wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 11:58 PM EDT

PDB ID	:	3AMO
Title	:	Time-resolved X-ray Crystal Structure Analysis of Enzymatic Reaction of Copper Amine Oxidase from Arthrobacter globiformis
Authors	:	Kataoka, M.; Oya, H.; Tominaga, A.; Otsu, M.; Okajima, T.; Tanizawa, K.; Yamaguchi, H.
Deposited on	:	2010-08-20
Resolution	:	2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

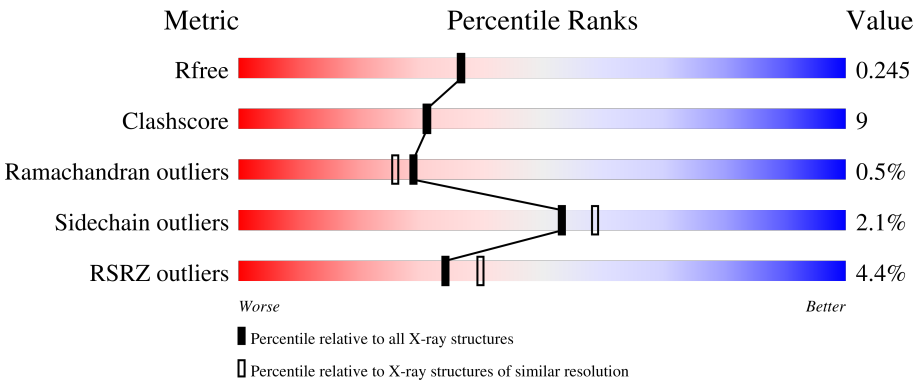
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	638	5% 82% 13% • •
2	B	638	4% 79% 15% • •

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
2	2TY	B	382	X	-	-	-
5	GOL	A	639	-	-	X	-
5	GOL	A	682	-	-	-	X
5	GOL	B	653	-	-	X	-
5	GOL	B	666	-	-	X	-
5	GOL	B	669	-	-	X	-
5	GOL	B	679	-	-	-	X
5	GOL	B	684	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11161 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 Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	619	4916	3105	868	934	9	0	5	0

- Molecule 2 is a protein called Phenylethylamine oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4915	3104	865	936	10	0	5	0

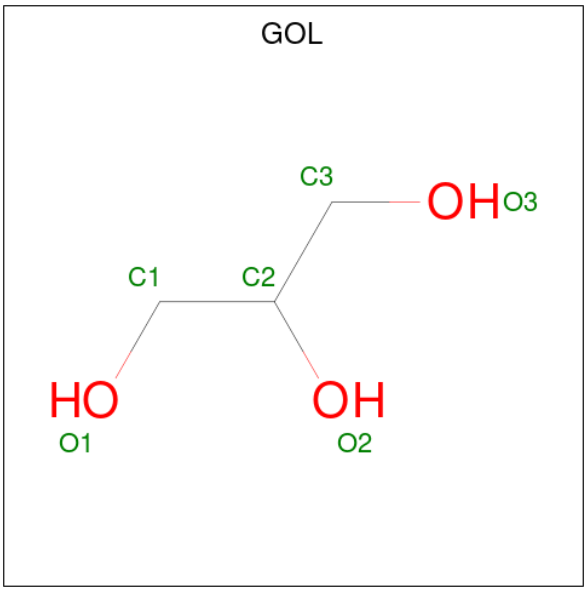
- Molecule 3 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	1	1	1	0	0
4	B	1	1	1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

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

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

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

- Molecule 6 is water.

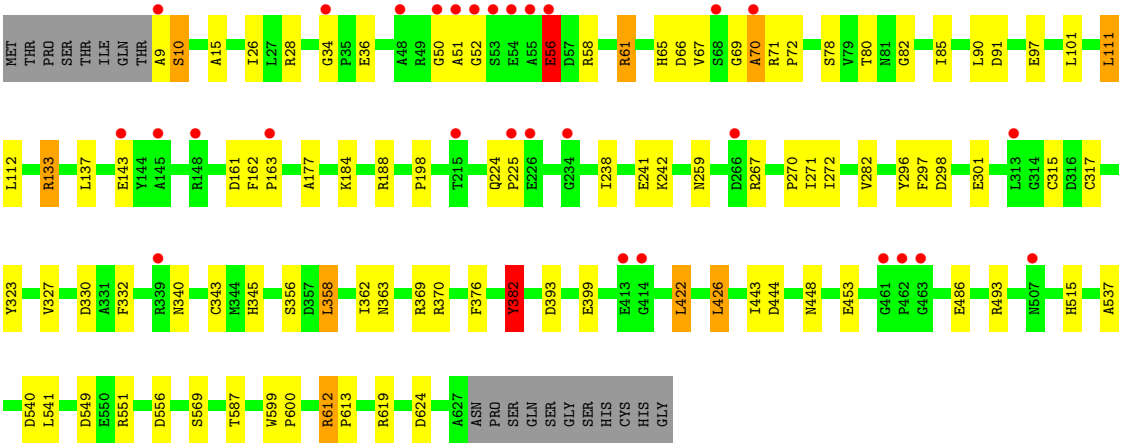
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	356	356	356	0	0
			Total	O		
6	B	388	388	388	0	0

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.

