0.84
2:A:619:THR:HG21	2:A:653:ASN:CB	2.08	0.83
2:A:26:TYR:HB2	2:A:33:GLN:HG3	1.60	0.80
2:A:619:THR:HG21	2:A:653:ASN:CA	2.12	0.80
1:B:263:LEU:HD12	1:B:265:LEU:CD2	2.11	0.79
2:A:183:LEU:HD12	2:A:202:MET:HE1	1.65	0.78
2:A:212:MET:O	2:A:215:ALA:HB3	1.82	0.77
2:A:25:LEU:HD23	2:A:25:LEU:N	2.01	0.74
2:A:59:PHE:HZ	2:A:95:TRP:CD2	2.07	0.72
2:A:631:THR:HB	2:A:636:MET:HE3	1.70	0.72
2:A:26:TYR:N	2:A:33:GLN:NE2	2.33	0.72
1:B:263:LEU:CD1	1:B:265:LEU:CD2	2.68	0.71
2:A:92:ASN:OD1	2:A:219:ALA:HB2	1.91	0.71
2:A:619:THR:HG21	2:A:653:ASN:HB2	1.70	0.71
2:A:627:PHE:HB2	2:A:636:MET:HE2	1.75	0.68
2:A:494:ASP:HB3	2:A:495:PRO:CD	2.26	0.66
2:A:16:ILE:O	2:A:19:PRO:HD2	1.97	0.65
1:B:96:LEU:HD22	1:B:118:ILE:CG1	2.27	0.64
2:A:59:PHE:CE2	2:A:98:TYR:CG	2.86	0.63
2:A:44:ASN:HD22	2:A:162:TRP:HZ2	1.48	0.61
2:A:522:VAL:HG21	2:A:545:MET:HE3	1.83	0.61
2:A:494:ASP:HB3	2:A:495:PRO:HD2	1.81	0.61
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.83	0.60
2:A:494:ASP:OD1	2:A:500:ALA:HA	2.04	0.58
1:B:61:SER:HB2	1:B:123:PRO:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:156:GLU:OE1	2:A:160:ARG:HD2	2.03	0.58
2:A:59:PHE:HE2	2:A:98:TYR:CG	2.22	0.58
2:A:26:TYR:H	2:A:33:GLN:HE22	1.49	0.58
1:B:61:SER:HB2	1:B:123:PRO:CG	2.32	0.58
2:A:90:VAL:O	2:A:94:LEU:HG	2.03	0.57
2:A:26:TYR:HB2	2:A:33:GLN:CG	2.30	0.57
2:A:522:VAL:HB	2:A:588:ASP:HB2	1.86	0.57
2:A:18:LYS:O	2:A:22:ARG:HG3	2.06	0.56
2:A:488:ALA:HB3	2:A:585:ALA:HB3	1.88	0.56
2:A:59:PHE:CE2	2:A:60:HIS:HB3	2.41	0.55
2:A:570:SER:HB2	2:A:601:GLU:CD	2.32	0.55
2:A:646:THR:O	2:A:650:GLU:HG3	2.07	0.55
2:A:284:THR:H	2:A:287:ASN:HD22	1.54	0.55
2:A:250:VAL:HB	2:A:633:ILE:HD11	1.88	0.55
2:A:709:LEU:HD11	2:A:742:PHE:CD2	2.42	0.55
2:A:724:ARG:O	2:A:727:TYR:HB3	2.07	0.55
2:A:56:PHE:CE1	2:A:94:LEU:HD23	2.43	0.54
2:A:59:PHE:CG	2:A:60:HIS:N	2.75	0.54
2:A:488:ALA:CB	2:A:585:ALA:HB3	2.38	0.54
2:A:743:PRO:O	2:A:746:VAL:HG22	2.08	0.54
1:B:8:LYS:HG2	1:B:60:TYR:CE2	2.43	0.53
2:A:213:LEU:C	2:A:215:ALA:H	2.16	0.53
2:A:169:LYS:HB2	2:A:171:ARG:NH1	2.23	0.53
2:A:660:ARG:HD2	2:A:765:ASP:OD2	2.08	0.53
