



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 05:32 AM EDT

PDB ID : 1Z8D  
Title : Crystal Structure of Human Muscle Glycogen Phosphorylase a with AMP and Glucose  
Authors : Lukacs, C.M.; Oikonomakos, N.G.; Crowther, R.L.; Hong, L.N.; Kammlott, R.U.; Levin, W.; Li, S.; Liu, C.M.; Lucas-McGady, D.; Pietranico, S.; Reik, L.  
Deposited on : 2005-03-30  
Resolution : 2.30 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

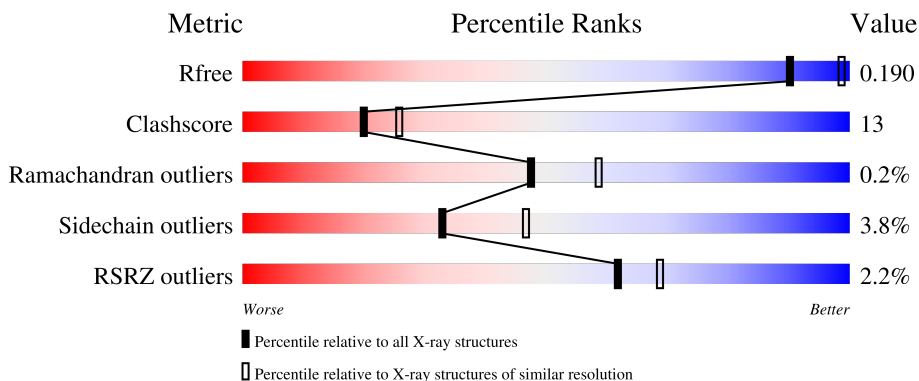
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	842	

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
1	SEP	A	14	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7121 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.

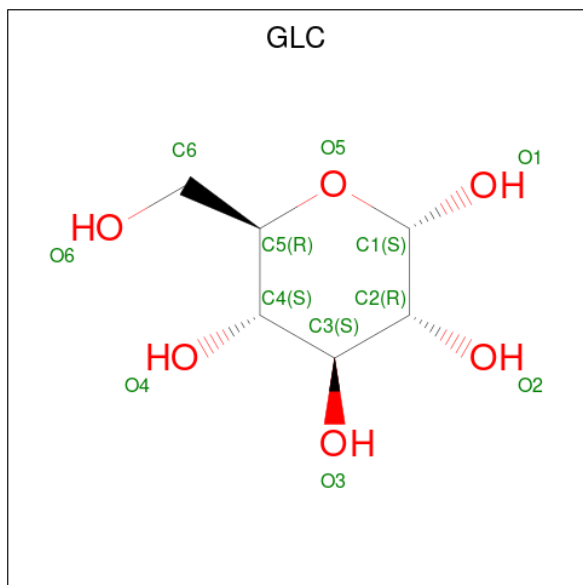
- Molecule 1 is a protein called Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	821	6707	4267	1187	1221	2	30	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	SEP	SER	engineered mutation	UNP P11217
A	680	LLP	LYS	engineered mutation	UNP P11217

- Molecule 2 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



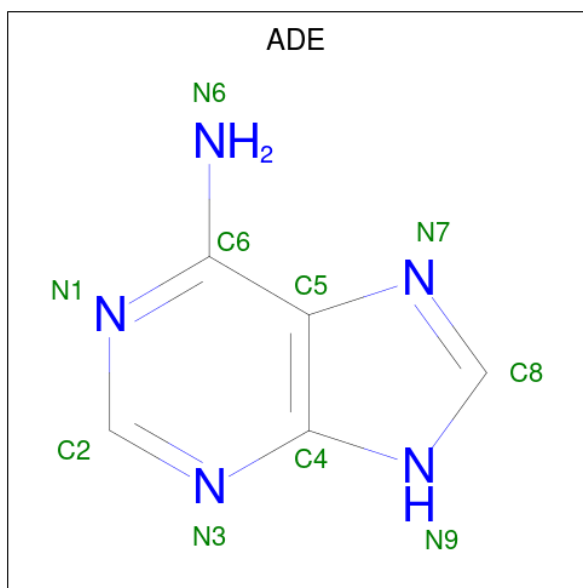
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	12	6	6	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	23	10	5	7	1	0	0