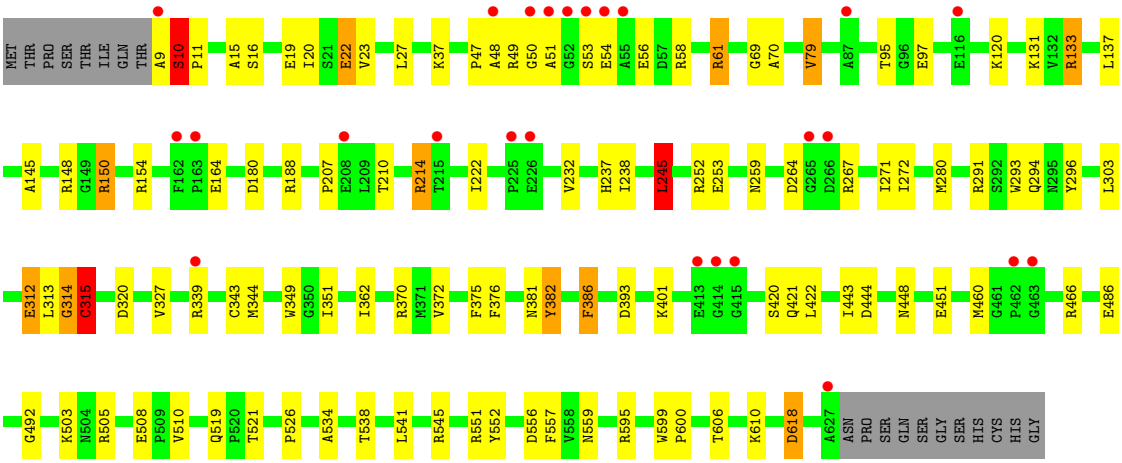
- Molecule 1: Phenylethylamine oxidase

Chain A:



- Molecule 2: Phenylethylamine oxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	190.87Å 63.63Å 157.56Å 90.00° 116.82° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 25.49 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.7 (50.00-2.10) 92.8 (25.49-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	5.73 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189 , 0.245 0.189 , 0.245	Depositor DCC
R_{free} test set	4577 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11161	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9833e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, 1TY, 2TY, NA, CU

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	1.00	2/5016 (0.0%)	0.92	7/6828 (0.1%)
2	B	1.07	9/5014 (0.2%)	0.98	20/6824 (0.3%)
All	All	1.04	11/10030 (0.1%)	0.95	27/13652 (0.2%)

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	0	2
2	B	1	4
All	All	1	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	CYS	CB-SG	-10.04	1.65	1.82
2	B	22	GLU	CG-CD	7.26	1.62	1.51
2	B	343	CYS	CB-SG	-7.23	1.70	1.82
2	B	315	CYS	CB-SG	-6.86	1.70	1.82
2	B	534	ALA	CA-CB	6.42	1.66	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	595	ARG	NE-CZ-NH2	-11.39	114.61	120.30
2	B	595	ARG	NE-CZ-NH1	10.70	125.65	120.30
2	B	133	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	358	LEU	CA-CB-CG	7.89	133.45	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	NE-CZ-NH2	-7.67	116.47	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	382	2TY	CA

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	1TY	Mainchain
1	A	56	GLU	Peptide
2	B	381	ASN	Peptide
2	B	382	2TY	Mainchain
2	B	9	ALA	Peptide

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	4916	0	4735	89	0
2	B	4915	0	4726	88	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	288	0	383	38	0
5	B	294	0	392	45	0
6	A	356	0	0	9	0
6	B	388	0	0	17	0
All	All	11161	0	10236	189	0

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

The worst 5 of 189 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:ARG:NH2	5:B:684:GOL:H32	1.63	1.12
1:A:619:ARG:HH11	5:A:652:GOL:H11	1.12	1.08
2:B:551:ARG:HH21	5:B:684:GOL:H32	1.02	1.06
1:A:612[A]:ARG:HH11	1:A:612[A]:ARG:HG2	0.87	1.02
5:B:640:GOL:H11	6:B:880:HOH:O	1.60	1.02