2:A:59:PHE:HZ	2:A:95:TRP:CE3	2.26	0.52
2:A:180:GLU:HG3	2:A:199:TYR:CE2	2.44	0.52
2:A:75:ILE:O	2:A:78:LEU:O	2.28	0.51
3:A:802:ANP:O1B	3:A:802:ANP:H5'1	2.10	0.51
2:A:23:ALA:HB1	2:A:155:ARG:HG2	1.93	0.51
1:B:130:PRO:HB3	1:B:145:PHE:CE1	2.46	0.51
2:A:647:ALA:HA	2:A:671:SER:OG	2.11	0.51
2:A:525:LEU:HD13	2:A:545:MET:HE2	1.93	0.50
2:A:272:ASP:OD1	2:A:449:SER:OG	2.23	0.50
2:A:518:MET:HB3	2:A:624:LEU:HD23	1.92	0.50
2:A:199:TYR:CE2	2:A:203:ARG:HD2	2.47	0.50
1:B:260:MET:HE3	1:B:274:TYR:HA	1.93	0.50
2:A:157:LEU:CD1	2:A:182:TYR:HB3	2.41	0.50
2:A:31:SER:O	2:A:57:SER:HB3	2.12	0.50
2:A:619:THR:HG23	2:A:653:ASN:OD1	2.12	0.50
2:A:567:ASP:O	2:A:608:ARG:NH2	2.44	0.50
2:A:101:ASP:HA	2:A:205:THR:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:101:ASP:HA	2:A:205:THR:HG22	1.93	0.49
2:A:549:PHE:CE2	2:A:588:ASP:HA	2.48	0.49
2:A:171:ARG:HB3	2:A:173:ASP:OD1	2.12	0.49
2:A:619:THR:CG2	2:A:653:ASN:CA	2.75	0.49
2:A:745:LEU:HD11	2:A:764:VAL:HG21	1.95	0.49
2:A:180:GLU:OE1	2:A:547:TYR:OH	2.23	0.48
2:A:284:THR:H	2:A:287:ASN:ND2	2.11	0.48
1:B:263:LEU:HD12	1:B:265:LEU:HD23	1.95	0.48
2:A:565:ILE:O	2:A:608:ARG:HD2	2.13	0.48
1:B:74:GLU:HB2	1:B:75:PRO:HD3	1.96	0.48
1:B:57:ALA:HB1	1:B:157:VAL:HG13	1.96	0.47
2:A:125:PRO:HG3	2:A:195:ILE:HD11	1.96	0.47
2:A:21:GLN:O	2:A:23:ALA:O	2.32	0.47
2:A:59:PHE:CD2	2:A:98:TYR:HB2	2.49	0.47
1:B:247:ILE:HG23	1:B:251:SER:CB	2.43	0.47
2:A:22:ARG:NH2	2:A:187:SER:O	2.46	0.47
2:A:688:ILE:HA	2:A:699:LEU:CD1	2.44	0.47
1:B:57:ALA:HA	1:B:158:TYR:O	2.15	0.47
2:A:525:LEU:HD22	2:A:588:ASP:HB3	1.95	0.47
1:B:220:PRO:HB3	1:B:247:ILE:HD12	1.96	0.47
2:A:26:TYR:HB3	2:A:36:ARG:HE	1.80	0.46
2:A:494:ASP:CB	2:A:495:PRO:CD	2.89	0.46
2:A:619:THR:CG2	2:A:653:ASN:CB	2.90	0.46
2:A:41:LEU:O	2:A:44:ASN:O	2.34	0.46
2:A:176:LEU:HB2	2:A:177:PRO:HD3	1.97	0.46
2:A:134:LEU:C	2:A:134:LEU:HD23	2.40	0.46
2:A:213:LEU:C	2:A:215:ALA:N	2.73	0.46
1:B:41:VAL:O	1:B:44:LEU:HB3	2.16	0.46
2:A:433:GLY:HA3	2:A:461:VAL:O	2.16	0.46
2:A:134:LEU:HD21	2:A:136:PHE:CE1	2.52	0.45
2:A:614:THR:HG21	2:A:618:LEU:HB2	1.98	0.45
