



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:28 am BST

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 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 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 : 2.11
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) : 2.11

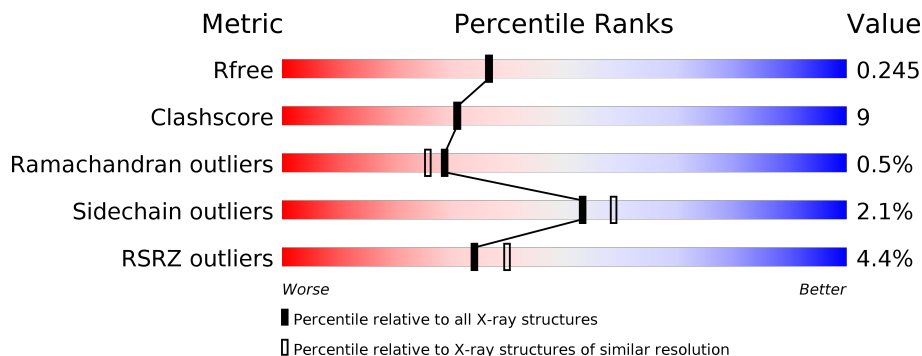
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 on 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	638	 5% (poor fit), 82% (0-1 outliers), 13% (2-3 outliers), ... (not modelled)
2	B	638	 4% (poor fit), 79% (0-1 outliers), 16% (2-3 outliers), ... (not modelled)

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
3	B	1	Total	Cu	0	0
			1	1		
3	A	1	Total	Cu	0	0
			1	1		

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

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

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

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

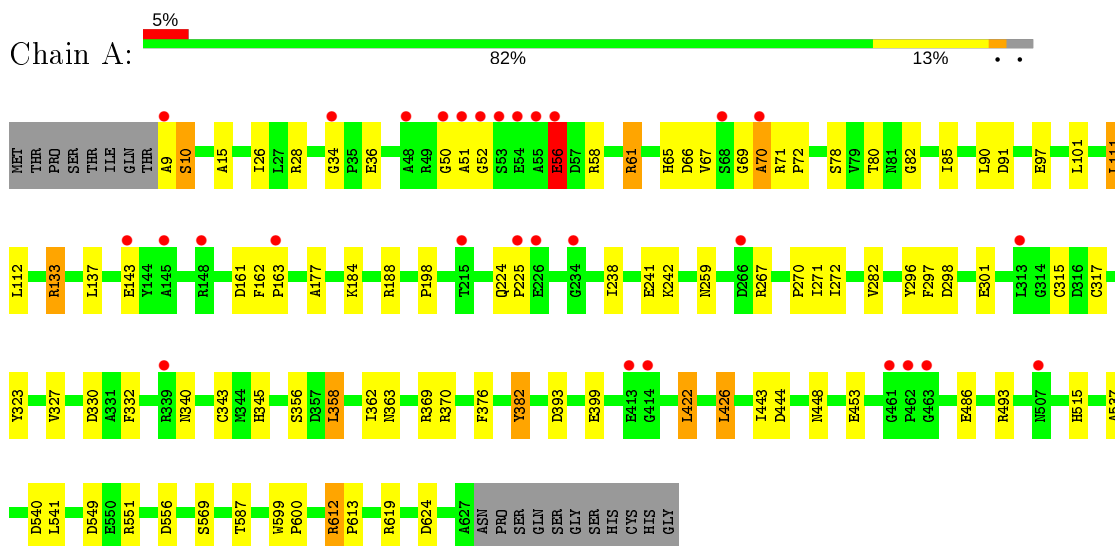
- Molecule 6 is water.

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

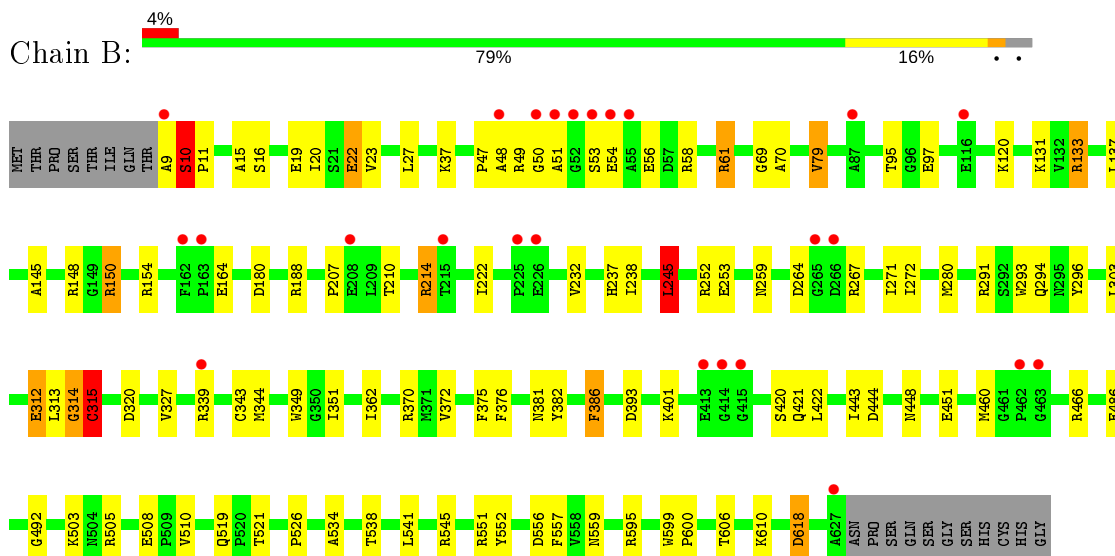
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



- Molecule 2: Phenylethylamine oxidase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	5.73 (at 2.10Å)	Xtrriage
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	Xtrriage
Anisotropy	0.027	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GOL, 1TY, 2TY, CU, NA

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

All (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
2	B	312	GLU	CG-CD	5.75	1.60	1.51
1	A	315	CYS	CB-SG	-5.25	1.73	1.81
2	B	164	GLU	CG-CD	5.24	1.59	1.51
2	B	253	GLU	CB-CG	5.19	1.62	1.52
2	B	552	TYR	CZ-OH	-5.12	1.29	1.37
2	B	510	VAL	CB-CG2	5.09	1.63	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	133	ARG	NE-CZ-NH2	-7.67	116.47	120.30
2	B	545	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	393	ASP	CB-CG-OD1	7.02	124.62	118.30
2	B	370	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	A	358	LEU	CB-CG-CD1	6.87	122.69	111.00
2	B	245	LEU	CB-CG-CD1	6.48	122.01	111.00
2	B	245	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	91	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	541	LEU	CA-CB-CG	-6.01	101.49	115.30
2	B	150	ARG	NE-CZ-NH1	5.96	123.28	120.30
2	B	541	LEU	CA-CB-CG	-5.89	101.75	115.30
2	B	133	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	B	214	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	B	618	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	B	393	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	595	ARG	CG-CD-NE	-5.53	100.18	111.80
2	B	545	ARG	NE-CZ-NH1	5.42	123.01	120.30
2	B	314	GLY	N-CA-C	-5.32	99.80	113.10
1	A	61	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	B	10	SER	N-CA-CB	-5.13	102.81	110.50
2	B	61	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	B	618	ASP	CB-CG-OD1	5.07	122.86	118.30
2	B	150	ARG	NE-CZ-NH2	-5.03	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	382	2TY	CA

All (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,Peptide
2	B	9	ALA	Peptide

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	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.