- Molecule 4 is ADENINE (three-letter code: ADE) (formula:  $C_5H_5N_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	10	5	5	0	0

- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	369	Total 369	O 369	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: Glycogen phosphorylase, muscle form



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.37Å 144.00Å 59.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.79 – 2.30 30.79 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.79-2.30) 97.7 (30.79-2.27)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.26Å)	Xtrriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.192 , 0.251 0.192 , 0.190	Depositor DCC
$R_{free}$ test set	934 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtrriage
Anisotropy	0.429	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: LLP, SEP, GLC, AMP, ADE

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	0.34	0/6822	0.60	1/9224 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	558	ASN	N-CA-C	-5.81	95.31	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	SEP	CA

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	6707	0	6634	169	1
2	A	12	0	12	0	0
3	A	23	0	12	0	0
4	A	10	0	4	0	0
5	A	369	0	0	7	0
All	All	7121	0	6662	169	1

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 13.

All (169) 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:549:LEU:HG	1:A:555:VAL:HG21	1.46	0.97
1:A:549:LEU:HB3	1:A:555:VAL:HG11	1.50	0.92
1:A:455:VAL:H	1:A:459:HIS:HD2	1.25	0.82
1:A:21:VAL:HG13	1:A:23:ASN:HB2	1.61	0.82
1:A:546:ALA:HB1	1:A:557:ILE:HG13	1.63	0.80
1:A:549:LEU:CG	1:A:555:VAL:HG21	2.12	0.80
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.65	0.77
1:A:235:ASN:HA	1:A:833:ARG:CG	2.16	0.75
1:A:455:VAL:HG22	1:A:484:ASN:OD1	1.85	0.74
1:A:558:ASN:O	1:A:560:ASN:N	2.20	0.72
1:A:554:LYS:HD3	1:A:555:VAL:N	2.04	0.72
1:A:311:PHE:CZ	1:A:323:ARG:HD3	2.25	0.72
1:A:565:ILE:HD12	1:A:660:ALA:HB2	1.72	0.71
1:A:591:LYS:HE2	1:A:633:ASP:OD2	1.90	0.71
1:A:287:GLU:HG2	1:A:289:LYS:HG2	1.74	0.70
1:A:565:ILE:HD13	1:A:656:VAL:HG22	1.74	0.70
1:A:355:ASP:OD2	1:A:398:ARG:HD3	1.93	0.69
1:A:100:VAL:HG21	1:A:494:LEU:HD21	1.75	0.68