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	621/638 (97%)	589 (95%)	29 (5%)	3 (0%)	29	26
2	B	621/638 (97%)	593 (96%)	25 (4%)	3 (0%)	29	26
All	All	1242/1276 (97%)	1182 (95%)	54 (4%)	6 (0%)	29	26

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	GLU
1	A	51	ALA
1	A	70	ALA
1	A	10	SER
2	B	10	SER

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	517/529 (98%)	504 (98%)	13 (2%)	47	52
2	B	517/529 (98%)	507 (98%)	10 (2%)	57	63
All	All	1034/1058 (98%)	1011 (98%)	23 (2%)	53	57

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	79	VAL
2	B	339	ARG
2	B	245	LEU
2	B	376	PHE
1	A	358	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	126	ASN
2	B	334	ASN
2	B	573	GLN
2	B	519	GLN
2	B	559	ASN

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	$\#\|Z\| > 2$
2	2TY	B	382	2	21,23,24	2.52	5 (23%)	23,30,32	1.41	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	1TY	A	382	1	21,23,24	1.29	3 (14%)	20,30,32	1.39	5 (25%)

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	2TY	B	382	2	1/1/1/3	2/11/12/14	0/2/2/2
1	1TY	A	382	1	-	2/11/28/30	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	382	2TY	CZ-CE2	6.62	1.50	1.40
2	B	382	2TY	O-C	5.07	1.39	1.20
2	B	382	2TY	CD1-CG	4.69	1.46	1.40
2	B	382	2TY	C1-NX1	3.62	1.34	1.26
2	B	382	2TY	CE2-NX1	-3.17	1.37	1.42

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	382	2TY	CB-CG-CD1	-4.04	116.46	121.05
1	A	382	1TY	CZ-CE1-CD1	3.01	123.56	120.30
2	B	382	2TY	CE2-NX1-C1	-2.73	113.12	119.79
1	A	382	1TY	CE1-CZ-CE2	-2.73	118.63	122.00
1	A	382	1TY	CD2-CG-CD1	2.70	120.58	118.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	382	2TY	CA

