



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 09:59 PM UTC

PDB ID : 6O4X / pdb_00006o4x
Title : Binary complex of native hAChE with 9-aminoacridine
Authors : Gerlits, O.; Kovalevsky, A.; Radic, Z.
Deposited on : 2019-03-01
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

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
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

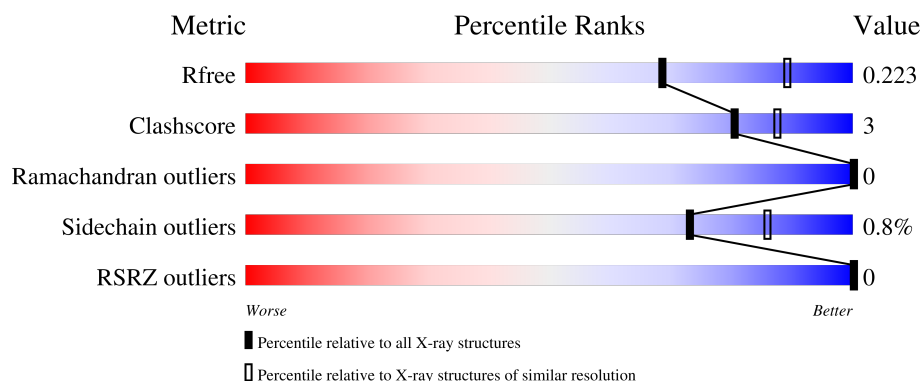
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

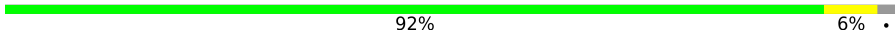
The reported resolution of this entry is 2.30 Å.

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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 ≥ 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	550	 91% 7% •
1	B	550	 92% 6% •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8996 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.

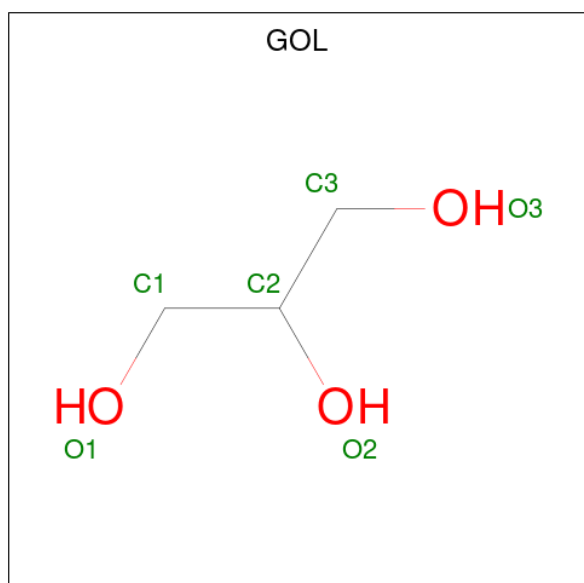
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4188	2686	732	757	13			
1	B	540	Total	C	N	O	S	0	0	0
			4188	2686	732	757	13			

There are 6 discrepancies between the modelled and reference sequences:

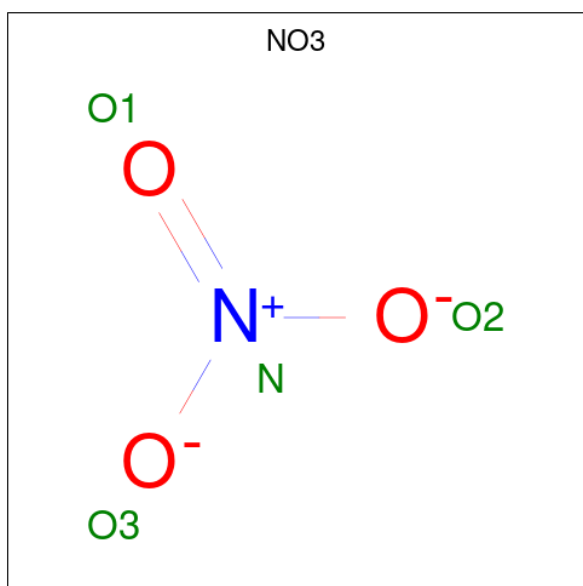
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P22303
A	-1	PRO	-	expression tag	UNP P22303
A	0	LEU	-	expression tag	UNP P22303
B	-2	GLY	-	expression tag	UNP P22303
B	-1	PRO	-	expression tag	UNP P22303
B	0	LEU	-	expression tag	UNP P22303

