



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:32 PM UTC

PDB ID : 3RAA / pdb_00003raa
Title : Structural studies of AAV8 capsid transitions associated with endosomal trafficking
Authors : Nam, H.-J.; Gurda, B.; McKenna, R.; Porter, M.; Byrne, B.; Salganik, M.; Muzyczka, N.; Agbandje-McKenna, M.
Deposited on : 2011-03-27
Resolution : 3.20 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

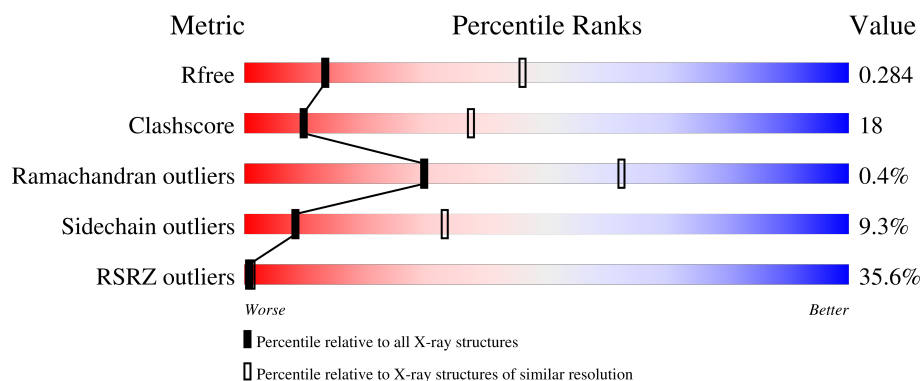
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	519	36% 64% 29% 7%

2 Entry composition [i](#)

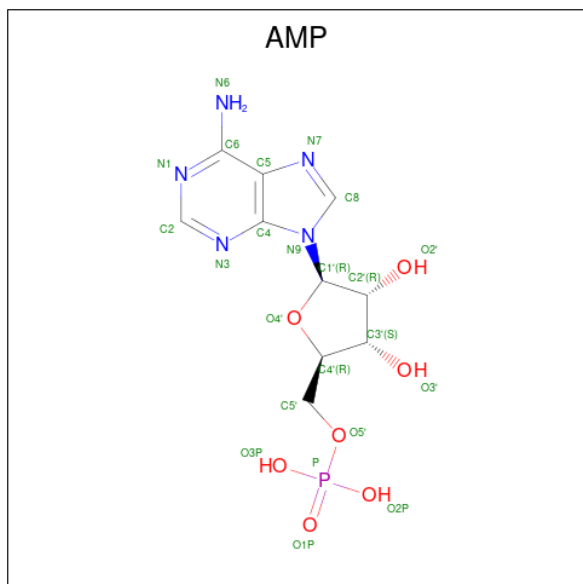
There are 2 unique types of molecules in this entry. The entry contains 4154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	4136	2609	716	798	13	0	0	0