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382	1TY	NX1-C1-C2-C1'
2	B	382	2TY	CD2-CE2-NX1-C1
2	B	382	2TY	CZ-CE2-NX1-C1
1	A	382	1TY	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382	1TY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 101 ligands modelled in this entry, 4 are monoatomic - leaving 97 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	$\#\|Z\| > 2$
5	GOL	A	668	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	B	656	-	5,5,5	0.42	0	5,5,5	0.23	0
5	GOL	A	641	-	5,5,5	0.34	0	5,5,5	0.52	0
5	GOL	A	667	-	5,5,5	0.40	0	5,5,5	0.37	0
5	GOL	A	680	-	5,5,5	0.50	0	5,5,5	0.71	0
5	GOL	B	661	-	5,5,5	0.33	0	5,5,5	0.34	0
5	GOL	B	679	-	5,5,5	0.44	0	5,5,5	0.43	0
5	GOL	B	677	-	5,5,5	0.34	0	5,5,5	0.54	0
5	GOL	B	683	-	5,5,5	0.31	0	5,5,5	0.34	0
5	GOL	B	687	-	5,5,5	0.50	0	5,5,5	0.49	0
5	GOL	B	666	-	5,5,5	0.42	0	5,5,5	1.08	1 (20%)
5	GOL	B	672	-	5,5,5	0.37	0	5,5,5	0.51	0
5	GOL	A	682	-	5,5,5	0.42	0	5,5,5	0.90	0
5	GOL	B	669	-	5,5,5	0.44	0	5,5,5	0.40	0
5	GOL	B	685	-	5,5,5	0.31	0	5,5,5	0.28	0
5	GOL	A	675	-	5,5,5	0.43	0	5,5,5	0.68	0
5	GOL	A	639	-	5,5,5	0.56	0	5,5,5	1.40	1 (20%)
5	GOL	A	658	-	5,5,5	0.37	0	5,5,5	0.80	0
5	GOL	A	683	-	5,5,5	0.25	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	B	657	-	5,5,5	0.54	0	5,5,5	1.34	1 (20%)
5	GOL	B	681	-	5,5,5	0.53	0	5,5,5	1.05	0
5	GOL	B	639	-	5,5,5	0.33	0	5,5,5	0.91	0
5	GOL	B	658	-	5,5,5	0.49	0	5,5,5	0.58	0
5	GOL	A	659	-	5,5,5	0.35	0	5,5,5	1.03	0
5	GOL	A	669	-	5,5,5	0.47	0	5,5,5	1.14	1 (20%)
5	GOL	B	663	-	5,5,5	0.42	0	5,5,5	0.68	0
5	GOL	B	667	-	5,5,5	0.57	0	5,5,5	0.57	0
5	GOL	B	682	-	5,5,5	0.59	0	5,5,5	1.19	0
5	GOL	B	671	-	5,5,5	0.40	0	5,5,5	0.23	0
5	GOL	B	678	-	5,5,5	0.45	0	5,5,5	0.26	0
5	GOL	B	652	-	5,5,5	0.28	0	5,5,5	1.09	1 (20%)
5	GOL	B	670	-	5,5,5	0.45	0	5,5,5	0.51	0
5	GOL	B	675	-	5,5,5	0.40	0	5,5,5	0.39	0
5	GOL	B	648	-	5,5,5	0.49	0	5,5,5	0.78	0
5	GOL	A	664	-	5,5,5	0.57	0	5,5,5	0.46	0
5	GOL	B	647	-	5,5,5	0.38	0	5,5,5	0.23	0
5	GOL	A	676	-	5,5,5	0.43	0	5,5,5	0.44	0
5	GOL	B	673	-	5,5,5	0.31	0	5,5,5	0.61	0
5	GOL	A	679	-	5,5,5	0.30	0	5,5,5	0.49	0
5	GOL	A	640	-	5,5,5	0.86	0	5,5,5	1.38	0
5	GOL	B	686	-	5,5,5	0.40	0	5,5,5	0.34	0
5	GOL	A	650	-	5,5,5	0.63	0	5,5,5	0.66	0
5	GOL	A	666	-	5,5,5	0.53	0	5,5,5	0.42	0
5	GOL	A	677	-	5,5,5	0.41	0	5,5,5	0.68	0
5	GOL	A	655	-	5,5,5	0.51	0	5,5,5	1.21	0
5	GOL	A	654	-	5,5,5	0.87	0	5,5,5	1.21	0
5	GOL	A	665	-	5,5,5	0.28	0	5,5,5	0.42	0
5	GOL	A	684	-	5,5,5	0.45	0	5,5,5	0.43	0
5	GOL	A	647	-	5,5,5	0.30	0	5,5,5	0.64	0