1:B:202:MET:HE2	1:B:204:ILE:HG13	1.98	0.45
2:A:59:PHE:CE2	2:A:98:TYR:CB	2.99	0.45
2:A:3:ILE:HD12	2:A:213:LEU:HD11	1.99	0.45
2:A:250:VAL:CG2	2:A:633:ILE:HD11	2.47	0.45
2:A:572:ARG:NH2	2:A:575:PRO:HG3	2.32	0.45
2:A:169:LYS:CB	2:A:171:ARG:NH1	2.80	0.44
2:A:250:VAL:HG13	2:A:258:TYR:HE2	1.82	0.44
2:A:18:LYS:HB2	2:A:19:PRO:HD3	2.00	0.44
2:A:520:GLY:O	2:A:589:ASP:HB2	2.18	0.43
2:A:367:LYS:O	2:A:370:ARG:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:92:ASN:CG	2:A:219:ALA:N	2.77	0.43
1:B:96:LEU:HD22	1:B:118:ILE:HG13	1.97	0.43
1:B:213:VAL:HG13	1:B:252:ILE:HD13	2.00	0.43
2:A:552:TYR:O	2:A:556:ILE:HG13	2.19	0.43
2:A:572:ARG:HG3	2:A:573:ASP:O	2.18	0.43
1:B:147:GLU:H	1:B:147:GLU:CD	2.27	0.43
1:B:133:VAL:O	1:B:141:SER:HA	2.19	0.42
2:A:634:TYR:CD1	2:A:634:TYR:C	2.97	0.42
2:A:338:VAL:HG13	2:A:342:GLU:HB2	2.00	0.42
2:A:272:ASP:OD1	2:A:434:ARG:NH1	2.50	0.42
2:A:593:VAL:C	2:A:599:ILE:HD11	2.44	0.42
1:B:21:ALA:HB2	1:B:216:SER:HB2	2.01	0.42
2:A:246:PHE:HD1	2:A:247:ILE:HG13	1.85	0.42
2:A:524:ARG:NH1	2:A:652:ARG:HD2	2.35	0.42
1:B:202:MET:CE	1:B:204:ILE:CG1	2.98	0.41
2:A:250:VAL:HG13	2:A:258:TYR:CE2	2.55	0.41
2:A:665:ASP:OD1	2:A:668:HIS:HD2	2.02	0.41
1:B:202:MET:HE2	1:B:204:ILE:CG1	2.51	0.41
2:A:713:ARG:NH1	2:A:762:TYR:O	2.52	0.41
2:A:59:PHE:CD2	2:A:60:HIS:N	2.89	0.41
2:A:524:ARG:CZ	2:A:652:ARG:HD2	2.51	0.41
1:B:76:ALA:HB2	1:B:285:PRO:HG3	2.03	0.41
2:A:250:VAL:HG12	2:A:251:SER:H	1.86	0.41
2:A:293:GLY:HA2	2:A:584:TYR:OH	2.21	0.41
2:A:503:GLU:HG2	2:A:507:MET:HE3	2.03	0.41
2:A:561:PHE:CD1	2:A:561:PHE:N	2.87	0.41
1:B:70:PRO:C	1:B:72:SER:H	2.29	0.41
2:A:12:LEU:HD23	2:A:175:LEU:HD23	2.02	0.41
2:A:171:ARG:HH22	2:A:174:ARG:NE	2.18	0.41
2:A:330:TYR:OH	2:A:366:ARG:HD2	2.21	0.41
2:A:490:TYR:CD1	2:A:491:PHE:N	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	B	238/289 (82%)	227 (95%)	11 (5%)	0	100	100
2	A	684/791 (86%)	644 (94%)	40 (6%)	0	100	100
All	All	922/1080 (85%)	871 (94%)	51 (6%)	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 X-ray entries followed by that with respect to entries of similar resolution.