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

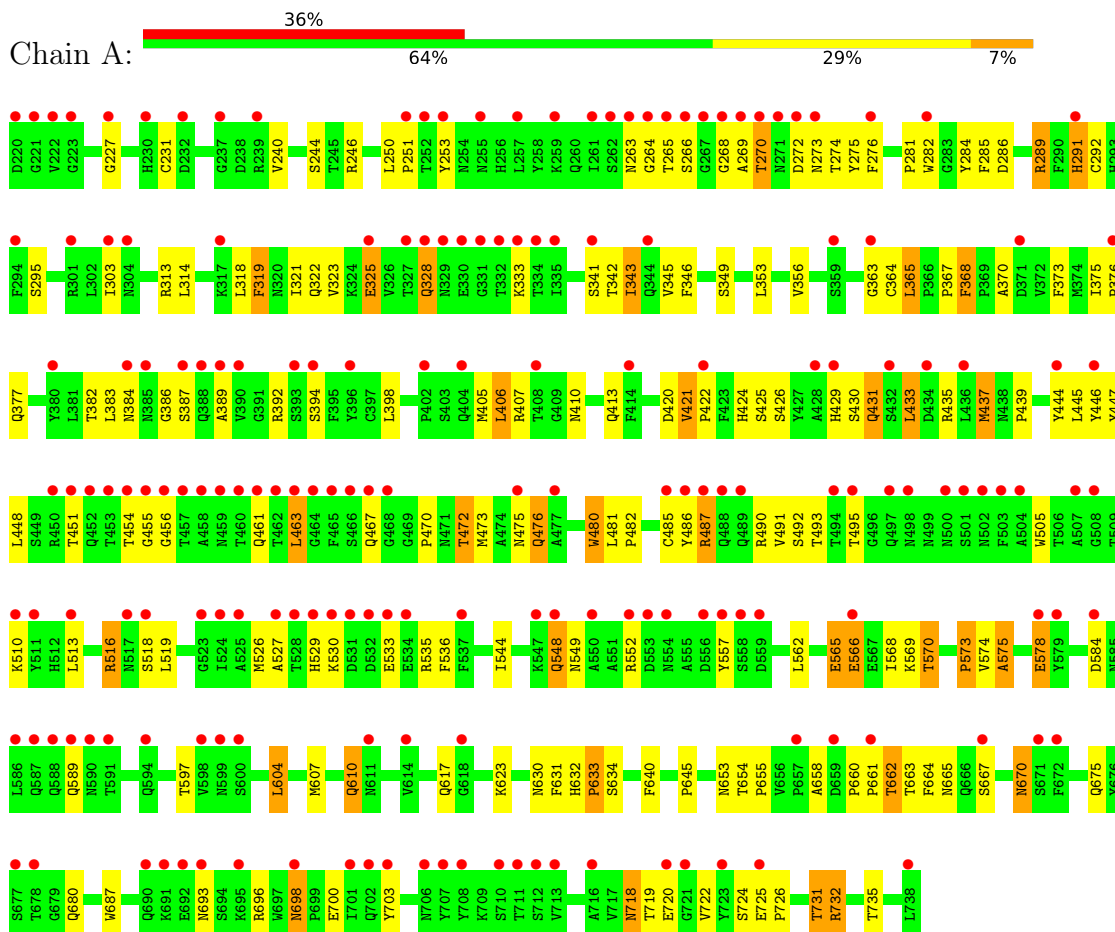


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	18	10	5	3	0	0

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 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: Capsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	256.40Å 256.40Å 447.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.84 – 3.20 34.84 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.0 (34.84-3.20) 88.9 (34.84-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.18Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.294 , 0.297 0.285 , 0.284	Depositor DCC
R_{free} test set	6363 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.24	EDS
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.38% 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: AMP

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	0.59	0/4259	1.14	37/5811 (0.6%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	GLN	OE1-CD-NE2	-9.99	112.61	122.60
1	A	328	GLN	OE1-CD-NE2	-9.54	113.06	122.60
1	A	548	GLN	OE1-CD-NE2	-8.95	113.65	122.60
1	A	719	THR	N-CA-C	-8.66	102.73	113.38
1	A	658	ALA	N-CA-C	-7.43	99.81	110.59
1	A	303	ILE	N-CA-C	7.03	119.83	111.05
1	A	292	CYS	N-CA-C	-6.88	104.35	112.89
1	A	319	PHE	N-CA-C	6.79	117.46	107.88
1	A	444	TYR	N-CA-C	-6.71	105.12	113.38
1	A	634	SER	CA-C-N	6.69	127.08	119.93
1	A	634	SER	C-N-CA	6.69	127.08	119.93
1	A	725	GLU	CA-C-N	6.58	128.07	119.84
1	A	725	GLU	C-N-CA	6.58	128.07	119.84
1	A	328	GLN	CG-CD-NE2	6.57	126.26	116.40
1	A	375	ILE	CA-C-N	6.53	126.51	119.78
1	A	375	ILE	C-N-CA	6.53	126.51	119.78
1	A	732	ARG	N-CA-C	6.43	120.08	108.17
1	A	548	GLN	CG-CD-NE2	6.34	125.91	116.40
1	A	375	ILE	N-CA-C	6.26	114.01	108.63
1	A	570	THR	N-CA-C	6.13	118.76	111.71
1	A	421	VAL	N-CA-C	-6.08	104.20	109.19
1	A	368	PHE	CA-C-N	6.04	126.20	119.32
1	A	368	PHE	C-N-CA	6.04	126.20	119.32
1	A	413	GLN	CG-CD-NE2	5.88	125.23	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	PHE	N-CA-C	5.56	118.08	110.24
1	A	634	SER	O-C-N	-5.54	116.49	121.31
1	A	573	PRO	CA-N-CD	-5.46	104.35	112.00
1	A	431	GLN	N-CA-C	-5.39	100.88	109.07
1	A	295	SER	N-CA-C	-5.30	102.33	110.07
1	A	343	ILE	N-CA-C	-5.16	101.97	109.29
1	A	281	PRO	N-CA-C	-5.15	109.33	114.68
1	A	476	GLN	N-CA-C	5.12	116.90	110.24
1	A	565	GLU	N-CA-C	-5.07	106.84	112.57
1	A	480	TRP	N-CA-C	5.06	116.69	109.14
1	A	365	LEU	CA-C-N	5.04	123.34	119.66
1	A	365	LEU	C-N-CA	5.04	123.34	119.66
1	A	575	ALA	N-CA-C	5.01	118.49	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4136	0	3893	142	0
2	A	18	0	10	0	0
All	All	4154	0	3903	142	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 18.