5	GOL	A	645	-	5,5,5	0.64	0	5,5,5	1.22	1 (20%)
5	GOL	B	654	-	5,5,5	0.57	0	5,5,5	0.84	0
5	GOL	A	651	-	5,5,5	0.60	0	5,5,5	0.89	0
5	GOL	A	681	-	5,5,5	0.50	0	5,5,5	0.41	0
5	GOL	A	685	-	5,5,5	0.40	0	5,5,5	0.60	0
5	GOL	B	641	-	5,5,5	0.97	0	5,5,5	1.43	1 (20%)
5	GOL	A	674	-	5,5,5	0.42	0	5,5,5	0.56	0
5	GOL	B	646	-	5,5,5	0.33	0	5,5,5	1.20	1 (20%)
5	GOL	B	664	-	5,5,5	0.49	0	5,5,5	0.65	0
5	GOL	A	663	-	5,5,5	0.43	0	5,5,5	0.72	0
5	GOL	B	645	-	5,5,5	0.69	0	5,5,5	1.62	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	GOL	A	671	-	5,5,5	0.42	0	5,5,5	0.23	0
5	GOL	B	653	-	5,5,5	0.30	0	5,5,5	0.91	0
5	GOL	B	676	-	5,5,5	0.42	0	5,5,5	0.74	0
5	GOL	B	655	-	5,5,5	0.66	0	5,5,5	0.82	0
5	GOL	A	670	-	5,5,5	0.33	0	5,5,5	0.66	0
5	GOL	B	659	-	5,5,5	0.41	0	5,5,5	0.61	0
5	GOL	B	644	-	5,5,5	0.40	0	5,5,5	1.00	0
5	GOL	A	657	-	5,5,5	0.43	0	5,5,5	0.63	0
5	GOL	A	646	-	5,5,5	0.54	0	5,5,5	0.36	0
5	GOL	A	649	-	5,5,5	0.58	0	5,5,5	0.94	0
5	GOL	A	660	-	5,5,5	0.56	0	5,5,5	0.95	0
5	GOL	B	674	-	5,5,5	0.53	0	5,5,5	0.27	0
5	GOL	B	642	-	5,5,5	0.65	0	5,5,5	0.87	0
5	GOL	A	643	-	5,5,5	0.37	0	5,5,5	0.78	0
5	GOL	A	656	-	5,5,5	0.49	0	5,5,5	1.32	1 (20%)
5	GOL	A	648	-	5,5,5	0.33	0	5,5,5	0.43	0
5	GOL	B	662	-	5,5,5	0.45	0	5,5,5	0.50	0
5	GOL	B	684	-	5,5,5	0.48	0	5,5,5	0.55	0
5	GOL	B	649	-	5,5,5	0.68	0	5,5,5	0.31	0
5	GOL	A	661	-	5,5,5	0.46	0	5,5,5	0.29	0
5	GOL	B	640	-	5,5,5	0.35	0	5,5,5	1.72	1 (20%)
5	GOL	A	673	-	5,5,5	0.52	0	5,5,5	1.37	1 (20%)
5	GOL	B	680	-	5,5,5	0.36	0	5,5,5	0.17	0
5	GOL	B	660	-	5,5,5	0.56	0	5,5,5	0.93	0
5	GOL	A	678	-	5,5,5	0.29	0	5,5,5	0.73	0
5	GOL	A	662	-	5,5,5	0.25	0	5,5,5	0.98	0
5	GOL	A	672	-	5,5,5	0.43	0	5,5,5	0.49	0
5	GOL	B	643	-	5,5,5	0.70	0	5,5,5	1.19	0
5	GOL	B	665	-	5,5,5	0.42	0	5,5,5	0.17	0
5	GOL	B	668	-	5,5,5	0.36	0	5,5,5	0.28	0
5	GOL	B	651	-	5,5,5	0.28	0	5,5,5	0.35	0
5	GOL	A	642	-	5,5,5	0.60	0	5,5,5	1.71	1 (20%)
5	GOL	B	650	-	5,5,5	0.64	0	5,5,5	0.66	0
5	GOL	A	686	-	5,5,5	0.26	0	5,5,5	0.60	0
5	GOL	A	644	-	5,5,5	0.42	0	5,5,5	0.70	0
5	GOL	A	652	-	5,5,5	0.31	0	5,5,5	0.80	0
5	GOL	A	653	-	5,5,5	0.39	0	5,5,5	0.32	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
5	GOL	A	668	-	-	0/4/4/4	-
5	GOL	B	656	-	-	2/4/4/4	-
5	GOL	A	641	-	-	3/4/4/4	-
5	GOL	A	667	-	-	2/4/4/4	-
5	GOL	A	680	-	-	1/4/4/4	-
5	GOL	B	661	-	-	4/4/4/4	-
5	GOL	B	679	-	-	2/4/4/4	-
5	GOL	B	677	-	-	1/4/4/4	-
5	GOL	B	683	-	-	2/4/4/4	-
5	GOL	B	687	-	-	0/4/4/4	-
5	GOL	B	666	-	-	4/4/4/4	-
5	GOL	B	672	-	-	2/4/4/4	-
5	GOL	A	682	-	-	2/4/4/4	-
5	GOL	B	669	-	-	3/4/4/4	-
5	GOL	B	685	-	-	0/4/4/4	-