1:A:82:ILE:HD11	1:A:827:VAL:HG21	1.76	0.67
1:A:16:ARG:NE	1:A:16:ARG:HA	2.11	0.65
1:A:7:GLN:HG3	1:A:8:GLU:N	2.11	0.65
1:A:96:GLN:HG2	1:A:494:LEU:HD22	1.78	0.64
1:A:455:VAL:HG13	1:A:674:SER:HB2	1.80	0.64
1:A:22:GLU:OE1	1:A:104:LEU:HD21	1.98	0.64
1:A:546:ALA:CB	1:A:557:ILE:HG21	2.27	0.64
1:A:550:GLU:HB2	1:A:555:VAL:HG12	1.79	0.64
1:A:687:LEU:HD13	1:A:800:MET:HE1	1.79	0.63
1:A:33:ARG:HG3	1:A:37:PHE:HD2	1.64	0.63
1:A:455:VAL:HG13	1:A:674:SER:CB	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:ND2	1:A:237:VAL:H	1.97	0.62
1:A:647:ASN:ND2	1:A:649:ARG:HE	1.97	0.62
1:A:12:GLN:O	1:A:14:SEP:N	2.33	0.61
1:A:455:VAL:HG22	1:A:484:ASN:CG	2.20	0.61
1:A:554:LYS:HD3	1:A:555:VAL:H	1.65	0.61
1:A:329:PHE:HB3	1:A:330:PRO:HD3	1.83	0.61
1:A:557:ILE:HD13	1:A:557:ILE:N	2.16	0.61
1:A:386:ARG:HD2	1:A:432:GLU:OE1	2.01	0.60
1:A:193:ARG:HB2	1:A:225:PRO:HG2	1.84	0.60
1:A:558:ASN:C	1:A:560:ASN:H	2.04	0.60
1:A:68:ILE:O	1:A:72:GLN:HG3	2.01	0.59
1:A:5:SER:OG	1:A:7:GLN:HG2	2.03	0.59
1:A:82:ILE:HD13	1:A:825:TRP:CE3	2.39	0.58
1:A:565:ILE:HD13	1:A:656:VAL:CG2	2.33	0.58
1:A:636:VAL:O	1:A:639:ARG:HD3	2.06	0.56
1:A:413:ARG:HD3	5:A:1258:HOH:O	2.05	0.56
1:A:192:ALA:HB1	1:A:224:MET:CE	2.36	0.56
1:A:246:ALA:O	1:A:247:LYS:HD3	2.07	0.55
1:A:741:VAL:HA	1:A:744:GLN:HE21	1.70	0.55
1:A:490:ARG:HA	1:A:494:LEU:HG	1.87	0.55
1:A:532:ARG:HG2	1:A:532:ARG:HH11	1.72	0.55
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.88	0.55
1:A:546:ALA:HB1	1:A:557:ILE:HG21	1.88	0.55
1:A:517:GLN:NE2	1:A:520:LYS:HE3	2.22	0.55
1:A:557:ILE:HD13	1:A:557:ILE:H	1.72	0.55
1:A:311:PHE:CE1	1:A:323:ARG:HD3	2.42	0.54
1:A:454:GLY:HA3	1:A:460:SER:OG	2.07	0.54
1:A:545:PHE:O	1:A:549:LEU:HB2	2.07	0.54
1:A:575:ARG:HD3	1:A:666:ILE:O	2.06	0.54
1:A:274:ASN:HA	1:A:277:ARG:CG	2.38	0.54
1:A:469:LYS:O	1:A:473:GLU:HG3	2.08	0.54
1:A:311:PHE:O	1:A:323:ARG:HD2	2.08	0.53
1:A:542:LYS:CE	1:A:661:ASP:OD2	2.57	0.53
1:A:555:VAL:HG13	1:A:556:HIS:N	2.23	0.53
1:A:35:LEU:HD13	1:A:35:LEU:O	2.09	0.53
1:A:6:ASP:O	1:A:10:ARG:HG3	2.09	0.53
1:A:547:ALA:O	1:A:551:ARG:HG2	2.08	0.53
1:A:35:LEU:HD13	1:A:35:LEU:C	2.29	0.52
1:A:405:GLU:O	1:A:409:ARG:HG2	2.08	0.52
1:A:617:LYS:HD3	5:A:1270:HOH:O	2.08	0.52