All (142) 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:382:THR:HG21	1:A:394:SER:H	1.23	1.01
1:A:698:ASN:HD22	1:A:698:ASN:H	1.01	0.99
1:A:566:GLU:O	1:A:569:LYS:HG3	1.66	0.96
1:A:632:HIS:N	1:A:633:PRO:HD3	1.82	0.93
1:A:632:HIS:N	1:A:633:PRO:CD	2.36	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:HIS:CD2	1:A:533:GLU:O	2.30	0.83
1:A:718:ASN:HB3	1:A:720:GLU:H	1.41	0.83
1:A:429:HIS:HB2	1:A:570:THR:HG21	1.60	0.82
1:A:264:GLY:HA3	1:A:387:SER:HB3	1.59	0.82
1:A:529:HIS:CG	1:A:533:GLU:O	2.33	0.81
1:A:718:ASN:HB2	1:A:722:VAL:H	1.46	0.81
1:A:264:GLY:CA	1:A:387:SER:HB3	2.13	0.78
1:A:665:ASN:HD21	1:A:667:SER:HB2	1.48	0.76
1:A:698:ASN:HD22	1:A:698:ASN:N	1.83	0.75
1:A:424:HIS:CD2	1:A:731:THR:HG21	2.22	0.75
1:A:670:ASN:H	1:A:670:ASN:HD22	1.35	0.73
1:A:426:SER:HA	1:A:731:THR:HG23	1.72	0.72
1:A:321:ILE:HD13	1:A:343:ILE:HD11	1.73	0.71
1:A:486:TYR:O	1:A:526:MET:HE1	1.91	0.70
1:A:631:PHE:C	1:A:633:PRO:HD3	2.16	0.70
1:A:698:ASN:H	1:A:698:ASN:ND2	1.78	0.69
1:A:270:THR:HG23	1:A:273:ASN:HD22	1.60	0.66
1:A:363:GLY:HA3	1:A:376:PRO:HG3	1.77	0.66
1:A:328:GLN:HE22	1:A:333:LYS:HB2	1.60	0.65
1:A:426:SER:HA	1:A:731:THR:CG2	2.27	0.65
1:A:424:HIS:NE2	1:A:731:THR:HG21	2.12	0.65
1:A:604:LEU:O	1:A:607:MET:HG3	1.97	0.64
1:A:610:GLN:HE21	1:A:610:GLN:CA	2.08	0.64
1:A:314:LEU:C	1:A:314:LEU:HD12	2.23	0.64
1:A:731:THR:HG22	1:A:732:ARG:HG3	1.80	0.64
1:A:406:LEU:N	1:A:406:LEU:HD23	2.14	0.63
1:A:510:LYS:HB3	1:A:518:SER:O	2.00	0.62
1:A:724:SER:O	1:A:726:PRO:HD3	2.01	0.60
1:A:291:HIS:CE1	1:A:367:PRO:HG3	2.36	0.60
1:A:610:GLN:HE21	1:A:610:GLN:HA	1.67	0.59
1:A:439:PRO:O	1:A:470:PRO:HB3	2.03	0.59
1:A:610:GLN:HA	1:A:610:GLN:NE2	2.17	0.59
1:A:662:THR:HG22	1:A:663:THR:HG23	1.86	0.57
1:A:268:GLY:O	1:A:269:ALA:C	2.46	0.56
1:A:382:THR:HG22	1:A:383:LEU:H	1.70	0.56
1:A:383:LEU:HD12	1:A:392:ARG:HB2	1.85	0.56
1:A:670:ASN:HD22	1:A:670:ASN:N	2.00	0.56
1:A:630:ASN:OD1	1:A:633:PRO:HG3	2.05	0.56
1:A:492:SER:HB2	1:A:536:PHE:CE2	2.41	0.55
1:A:365:LEU:HD22	1:A:373:PHE:CZ	2.41	0.55
1:A:490:ARG:HD2	1:A:536:PHE:CG	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:TRP:CE2	1:A:510:LYS:HE2	2.42	0.55
1:A:670:ASN:H	1:A:670:ASN:ND2	2.05	0.55
1:A:285:PHE:CZ	1:A:318:LEU:HD21	2.42	0.55
1:A:665:ASN:ND2	1:A:667:SER:HB2	2.21	0.54
1:A:289:ARG:HD2	1:A:364:CYS:SG	2.48	0.53
1:A:405:MET:C	1:A:406:LEU:HD23	2.33	0.53
1:A:703:TYR:CD2	1:A:703:TYR:C	2.86	0.53
1:A:435:ARG:NE	1:A:473:MET:HE3	2.23	0.53
1:A:700:GLU:OE1	1:A:735:THR:HG23	2.09	0.53
1:A:272:ASP:HA	1:A:516:ARG:HB2	1.91	0.53
1:A:276:PHE:CZ	1:A:389:ALA:HB2	2.44	0.53
1:A:527:ALA:HB3	1:A:574:VAL:HA	1.91	0.52
1:A:328:GLN:HA	1:A:328:GLN:OE1	2.10	0.52
1:A:321:ILE:HD13	1:A:343:ILE:CD1	2.40	0.51
1:A:610:GLN:CA	1:A:610:GLN:NE2	2.73	0.51
1:A:328:GLN:NE2	1:A:333:LYS:HB2	2.24	0.51
1:A:472:THR:HG22	1:A:475:ASN:HD22	1.76	0.51
1:A:275:TYR:C	1:A:275:TYR:CD1	2.88	0.50
1:A:342:THR:HG22	1:A:407:ARG:HG2	1.94	0.50
1:A:535:ARG:HH11	1:A:535:ARG:HG2	1.76	0.50
1:A:353:LEU:HD11	1:A:398:LEU:HD22	1.92	0.50
1:A:433:LEU:HD21	1:A:480:TRP:HB2	1.93	0.50
1:A:529:HIS:HD2	1:A:530:LYS:O	1.95	0.50
1:A:526:MET:HB2	1:A:575:ALA:HB2	1.93	0.49
1:A:231:CYS:HA	1:A:244:SER:HA	1.95	0.49
1:A:264:GLY:N	1:A:387:SER:HB3	2.27	0.49