5	GOL	A	675	-	-	0/4/4/4	-
5	GOL	A	639	-	-	2/4/4/4	-
5	GOL	A	658	-	-	2/4/4/4	-
5	GOL	A	683	-	-	1/4/4/4	-
5	GOL	B	657	-	-	2/4/4/4	-
5	GOL	B	681	-	-	3/4/4/4	-
5	GOL	B	639	-	-	2/4/4/4	-
5	GOL	B	658	-	-	0/4/4/4	-
5	GOL	A	659	-	-	1/4/4/4	-
5	GOL	A	669	-	-	3/4/4/4	-
5	GOL	B	663	-	-	2/4/4/4	-
5	GOL	B	667	-	-	1/4/4/4	-
5	GOL	B	682	-	-	2/4/4/4	-
5	GOL	B	671	-	-	0/4/4/4	-
5	GOL	B	678	-	-	2/4/4/4	-
5	GOL	B	652	-	-	4/4/4/4	-
5	GOL	B	670	-	-	0/4/4/4	-
5	GOL	B	675	-	-	2/4/4/4	-
5	GOL	B	648	-	-	2/4/4/4	-
5	GOL	A	664	-	-	0/4/4/4	-
5	GOL	B	647	-	-	0/4/4/4	-
5	GOL	A	676	-	-	4/4/4/4	-
5	GOL	B	673	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	679	-	-	2/4/4/4	-
5	GOL	A	640	-	-	3/4/4/4	-
5	GOL	B	686	-	-	4/4/4/4	-
5	GOL	A	650	-	-	0/4/4/4	-
5	GOL	A	666	-	-	2/4/4/4	-
5	GOL	A	677	-	-	2/4/4/4	-
5	GOL	A	655	-	-	4/4/4/4	-
5	GOL	A	654	-	-	4/4/4/4	-
5	GOL	A	665	-	-	2/4/4/4	-
5	GOL	A	684	-	-	3/4/4/4	-
5	GOL	A	647	-	-	4/4/4/4	-
5	GOL	A	645	-	-	3/4/4/4	-
5	GOL	B	654	-	-	4/4/4/4	-
5	GOL	A	651	-	-	4/4/4/4	-
5	GOL	A	681	-	-	1/4/4/4	-
5	GOL	A	685	-	-	0/4/4/4	-
5	GOL	B	641	-	-	2/4/4/4	-
5	GOL	A	674	-	-	3/4/4/4	-
5	GOL	B	646	-	-	2/4/4/4	-
5	GOL	B	664	-	-	1/4/4/4	-
5	GOL	A	663	-	-	2/4/4/4	-
5	GOL	B	645	-	-	2/4/4/4	-
5	GOL	A	671	-	-	2/4/4/4	-
5	GOL	B	653	-	-	4/4/4/4	-
5	GOL	B	676	-	-	0/4/4/4	-
5	GOL	B	655	-	-	2/4/4/4	-
5	GOL	A	670	-	-	2/4/4/4	-
5	GOL	B	659	-	-	2/4/4/4	-
5	GOL	B	644	-	-	2/4/4/4	-
5	GOL	A	657	-	-	2/4/4/4	-
5	GOL	A	646	-	-	0/4/4/4	-
5	GOL	A	649	-	-	2/4/4/4	-
5	GOL	A	660	-	-	4/4/4/4	-
5	GOL	B	674	-	-	4/4/4/4	-
5	GOL	B	642	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	643	-	-	2/4/4/4	-
5	GOL	A	656	-	-	4/4/4/4	-
5	GOL	A	648	-	-	2/4/4/4	-
5	GOL	B	662	-	-	0/4/4/4	-
5	GOL	B	684	-	-	4/4/4/4	-
5	GOL	B	649	-	-	2/4/4/4	-
5	GOL	A	661	-	-	2/4/4/4	-
5	GOL	B	640	-	-	4/4/4/4	-
5	GOL	A	673	-	-	2/4/4/4	-
5	GOL	B	680	-	-	1/4/4/4	-
5	GOL	B	660	-	-	2/4/4/4	-
5	GOL	A	678	-	-	4/4/4/4	-
5	GOL	A	662	-	-	2/4/4/4	-
5	GOL	A	672	-	-	0/4/4/4	-
5	GOL	B	643	-	-	2/4/4/4	-
5	GOL	B	665	-	-	4/4/4/4	-
5	GOL	B	668	-	-	0/4/4/4	-
5	GOL	B	651	-	-	2/4/4/4	-
5	GOL	A	642	-	-	1/4/4/4	-
5	GOL	B	650	-	-	2/4/4/4	-
5	GOL	A	686	-	-	4/4/4/4	-
5	GOL	A	644	-	-	2/4/4/4	-
5	GOL	A	652	-	-	2/4/4/4	-
5	GOL	A	653	-	-	4/4/4/4	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	642	GOL	C3-C2-C1	-3.68	98.32	111.80
5	B	640	GOL	C3-C2-C1	-3.63	98.48	111.80
5	B	641	GOL	O2-C2-C3	2.87	121.06	109.18
5	A	639	GOL	O1-C1-C2	-2.59	98.72	110.38
5	B	645	GOL	C3-C2-C1	-2.44	102.83	111.80