1:A:388:PRO:HB2	1:A:390:HIS:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:O	1:A:16:ARG:HG2	2.09	0.52
1:A:91:MET:HB2	1:A:129:ALA:HB3	1.91	0.52
1:A:538:LYS:CE	1:A:660:ALA:O	2.58	0.52
1:A:682:MET:HE1	1:A:699:MET:HG2	1.91	0.52
1:A:517:GLN:HE21	1:A:520:LYS:HE3	1.76	0.51
1:A:517:GLN:HG2	5:A:1162:HOH:O	2.09	0.51
1:A:546:ALA:HB1	1:A:557:ILE:CG1	2.36	0.51
1:A:830:SER:OG	1:A:832:GLN:HG2	2.11	0.51
1:A:598:PHE:HD2	1:A:639:ARG:HH21	1.59	0.51
1:A:16:ARG:HA	1:A:16:ARG:HE	1.74	0.50
1:A:458:ILE:O	1:A:462:ILE:HG13	2.11	0.50
1:A:622:LEU:HD22	1:A:626:ILE:HG13	1.94	0.50
1:A:192:ALA:HB1	1:A:224:MET:HE2	1.92	0.49
1:A:23:ASN:HB3	1:A:26:GLU:H	1.78	0.49
1:A:538:LYS:HE2	1:A:660:ALA:O	2.11	0.49
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.34	0.49
1:A:81:ARG:NE	1:A:310:ARG:HD3	2.28	0.49
1:A:177:GLU:H	1:A:177:GLU:CD	2.15	0.49
1:A:274:ASN:HA	1:A:277:ARG:HG3	1.96	0.48
1:A:21:VAL:HG12	1:A:26:GLU:HG3	1.96	0.48
1:A:532:ARG:NH1	1:A:533:ASP:OD1	2.47	0.48
1:A:303:THR:O	1:A:307:ILE:HG13	2.13	0.48
1:A:833:ARG:N	1:A:833:ARG:HD3	2.29	0.48
1:A:648:TYR:HA	1:A:652:LEU:HD23	1.95	0.47
1:A:67:TRP:HA	1:A:238:VAL:HB	1.97	0.47
1:A:21:VAL:CG1	1:A:26:GLU:HG3	2.45	0.47
1:A:119:MET:O	1:A:123:GLU:HG3	2.14	0.47
1:A:713:MET:HG3	1:A:776:ASP:OD1	2.15	0.47
1:A:21:VAL:CG1	1:A:23:ASN:HB2	2.41	0.47
1:A:291:LEU:O	1:A:295:GLN:HG3	2.14	0.46
1:A:143:PHE:O	1:A:147:MET:HG3	2.16	0.46
1:A:4:LEU:O	1:A:9:LYS:HE3	2.15	0.46
1:A:67:TRP:HD1	1:A:238:VAL:HG12	1.80	0.46
1:A:525:VAL:O	1:A:799:ARG:HD2	2.16	0.46
1:A:378:THR:HG22	5:A:1095:HOH:O	2.16	0.46
1:A:62:HIS:O	1:A:66:ARG:HG2	2.16	0.46
1:A:85:LEU:HD13	1:A:335:ILE:HG23	1.97	0.46
1:A:194:PRO:HB3	1:A:224:MET:HE1	1.98	0.45
1:A:60:ARG:HD2	1:A:188:PRO:O	2.16	0.45
1:A:311:PHE:CE2	1:A:323:ARG:HD3	2.51	0.45
1:A:4:LEU:HG	1:A:8:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASP:O	1:A:517:GLN:HB2	2.17	0.45
1:A:21:VAL:C	1:A:23:ASN:H	2.19	0.45
1:A:60:ARG:O	1:A:64:VAL:HG23	2.16	0.45
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.99	0.45
1:A:235:ASN:CA	1:A:833:ARG:HG3	2.41	0.44
1:A:587:TYR:CD1	1:A:630:VAL:HG22	2.52	0.44
1:A:66:ARG:HB2	1:A:238:VAL:HG21	1.99	0.44
1:A:411:LEU:HD12	1:A:411:LEU:HA	1.78	0.44
1:A:457:ARG:HH22	1:A:701:GLU:CD	2.21	0.44
1:A:692:MET:HG3	1:A:714:ARG:NE	2.33	0.44