All (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
1:A:612[A]:ARG:HG2	1:A:612[A]:ARG:NH1	1.70	0.98
1:A:612[A]:ARG:CG	1:A:612[A]:ARG:HH11	1.76	0.97
2:B:443:ILE:H	2:B:448:ASN:HD21	1.13	0.94
1:A:619:ARG:NH1	5:A:652:GOL:H11	1.85	0.91
2:B:351:ILE:O	5:B:682:GOL:H12	1.73	0.89
1:A:56:GLU:HB2	6:A:913:HOH:O	1.74	0.86
1:A:540:ASP:OD2	5:A:649:GOL:H12	1.76	0.85
2:B:37:LYS:HE3	6:B:813:HOH:O	1.75	0.85
2:B:401:LYS:HD3	5:B:666:GOL:H11	1.60	0.81
1:A:66:ASP:OD2	1:A:70:ALA:HB3	1.79	0.81
1:A:298:ASP:OD1	1:A:382:1TY:H11	1.80	0.81
1:A:612[B]:ARG:HB2	1:A:613:PRO:HD2	1.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:551:ARG:HH21	5:B:684:GOL:C3	1.92	0.79
5:B:654:GOL:H11	5:B:684:GOL:H31	1.65	0.78
1:A:282:VAL:HG21	6:A:744:HOH:O	1.84	0.78
1:A:569:SER:OG	5:A:677:GOL:H11	1.82	0.78
1:A:327:VAL:O	5:A:642:GOL:H12	1.84	0.77
5:B:659:GOL:O3	5:B:666:GOL:H31	1.87	0.74
1:A:28[A]:ARG:NH2	6:A:997:HOH:O	2.15	0.74
1:A:72:PRO:HG2	1:A:90:LEU:HB2	1.70	0.74
1:A:370:ARG:HH12	5:A:639:GOL:H32	1.51	0.73
2:B:238:ILE:HB	2:B:245:LEU:HD13	1.70	0.73
2:B:618:ASP:HB2	5:B:653:GOL:H32	1.69	0.73
1:A:399:GLU:OE2	5:A:639:GOL:H31	1.88	0.72
2:B:618:ASP:H	5:B:653:GOL:C3	2.01	0.72
1:A:443:ILE:H	1:A:448:ASN:HD21	1.36	0.72
2:B:443:ILE:H	2:B:448:ASN:ND2	1.87	0.72
2:B:420:SER:HA	5:B:658:GOL:H32	1.73	0.71
1:A:28[B]:ARG:NH2	6:A:1001:HOH:O	2.02	0.70
2:B:505:ARG:HB2	5:B:662:GOL:H31	1.74	0.70
2:B:349:TRP:HE1	5:B:669:GOL:H11	1.57	0.69
2:B:443:ILE:N	2:B:448:ASN:HD21	1.89	0.69
2:B:97:GLU:OE1	6:B:970:HOH:O	2.11	0.68
2:B:207:PRO:HA	2:B:210:THR:OG1	1.95	0.67
2:B:606:THR:O	5:B:672:GOL:H2	1.95	0.67
1:A:137:LEU:HD22	1:A:296:TYR:CZ	2.31	0.65
5:A:660:GOL:H32	2:B:312:GLU:OE1	1.95	0.65
2:B:421:GLN:H	5:B:658:GOL:H2	1.61	0.64
1:A:15:ALA:HB3	5:A:642:GOL:H11	1.80	0.64
2:B:599:TRP:CD2	2:B:600:PRO:HA	2.33	0.64
1:A:619:ARG:HH11	5:A:652:GOL:C1	2.01	0.63
2:B:22:GLU:OE2	6:B:982:HOH:O	2.15	0.63
2:B:264:ASP:OD1	5:B:653:GOL:H2	2.01	0.61
1:A:317:CYS:HA	5:A:674:GOL:H12	1.81	0.61
2:B:48:ALA:O	2:B:51:ALA:HB3	2.00	0.61
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.35	0.61
1:A:82:GLY:O	5:A:676:GOL:H31	2.01	0.60
2:B:10:SER:CB	6:B:879:HOH:O	2.50	0.60
2:B:349:TRP:HE1	5:B:669:GOL:C1	2.14	0.60
1:A:71:ARG:O	6:A:1025:HOH:O	2.16	0.60
1:A:612[B]:ARG:NH1	5:A:656:GOL:H11	2.16	0.60
1:A:612[B]:ARG:NH1	5:A:656:GOL:C1	2.65	0.60
2:B:49:ARG:HB3	5:B:685:GOL:H12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:SER:HB2	1:A:85:ILE:HD11	1.85	0.59
1:A:271:ILE:HG22	1:A:272:ILE:HG13	1.83	0.59
2:B:618:ASP:H	5:B:653:GOL:H31	1.68	0.58
1:A:137:LEU:HD22	1:A:296:TYR:OH	2.03	0.58
1:A:241:GLU:O	1:A:242:LYS:HB2	2.04	0.57
2:B:61:ARG:HH22	2:B:556:ASP:CG	2.08	0.57
1:A:34:GLY:HA2	5:A:681:GOL:H11	1.87	0.57
1:A:56:GLU:HG3	1:A:58:ARG:HG2	1.85	0.57
1:A:356:SER:HA	1:A:363:ASN:HD22	1.69	0.57
1:A:612[B]:ARG:HH11	5:A:656:GOL:C1	2.17	0.57
2:B:19:GLU:HG2	2:B:79:VAL:HG11	1.87	0.57
2:B:422:LEU:HD13	2:B:599:TRP:HB2	1.87	0.57
2:B:137:LEU:HD22	2:B:296:TYR:CZ	2.40	0.56
1:A:162:PHE:HB2	1:A:163:PRO:CD	2.36	0.56
1:A:345:HIS:CE1	5:A:674:GOL:H11	2.41	0.56
2:B:148[A]:ARG:N	2:B:148[A]:ARG:HD3	2.21	0.56
2:B:10:SER:CA	6:B:879:HOH:O	2.54	0.55
2:B:291:ARG:O	2:B:294:GLN:HG2	2.06	0.55
5:A:670:GOL:H32	5:B:657:GOL:H32	1.88	0.54
1:A:443:ILE:H	1:A:448:ASN:ND2	2.06	0.54
1:A:9:ALA:O	1:A:10:SER:HB3	2.08	0.54
1:A:370:ARG:NH1	5:A:639:GOL:H32	2.22	0.53
5:B:643:GOL:C1	6:B:928:HOH:O	2.56	0.53
1:A:56:GLU:CG	1:A:58:ARG:HG2	2.38	0.53
5:A:643:GOL:C3	6:A:1022:HOH:O	2.57	0.53
5:B:666:GOL:H12	6:B:920:HOH:O	2.09	0.53
1:A:97:GLU:OE2	5:A:686:GOL:H31	2.09	0.53
2:B:349:TRP:NE1	5:B:669:GOL:H11	2.24	0.53
1:A:267:ARG:NH2	6:A:955:HOH:O	2.42	0.52
1:A:28[B]:ARG:HG3	1:A:28[B]:ARG:HH11	1.74	0.52
5:B:643:GOL:H12	6:B:928:HOH:O	2.10	0.52
2:B:538:THR:HG21	5:B:678:GOL:H11	1.91	0.52
2:B:312:GLU:O	2:B:314:GLY:O	2.26	0.52
1:A:370:ARG:HH22	5:A:639:GOL:H32	1.74	0.52
1:A:356:SER:HB3	1:A:363:ASN:ND2	2.25	0.51
2:B:58:ARG:HD2	5:B:644:GOL:H31	1.92	0.51
5:B:645:GOL:H31	5:B:666:GOL:O3	2.11	0.51
1:A:551:ARG:HG2	5:A:655:GOL:O3	2.11	0.51
1:A:72:PRO:HD3	5:A:686:GOL:H11	1.93	0.51
