



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 AM UTC

PDB ID : 6I7E / pdb_00006i7e
Title : Plasmodium falciparum Myosin A, Pre-powerstroke
Authors : Robert-Paganin, J.; Auguin, D.; Moussaoui, D.; Jousset, G.; Baum, J.; Trybus, K.M.; Houdusse, A.
Deposited on : 2018-11-16
Resolution : 3.49 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)
Xtriage (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

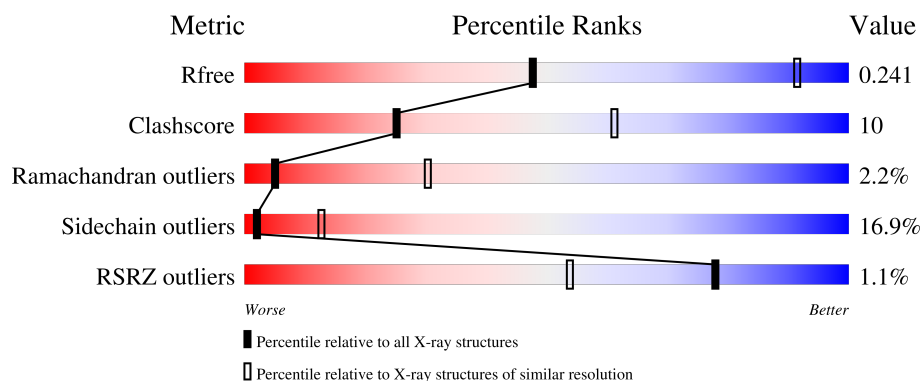
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	A	768	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	VO4	A	803	-	-	X	-

2 Entry composition [i](#)

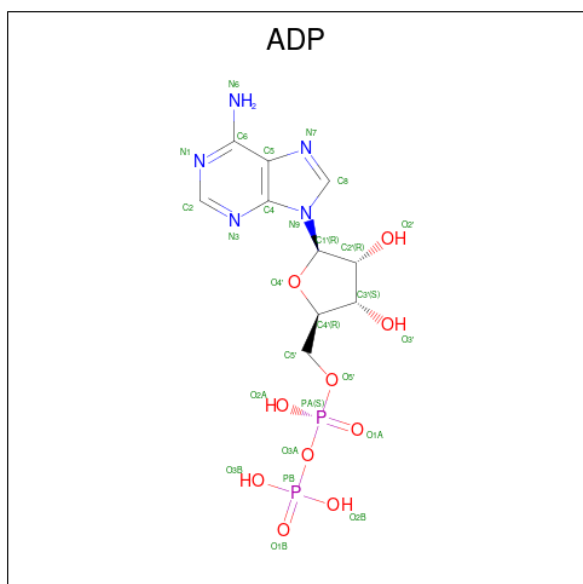
There are 4 unique types of molecules in this entry. The entry contains 6061 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Myosin-A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	P	S	0	1	0
			6028	3835	1014	1147	1	31			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

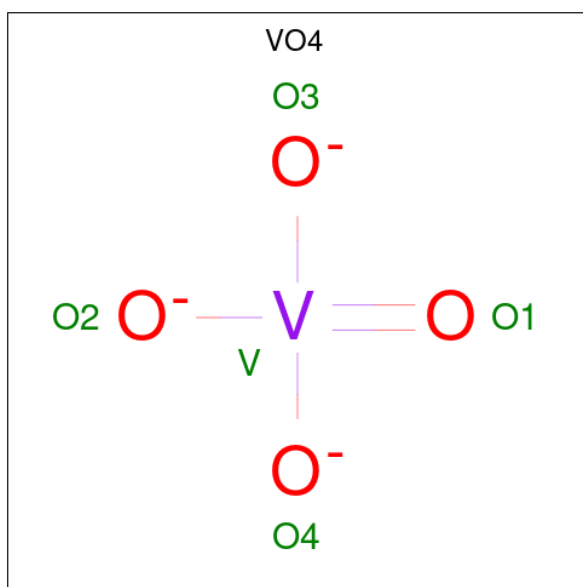


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is VANADATE ION (CCD ID: VO4) (formula: O_4V).