1:A:368:PHE:CE2	1:A:370:ALA:HB3	2.48	0.48
1:A:544:ILE:HG12	1:A:562:LEU:HD22	1.94	0.48
1:A:718:ASN:HB3	1:A:720:GLU:N	2.20	0.48
1:A:246:ARG:HG3	1:A:365:LEU:HB3	1.96	0.47
1:A:670:ASN:N	1:A:670:ASN:ND2	2.63	0.47
1:A:446:TYR:CE2	1:A:467:GLN:HG3	2.50	0.47
1:A:244:SER:HB2	1:A:246:ARG:HH12	1.78	0.47
1:A:623:LYS:HB2	1:A:645:PRO:HG3	1.96	0.47
1:A:286:ASP:O	1:A:364:CYS:HA	2.15	0.47
1:A:382:THR:HG21	1:A:394:SER:N	2.08	0.47
1:A:630:ASN:CG	1:A:633:PRO:HG3	2.40	0.47
1:A:437:MET:HG2	1:A:476:GLN:OE1	2.14	0.47
1:A:435:ARG:HD2	1:A:473:MET:CE	2.45	0.47
1:A:535:ARG:HG2	1:A:535:ARG:NH1	2.30	0.47
1:A:227:GLY:HA3	1:A:319:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:CA	1:A:731:THR:HG23	2.42	0.46
1:A:426:SER:CB	1:A:731:THR:HG23	2.45	0.46
1:A:435:ARG:HD2	1:A:473:MET:HE1	1.98	0.46
1:A:282:TRP:CG	1:A:398:LEU:HD12	2.51	0.46
1:A:325:GLU:HA	1:A:675:GLN:HB3	1.97	0.46
1:A:461:GLN:H	1:A:461:GLN:CD	2.23	0.46
1:A:492:SER:HB2	1:A:536:PHE:HE2	1.78	0.46
1:A:314:LEU:HD12	1:A:314:LEU:O	2.15	0.46
1:A:454:THR:O	1:A:456:GLY:N	2.49	0.46
1:A:345:VAL:HG12	1:A:346:PHE:N	2.31	0.46
1:A:578:GLU:HB3	1:A:597:THR:HG23	1.98	0.46
1:A:451:THR:HG22	1:A:451:THR:O	2.16	0.45
1:A:529:HIS:CB	1:A:533:GLU:O	2.63	0.45
1:A:482:PRO:O	1:A:607:MET:HE2	2.17	0.45
1:A:557:TYR:CD2	1:A:557:TYR:C	2.94	0.45
1:A:447:TYR:OH	1:A:472:THR:HG21	2.17	0.45
1:A:321:ILE:HD12	1:A:406:LEU:HD12	1.98	0.45
1:A:319:PHE:N	1:A:319:PHE:CD2	2.85	0.45
1:A:274:THR:HB	1:A:386:GLY:O	2.17	0.44
1:A:353:LEU:CD1	1:A:398:LEU:HD22	2.47	0.44
1:A:654:THR:HA	1:A:655:PRO:HD3	1.86	0.44
1:A:696:ARG:HD3	1:A:700:GLU:HG2	2.00	0.44
1:A:328:GLN:OE1	1:A:333:LYS:HB2	2.17	0.44
1:A:250:LEU:HD23	1:A:653:ASN:ND2	2.33	0.44
1:A:263:ASN:HD21	1:A:269:ALA:HB2	1.83	0.44
1:A:244:SER:HB2	1:A:246:ARG:NH1	2.33	0.44
1:A:284:TYR:CE2	1:A:376:PRO:HB2	2.54	0.43
1:A:421:VAL:HG21	1:A:640:PHE:HB3	1.98	0.43
1:A:406:LEU:HB3	1:A:410:ASN:HB3	2.01	0.43
1:A:291:HIS:NE2	1:A:367:PRO:HG3	2.34	0.43
1:A:632:HIS:N	1:A:633:PRO:HD2	2.27	0.43
1:A:718:ASN:HB2	1:A:722:VAL:N	2.22	0.43
1:A:289:ARG:NH1	1:A:617:GLN:O	2.51	0.43
1:A:253:TYR:CE1	1:A:377:GLN:HB2	2.54	0.42
1:A:313:ARG:HB3	1:A:313:ARG:NH1	2.34	0.42
1:A:431:GLN:O	1:A:570:THR:OG1	2.37	0.42
1:A:435:ARG:CD	1:A:473:MET:HE3	2.50	0.42
1:A:421:VAL:HG22	1:A:422:PRO:HD2	2.02	0.41
1:A:463:LEU:HD12	1:A:463:LEU:HA	1.84	0.41
1:A:240:VAL:CG1	1:A:687:TRP:HB2	2.51	0.41
1:A:700:GLU:OE1	1:A:735:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:CYS:SG	1:A:244:SER:HA	2.61	0.41
1:A:660:PRO:HB2	1:A:661:PRO:HD2	2.02	0.41
1:A:430:SER:HB3	1:A:735:THR:HB	2.03	0.41
1:A:529:HIS:HB2	1:A:533:GLU:O	2.20	0.41
1:A:289:ARG:CG	1:A:289:ARG:HH11	2.34	0.41
1:A:693:ASN:O	1:A:693:ASN:CG	2.64	0.41
1:A:250:LEU:HD12	1:A:251:PRO:HD2	2.01	0.40
1:A:487:ARG:HH11	1:A:487:ARG:HD2	1.78	0.40
1:A:565:GLU:O	1:A:568:ILE:HG12	2.22	0.40
1:A:276:PHE:CB	1:A:384:ASN:HB3	2.51	0.40
1:A:435:ARG:CZ	1:A:473:MET:HE3	2.51	0.40
1:A:323:VAL:HG11	1:A:341:SER:HB2	2.03	0.40
1:A:493:THR:HG22	1:A:557:TYR:CE1	2.56	0.40
1:A:718:ASN:HD22	1:A:718:ASN:HA	1.52	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	517/519 (100%)	491 (95%)	24 (5%)	2 (0%)	30 62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	GLY
1	A	633	PRO