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	B	211/240 (88%)	198 (94%)	13 (6%)	16	38
2	A	595/665 (90%)	558 (94%)	37 (6%)	16	38
All	All	806/905 (89%)	756 (94%)	50 (6%)	16	38

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	THR
1	B	38	GLN
1	B	92	THR
1	B	96	LEU
1	B	143	ILE
1	B	147	GLU
1	B	157	VAL
1	B	199	PHE
1	B	213	VAL
1	B	222	LYS
1	B	247	ILE
1	B	263	LEU
1	B	265	LEU
2	A	20	VAL
2	A	25	LEU

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Mol	Chain	Res	Type
2	A	31	SER
2	A	45	THR
2	A	67	ASN
2	A	79	SER
2	A	91	LEU
2	A	133	GLU
2	A	151	SER
2	A	157	LEU
2	A	162	TRP
2	A	170	LEU
2	A	184	THR
2	A	189	VAL
2	A	195	ILE
2	A	227	CYS
2	A	249	ARG
2	A	251	SER
2	A	345	ARG
2	A	354	GLU
2	A	364	THR
2	A	427	PRO
2	A	428	LYS
2	A	429	LEU
2	A	487	VAL
2	A	499	VAL
2	A	537	LYS
2	A	553	ILE
2	A	570	SER
2	A	608	ARG
2	A	633	ILE
2	A	638	ASP
2	A	648	LYS
2	A	654	ARG
2	A	687	ARG
2	A	728	LEU
2	A	744	GLU

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

Mol	Chain	Res	Type
1	B	36	HIS
1	B	200	HIS
2	A	21	GLN

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Mol	Chain	Res	Type
2	A	33	GLN
2	A	67	ASN
2	A	287	ASN
2	A	291	ASN
2	A	472	ASN
2	A	668	HIS
2	A	675	ASN
2	A	692	ASN
2	A	759	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
3	ANP	A	802	4	33,33,33	1.15	4 (12%)	45,52,52	0.95	3 (6%)
3	ANP	A	801	4	33,33,33	1.07	4 (12%)	45,52,52	0.97	3 (6%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	802	4	-	4/18/38/38	0/3/3/3
3	ANP	A	801	4	-	1/18/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ANP	PB-O1B	3.27	1.51	1.46
3	A	801	ANP	PB-O1B	3.13	1.50	1.46
3	A	802	ANP	PG-O1G	2.93	1.50	1.46
3	A	801	ANP	PG-O1G	2.78	1.50	1.46
3	A	801	ANP	PB-O2B	-2.41	1.50	1.56
3	A	801	ANP	PG-O3G	-2.26	1.50	1.56
3	A	802	ANP	PB-O2B	-2.17	1.51	1.56
3	A	802	ANP	PG-O3G	-2.08	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	O2B-PB-O1B	4.16	118.78	109.87
3	A	802	ANP	O2B-PB-O1B	3.73	117.86	109.87
3	A	802	ANP	O3G-PG-O1G	-3.31	105.14	113.45
3	A	801	ANP	O1G-PG-N3B	-2.62	107.91	111.77
3	A	802	ANP	O2G-PG-O1G	-2.47	107.25	113.45
3	A	801	ANP	O3G-PG-O1G	-2.15	108.06	113.45

There are no chirality outliers.