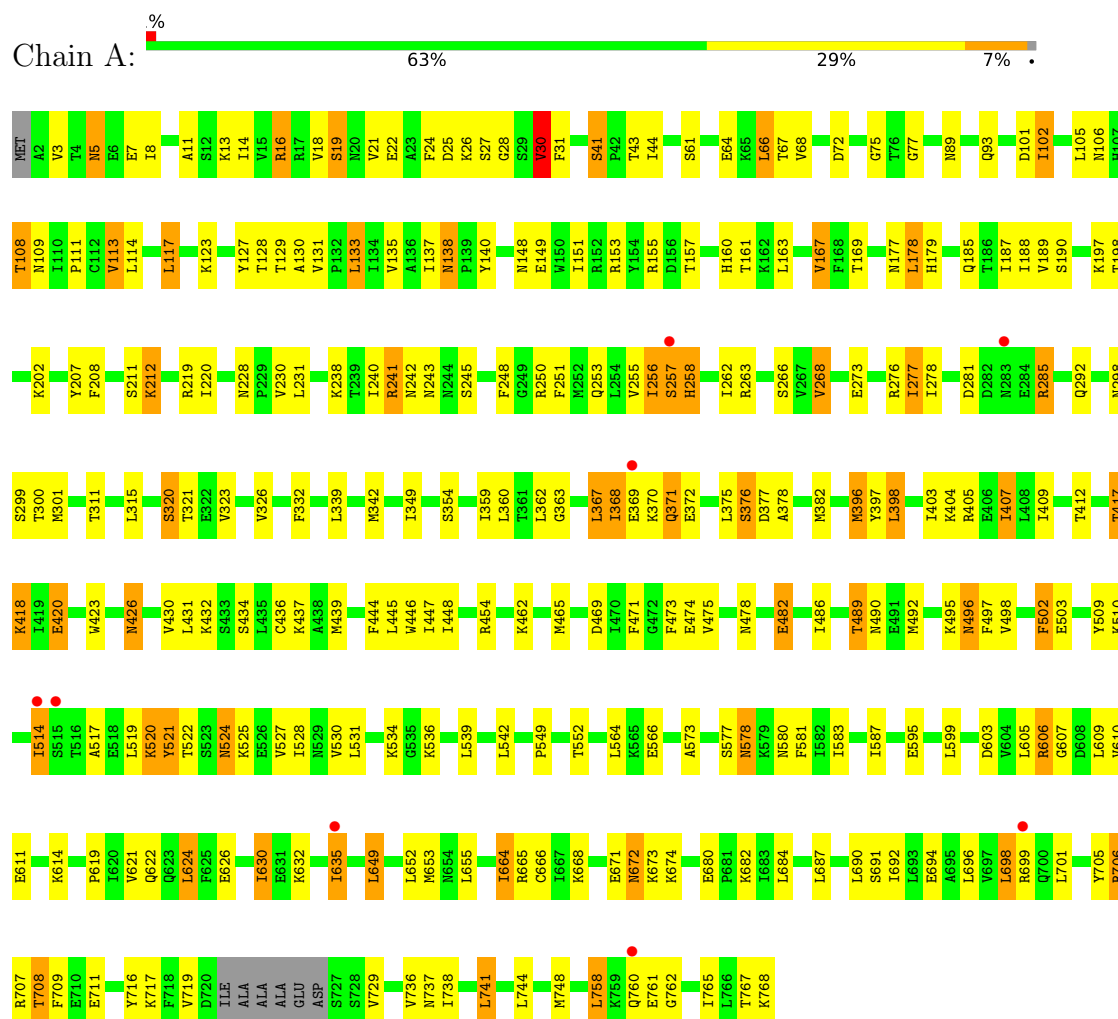


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	V	0	0
			5	4	1		

3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Myosin-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.46Å 197.46Å 178.14Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.17 – 3.49 25.17 – 3.49	Depositor EDS
% Data completeness (in resolution range)	58.7 (25.17-3.49) 58.6 (25.17-3.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.46Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.193 , 0.233 0.211 , 0.241	Depositor DCC
R_{free} test set	774 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	139.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 167.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6061	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MG, VO4, ADP