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	453/453 (100%)	411 (91%)	42 (9%)	8 33

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	THR
1	A	266	SER
1	A	270	THR
1	A	289	ARG
1	A	291	HIS
1	A	322	GLN
1	A	325	GLU
1	A	349	SER
1	A	356	VAL
1	A	406	LEU
1	A	420	ASP
1	A	425	SER
1	A	433	LEU
1	A	437	MET
1	A	445	LEU
1	A	448	LEU
1	A	463	LEU
1	A	472	THR
1	A	481	LEU
1	A	485	CYS
1	A	487	ARG
1	A	491	VAL
1	A	495	THR
1	A	513	LEU
1	A	516	ARG
1	A	519	LEU
1	A	548	GLN
1	A	549	ASN
1	A	552	ARG
1	A	566	GLU

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Mol	Chain	Res	Type
1	A	573	PRO
1	A	578	GLU
1	A	584	ASP
1	A	589	GLN
1	A	604	LEU
1	A	610	GLN
1	A	662	THR
1	A	670	ASN
1	A	680	GLN
1	A	698	ASN
1	A	718	ASN
1	A	731	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	HIS
1	A	260	GLN
1	A	263	ASN
1	A	273	ASN
1	A	300	GLN
1	A	322	GLN
1	A	361	HIS
1	A	410	ASN
1	A	429	HIS
1	A	467	GLN
1	A	475	ASN
1	A	499	ASN
1	A	521	ASN
1	A	529	HIS
1	A	548	GLN
1	A	549	ASN
1	A	610	GLN
1	A	653	ASN
1	A	665	ASN
1	A	666	GLN
1	A	670	ASN
1	A	698	ASN
1	A	718	ASN
1	A	737	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand 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	$\# Z > 2$
2	AMP	A	2	-	20,20,25	0.39	0	29,29,38	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	A	2	-	-	1/6/18/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