All (5) torsion outliers are listed below:

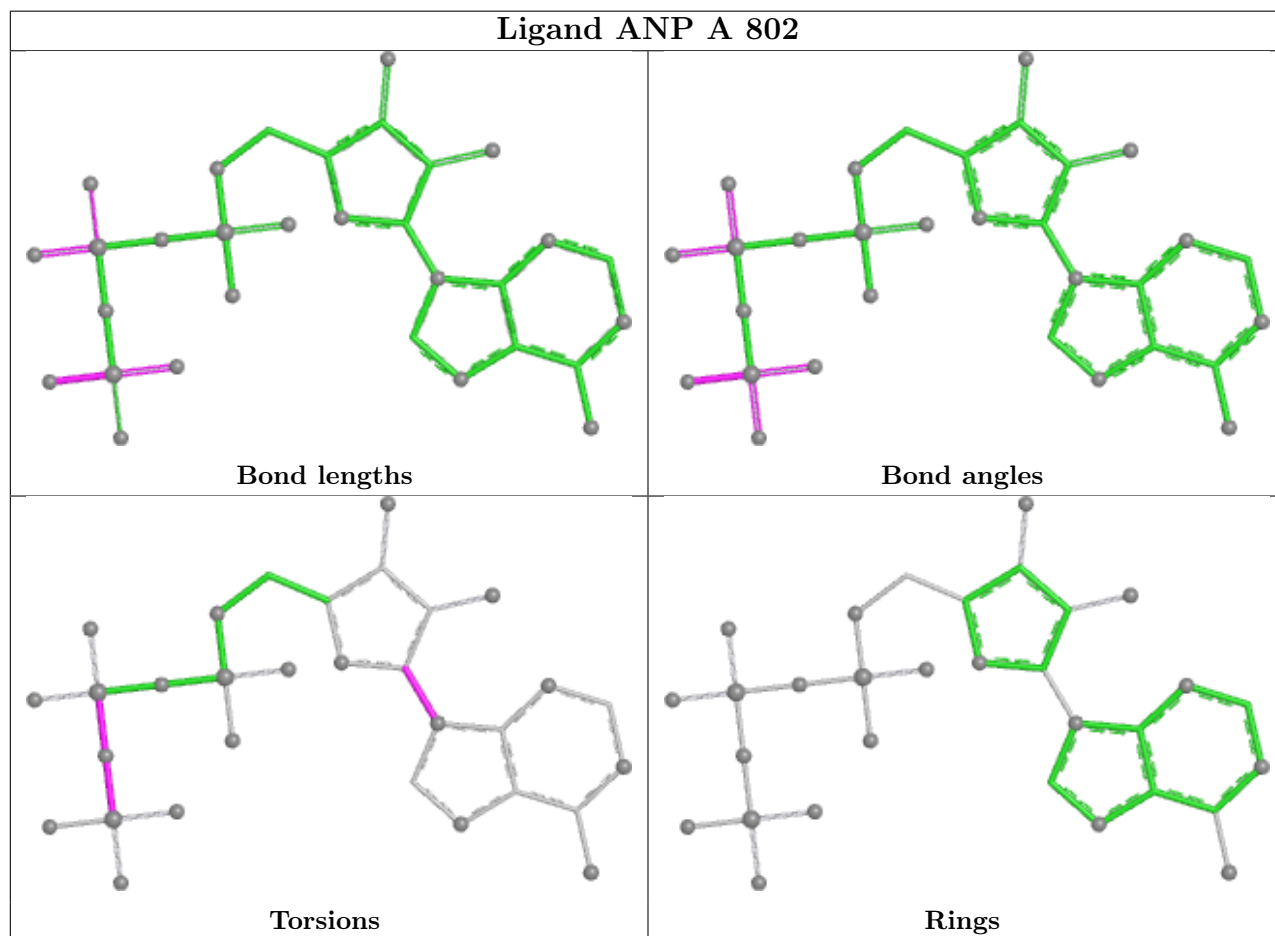
Mol	Chain	Res	Type	Atoms
3	A	802	ANP	PB-N3B-PG-O1G
3	A	802	ANP	PG-N3B-PB-O1B
3	A	802	ANP	PG-N3B-PB-O3A
3	A	801	ANP	PB-O3A-PA-O5'
3	A	802	ANP	C2'-C1'-N9-C8

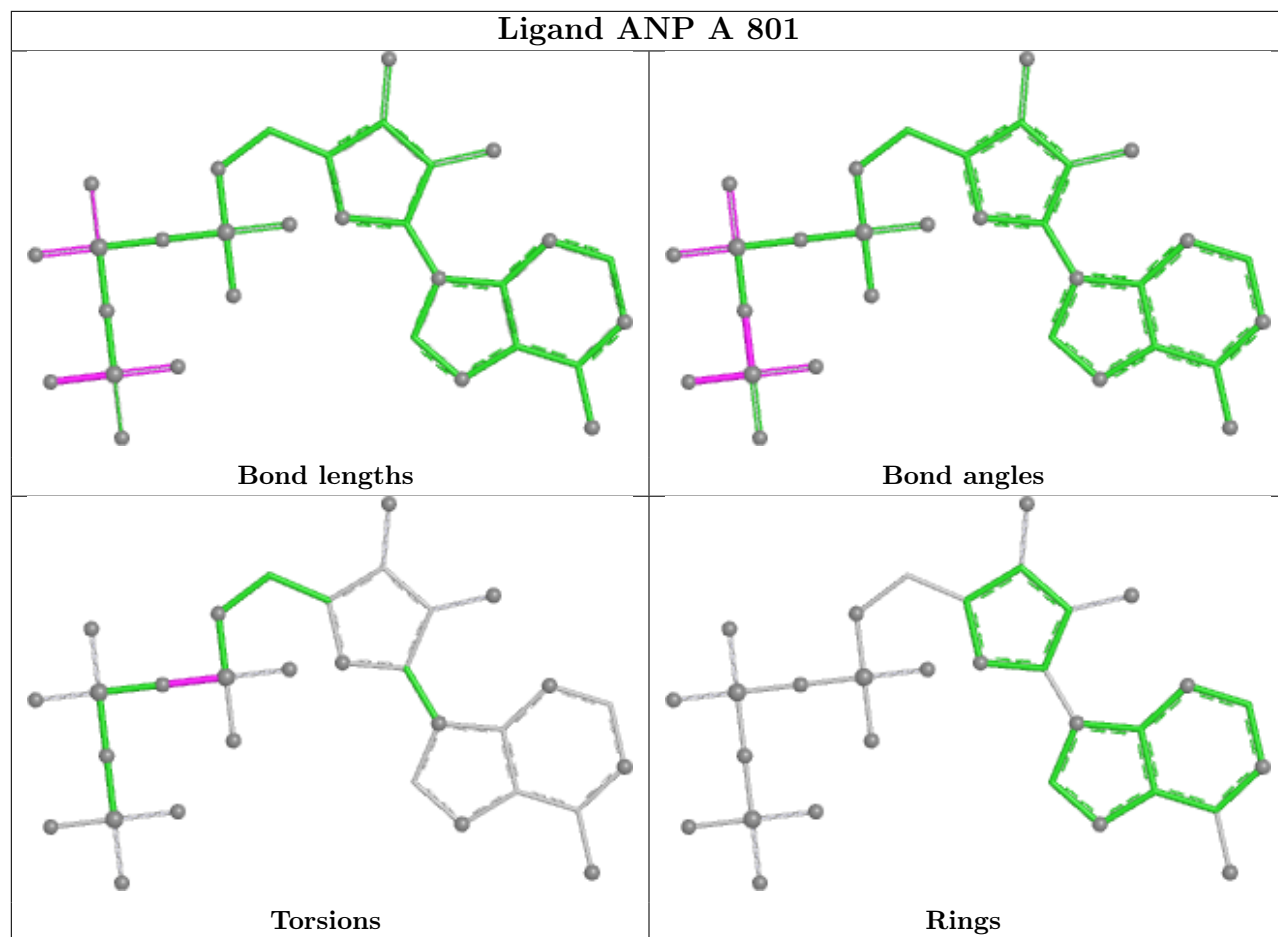
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ANP	1	0

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





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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	250/289 (86%)	0.22	13 (5%) 33 29	56, 87, 137, 176	0