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	0.83	0/6122	1.47	50/8255 (0.6%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	517	ALA	N-CA-C	-8.29	102.72	113.17
1	A	407	ILE	N-CA-C	-7.51	99.01	109.45
1	A	478	ASN	CA-CB-CG	7.07	119.67	112.60
1	A	377	ASP	CA-C-N	6.47	130.95	121.31
1	A	377	ASP	C-N-CA	6.47	130.95	121.31
1	A	444	PHE	CA-CB-CG	6.26	120.06	113.80
1	A	502	PHE	CA-CB-CG	6.07	119.87	113.80
1	A	496	ASN	CA-C-N	6.01	128.26	120.44
1	A	496	ASN	C-N-CA	6.01	128.26	120.44
1	A	281	ASP	CA-CB-CG	5.90	118.50	112.60
1	A	382	MET	CA-C-N	5.88	128.48	120.54
1	A	382	MET	C-N-CA	5.88	128.48	120.54
1	A	603	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	167	VAL	N-CA-C	-5.83	104.64	111.00
1	A	257	SER	CA-C-N	5.79	132.60	121.54
1	A	257	SER	C-N-CA	5.79	132.60	121.54
1	A	117	LEU	CA-C-N	5.77	128.27	120.65
1	A	117	LEU	C-N-CA	5.77	128.27	120.65
1	A	542	LEU	N-CA-C	-5.73	105.96	113.12
1	A	517	ALA	CA-C-N	5.72	130.47	122.41
1	A	517	ALA	C-N-CA	5.72	130.47	122.41
1	A	729	VAL	N-CA-C	-5.69	108.31	113.71
1	A	403	ILE	N-CA-C	-5.66	105.00	110.72
1	A	371	GLN	CA-C-N	5.52	132.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	371	GLN	C-N-CA	5.52	132.09	121.54
1	A	403	ILE	CA-C-N	5.50	127.65	120.28
1	A	403	ILE	C-N-CA	5.50	127.65	120.28
1	A	578	ASN	CA-CB-CG	5.47	118.08	112.60
1	A	716	TYR	CA-C-N	5.36	131.77	121.54
1	A	716	TYR	C-N-CA	5.36	131.77	121.54
1	A	123	LYS	CA-C-N	5.33	132.14	123.93
1	A	123	LYS	C-N-CA	5.33	132.14	123.93
1	A	26	LYS	CA-C-N	5.33	127.68	120.65
1	A	26	LYS	C-N-CA	5.33	127.68	120.65
1	A	5	ASN	CA-C-N	5.32	129.68	120.58
1	A	5	ASN	C-N-CA	5.32	129.68	120.58
1	A	277	ILE	CA-C-N	5.26	127.29	120.56
1	A	277	ILE	C-N-CA	5.26	127.29	120.56
1	A	72	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	709	PHE	CA-C-N	5.18	127.23	120.28
1	A	709	PHE	C-N-CA	5.18	127.23	120.28
1	A	564	LEU	CA-C-N	5.16	127.50	120.54
1	A	564	LEU	C-N-CA	5.16	127.50	120.54
1	A	13	LYS	CA-C-N	5.11	127.45	120.46
1	A	13	LYS	C-N-CA	5.11	127.45	120.46
1	A	760	GLN	CA-C-N	5.11	129.31	120.58
1	A	760	GLN	C-N-CA	5.11	129.31	120.58
1	A	157	THR	CA-C-N	5.02	126.97	120.44
1	A	157	THR	C-N-CA	5.02	126.97	120.44
1	A	177	ASN	CA-CB-CG	5.01	117.61	112.60