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



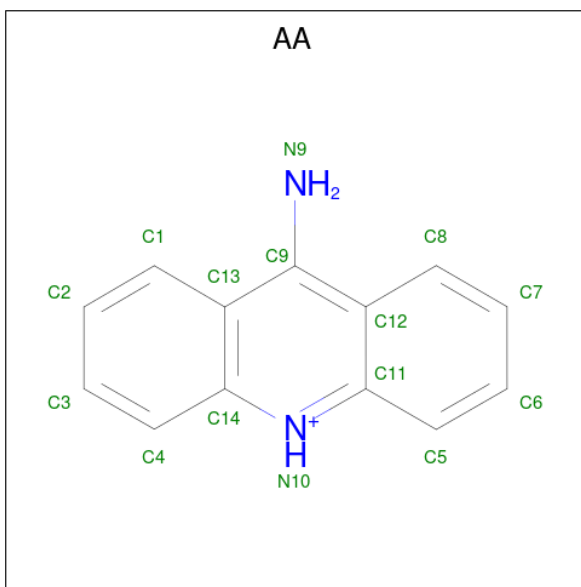
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is 9-AMINOACRIDINE (CCD ID: AA) (formula: $\text{C}_{13}\text{H}_{11}\text{N}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			15	13	2		
4	B	1	Total	C	N	0	0
			15	13	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total	O	0	0
			278	278		
5	B	278	Total	O	0	0
			278	278		

i

- Molecule 1: Acetylcholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	124.63Å 124.63Å 129.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.46 – 2.30 31.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	73.2 (31.46-2.30) 73.2 (31.46-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11_2567)	Depositor
R, R_{free}	0.190 , 0.223 0.192 , 0.223	Depositor DCC
R_{free} test set	3678 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 22.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l 0.068 for h,-h-k,-l 0.480 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8996	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: NO3, GOL, AA

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	0.12	0/4317	0.32	0/5903
1	B	0.12	0/4317	0.32	0/5903
All	All	0.12	0/8634	0.32	0/11806

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4188	0	4068	23	0
1	B	4188	0	4068	19	0
2	A	18	0	24	3	0
2	B	12	0	16	0	0
3	A	4	0	0	0	0
4	A	15	0	11	1	0
4	B	15	0	11	1	0
5	A	278	0	0	6	0
5	B	278	0	0	2	0
All	All	8996	0	8198	44	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 3.

All (44) 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:7:GLU:HG3	1:A:105:TYR:HE1	1.58	0.68
1:A:437:LEU:HA	2:A:602:GOL:H32	1.76	0.68
4:A:605:AA:H1	5:A:804:HOH:O	1.94	0.66
1:A:429:VAL:HG11	2:A:603:GOL:H11	1.77	0.65
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.82	0.60
1:B:113:PRO:HG3	1:B:485:ARG:HG2	1.88	0.56
1:B:180:LEU:HD21	1:B:199:LEU:HD21	1.87	0.55
1:B:138:LEU:HD23	1:B:146:LEU:HD22	1.89	0.53
1:A:113:PRO:HG3	1:A:485:ARG:HG2	1.91	0.52
1:B:116:VAL:HB	1:B:199:LEU:HD23	1.93	0.51
1:A:81:GLU:HG2	5:A:875:HOH:O	2.11	0.50
1:B:4:GLU:N	1:B:105:TYR:HH	2.10	0.49
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.93	0.49
1:B:135:GLY:HA3	1:B:146:LEU:HD23	1.94	0.48
1:B:433:ARG:HG3	1:B:437:LEU:HD23	1.96	0.48
1:A:7:GLU:HG3	1:A:105:TYR:CE1	2.44	0.48
1:A:306:ASP:HB3	5:A:793:HOH:O	2.13	0.48
1:A:381:HIS:HD2	5:A:953:HOH:O	1.99	0.46
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.51	0.46
4:B:603:AA:H8	5:B:848:HOH:O	2.16	0.45
1:A:252:ALA:HB1	1:A:257:CYS:HB2	1.98	0.44
1:A:4:GLU:CD	1:A:21:ARG:HH22	2.25	0.44
1:A:162:PRO:HB2	1:A:241:MET:HE3	1.98	0.44
1:A:25:PRO:HG3	1:A:461:PRO:HG3	1.99	0.44
1:A:525:ARG:HE	2:A:603:GOL:H31	1.82	0.43
1:B:460:ASP:HB3	1:B:463:ARG:HG3	2.00	0.43
1:B:226:VAL:HG22	1:B:327:LEU:HB3	2.00	0.43
1:B:306:ASP:HB3	5:B:786:HOH:O	2.18	0.43
1:B:200:PHE:CB	1:B:226:VAL:HB	2.49	0.43
1:B:202:GLU:HA	1:B:228:GLN:O	2.19	0.43
1:A:319:GLY:O	1:A:421:GLN:NE2	2.52	0.43
1:A:475:ARG:HG3	5:A:915:HOH:O	2.19	0.42
1:A:66:GLN:HG3	1:A:98:TYR:CD2	2.54	0.42
1:A:177:ARG:NH1	5:A:704:HOH:O	2.37	0.42
1:A:200:PHE:CB	1:A:226:VAL:HB	2.48	0.42
1:A:56:TRP:CD1	1:A:60:VAL:HG23	2.55	0.41
1:B:227:LEU:HB2	1:B:328:VAL:HG12	2.03	0.41
1:B:458:PRO:HA	1:B:465:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:HG21	1:B:415:ALA:HB2	2.02	0.41
1:A:260:GLY:HA2	1:A:261:GLY:HA2	1.55	0.41
1:A:305:GLY:HA2	1:A:309:SER:HA	2.02	0.41
1:B:507:ALA:HA	1:B:522:ARG:HH21	1.85	0.41
1:B:17:LEU:HD23	1:B:60:VAL:HB	2.03	0.40
1:B:501:PRO:HA	1:B:502:PRO:HD3	1.98	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	538/550 (98%)	520 (97%)	18 (3%)	0	100	100
1	B	538/550 (98%)	516 (96%)	22 (4%)	0	100	100
All	All	1076/1100 (98%)	1036 (96%)	40 (4%)	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	A	436/444 (98%)	433 (99%)	3 (1%)	76	87
1	B	436/444 (98%)	432 (99%)	4 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	872/888 (98%)	865 (99%)	7 (1%)	73	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	200	PHE
1	A	337	TYR
1	B	200	PHE
1	B	337	TYR
1	B	380	LEU
1	B	516	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	HIS
1	A	421	GLN
1	A	508	GLN
1	A	509	GLN
1	B	253	HIS
1	B	279	GLN
1	B	325	GLN
1	B	509	GLN