2:B:47:PRO:HD3	5:B:644:GOL:H2	1.92	0.51
1:A:161:ASP:OD2	5:A:643:GOL:O3	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:666:GOL:C1	6:B:920:HOH:O	2.59	0.50
5:A:660:GOL:H31	2:B:315:CYS:SG	2.52	0.50
1:A:422:LEU:HD13	1:A:599:TRP:HB2	1.93	0.50
1:A:297:PHE:HB2	1:A:301:GLU:HG3	1.94	0.49
1:A:612[A]:ARG:CG	1:A:612[A]:ARG:NH1	2.48	0.49
2:B:10:SER:HB3	6:B:879:HOH:O	2.11	0.49
2:B:259:ASN:ND2	6:B:731:HOH:O	2.11	0.48
2:B:375:PHE:CE2	2:B:386:PHE:HB2	2.48	0.48
5:A:659:GOL:H11	5:A:662:GOL:O3	2.13	0.48
1:A:327:VAL:O	5:A:642:GOL:C1	2.58	0.48
1:A:515:HIS:NE2	1:A:612[A]:ARG:HD3	2.28	0.48
2:B:16:SER:HA	5:B:643:GOL:O2	2.15	0.47
1:A:61:ARG:HH22	1:A:556:ASP:CG	2.18	0.47
1:A:36:GLU:O	1:A:67:VAL:HG22	2.15	0.47
2:B:145:ALA:O	2:B:148[A]:ARG:HG2	2.15	0.47
2:B:267:ARG:NH2	5:B:671:GOL:O2	2.40	0.47
5:A:646:GOL:H32	2:B:362:ILE:HD12	1.96	0.47
2:B:20:ILE:HD12	2:B:327:VAL:HG12	1.97	0.46
1:A:537:ALA:HA	1:A:587:THR:HG21	1.97	0.46
2:B:188:ARG:HD3	6:B:925:HOH:O	2.16	0.46
1:A:551:ARG:NE	5:A:651:GOL:O3	2.48	0.46
2:B:280[A]:MET:HG3	2:B:280[A]:MET:O	2.15	0.46
2:B:610:LYS:NZ	5:B:669:GOL:H32	2.30	0.46
2:B:460:MET:HE2	2:B:466:ARG:C	2.36	0.46
2:B:508:GLU:HB3	5:B:668:GOL:H12	1.98	0.46
2:B:10:SER:HA	2:B:11:PRO:HD2	1.93	0.45
2:B:95:THR:O	2:B:557:PHE:HB2	2.16	0.45
1:A:362:ILE:HD12	6:B:1067:HOH:O	2.15	0.45
1:A:69:GLY:C	1:A:70:ALA:O	2.54	0.45
2:B:451:GLU:OE1	6:B:812:HOH:O	2.21	0.45
1:A:65:HIS:CD2	1:A:101:LEU:HD11	2.52	0.45
1:A:133:ARG:HA	1:A:133:ARG:HD3	1.55	0.45
1:A:50:GLY:O	1:A:52:GLY:N	2.49	0.45
2:B:51:ALA:C	2:B:53:SER:H	2.19	0.45
1:A:515:HIS:CD2	1:A:612[A]:ARG:HD3	2.50	0.45
5:A:648:GOL:H12	6:A:1007:HOH:O	2.16	0.45
2:B:267:ARG:HH12	5:B:671:GOL:H11	1.82	0.45
1:A:515:HIS:HB3	5:A:664:GOL:H11	1.98	0.45
1:A:323:TYR:CD1	1:A:340:ASN:HB3	2.51	0.45
2:B:313:LEU:C	2:B:314:GLY:O	2.54	0.45
2:B:492:GLY:HA2	5:B:660:GOL:H32	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ILE:HD11	1:A:82:GLY:HA2	1.98	0.45
1:A:612[B]:ARG:HB2	1:A:613:PRO:CD	2.40	0.44
1:A:369:ARG:HH21	5:A:658:GOL:H2	1.82	0.44
2:B:486:GLU:HB2	5:B:657:GOL:H11	1.98	0.44
1:A:259:ASN:ND2	5:A:673:GOL:O2	2.46	0.44
1:A:111:LEU:HD21	1:A:184:LYS:HA	2.00	0.44
2:B:526:PRO:HB3	5:B:678:GOL:H12	1.99	0.44
2:B:154:ARG:HD2	2:B:293:TRP:CE3	2.53	0.44
2:B:137:LEU:HD22	2:B:296:TYR:OH	2.18	0.44
2:B:344:MET:HA	2:B:372:VAL:O	2.18	0.44
1:A:9:ALA:O	1:A:10:SER:CB	2.65	0.44
2:B:58:ARG:HA	5:B:644:GOL:H31	1.99	0.44
2:B:401:LYS:HG2	2:B:606:THR:HG22	2.00	0.44
2:B:252:ARG:HB2	2:B:303:LEU:HD22	1.99	0.44
2:B:314:GLY:O	2:B:315:CYS:CB	2.60	0.43
2:B:23:VAL:O	2:B:27:LEU:HG	2.18	0.43
5:A:679:GOL:HO3	5:A:684:GOL:HO2	1.66	0.43
2:B:150:ARG:HD3	2:B:180:ASP:OD2	2.19	0.43
1:A:443:ILE:N	1:A:448:ASN:HD21	2.12	0.43
2:B:148[A]:ARG:CD	2:B:148[A]:ARG:N	2.81	0.43
2:B:15:ALA:HB3	5:B:640:GOL:H12	2.00	0.43
1:A:112:LEU:HD21	1:A:177:ALA:HB1	1.99	0.43
2:B:320:ASP:OD2	5:B:679:GOL:H2	2.18	0.43
2:B:222:ILE:HD13	5:B:664:GOL:H32	2.00	0.43
2:B:521:THR:OG1	5:B:657:GOL:C3	2.67	0.43
2:B:503:LYS:O	5:B:671:GOL:H32	2.19	0.43
1:A:453:GLU:O	1:A:493:ARG:HA	2.19	0.42
2:B:271:ILE:HG22	2:B:272:ILE:HG13	2.01	0.42
1:A:198:PRO:HG2	1:A:426:LEU:HD23	2.01	0.42
1:A:370:ARG:HH12	5:A:639:GOL:C3	2.26	0.42
1:A:56:GLU:CB	6:A:913:HOH:O	2.49	0.42
2:B:133:ARG:HD3	2:B:133:ARG:HA	1.78	0.42
2:B:150:ARG:HA	5:B:639:GOL:H11	2.01	0.42
2:B:50:GLY:O	2:B:54:GLU:HG2	2.20	0.42
2:B:232:VAL:HA	2:B:237:HIS:O	2.20	0.42
1:A:162:PHE:HB2	1:A:163:PRO:HD2	2.02	0.41
1:A:345:HIS:CD2	5:A:662:GOL:O1	2.73	0.41
1:A:399:GLU:OE2	5:A:639:GOL:C3	2.65	0.41
2:B:131:LYS:HA	6:B:776:HOH:O	2.19	0.41
1:A:241:GLU:O	1:A:242:LYS:CB	2.68	0.41
2:B:69:GLY:C	2:B:70:ALA:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28[B]:ARG:NH1	1:A:28[B]:ARG:HG3	2.34	0.41
1:A:330:ASP:OD1	1:A:332:PHE:N	2.48	0.41
1:A:624:ASP:O	2:B:214:ARG:HG3	2.20	0.41
1:A:224:GLN:HA	1:A:225:PRO:HD2	1.95	0.41
2:B:451:GLU:HG3	6:B:812:HOH:O	2.20	0.41
2:B:148[A]:ARG:NH1	5:B:661:GOL:O1	2.54	0.40
1:A:270:PRO:HD2	1:A:444:ASP:HA	2.02	0.40
1:A:549:ASP:N	1:A:549:ASP:OD1	2.51	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	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