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	6028	0	6095	114	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	4	0
All	All	6061	0	6107	118	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 (118) 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:315:LEU:HD11	1:A:363:GLY:HA3	1.60	0.82
1:A:16:ARG:HH12	1:A:109:ASN:HA	1.47	0.79
1:A:489:THR:HA	1:A:649:LEU:HD11	1.66	0.76
1:A:581:PHE:HE2	1:A:583:ILE:HD11	1.53	0.74
1:A:109:ASN:HD22	1:A:111:PRO:HD2	1.58	0.67
1:A:492:MET:HG2	1:A:528:ILE:HD11	1.76	0.67
1:A:250:ARG:HB3	1:A:469:ASP:HB3	1.78	0.66
1:A:256:ILE:HG23	1:A:262:ILE:HG13	1.77	0.66
1:A:630:ILE:H	1:A:630:ILE:HD13	1.61	0.65
1:A:198:THR:HG22	1:A:202:LYS:HD2	1.78	0.64
4:A:803:VO4:O4	4:A:803:VO4:V	1.54	0.64
1:A:397:TYR:HB2	1:A:621:VAL:HG21	1.79	0.64
4:A:803:VO4:V	4:A:803:VO4:O3	1.56	0.63
1:A:253:GLN:HB2	1:A:266:SER:HB3	1.82	0.62
1:A:376:SER:C	1:A:378:ALA:H	2.05	0.62
4:A:803:VO4:V	4:A:803:VO4:O1	1.56	0.62
1:A:16:ARG:NH1	1:A:109:ASN:HA	2.15	0.62
4:A:803:VO4:V	4:A:803:VO4:O2	1.56	0.62
1:A:495:LYS:HD2	1:A:524:ASN:HB3	1.82	0.61
1:A:292:GLN:HB3	1:A:332:PHE:HB2	1.81	0.61
1:A:179:HIS:CE1	1:A:258:HIS:H	2.19	0.60
1:A:368:ILE:HD13	1:A:369:GLU:H	1.68	0.59
1:A:605:LEU:HD23	1:A:610:VAL:HG22	1.85	0.59
1:A:502:PHE:HB3	1:A:520:LYS:HB3	1.85	0.58
1:A:606:ARG:HH21	1:A:635:ILE:HA	1.68	0.58
1:A:396:MET:HE2	1:A:398:LEU:HD11	1.86	0.58
1:A:434:SER:HA	1:A:437:LYS:HD2	1.85	0.58
1:A:278:ILE:HG13	1:A:437:LYS:HE2	1.85	0.58
1:A:519:LEU:HA	1:A:698:LEU:HD22	1.84	0.58
1:A:24:PHE:HE2	1:A:61:SER:O	1.86	0.58
1:A:581:PHE:CE2	1:A:583:ILE:HD11	2.37	0.58
1:A:323:VAL:HB	1:A:326:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ASN:O	1:A:741:LEU:HG	2.06	0.56
1:A:396:MET:HE3	1:A:439:MET:HG3	1.88	0.55
1:A:339:LEU:HA	1:A:342:MET:HE2	1.89	0.55
1:A:256:ILE:HD11	1:A:465:MET:HB2	1.89	0.54
1:A:510:LYS:HG3	1:A:514:ILE:HD13	1.89	0.54
1:A:525:LYS:HA	1:A:528:ILE:HG22	1.90	0.54
1:A:495:LYS:HB2	1:A:524:ASN:ND2	2.24	0.53
1:A:208:PHE:HB3	1:A:256:ILE:HG21	1.89	0.53
1:A:502:PHE:HB3	1:A:520:LYS:HD3	1.91	0.53
1:A:521:TYR:OH	1:A:691:SER:HA	2.08	0.53
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.91	0.52
1:A:273:GLU:HG3	1:A:482:GLU:HG2	1.93	0.51
1:A:61:SER:HB3	1:A:66:LEU:HA	1.93	0.51
1:A:130:ALA:HB3	1:A:133:LEU:HB2	1.92	0.50
1:A:178:LEU:HD12	1:A:185:GLN:H	1.76	0.50
1:A:671:GLU:HB2	1:A:682:LYS:HE3	1.92	0.50
1:A:744:LEU:HD23	1:A:748:MET:HB3	1.93	0.50
1:A:509:TYR:HB3	1:A:514:ILE:HA	1.93	0.50
1:A:187:ILE:HG23	1:A:664:ILE:HD13	1.93	0.49
1:A:531:LEU:HD21	1:A:583:ILE:HG21	1.95	0.49
1:A:114:LEU:HD22	1:A:680:GLU:HG2	1.94	0.49
1:A:133:LEU:H	1:A:133:LEU:HD12	1.78	0.49
1:A:138:ASN:HD22	1:A:140:TYR:H	1.60	0.48
1:A:238:LYS:HG2	1:A:243:ASN:HA	1.95	0.48
1:A:521:TYR:CZ	1:A:694:GLU:HB2	2.48	0.48
1:A:426:ASN:H	1:A:426:ASN:HD22	1.61	0.48