1:A:227:ASP:OD1	1:A:242:ARG:CD	2.66	0.44
1:A:740:GLN:O	1:A:744:GLN:HG3	2.18	0.44
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.18	0.43
1:A:558:ASN:C	1:A:560:ASN:N	2.69	0.43
1:A:575:ARG:NH2	1:A:776:ASP:OD2	2.36	0.43
1:A:45:VAL:HG22	1:A:45:VAL:O	2.18	0.43
1:A:557:ILE:N	1:A:557:ILE:CD1	2.81	0.43
1:A:515:LEU:HD22	1:A:812:SER:HB2	2.00	0.43
1:A:94:THR:HG23	5:A:963:HOH:O	2.19	0.43
1:A:351:ARG:CD	1:A:398:ARG:HG2	2.49	0.43
1:A:397:PRO:O	1:A:401:GLN:HG3	2.19	0.43
1:A:235:ASN:HD22	1:A:236:ASN:N	2.17	0.43
1:A:455:VAL:HG13	1:A:674:SER:HB3	2.00	0.43
1:A:555:VAL:CG1	1:A:556:HIS:N	2.81	0.42
1:A:49:ARG:HA	1:A:125:ILE:HG21	2.02	0.42
1:A:235:ASN:HD22	1:A:235:ASN:H	1.66	0.42
1:A:183:LEU:HB2	5:A:971:HOH:O	2.19	0.42
1:A:538:LYS:HA	1:A:538:LYS:HD2	1.79	0.42
1:A:815:ARG:HD2	1:A:815:ARG:C	2.40	0.42
1:A:605:ILE:O	1:A:644:PHE:HA	2.20	0.42
1:A:361:TRP:CH2	1:A:405:GLU:HG2	2.55	0.42
1:A:522:LEU:HD13	1:A:806:ALA:CB	2.50	0.42
1:A:546:ALA:CB	1:A:557:ILE:HG13	2.41	0.42
1:A:589:ARG:HD2	1:A:737:GLU:OE2	2.19	0.42
1:A:103:ALA:HB2	1:A:234:ARG:HD2	2.02	0.41
1:A:138:ARG:HA	1:A:138:ARG:HD2	1.88	0.41
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.20	0.41
1:A:517:GLN:NE2	1:A:520:LYS:CE	2.83	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.92	0.41
1:A:21:VAL:O	1:A:23:ASN:N	2.43	0.41
1:A:235:ASN:HA	1:A:833:ARG:HG2	1.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ARG:NH1	1:A:432:GLU:OE2	2.53	0.41
1:A:548:TYR:CD1	1:A:548:TYR:C	2.93	0.41
1:A:33:ARG:HG3	1:A:37:PHE:CD2	2.50	0.41
1:A:390:HIS:HA	5:A:927:HOH:O	2.20	0.41
1:A:421:ASP:OD1	1:A:424:ARG:HB2	2.21	0.41
1:A:633:ASP:HA	1:A:634:PRO:HD2	1.96	0.41
1:A:13:ILE:O	1:A:14:SEP:CB	2.69	0.41
1:A:463:LEU:CD2	1:A:467:ILE:HD11	2.51	0.41
1:A:157:TYR:CE2	1:A:242:ARG:HG2	2.56	0.41
1:A:455:VAL:HG22	1:A:484:ASN:ND2	2.35	0.41
1:A:682:MET:HE1	1:A:811:PHE:CD2	2.56	0.41
1:A:308:ILE:CD1	1:A:352:ILE:HG21	2.50	0.41
1:A:706:GLU:H	1:A:706:GLU:CD	2.23	0.41
1:A:80:LYS:HE2	1:A:334:ALA:HB2	2.03	0.40
1:A:351:ARG:HD2	1:A:398:ARG:HG2	2.02	0.40
1:A:568:LYS:HB3	1:A:568:LYS:HE2	1.90	0.40
1:A:455:VAL:CG2	1:A:484:ASN:OD1	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:ND2	1:A:270:ASN:ND2[2_655]	1.71	0.49