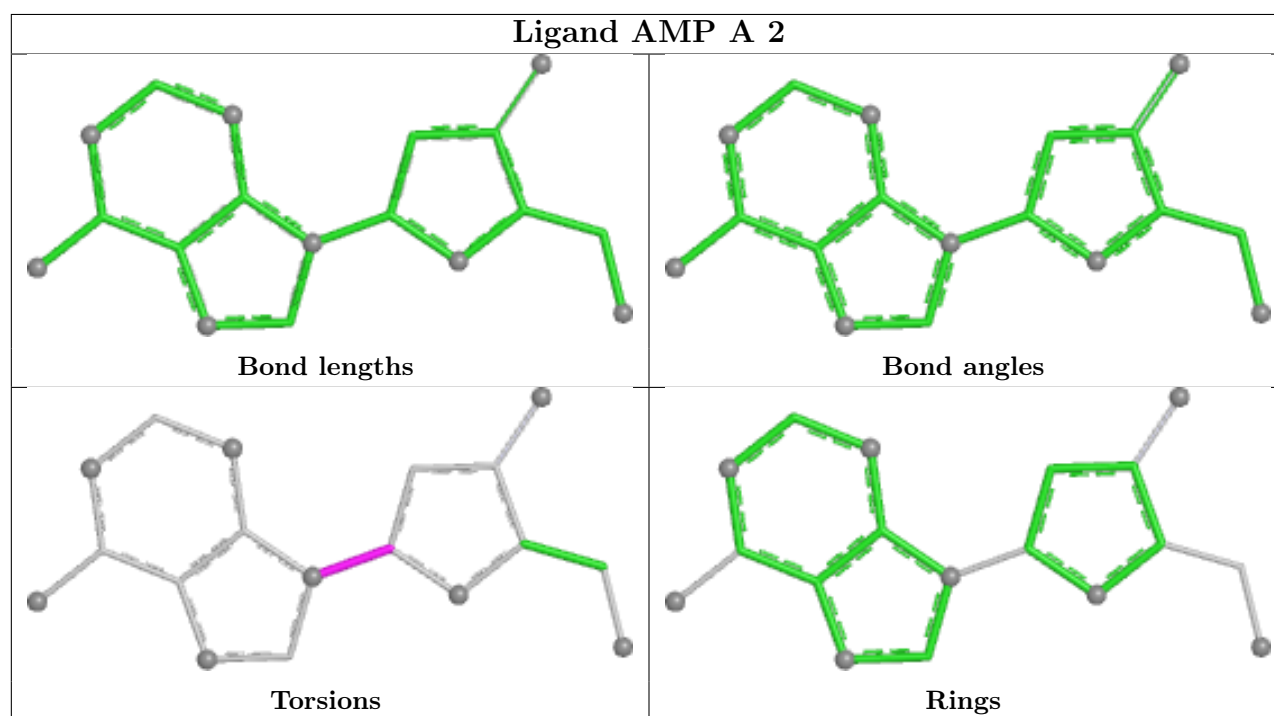
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2	AMP	C2'-C1'-N9-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	A	519/519 (100%)	1.79	185 (35%) ⓘ ⓘ	28, 42, 67, 96	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	GLY	10.4
1	A	328	GLN	7.4
1	A	330	GLU	6.1
1	A	265	THR	5.4
1	A	553	ASP	5.3
1	A	220	ASP	5.3
1	A	266	SER	4.7
1	A	589	GLN	4.5
1	A	618	GLY	4.4
1	A	329	ASN	4.4
1	A	706	ASN	4.3
1	A	263	ASN	4.2
1	A	460	THR	4.1
1	A	388	GLN	4.1
1	A	456	GLY	4.1
1	A	271	ASN	4.0
1	A	325	GLU	4.0
1	A	251	PRO	4.0
1	A	500	ASN	4.0
1	A	262	SER	4.0
1	A	534	GLU	3.9
1	A	331	GLY	3.8
1	A	720	GLU	3.7
1	A	710	SER	3.7
1	A	264	GLY	3.7
1	A	548	GLN	3.7
1	A	485	CYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	458	ALA	3.6
1	A	533	GLU	3.6
1	A	503	PHE	3.5
1	A	332	THR	3.5
1	A	255	ASN	3.5
1	A	550	ALA	3.4
1	A	532	ASP	3.4
1	A	486	TYR	3.4
1	A	270	THR	3.4
1	A	334	THR	3.4
1	A	455	GLY	3.4
1	A	691	LYS	3.3
1	A	268	GLY	3.3
1	A	461	GLN	3.3
1	A	578	GLU	3.3
1	A	497	GLN	3.3
1	A	389	ALA	3.2
1	A	513	LEU	3.2
1	A	272	ASP	3.2
1	A	504	ALA	3.2
1	A	459	ASN	3.2
1	A	707	TYR	3.2
1	A	558	SER	3.2
1	A	587	GLN	3.1
1	A	695	LYS	3.1
1	A	384	ASN	3.1
1	A	462	THR	3.1
1	A	390	VAL	3.0
1	A	394	SER	3.0
1	A	475	ASN	3.0
1	A	712	SER	3.0
1	A	385	ASN	3.0
1	A	590	ASN	3.0
1	A	692	GLU	3.0
1	A	232	ASP	3.0
1	A	477	ALA	2.9
1	A	452	GLN	2.9
1	A	667	SER	2.9
1	A	508	GLY	2.9
1	A	393	SER	2.9
1	A	450	ARG	2.9
1	A	721	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	408	THR	2.8
1	A	708	TYR	2.8
1	A	269	ALA	2.8
1	A	527	ALA	2.8
1	A	467	GLN	2.8
1	A	380	TYR	2.8
1	A	678	THR	2.8
1	A	698	ASN	2.7
1	A	657	PRO	2.7
1	A	223	GLY	2.7
1	A	711	THR	2.7
1	A	282	TRP	2.7
1	A	498	ASN	2.7
1	A	588	GLN	2.7
1	A	363	GLY	2.7
1	A	259	LYS	2.7
1	A	327	THR	2.7