There are no chirality outliers.

5 of 204 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	639	GOL	O1-C1-C2-C3
5	A	640	GOL	C1-C2-C3-O3
5	A	641	GOL	O1-C1-C2-C3
5	A	643	GOL	O1-C1-C2-C3
5	A	645	GOL	O1-C1-C2-O2

There are no ring outliers.

48 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	661	GOL	1	0
5	B	679	GOL	1	0
5	B	666	GOL	5	0
5	B	672	GOL	1	0
5	B	669	GOL	4	0
5	B	685	GOL	1	0
5	A	639	GOL	6	0
5	A	658	GOL	1	0
5	B	657	GOL	3	0
5	B	639	GOL	1	0
5	B	658	GOL	2	0
5	A	659	GOL	1	0
5	B	682	GOL	1	0
5	B	671	GOL	3	0
5	B	678	GOL	2	0
5	A	664	GOL	1	0
5	A	676	GOL	1	0
5	A	679	GOL	1	0
5	A	677	GOL	1	0
5	A	655	GOL	1	0
5	A	684	GOL	1	0
5	B	654	GOL	1	0
5	A	651	GOL	1	0
5	A	681	GOL	1	0
5	A	674	GOL	2	0
5	B	664	GOL	1	0
5	B	645	GOL	1	0
5	B	653	GOL	4	0
5	A	670	GOL	1	0
5	B	659	GOL	1	0
5	B	644	GOL	3	0
5	A	646	GOL	1	0
5	A	649	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	660	GOL	2	0
5	A	643	GOL	2	0
5	A	656	GOL	3	0
5	A	648	GOL	1	0
5	B	662	GOL	1	0
5	B	684	GOL	4	0
5	B	640	GOL	2	0
5	A	673	GOL	1	0
5	B	660	GOL	1	0
5	A	662	GOL	2	0
5	B	643	GOL	3	0
5	B	668	GOL	1	0
5	A	642	GOL	3	0
5	A	686	GOL	2	0
5	A	652	GOL	3	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	618/638 (96%)	-0.01	29 (4%)	31	37	14, 26, 43, 74	1 (0%)
2	B	618/638 (96%)	-0.15	25 (4%)	38	44	11, 23, 38, 72	2 (0%)
All	All	1236/1276 (96%)	-0.08	54 (4%)	34	40	11, 24, 41, 74	3 (0%)