All (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
2	B	315	CYS

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

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	80	THR
1	A	111	LEU
1	A	143	GLU
1	A	188	ARG
1	A	238	ILE
1	A	358	LEU
1	A	376	PHE
1	A	422	LEU
1	A	426	LEU
1	A	486	GLU
1	A	612[A]	ARG
1	A	612[B]	ARG
2	B	10	SER
2	B	79	VAL
2	B	120	LYS
2	B	245	LEU
2	B	339	ARG
2	B	376	PHE
2	B	386	PHE
2	B	444	ASP
2	B	519	GLN
2	B	559	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	ASN
1	A	334	ASN
1	A	363	ASN
1	A	448	ASN
1	A	518	ASN
1	A	573	GLN
2	B	24	GLN
2	B	126	ASN
2	B	334	ASN
2	B	421	GLN
2	B	448	ASN
2	B	519	GLN
2	B	559	ASN
2	B	573	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	1TY	A	382	1	20,23,24	1.33	3 (15%)	21,30,32	1.37	5 (23%)
2	2TY	B	382	2	21,23,24	2.40	5 (23%)	24,30,32	1.75	6 (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
1	1TY	A	382	1	-	2/11/28/30	0/2/2/2
2	2TY	B	382	2	1/1/1/3	2/11/12/14	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	382	2TY	CZ-CE2	6.28	1.50	1.40
2	B	382	2TY	O-C	4.83	1.39	1.19
2	B	382	2TY	CD1-CG	4.49	1.46	1.40
1	A	382	1TY	CE1-CZ	3.58	1.41	1.35
2	B	382	2TY	C1-NX1	3.49	1.34	1.26
2	B	382	2TY	CE2-NX1	-3.16	1.37	1.42
1	A	382	1TY	CD2-CG	2.53	1.41	1.34
1	A	382	1TY	CB-CA	-2.07	1.49	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	382	2TY	CB-CG-CD1	-4.29	116.46	120.95
2	B	382	2TY	CG-CB-CA	-4.11	108.18	114.53
1	A	382	1TY	CB-CA-C	-3.00	105.84	111.47
1	A	382	1TY	CZ-CE1-CD1	2.94	123.56	120.30
2	B	382	2TY	CZ-CE2-NX1	2.73	120.90	115.35
2	B	382	2TY	CB-CA-C	-2.56	106.67	111.47
1	A	382	1TY	CD2-CG-CD1	2.53	120.58	118.64
2	B	382	2TY	CE2-NX1-C1	-2.51	113.12	119.82
1	A	382	1TY	C1-NX1-CE2	2.51	126.95	121.36
1	A	382	1TY	CE1-CZ-CE2	-2.37	118.63	121.75
2	B	382	2TY	CB-CG-CD2	2.22	123.70	119.77