2	A	704/791 (89%)	0.27	41 (5%) 29 26	56, 87, 141, 195	0
All	All	954/1080 (88%)	0.26	54 (5%) 29 26	56, 87, 142, 195	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	427	PRO	5.5
2	A	225	GLY	5.3
1	B	134	LEU	5.2
2	A	220	GLU	4.6
2	A	11	GLY	4.2
2	A	729	THR	4.1
1	B	149	ILE	3.8
1	B	179	LEU	3.7
2	A	113	PRO	3.6
2	A	59	PHE	3.6
2	A	53	LEU	3.4
1	B	79	GLY	3.3
2	A	504	GLU	3.2
2	A	323	ARG	3.0
1	B	90	TYR	2.9
2	A	748	ILE	2.9
2	A	170	LEU	2.8
2	A	728	LEU	2.8
2	A	146	VAL	2.8
2	A	250	VAL	2.7
1	B	17	ASP	2.6
2	A	723	VAL	2.6
2	A	422	LEU	2.6
1	B	114	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	A	171	ARG	2.6
2	A	219	ALA	2.6
2	A	726	ALA	2.5
2	A	15	ASP	2.5
1	B	194	LEU	2.5
2	A	10	GLY	2.5
2	A	3	ILE	2.5
2	A	746	VAL	2.5
2	A	419	LEU	2.5
2	A	428	LYS	2.4
2	A	715	LEU	2.3
2	A	25	LEU	2.3
2	A	727	TYR	2.3
2	A	347	GLY	2.3
2	A	552	TYR	2.3
2	A	776	ARG	2.2
2	A	149	ILE	2.2
2	A	159	LYS	2.2
2	A	343	PHE	2.2
2	A	739	SER	2.2
2	A	175	LEU	2.1
1	B	287	GLY	2.1
1	B	141	SER	2.1
1	B	195	PHE	2.1
2	A	6	LEU	2.1
2	A	178	VAL	2.1
2	A	217	CYS	2.1
1	B	15	PHE	2.0
2	A	48	ALA	2.0
1	B	96	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

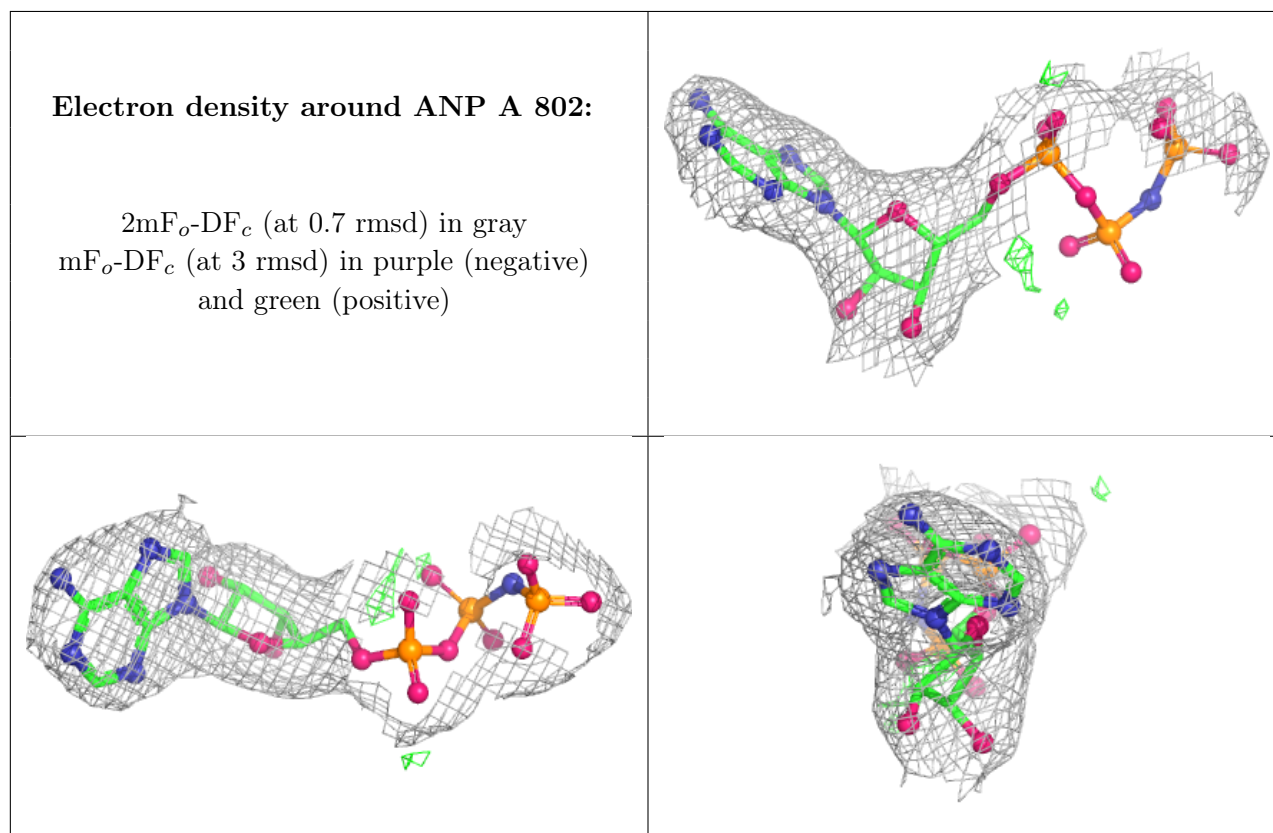
There are no oligosaccharides in this entry.