1:A:665:ARG:HB3	1:A:690:LEU:HD22	1.95	0.48
1:A:473:PHE:CE2	1:A:490:ASN:HB3	2.49	0.48
1:A:25:ASP:HB3	1:A:28:GLY:O	2.14	0.48
1:A:611:GLU:HG2	1:A:630:ILE:HG21	1.95	0.48
1:A:155:ARG:HH12	1:A:212:LYS:N	2.12	0.47
1:A:417:THR:HA	1:A:418:LYS:HZ1	1.79	0.47
1:A:474:GLU:HG3	1:A:486:ILE:HG21	1.96	0.47
1:A:672:ASN:HB3	1:A:674:LYS:HE2	1.96	0.46
1:A:367:LEU:HD12	1:A:432:LYS:HD3	1.96	0.46
1:A:228:ASN:HA	1:A:250:ARG:HH22	1.80	0.46
1:A:102:ILE:HG21	1:A:113:VAL:HG13	1.97	0.46
1:A:127:TYR:HA	1:A:135:VAL:O	2.15	0.46
1:A:160:HIS:HA	1:A:163:LEU:HD12	1.98	0.46
1:A:18:VAL:HG23	1:A:19:SEP:H	1.80	0.46
1:A:255:VAL:HG12	1:A:263:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:ILE:HG23	1:A:436:CYS:HB3	1.98	0.45
1:A:248:PHE:HE2	1:A:250:ARG:HB2	1.81	0.45
1:A:497:PHE:CE2	1:A:691:SER:HB2	2.50	0.45
1:A:573:ALA:HB3	1:A:577:SER:HA	1.98	0.45
1:A:140:TYR:CZ	1:A:673:LYS:HA	2.51	0.45
1:A:248:PHE:CE2	1:A:250:ARG:HB2	2.52	0.45
1:A:502:PHE:CD2	1:A:520:LYS:HB3	2.52	0.45
1:A:405:ARG:O	1:A:409:ILE:HB	2.16	0.45
1:A:495:LYS:HA	1:A:498:VAL:HG22	1.99	0.44
1:A:497:PHE:HE2	1:A:691:SER:HB2	1.82	0.44
1:A:619:PRO:HA	1:A:622:GLN:HE21	1.82	0.44
1:A:607:GLY:HA2	1:A:632:LYS:HA	1.99	0.44
1:A:11:ALA:HA	1:A:14:ILE:HD12	1.99	0.44
1:A:404:LYS:O	1:A:407:ILE:O	2.36	0.44
1:A:285:ARG:HG3	1:A:320:SER:O	2.17	0.44
1:A:376:SER:C	1:A:378:ALA:N	2.73	0.44
1:A:75:GLY:C	1:A:77:GLY:H	2.26	0.44
1:A:240:ILE:HG22	1:A:241:ARG:HH12	1.82	0.44
1:A:684:LEU:HA	1:A:687:LEU:HD12	1.99	0.43
1:A:423:TRP:HA	1:A:423:TRP:CE3	2.53	0.43
1:A:151:ILE:HG23	1:A:207:TYR:CD1	2.54	0.43
1:A:251:PHE:HB3	1:A:268:VAL:HG23	2.00	0.43
1:A:611:GLU:HA	1:A:614:LYS:HB2	2.00	0.43
1:A:5:ASN:HA	1:A:8:ILE:HD12	2.01	0.42
1:A:717:LYS:HD2	1:A:717:LYS:H	1.84	0.42
1:A:117:LEU:HD22	1:A:137:ILE:HD11	2.02	0.42
1:A:495:LYS:CD	1:A:524:ASN:HB3	2.49	0.42
1:A:28:GLY:C	1:A:30:VAL:H	2.28	0.42
1:A:41:SER:HB3	1:A:44:ILE:HD12	2.02	0.42
1:A:298:ASN:ND2	1:A:301:MET:HE3	2.34	0.42
1:A:748:MET:SD	1:A:762:GLY:CA	3.08	0.42
1:A:762:GLY:HA2	1:A:765:ILE:HD12	2.01	0.42
1:A:446:TRP:HE3	1:A:447:ILE:HG13	1.85	0.42
1:A:527:VAL:HA	1:A:530:VAL:HG12	2.01	0.42
1:A:708:THR:HG22	1:A:711:GLU:HG3	2.02	0.42
1:A:19:SEP:HB3	1:A:89:ASN:HD22	1.85	0.41
1:A:108:THR:HB	1:A:696:LEU:HD13	2.02	0.41
1:A:707:ARG:HD3	1:A:711:GLU:OE1	2.21	0.41
1:A:315:LEU:HD13	1:A:360:LEU:HA	2.03	0.41
1:A:230:VAL:HG11	1:A:342:MET:HE1	2.01	0.41
1:A:621:VAL:O	1:A:624:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:573:ALA:HB2	1:A:580:ASN:HB2	2.03	0.40
1:A:705:TYR:CB	1:A:758:LEU:HB2	2.51	0.40
1:A:148:ASN:HA	1:A:151:ILE:HD12	2.03	0.40
1:A:694:GLU:C	1:A:696:LEU:H	2.29	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 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	A	757/768 (99%)	652 (86%)	88 (12%)	17 (2%)	5	30