1	A	468	GLY	2.7
1	A	525	ALA	2.7
1	A	716	ALA	2.7
1	A	584	ASP	2.7
1	A	304	ASN	2.7
1	A	725	GLU	2.6
1	A	451	THR	2.6
1	A	294	PHE	2.6
1	A	579	TYR	2.6
1	A	529	HIS	2.6
1	A	557	TYR	2.6
1	A	556	ASP	2.6
1	A	659	ASP	2.6
1	A	273	ASN	2.6
1	A	554	ASN	2.6
1	A	261	ILE	2.5
1	A	446	TYR	2.5
1	A	453	THR	2.5
1	A	402	PRO	2.5
1	A	671	SER	2.5
1	A	690	GLN	2.5
1	A	511	TYR	2.5
1	A	518	SER	2.5
1	A	614	VAL	2.5
1	A	586	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	594	GLN	2.5
1	A	317	LYS	2.5
1	A	661	PRO	2.5
1	A	428	ALA	2.4
1	A	530	LYS	2.4
1	A	723	TYR	2.4
1	A	466	SER	2.4
1	A	465	PHE	2.4
1	A	222	VAL	2.4
1	A	537	PHE	2.4
1	A	341	SER	2.4
1	A	252	THR	2.4
1	A	531	ASP	2.4
1	A	230	HIS	2.4
1	A	487	ARG	2.4
1	A	371	ASP	2.4
1	A	591	THR	2.3
1	A	387	SER	2.3
1	A	457	THR	2.3
1	A	528	THR	2.3
1	A	611	ASN	2.3
1	A	301	ARG	2.3
1	A	559	ASP	2.3
1	A	333	LYS	2.3
1	A	335	ILE	2.3
1	A	429	HIS	2.3
1	A	227	GLY	2.3
1	A	436	LEU	2.3
1	A	599	ASN	2.3
1	A	552	ARG	2.3
1	A	434	ASP	2.3
1	A	713	VAL	2.3
1	A	303	ILE	2.2
1	A	253	TYR	2.2
1	A	344	GLN	2.2
1	A	489	GLN	2.2
1	A	494	THR	2.2
1	A	359	SER	2.2
1	A	432	SER	2.2
1	A	738	LEU	2.2
1	A	547	LYS	2.2
1	A	672	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	444	TYR	2.2
1	A	703	TYR	2.2
1	A	507	ALA	2.2
1	A	677	SER	2.2
1	A	523	GLY	2.2
1	A	495	THR	2.1
1	A	237	GLY	2.1
1	A	422	PRO	2.1
1	A	276	PHE	2.1
1	A	414	PHE	2.1
1	A	598	VAL	2.1
1	A	404	GLN	2.1
1	A	488	GLN	2.1
1	A	239	ARG	2.1
1	A	396	TYR	2.1
1	A	566	GLU	2.1
1	A	517	ASN	2.1
1	A	221	GLY	2.1
1	A	464	GLY	2.1
1	A	702	GLN	2.1
1	A	502	ASN	2.0
1	A	693	ASN	2.0
1	A	376	PRO	2.0
1	A	257	LEU	2.0
1	A	501	SER	2.0
1	A	600	SER	2.0
1	A	701	ILE	2.0
1	A	291	HIS	2.0
1	A	454	THR	2.0
1	A	510	LYS	2.0
1	A	463	LEU	2.0
1	A	524	ILE	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](#)