## 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	813/842 (97%)	777 (96%)	34 (4%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	559	PRO
1	A	13	ILE

### 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	A	710/727 (98%)	683 (96%)	27 (4%)	33 47

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	63	LEU
1	A	90	TYR
1	A	95	LEU
1	A	128	ASP
1	A	211	GLN
1	A	235	ASN
1	A	242	ARG
1	A	277	ARG
1	A	291	LEU
1	A	337	LEU
1	A	384	LEU
1	A	400	LEU
1	A	411	LEU
1	A	425	LEU
1	A	455	VAL
1	A	492	LEU
1	A	522	LEU
1	A	557	ILE
1	A	579	ASN
1	A	613	TYR
1	A	622	LEU
1	A	649	ARG
1	A	683	LEU
1	A	706	GLU

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Mol	Chain	Res	Type
1	A	708	PHE
1	A	831	ARG

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	23	ASN
1	A	97	ASN
1	A	211	GLN
1	A	235	ASN
1	A	239	ASN
1	A	450	HIS
1	A	459	HIS
1	A	481	ASN
1	A	517	GLN
1	A	558	ASN
1	A	566	GLN
1	A	579	ASN
1	A	588	ASN
1	A	744	GLN
1	A	763	ASN
1	A	832	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	A	14	1	8,9,10	1.77	2 (25%)	8,12,14	1.12	1 (12%)
1	LLP	A	680	1	23,24,25	1.64	6 (26%)	25,32,34	3.18	9 (36%)

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	14	1	1/1/2/3	1/5/8/10	-
1	LLP	A	680	1	-	2/16/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	C4-C4'	4.67	1.55	1.46
1	A	14	SEP	P-OG	-3.89	1.47	1.60
1	A	680	LLP	C2-N1	2.80	1.39	1.33
1	A	680	LLP	C4'-NZ	2.54	1.35	1.27
1	A	680	LLP	C3-C2	-2.18	1.38	1.40
1	A	14	SEP	P-O3P	-2.17	1.46	1.54
1	A	680	LLP	C6-N1	2.03	1.38	1.34
1	A	680	LLP	P-OP3	-2.00	1.47	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	OP3-P-OP4	-8.25	84.78	106.73
1	A	680	LLP	OP3-P-OP1	-6.69	84.50	110.68
1	A	680	LLP	OP3-P-OP2	-5.49	86.66	107.64
1	A	680	LLP	C4-C3-C2	5.04	123.31	120.19
1	A	680	LLP	OP2-P-OP4	4.26	118.08	106.73
1	A	680	LLP	C2'-C2-C3	4.15	126.01	120.89
1	A	680	LLP	OP4-P-OP1	3.88	117.35	106.47
1	A	680	LLP	OP4-C5'-C5	3.48	115.98	109.35
1	A	680	LLP	OP2-P-OP1	3.04	122.59	110.68
1	A	14	SEP	O3P-P-O2P	2.35	116.64	107.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	SEP	CA

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	680	LLP	C5'-OP4-P-OP2
1	A	680	LLP	C5'-OP4-P-OP3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	14	SEP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ADE	A	902	-	9,11,11	1.12	1 (11%)	7,15,15	2.20	4 (57%)
2	GLC	A	901	-	12,12,12	0.39	0	17,17,17	0.34	0
3	AMP	A	900	-	22,25,25	2.26	6 (27%)	25,38,38	1.64	5 (20%)

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
4	ADE	A	902	-	-	-	0/2/2/2
2	GLC	A	901	-	-	0/2/22/22	0/1/1/1
3	AMP	A	900	-	-	0/6/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	AMP	C2'-C1'	5.88	1.62	1.53
3	A	900	AMP	C3'-C4'	5.69	1.67	1.53
3	A	900	AMP	O3'-C3'	3.42	1.51	1.43
3	A	900	AMP	C2'-C3'	2.78	1.60	1.53
3	A	900	AMP	O4'-C1'	2.66	1.44	1.41
4	A	902	ADE	C2-N3	2.61	1.36	1.32
3	A	900	AMP	C2-N3	2.60	1.36	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	AMP	C4-C5-N7	4.20	113.78	109.40
4	A	902	ADE	N6-C6-N1	3.51	125.85	118.57
3	A	900	AMP	N6-C6-N1	3.14	125.09	118.57
3	A	900	AMP	C2'-C3'-C4'	-2.87	97.07	102.64
3	A	900	AMP	C2-N1-C6	2.59	123.18	118.75
4	A	902	ADE	N3-C2-N1	-2.45	124.84	128.68
4	A	902	ADE	C2-N1-C6	2.44	122.92	118.75
3	A	900	AMP	N3-C2-N1	-2.35	125.00	128.68
4	A	902	ADE	C5-C6-N1	-2.26	115.22	120.35

There are no chirality outliers.