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	VAL
1	A	258	HIS
1	A	595	GLU
1	A	219	ARG
1	A	719	VAL
1	A	93	GLN
1	A	299	SER
1	A	420	GLU
1	A	520	LYS
1	A	626	GLU
1	A	672	ASN
1	A	131	VAL
1	A	376	SER
1	A	372	GLU
1	A	549	PRO
1	A	706	ARG
1	A	41	SER

5.3.2 Protein sidechains ⓘ

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	A	675/679 (99%)	561 (83%)	114 (17%)	2 13

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	GLU
1	A	16	ARG
1	A	21	VAL
1	A	22	GLU
1	A	27	SER
1	A	30	VAL
1	A	31	PHE
1	A	43	THR
1	A	64	GLU
1	A	66	LEU
1	A	67	THR
1	A	68	VAL
1	A	101	ASP
1	A	102	ILE
1	A	105	LEU
1	A	106	ASN
1	A	108	THR
1	A	113	VAL
1	A	128	THR
1	A	129	THR
1	A	133	LEU
1	A	138	ASN
1	A	149	GLU
1	A	153	ARG
1	A	161	THR
1	A	167	VAL
1	A	169	THR
1	A	178	LEU
1	A	188	ILE

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Mol	Chain	Res	Type
1	A	189	VAL
1	A	190	SER
1	A	197	LYS
1	A	211	SER
1	A	212	LYS
1	A	220	ILE
1	A	231	LEU
1	A	241	ARG
1	A	242	ASN
1	A	245	SER
1	A	256	ILE
1	A	257	SER
1	A	268	VAL
1	A	276	ARG
1	A	277	ILE
1	A	285	ARG
1	A	300	THR
1	A	311	THR
1	A	320	SER
1	A	321	THR
1	A	349	ILE
1	A	354	SER
1	A	362	LEU
1	A	367	LEU
1	A	368	ILE
1	A	370	LYS
1	A	371	GLN
1	A	375	LEU
1	A	396	MET
1	A	398	LEU
1	A	412	THR
1	A	417	THR
1	A	418	LYS
1	A	420	GLU
1	A	426	ASN
1	A	430	VAL
1	A	431	LEU
1	A	445	LEU
1	A	448	ILE
1	A	454	ARG
1	A	462	LYS
1	A	471	PHE

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Mol	Chain	Res	Type
1	A	475	VAL
1	A	482	GLU
1	A	489	THR
1	A	496	ASN
1	A	503	GLU
1	A	514	ILE
1	A	521	TYR
1	A	522	THR
1	A	524	ASN
1	A	534	LYS
1	A	536	LYS
1	A	539	LEU
1	A	552	THR
1	A	566	GLU
1	A	578	ASN
1	A	587	ILE
1	A	599	LEU
1	A	606	ARG
1	A	609	LEU
1	A	624	LEU
1	A	630	ILE
1	A	635	ILE
1	A	649	LEU
1	A	652	LEU
1	A	653	MET
1	A	655	LEU
1	A	664	ILE
1	A	666	CYS
1	A	668	LYS
1	A	692	ILE
1	A	698	LEU
1	A	699	ARG
1	A	701	LEU
1	A	706	ARG
1	A	708	THR
1	A	736	VAL
1	A	738	ILE
1	A	741	LEU
1	A	758	LEU
1	A	761	GLU
1	A	767	THR
1	A	768	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	59	GLN
1	A	91	ASN
1	A	109	ASN
1	A	138	ASN
1	A	341	ASN
1	A	390	ASN
1	A	424	ASN
1	A	426	ASN
1	A	478	ASN
1	A	479	ASN
1	A	496	ASN
1	A	524	ASN
1	A	545	GLN
1	A	580	ASN
1	A	622	GLN
1	A	647	ASN
1	A	648	GLN
1	A	657	ASN
1	A	700	GLN
1	A	732	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	SEP	A	19	1	8,9,10	1.07	1 (12%)	7,12,14	2.47	1 (14%)