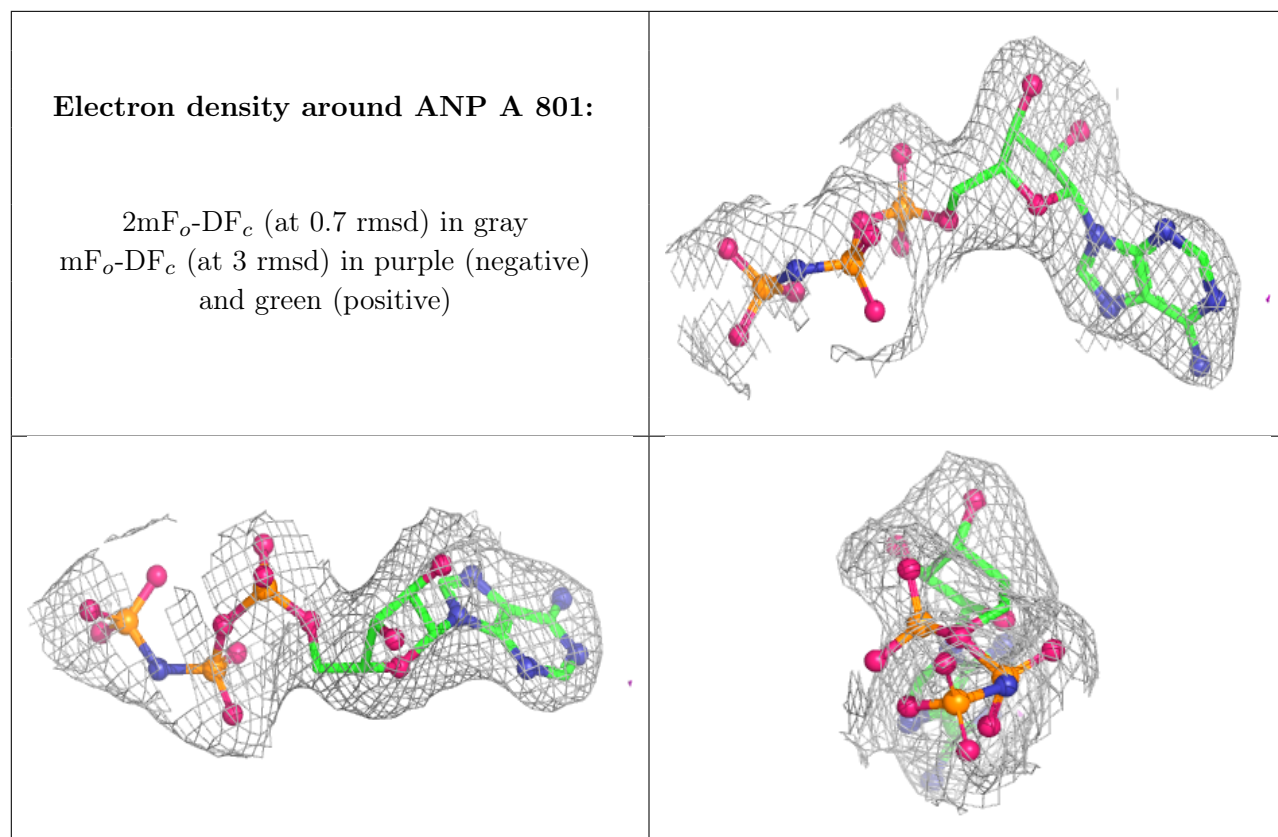
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ANP	A	802	31/31	0.90	0.07	56,71,116,120	0
4	MN	A	805	1/1	0.92	0.10	149,149,149,149	0
3	ANP	A	801	31/31	0.98	0.05	59,69,74,75	0
4	MN	A	804	1/1	0.99	0.04	72,72,72,72	0
4	MN	A	803	1/1	1.00	0.01	70,70,70,70	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.