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 carbohydrates 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	645	-	5,5,5	0.62	0	5,5,5	1.16	0
5	GOL	A	666	-	5,5,5	0.50	0	5,5,5	0.41	0
5	GOL	B	662	-	5,5,5	0.44	0	5,5,5	0.45	0
5	GOL	B	675	-	5,5,5	0.39	0	5,5,5	0.35	0
5	GOL	A	655	-	5,5,5	0.49	0	5,5,5	1.14	0
5	GOL	B	654	-	5,5,5	0.55	0	5,5,5	0.77	0
5	GOL	A	668	-	5,5,5	0.37	0	5,5,5	0.27	0
5	GOL	A	661	-	5,5,5	0.45	0	5,5,5	0.27	0
5	GOL	B	642	-	5,5,5	0.63	0	5,5,5	0.83	0
5	GOL	A	671	-	5,5,5	0.41	0	5,5,5	0.20	0
5	GOL	A	676	-	5,5,5	0.42	0	5,5,5	0.44	0
5	GOL	A	641	-	5,5,5	0.33	0	5,5,5	0.48	0
5	GOL	B	668	-	5,5,5	0.35	0	5,5,5	0.25	0
5	GOL	B	685	-	5,5,5	0.31	0	5,5,5	0.26	0
5	GOL	A	677	-	5,5,5	0.40	0	5,5,5	0.64	0
5	GOL	A	640	-	5,5,5	0.84	0	5,5,5	1.29	0
5	GOL	B	674	-	5,5,5	0.51	0	5,5,5	0.25	0
5	GOL	A	675	-	5,5,5	0.42	0	5,5,5	0.61	0
5	GOL	B	656	-	5,5,5	0.41	0	5,5,5	0.21	0
5	GOL	A	680	-	5,5,5	0.48	0	5,5,5	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	678	-	5,5,5	0.44	0	5,5,5	0.24	0
5	GOL	A	672	-	5,5,5	0.42	0	5,5,5	0.44	0
5	GOL	B	653	-	5,5,5	0.29	0	5,5,5	0.85	0
5	GOL	B	660	-	5,5,5	0.53	0	5,5,5	0.88	0
5	GOL	B	670	-	5,5,5	0.44	0	5,5,5	0.48	0
5	GOL	B	667	-	5,5,5	0.55	0	5,5,5	0.56	0
5	GOL	B	669	-	5,5,5	0.43	0	5,5,5	0.37	0
5	GOL	B	652	-	5,5,5	0.27	0	5,5,5	1.02	1 (20%)
5	GOL	B	641	-	5,5,5	0.93	0	5,5,5	1.35	1 (20%)
5	GOL	B	686	-	5,5,5	0.39	0	5,5,5	0.31	0
5	GOL	A	674	-	5,5,5	0.41	0	5,5,5	0.54	0
5	GOL	B	664	-	5,5,5	0.47	0	5,5,5	0.63	0
5	GOL	B	683	-	5,5,5	0.31	0	5,5,5	0.32	0
5	GOL	A	643	-	5,5,5	0.37	0	5,5,5	0.71	0
5	GOL	B	644	-	5,5,5	0.39	0	5,5,5	0.93	0
5	GOL	B	640	-	5,5,5	0.34	0	5,5,5	1.61	1 (20%)
5	GOL	A	673	-	5,5,5	0.49	0	5,5,5	1.30	1 (20%)
5	GOL	B	663	-	5,5,5	0.41	0	5,5,5	0.64	0
5	GOL	A	681	-	5,5,5	0.49	0	5,5,5	0.40	0
5	GOL	A	649	-	5,5,5	0.57	0	5,5,5	0.89	0
5	GOL	B	645	-	5,5,5	0.66	0	5,5,5	1.50	1 (20%)
5	GOL	A	679	-	5,5,5	0.30	0	5,5,5	0.45	0
5	GOL	A	646	-	5,5,5	0.53	0	5,5,5	0.34	0
5	GOL	A	654	-	5,5,5	0.84	0	5,5,5	1.15	0
5	GOL	B	682	-	5,5,5	0.58	0	5,5,5	1.13	0
5	GOL	A	669	-	5,5,5	0.45	0	5,5,5	1.08	1 (20%)
5	GOL	B	665	-	5,5,5	0.41	0	5,5,5	0.16	0
5	GOL	A	684	-	5,5,5	0.44	0	5,5,5	0.42	0
5	GOL	B	684	-	5,5,5	0.47	0	5,5,5	0.52	0
5	GOL	B	639	-	5,5,5	0.32	0	5,5,5	0.84	0
5	GOL	A	651	-	5,5,5	0.58	0	5,5,5	0.85	0
5	GOL	A	663	-	5,5,5	0.41	0	5,5,5	0.68	0
5	GOL	A	678	-	5,5,5	0.29	0	5,5,5	0.68	0
5	GOL	B	646	-	5,5,5	0.32	0	5,5,5	1.12	1 (20%)
5	GOL	B	687	-	5,5,5	0.47	0	5,5,5	0.47	0
5	GOL	A	659	-	5,5,5	0.34	0	5,5,5	0.99	0
5	GOL	A	686	-	5,5,5	0.26	0	5,5,5	0.56	0
5	GOL	B	661	-	5,5,5	0.32	0	5,5,5	0.32	0
5	GOL	B	681	-	5,5,5	0.52	0	5,5,5	0.98	0
5	GOL	B	649	-	5,5,5	0.66	0	5,5,5	0.30	0
5	GOL	B	647	-	5,5,5	0.37	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	673	-	5,5,5	0.31	0	5,5,5	0.55	0
5	GOL	A	652	-	5,5,5	0.30	0	5,5,5	0.75	0
5	GOL	A	639	-	5,5,5	0.54	0	5,5,5	1.30	1 (20%)
5	GOL	B	666	-	5,5,5	0.40	0	5,5,5	1.03	0
5	GOL	A	670	-	5,5,5	0.32	0	5,5,5	0.64	0
5	GOL	A	683	-	5,5,5	0.24	0	5,5,5	0.47	0
5	GOL	A	667	-	5,5,5	0.39	0	5,5,5	0.35	0
5	GOL	B	643	-	5,5,5	0.67	0	5,5,5	1.13	0
5	GOL	B	677	-	5,5,5	0.33	0	5,5,5	0.49	0
5	GOL	B	658	-	5,5,5	0.48	0	5,5,5	0.56	0
5	GOL	A	656	-	5,5,5	0.48	0	5,5,5	1.24	0
5	GOL	B	657	-	5,5,5	0.53	0	5,5,5	1.27	1 (20%)
5	GOL	A	660	-	5,5,5	0.55	0	5,5,5	0.91	0
5	GOL	B	680	-	5,5,5	0.36	0	5,5,5	0.16	0
5	GOL	A	657	-	5,5,5	0.42	0	5,5,5	0.58	0
5	GOL	B	679	-	5,5,5	0.43	0	5,5,5	0.42	0
5	GOL	A	658	-	5,5,5	0.37	0	5,5,5	0.75	0
5	GOL	A	647	-	5,5,5	0.29	0	5,5,5	0.61	0
5	GOL	B	659	-	5,5,5	0.40	0	5,5,5	0.57	0
5	GOL	B	676	-	5,5,5	0.41	0	5,5,5	0.67	0
5	GOL	A	644	-	5,5,5	0.40	0	5,5,5	0.67	0
5	GOL	A	685	-	5,5,5	0.39	0	5,5,5	0.57	0
5	GOL	B	671	-	5,5,5	0.39	0	5,5,5	0.22	0