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	ALA	9.9
2	B	52	GLY	9.8
2	B	55	ALA	9.7
2	B	53	SER	9.1
1	A	52	GLY	8.6

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	1TY	A	382	22/23	0.94	0.13	21,30,41,43	0
2	2TY	B	382	22/23	0.95	0.12	17,27,36,38	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, 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
5	GOL	A	682	6/6	0.22	0.47	86,88,89,89	0
5	GOL	B	677	6/6	0.52	0.27	70,71,72,72	0
5	GOL	A	671	6/6	0.63	0.31	68,72,73,73	0
5	GOL	A	666	6/6	0.64	0.27	68,71,72,72	0
5	GOL	A	668	6/6	0.67	0.34	74,76,77,77	0
5	GOL	B	665	6/6	0.69	0.23	61,65,66,66	0
5	GOL	B	656	6/6	0.69	0.29	74,75,75,75	0
5	GOL	B	643	6/6	0.70	0.23	43,55,56,57	0
5	GOL	B	679	6/6	0.73	0.48	67,70,71,71	0
5	GOL	A	660	6/6	0.74	0.22	55,59,61,61	0
5	GOL	A	667	6/6	0.74	0.27	59,60,61,61	0
5	GOL	B	687	6/6	0.74	0.38	45,56,61,62	0
5	GOL	A	663	6/6	0.76	0.34	55,61,63,63	0
5	GOL	A	654	6/6	0.77	0.28	33,44,45,50	0
5	GOL	A	677	6/6	0.77	0.23	60,62,64,66	0
5	GOL	A	670	6/6	0.77	0.24	58,63,64,65	0
5	GOL	A	665	6/6	0.78	0.22	54,56,57,60	0
5	GOL	A	679	6/6	0.78	0.29	63,64,65,66	0
5	GOL	B	683	6/6	0.78	0.35	72,74,75,76	0
5	GOL	A	673	6/6	0.78	0.19	45,47,51,54	0
5	GOL	B	658	6/6	0.79	0.19	50,54,56,56	0
5	GOL	B	663	6/6	0.79	0.28	56,58,58,59	0
5	GOL	A	653	6/6	0.79	0.30	60,63,65,67	0
5	GOL	B	674	6/6	0.79	0.20	62,63,63,63	0
5	GOL	A	680	6/6	0.80	0.15	47,52,53,56	0
5	GOL	A	684	6/6	0.81	0.31	61,63,64,64	0
5	GOL	B	678	6/6	0.81	0.28	60,62,64,64	0
5	GOL	A	672	6/6	0.81	0.25	55,61,64,67	0
5	GOL	B	647	6/6	0.81	0.17	68,69,70,70	0
5	GOL	B	685	6/6	0.81	0.33	56,58,58,60	0
5	GOL	A	676	6/6	0.81	0.30	60,63,63,64	0
5	GOL	B	676	6/6	0.82	0.33	55,58,59,60	0
5	GOL	B	668	6/6	0.82	0.23	61,66,66,67	0
5	GOL	B	680	6/6	0.82	0.23	63,64,64,65	0
5	GOL	B	657	6/6	0.83	0.19	39,41,42,45	0
5	GOL	B	686	6/6	0.83	0.24	57,62,62,63	0
5	GOL	B	662	6/6	0.83	0.17	65,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	672	6/6	0.84	0.19	43,50,52,54	0
5	GOL	A	678	6/6	0.84	0.24	49,53,54,58	0
5	GOL	B	675	6/6	0.84	0.18	62,63,65,65	0
5	GOL	A	669	6/6	0.84	0.15	42,47,48,48	0
5	GOL	A	683	6/6	0.84	0.23	47,51,52,52	0
5	GOL	B	660	6/6	0.84	0.14	32,38,42,45	0
5	GOL	A	686	6/6	0.85	0.17	55,57,58,59	0
5	GOL	A	647	6/6	0.85	0.25	54,57,58,59	0
5	GOL	A	661	6/6	0.85	0.23	58,62,63,63	0
5	GOL	B	655	6/6	0.85	0.22	42,45,47,47	0
5	GOL	B	646	6/6	0.86	0.16	33,43,45,50	0
5	GOL	A	657	6/6	0.86	0.17	36,41,43,48	0
5	GOL	B	649	6/6	0.86	0.19	40,49,50,51	0
5	GOL	A	658	6/6	0.86	0.20	46,50,51,51	0
5	GOL	A	685	6/6	0.87	0.23	58,59,60,61	0
5	GOL	B	681	6/6	0.87	0.34	46,53,54,58	0
5	GOL	B	667	6/6	0.87	0.19	36,46,47,48	0
5	GOL	A	651	6/6	0.88	0.16	39,41,43,44	0
5	GOL	B	670	6/6	0.88	0.26	58,60,60,60	0
5	GOL	B	684	6/6	0.88	0.18	65,66,67,67	0
5	GOL	B	661	6/6	0.88	0.17	46,47,48,51	0
5	GOL	B	666	6/6	0.88	0.22	43,50,50,53	0
5	GOL	A	655	6/6	0.88	0.16	46,48,49,52	0
5	GOL	A	664	6/6	0.89	0.17	37,46,48,51	0
5	GOL	B	645	6/6	0.90	0.20	33,37,40,46	0
5	GOL	B	664	6/6	0.90	0.18	43,48,49,49	0
5	GOL	A	639	6/6	0.90	0.15	34,39,41,44	0
5	GOL	A	681	6/6	0.90	0.26	44,49,51,52	0
5	GOL	A	640	6/6	0.90	0.15	34,38,40,43	0
5	GOL	B	653	6/6	0.90	0.15	31,36,39,39	0
5	GOL	A	644	6/6	0.90	0.22	40,45,46,50	0
5	GOL	A	643	6/6	0.91	0.15	46,49,50,51	0
5	GOL	B	639	6/6	0.91	0.16	28,38,40,44	0
5	GOL	B	671	6/6	0.91	0.30	54,56,58,58	0
5	GOL	A	648	6/6	0.91	0.15	49,51,53,54	0
5	GOL	B	673	6/6	0.91	0.12	52,53,54,54	0
5	GOL	B	644	6/6	0.91	0.29	34,42,44,48	0
5	GOL	A	659	6/6	0.91	0.13	32,39,40,42	0
5	GOL	A	645	6/6	0.91	0.20	36,41,44,46	0
5	GOL	A	675	6/6	0.91	0.29	61,62,63,65	0
5	GOL	B	640	6/6	0.92	0.18	23,34,36,38	0
5	GOL	A	650	6/6	0.92	0.14	38,40,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	654	6/6	0.92	0.14	39,44,46,47	0
5	GOL	A	652	6/6	0.92	0.21	34,40,43,43	0
5	GOL	B	682	6/6	0.92	0.26	43,46,48,50	0
5	GOL	B	648	6/6	0.93	0.19	38,44,45,45	0
5	GOL	A	649	6/6	0.93	0.14	41,46,48,49	0
5	GOL	A	662	6/6	0.93	0.21	52,54,55,56	0
5	GOL	A	656	6/6	0.93	0.13	29,36,40,43	0
5	GOL	A	641	6/6	0.93	0.29	40,51,53,55	0
5	GOL	A	674	6/6	0.94	0.14	38,46,48,49	0
5	GOL	B	651	6/6	0.94	0.09	43,45,46,46	0
5	GOL	B	669	6/6	0.94	0.24	48,50,51,53	0
5	GOL	B	652	6/6	0.94	0.14	40,40,41,43	0
5	GOL	B	641	6/6	0.94	0.12	27,29,30,30	0
5	GOL	B	659	6/6	0.94	0.16	36,37,40,45	0
5	GOL	B	642	6/6	0.94	0.14	29,36,38,38	0
5	GOL	A	642	6/6	0.95	0.20	26,33,37,39	0
5	GOL	A	646	6/6	0.95	0.18	21,31,34,36	0
5	GOL	B	650	6/6	0.98	0.12	29,31,32,34	0
4	NA	B	703	1/1	0.99	0.09	11,11,11,11	0
4	NA	A	703	1/1	0.99	0.17	15,15,15,15	0
3	CU	B	701	1/1	1.00	0.06	20,20,20,20	0
3	CU	A	701	1/1	1.00	0.06	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.