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
1	SEP	A	19	1	-	3/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	SEP	P-OG	-2.46	1.52	1.60

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	SEP	OG-CB-CA	6.06	114.04	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	SEP	N-CA-CB-OG
1	A	19	SEP	C-CA-CB-OG
1	A	19	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	19	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
2	ADP	A	801	4	28,29,29	0.42	0	43,45,45	0.47	0
4	VO4	A	803	3,2	0,4,4	-	-	-		

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	ADP	A	801	4	-	8/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O3B
2	A	801	ADP	C5'-O5'-PA-O2A
2	A	801	ADP	C5'-O5'-PA-O3A
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	C5'-O5'-PA-O1A
2	A	801	ADP	C4'-C5'-O5'-PA
2	A	801	ADP	PB-O3A-PA-O2A
2	A	801	ADP	PB-O3A-PA-O1A

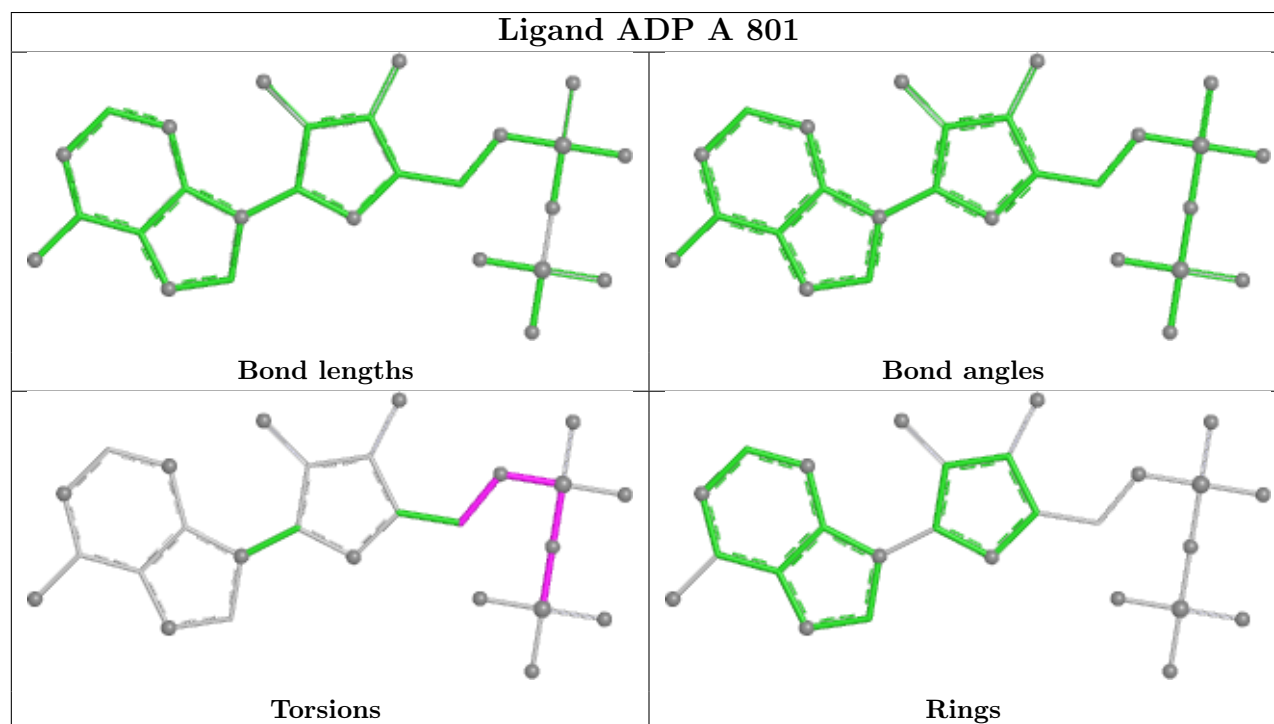
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	VO4	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	760/768 (98%)	-0.23	8 (1%) 78 54	77, 148, 194, 233	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	635	ILE	3.5
1	A	515	SER	3.3
1	A	283	ASN	2.5
1	A	514	ILE	2.4
1	A	369	GLU	2.4
1	A	760	GLN	2.4
1	A	257	SER	2.4
1	A	699	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	19	10/11	0.79	0.10	162,164,174,174	0