5	GOL	A	642	-	5,5,5	0.58	0	5,5,5	1.60	1 (20%)
5	GOL	A	650	-	5,5,5	0.61	0	5,5,5	0.62	0
5	GOL	B	651	-	5,5,5	0.28	0	5,5,5	0.31	0
5	GOL	B	655	-	5,5,5	0.65	0	5,5,5	0.79	0
5	GOL	A	662	-	5,5,5	0.24	0	5,5,5	0.92	0
5	GOL	A	665	-	5,5,5	0.28	0	5,5,5	0.39	0
5	GOL	A	682	-	5,5,5	0.40	0	5,5,5	0.86	0
5	GOL	B	672	-	5,5,5	0.36	0	5,5,5	0.47	0
5	GOL	B	650	-	5,5,5	0.61	0	5,5,5	0.64	0
5	GOL	A	648	-	5,5,5	0.32	0	5,5,5	0.38	0
5	GOL	A	664	-	5,5,5	0.56	0	5,5,5	0.42	0
5	GOL	A	653	-	5,5,5	0.38	0	5,5,5	0.29	0
5	GOL	B	648	-	5,5,5	0.48	0	5,5,5	0.72	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	645	-	-	3/4/4/4	-
5	GOL	A	666	-	-	2/4/4/4	-
5	GOL	B	662	-	-	0/4/4/4	-
5	GOL	B	675	-	-	2/4/4/4	-
5	GOL	A	655	-	-	4/4/4/4	-
5	GOL	B	654	-	-	4/4/4/4	-
5	GOL	A	668	-	-	0/4/4/4	-
5	GOL	A	661	-	-	3/4/4/4	-
5	GOL	B	642	-	-	4/4/4/4	-
5	GOL	A	671	-	-	2/4/4/4	-
5	GOL	A	676	-	-	4/4/4/4	-
5	GOL	A	641	-	-	2/4/4/4	-
5	GOL	B	668	-	-	0/4/4/4	-
5	GOL	B	685	-	-	0/4/4/4	-
5	GOL	A	677	-	-	2/4/4/4	-
5	GOL	A	640	-	-	3/4/4/4	-
5	GOL	B	674	-	-	4/4/4/4	-
5	GOL	A	675	-	-	0/4/4/4	-
5	GOL	B	656	-	-	3/4/4/4	-
5	GOL	A	680	-	-	1/4/4/4	-
5	GOL	B	678	-	-	2/4/4/4	-
5	GOL	A	672	-	-	0/4/4/4	-
5	GOL	B	653	-	-	4/4/4/4	-
5	GOL	B	660	-	-	2/4/4/4	-
5	GOL	B	670	-	-	0/4/4/4	-
5	GOL	B	667	-	-	2/4/4/4	-
5	GOL	B	669	-	-	3/4/4/4	-
5	GOL	B	652	-	-	4/4/4/4	-
5	GOL	B	641	-	-	2/4/4/4	-
5	GOL	B	686	-	-	4/4/4/4	-
5	GOL	A	674	-	-	3/4/4/4	-
5	GOL	B	664	-	-	2/4/4/4	-
5	GOL	B	683	-	-	2/4/4/4	-
5	GOL	A	643	-	-	2/4/4/4	-
5	GOL	B	644	-	-	3/4/4/4	-
5	GOL	B	640	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	673	-	-	2/4/4/4	-
5	GOL	B	663	-	-	2/4/4/4	-
5	GOL	A	681	-	-	1/4/4/4	-
5	GOL	A	649	-	-	2/4/4/4	-
5	GOL	B	645	-	-	2/4/4/4	-
5	GOL	A	679	-	-	2/4/4/4	-
5	GOL	A	646	-	-	0/4/4/4	-
5	GOL	A	654	-	-	4/4/4/4	-
5	GOL	B	682	-	-	2/4/4/4	-
5	GOL	A	669	-	-	3/4/4/4	-
5	GOL	B	665	-	-	4/4/4/4	-
5	GOL	A	684	-	-	4/4/4/4	-
5	GOL	B	684	-	-	4/4/4/4	-
5	GOL	B	639	-	-	2/4/4/4	-
5	GOL	A	651	-	-	4/4/4/4	-
5	GOL	A	663	-	-	2/4/4/4	-
5	GOL	A	678	-	-	4/4/4/4	-
5	GOL	B	646	-	-	2/4/4/4	-
5	GOL	B	687	-	-	0/4/4/4	-
5	GOL	A	659	-	-	1/4/4/4	-
5	GOL	A	686	-	-	4/4/4/4	-
5	GOL	B	661	-	-	4/4/4/4	-
5	GOL	B	681	-	-	3/4/4/4	-
5	GOL	B	649	-	-	2/4/4/4	-
5	GOL	B	647	-	-	0/4/4/4	-
5	GOL	B	673	-	-	3/4/4/4	-
5	GOL	A	652	-	-	2/4/4/4	-
5	GOL	A	639	-	-	2/4/4/4	-
5	GOL	B	666	-	-	4/4/4/4	-
5	GOL	A	670	-	-	2/4/4/4	-
5	GOL	A	683	-	-	0/4/4/4	-
5	GOL	A	667	-	-	2/4/4/4	-
5	GOL	B	643	-	-	2/4/4/4	-
5	GOL	B	677	-	-	1/4/4/4	-
5	GOL	B	658	-	-	0/4/4/4	-
5	GOL	A	656	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	657	-	-	2/4/4/4	-
5	GOL	A	660	-	-	4/4/4/4	-
5	GOL	B	680	-	-	1/4/4/4	-
5	GOL	A	657	-	-	2/4/4/4	-
5	GOL	B	679	-	-	2/4/4/4	-
5	GOL	A	658	-	-	2/4/4/4	-
5	GOL	A	647	-	-	2/4/4/4	-
5	GOL	B	659	-	-	2/4/4/4	-
5	GOL	B	676	-	-	0/4/4/4	-
5	GOL	A	644	-	-	2/4/4/4	-
5	GOL	A	685	-	-	0/4/4/4	-
5	GOL	B	671	-	-	0/4/4/4	-
5	GOL	A	642	-	-	1/4/4/4	-
5	GOL	A	650	-	-	0/4/4/4	-
5	GOL	B	651	-	-	2/4/4/4	-
5	GOL	B	655	-	-	2/4/4/4	-
5	GOL	A	662	-	-	2/4/4/4	-
5	GOL	A	665	-	-	2/4/4/4	-
5	GOL	A	682	-	-	2/4/4/4	-
5	GOL	B	672	-	-	2/4/4/4	-
5	GOL	B	650	-	-	2/4/4/4	-
5	GOL	A	648	-	-	2/4/4/4	-
5	GOL	A	664	-	-	0/4/4/4	-
5	GOL	A	653	-	-	4/4/4/4	-
5	GOL	B	648	-	-	2/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	642	GOL	C3-C2-C1	-3.44	98.32	111.70
5	B	640	GOL	C3-C2-C1	-3.40	98.48	111.70
5	B	641	GOL	O2-C2-C3	2.71	121.06	109.12
5	A	639	GOL	O1-C1-C2	-2.39	98.72	110.20
5	B	645	GOL	C3-C2-C1	-2.28	102.83	111.70
5	A	673	GOL	O2-C2-C3	2.27	119.10	109.12
5	B	646	GOL	O2-C2-C3	2.14	118.55	109.12
5	A	669	GOL	O3-C3-C2	2.08	120.16	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	657	GOL	O3-C3-C2	2.07	120.15	110.20
5	B	652	GOL	C3-C2-C1	-2.06	103.70	111.70