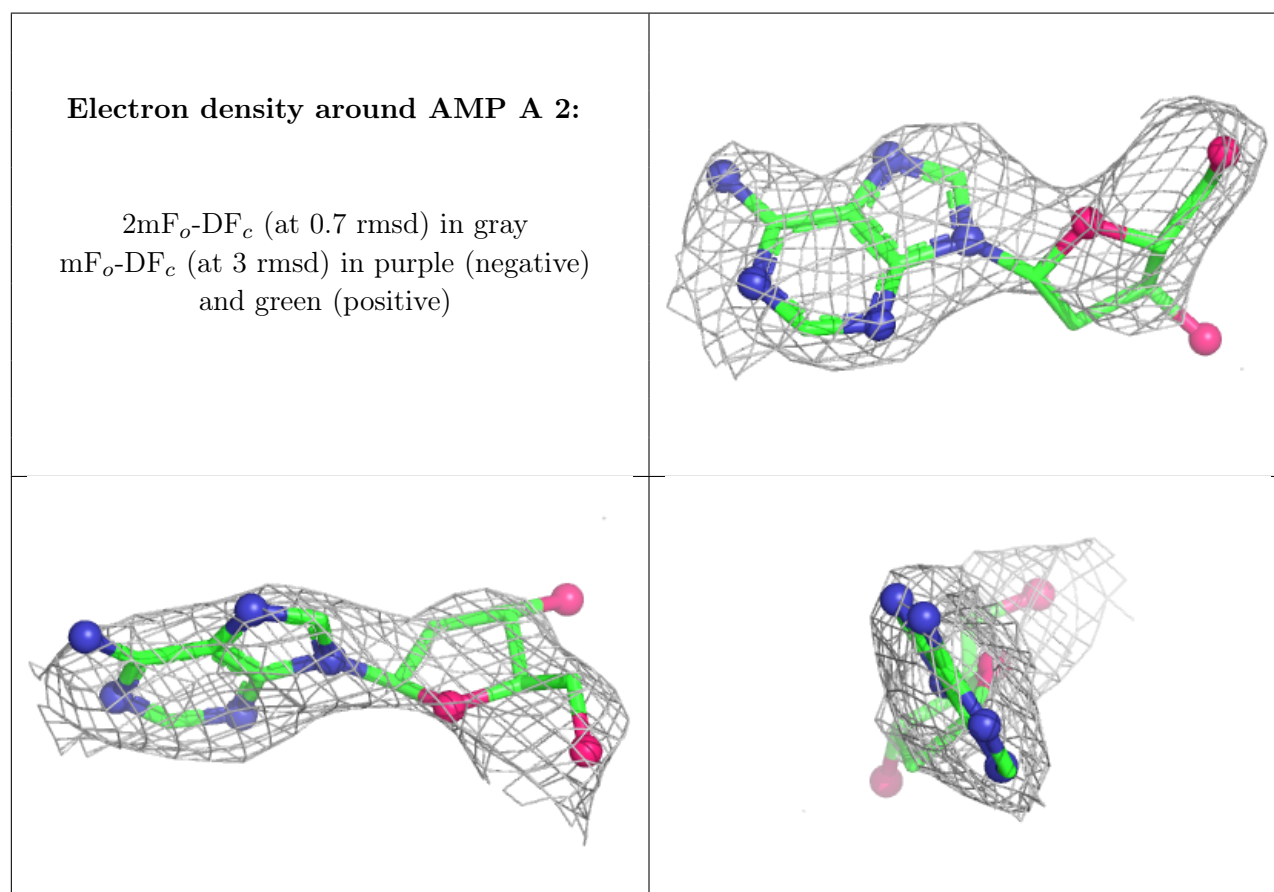
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	AMP	A	2	18/23	0.88	0.23	32,36,42,43	18

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.