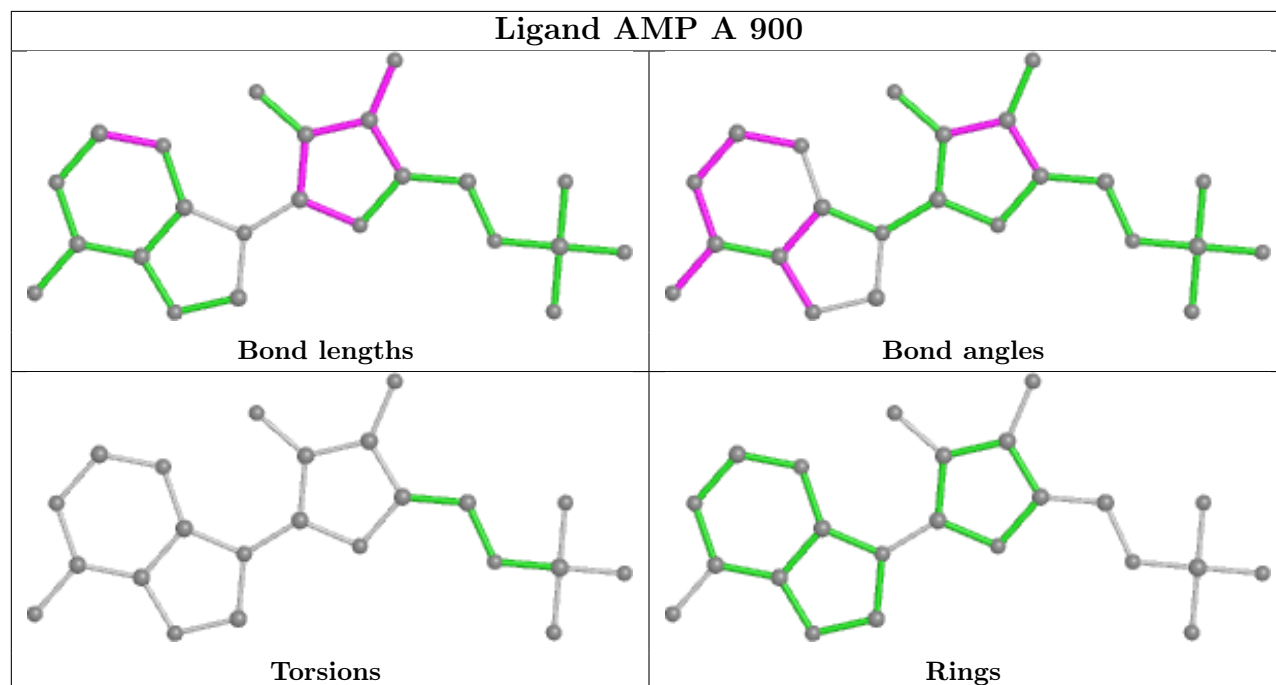
There are no torsion outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	819/842 (97%)	-0.16	18 (2%) 62 69	6, 15, 32, 68	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	ILE	6.5
1	A	556	HIS	5.5
1	A	555	VAL	5.5
1	A	21	VAL	4.4
1	A	550	GLU	3.3
1	A	3	PRO	3.3
1	A	595	ASN	3.2
1	A	558	ASN	3.1
1	A	560	ASN	2.9
1	A	23	ASN	2.9
1	A	549	LEU	2.9
1	A	548	TYR	2.9
1	A	551	ARG	2.8
1	A	547	ALA	2.8
1	A	7	GLN	2.7
1	A	594	PRO	2.6
1	A	319	ARG	2.4
1	A	554	LYS	2.2

### 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, 95<sup>th</sup> 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
1	SEP	A	14	10/11	0.93	0.16	20,22,23,24	0
1	LLP	A	680	24/25	0.96	0.16	8,11,21,24	0