There are no chirality outliers.

All (206) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	645	GOL	O1-C1-C2-O2
5	B	675	GOL	O1-C1-C2-C3
5	A	655	GOL	O1-C1-C2-O2
5	B	654	GOL	O1-C1-C2-O2
5	A	661	GOL	O1-C1-C2-C3
5	A	671	GOL	C1-C2-C3-O3
5	A	676	GOL	C1-C2-C3-O3
5	A	641	GOL	O1-C1-C2-C3
5	A	677	GOL	O1-C1-C2-C3
5	A	640	GOL	C1-C2-C3-O3
5	B	674	GOL	O1-C1-C2-C3
5	B	674	GOL	C1-C2-C3-O3
5	B	653	GOL	C1-C2-C3-O3
5	B	660	GOL	O1-C1-C2-C3
5	B	652	GOL	O1-C1-C2-O2
5	B	652	GOL	O1-C1-C2-C3
5	B	641	GOL	O1-C1-C2-C3
5	B	686	GOL	O1-C1-C2-C3
5	A	674	GOL	C1-C2-C3-O3
5	A	643	GOL	O1-C1-C2-C3
5	B	640	GOL	O1-C1-C2-C3
5	B	640	GOL	C1-C2-C3-O3
5	A	649	GOL	O1-C1-C2-C3
5	A	654	GOL	O1-C1-C2-C3
5	A	654	GOL	C1-C2-C3-O3
5	B	682	GOL	O1-C1-C2-C3
5	A	669	GOL	O1-C1-C2-C3
5	B	665	GOL	O1-C1-C2-C3
5	B	665	GOL	C1-C2-C3-O3
5	A	684	GOL	C1-C2-C3-O3
5	A	651	GOL	O1-C1-C2-C3
5	A	663	GOL	C1-C2-C3-O3
5	A	678	GOL	O1-C1-C2-C3
5	B	646	GOL	O1-C1-C2-C3
5	A	686	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	686	GOL	O1-C1-C2-C3
5	B	661	GOL	O1-C1-C2-C3
5	B	681	GOL	O2-C2-C3-O3
5	B	649	GOL	O1-C1-C2-C3
5	B	673	GOL	C1-C2-C3-O3
5	A	652	GOL	O1-C1-C2-C3
5	A	639	GOL	O1-C1-C2-C3
5	B	666	GOL	C1-C2-C3-O3
5	A	670	GOL	C1-C2-C3-O3
5	A	667	GOL	O1-C1-C2-C3
5	B	643	GOL	O1-C1-C2-C3
5	A	656	GOL	O1-C1-C2-O2
5	A	656	GOL	O1-C1-C2-C3
5	A	656	GOL	C1-C2-C3-O3
5	B	657	GOL	C1-C2-C3-O3
5	A	660	GOL	O1-C1-C2-C3
5	A	660	GOL	C1-C2-C3-O3
5	A	657	GOL	O1-C1-C2-C3
5	A	658	GOL	O1-C1-C2-C3
5	B	659	GOL	C1-C2-C3-O3
5	B	659	GOL	O2-C2-C3-O3
5	B	651	GOL	O1-C1-C2-C3
5	A	662	GOL	O1-C1-C2-C3
5	A	682	GOL	O1-C1-C2-C3
5	B	672	GOL	C1-C2-C3-O3
5	B	672	GOL	O2-C2-C3-O3
5	A	653	GOL	O1-C1-C2-C3
5	B	654	GOL	O2-C2-C3-O3
5	A	671	GOL	O2-C2-C3-O3
5	B	674	GOL	O2-C2-C3-O3
5	A	686	GOL	O2-C2-C3-O3
5	A	653	GOL	O2-C2-C3-O3
5	A	645	GOL	O1-C1-C2-C3
5	A	645	GOL	C1-C2-C3-O3
5	A	666	GOL	O1-C1-C2-C3
5	A	655	GOL	O1-C1-C2-C3
5	A	655	GOL	C1-C2-C3-O3
5	B	654	GOL	O1-C1-C2-C3
5	B	654	GOL	C1-C2-C3-O3
5	B	642	GOL	O1-C1-C2-C3
5	B	642	GOL	C1-C2-C3-O3
5	A	676	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	640	GOL	O1-C1-C2-C3
5	B	678	GOL	O1-C1-C2-C3
5	B	653	GOL	O1-C1-C2-C3
5	B	669	GOL	O1-C1-C2-C3
5	B	669	GOL	C1-C2-C3-O3
5	B	652	GOL	C1-C2-C3-O3
5	B	686	GOL	C1-C2-C3-O3
5	B	683	GOL	C1-C2-C3-O3
5	A	673	GOL	O1-C1-C2-C3
5	B	663	GOL	O1-C1-C2-C3
5	B	645	GOL	C1-C2-C3-O3
5	A	679	GOL	C1-C2-C3-O3
5	B	684	GOL	C1-C2-C3-O3
5	B	639	GOL	C1-C2-C3-O3
5	A	651	GOL	C1-C2-C3-O3
5	A	678	GOL	C1-C2-C3-O3
5	A	659	GOL	O1-C1-C2-C3
5	A	686	GOL	C1-C2-C3-O3
5	B	661	GOL	C1-C2-C3-O3
5	B	681	GOL	O1-C1-C2-C3
5	B	681	GOL	C1-C2-C3-O3
5	B	666	GOL	O1-C1-C2-C3
5	B	677	GOL	O1-C1-C2-C3
5	B	679	GOL	O1-C1-C2-C3
5	A	647	GOL	C1-C2-C3-O3
5	A	642	GOL	O1-C1-C2-C3
5	B	655	GOL	O1-C1-C2-C3
5	A	665	GOL	O1-C1-C2-C3
5	B	650	GOL	O1-C1-C2-C3
5	A	648	GOL	C1-C2-C3-O3
5	A	653	GOL	C1-C2-C3-O3
5	B	648	GOL	C1-C2-C3-O3
5	B	675	GOL	O1-C1-C2-O2