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

8 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	AA	A	605	-	15,17,17	1.67	3 (20%)	18,24,24	1.05	0
2	GOL	A	601	-	5,5,5	0.38	0	5,5,5	0.27	0
2	GOL	A	603	-	5,5,5	0.36	0	5,5,5	0.34	0
4	AA	B	603	-	15,17,17	1.68	3 (20%)	18,24,24	1.13	2 (11%)
2	GOL	A	602	-	5,5,5	0.37	0	5,5,5	0.20	0
3	NO3	A	604	-	1,3,3	0.55	0	0,3,3	-	-
2	GOL	B	601	-	5,5,5	0.38	0	5,5,5	0.30	0
2	GOL	B	602	-	5,5,5	0.38	0	5,5,5	0.12	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
4	AA	A	605	-	-	-	0/2/3/3
2	GOL	A	601	-	-	2/4/4/4	-
2	GOL	A	603	-	-	1/4/4/4	-
4	AA	B	603	-	-	-	0/2/3/3
2	GOL	A	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	B	602	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	AA	C13-C9	-3.70	1.40	1.46
4	A	605	AA	C14-N10	-3.69	1.32	1.39
4	B	603	AA	C13-C9	-3.69	1.40	1.46
4	B	603	AA	C14-N10	-3.66	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	603	AA	C9-N9	3.30	1.42	1.35
4	A	605	AA	C9-N9	3.19	1.41	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	603	AA	C11-C12-C8	2.19	120.64	117.58
4	B	603	AA	C7-C8-C12	-2.09	119.74	121.80

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	GOL	O1-C1-C2-C3
2	A	601	GOL	O1-C1-C2-C3
2	A	603	GOL	C1-C2-C3-O3
2	B	602	GOL	O1-C1-C2-C3
2	B	601	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-C3
2	B	602	GOL	O1-C1-C2-O2
2	A	601	GOL	O1-C1-C2-O2
2	A	602	GOL	O1-C1-C2-O2
2	B	602	GOL	C1-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	AA	1	0
2	A	603	GOL	2	0
4	B	603	AA	1	0
2	A	602	GOL	1	0

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	540/550 (98%)	-1.35	0 100 100	17, 35, 59, 117	0
1	B	540/550 (98%)	-1.35	0 100 100	20, 35, 61, 126	0
All	All	1080/1100 (98%)	-1.35	0 100 100	17, 35, 60, 126	0

There are no RSRZ outliers to report.

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
2	GOL	A	601	6/6	0.99	0.03	35,40,44,48	0
2	GOL	A	602	6/6	0.99	0.04	41,44,52,59	0
2	GOL	A	603	6/6	0.99	0.05	43,51,55,61	0
2	GOL	B	601	6/6	0.99	0.04	41,43,46,48	0
2	GOL	B	602	6/6	0.99	0.04	33,37,46,48	0
3	NO3	A	604	4/4	0.99	0.05	43,47,50,54	4
4	AA	A	605	15/15	0.99	0.04	18,24,31,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AA	B	603	15/15	1.00	0.03	23,27,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.