6.3 Carbohydrates [i](#)

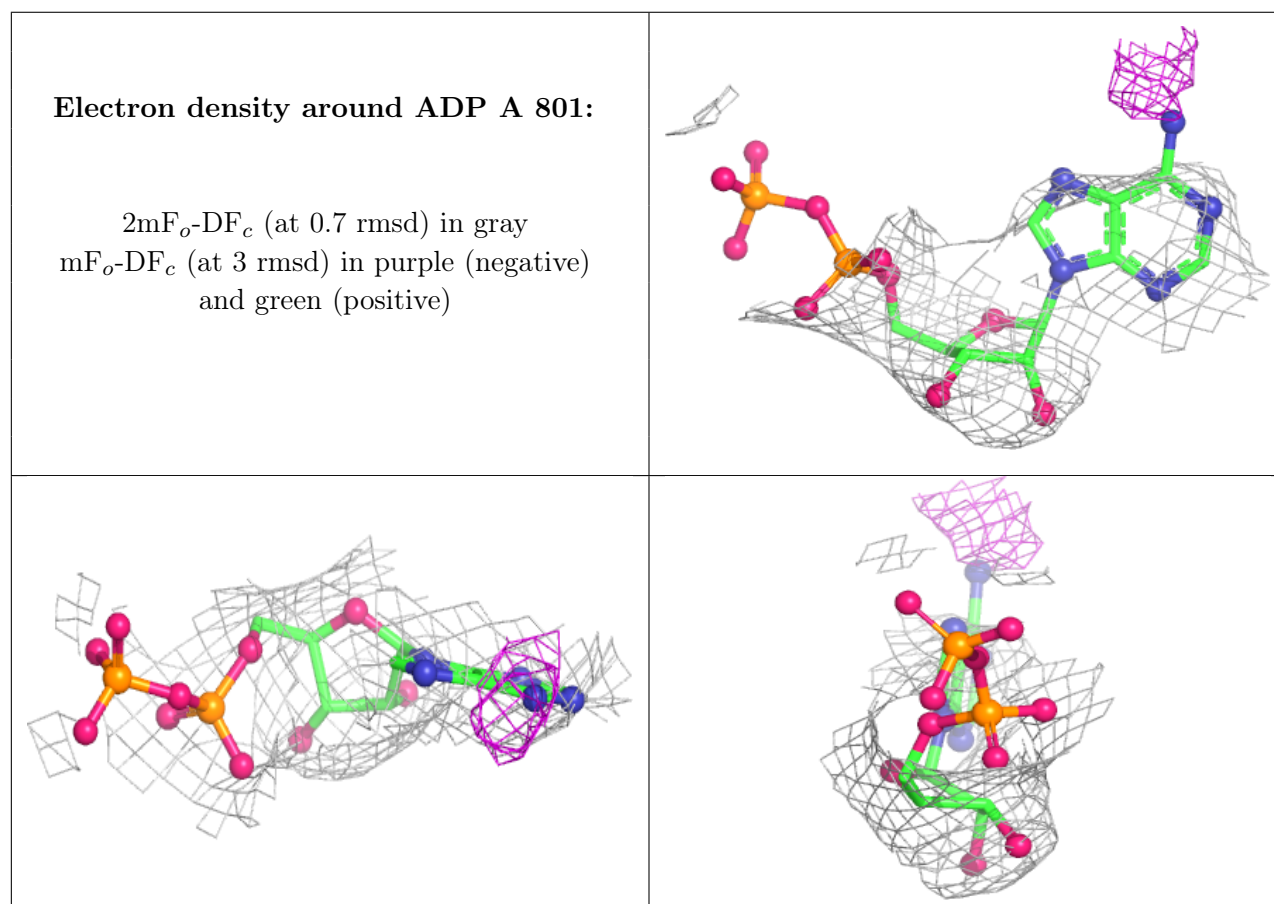
There are no oligosaccharides in this entry.

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
2	ADP	A	801	27/27	0.97	0.07	126,142,145,147	0
3	MG	A	802	1/1	0.97	0.10	109,109,109,109	0
4	VO4	A	803	5/5	0.99	0.05	144,144,145,145	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.