### 6.3 Carbohydrates [i](#)

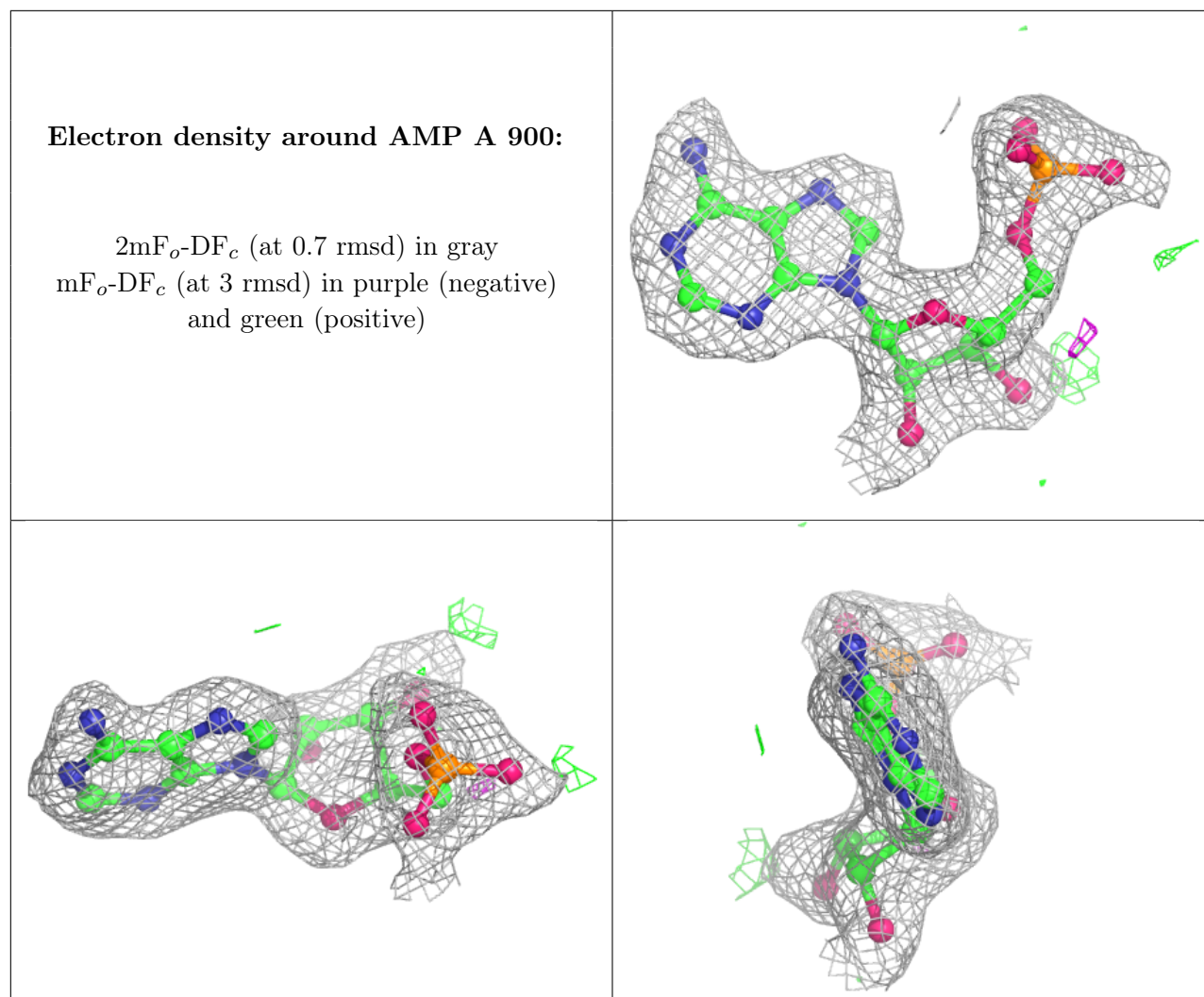
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> 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
4	ADE	A	902	10/10	0.87	0.20	28,30,32,33	0
3	AMP	A	900	23/23	0.96	0.11	11,14,18,20	0
2	GLC	A	901	12/12	0.97	0.12	7,9,11,12	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.