5	B	642	GOL	O2-C2-C3-O3
5	A	676	GOL	O2-C2-C3-O3
5	A	641	GOL	O1-C1-C2-O2
5	A	677	GOL	O1-C1-C2-O2
5	B	678	GOL	O1-C1-C2-O2
5	B	653	GOL	O2-C2-C3-O3
5	B	660	GOL	O1-C1-C2-O2
5	B	641	GOL	O1-C1-C2-O2
5	B	686	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	674	GOL	O2-C2-C3-O3
5	B	640	GOL	O1-C1-C2-O2
5	A	649	GOL	O1-C1-C2-O2
5	A	679	GOL	O2-C2-C3-O3
5	A	654	GOL	O1-C1-C2-O2
5	B	682	GOL	O1-C1-C2-O2
5	A	669	GOL	O1-C1-C2-O2
5	A	684	GOL	O2-C2-C3-O3
5	A	651	GOL	O1-C1-C2-O2
5	A	678	GOL	O1-C1-C2-O2
5	B	649	GOL	O1-C1-C2-O2
5	B	673	GOL	O2-C2-C3-O3
5	A	652	GOL	O1-C1-C2-O2
5	B	666	GOL	O1-C1-C2-O2
5	B	666	GOL	O2-C2-C3-O3
5	A	670	GOL	O2-C2-C3-O3
5	A	667	GOL	O1-C1-C2-O2
5	B	643	GOL	O1-C1-C2-O2
5	A	656	GOL	O2-C2-C3-O3
5	B	657	GOL	O2-C2-C3-O3
5	A	660	GOL	O2-C2-C3-O3
5	A	657	GOL	O1-C1-C2-O2
5	A	658	GOL	O1-C1-C2-O2
5	B	651	GOL	O1-C1-C2-O2
5	A	655	GOL	O2-C2-C3-O3
5	A	640	GOL	O2-C2-C3-O3
5	A	643	GOL	O1-C1-C2-O2
5	B	644	GOL	O2-C2-C3-O3
5	B	640	GOL	O2-C2-C3-O3
5	A	654	GOL	O2-C2-C3-O3
5	B	665	GOL	O2-C2-C3-O3
5	B	684	GOL	O2-C2-C3-O3
5	B	661	GOL	O1-C1-C2-O2
5	A	639	GOL	O1-C1-C2-O2
5	A	682	GOL	O1-C1-C2-O2
5	B	650	GOL	O1-C1-C2-O2
5	A	648	GOL	O2-C2-C3-O3
5	B	644	GOL	O1-C1-C2-C3
5	A	676	GOL	O1-C1-C2-O2
5	B	674	GOL	O1-C1-C2-O2
5	A	680	GOL	O1-C1-C2-O2
5	B	665	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	B	684	GOL	O1-C1-C2-O2
5	A	651	GOL	O2-C2-C3-O3
5	A	663	GOL	O2-C2-C3-O3
5	B	661	GOL	O2-C2-C3-O3
5	A	660	GOL	O1-C1-C2-O2
5	A	647	GOL	O2-C2-C3-O3
5	A	644	GOL	O2-C2-C3-O3
5	B	655	GOL	O1-C1-C2-O2
5	A	662	GOL	O1-C1-C2-O2
5	A	653	GOL	O1-C1-C2-O2
5	A	666	GOL	O2-C2-C3-O3
5	B	642	GOL	O1-C1-C2-O2
5	B	656	GOL	O2-C2-C3-O3
5	B	653	GOL	O1-C1-C2-O2
5	B	667	GOL	O1-C1-C2-O2
5	B	652	GOL	O2-C2-C3-O3
5	B	664	GOL	O2-C2-C3-O3
5	B	683	GOL	O2-C2-C3-O3
5	A	673	GOL	O2-C2-C3-O3
5	A	684	GOL	O1-C1-C2-O2
5	A	665	GOL	O1-C1-C2-O2
5	B	656	GOL	O1-C1-C2-C3
5	A	681	GOL	C1-C2-C3-O3
5	B	684	GOL	O1-C1-C2-C3
5	A	644	GOL	C1-C2-C3-O3
5	A	661	GOL	O1-C1-C2-O2
5	B	679	GOL	O1-C1-C2-O2
5	B	669	GOL	O1-C1-C2-O2
5	B	645	GOL	O2-C2-C3-O3
5	B	656	GOL	C1-C2-C3-O3
5	B	667	GOL	O1-C1-C2-C3
5	B	664	GOL	C1-C2-C3-O3
5	B	644	GOL	C1-C2-C3-O3
5	A	684	GOL	O1-C1-C2-C3
5	B	646	GOL	C1-C2-C3-O3
5	B	686	GOL	O2-C2-C3-O3
5	A	678	GOL	O2-C2-C3-O3
5	B	663	GOL	O1-C1-C2-O2
5	A	669	GOL	O2-C2-C3-O3
5	B	639	GOL	O2-C2-C3-O3
5	B	648	GOL	O2-C2-C3-O3
5	A	661	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	674	GOL	O1-C1-C2-C3
5	B	680	GOL	C1-C2-C3-O3
5	B	673	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	662	GOL	1	0
5	A	655	GOL	1	0
5	B	654	GOL	1	0
5	A	676	GOL	1	0
5	B	668	GOL	1	0
5	B	685	GOL	1	0
5	A	677	GOL	1	0
5	B	678	GOL	2	0
5	B	653	GOL	4	0
5	B	660	GOL	1	0
5	B	669	GOL	4	0
5	A	674	GOL	2	0
5	B	664	GOL	1	0
5	A	643	GOL	2	0
5	B	644	GOL	3	0
5	B	640	GOL	2	0
5	A	673	GOL	1	0
5	A	681	GOL	1	0
5	A	649	GOL	1	0
5	B	645	GOL	1	0
5	A	679	GOL	1	0
5	A	646	GOL	1	0
5	B	682	GOL	1	0
5	A	684	GOL	1	0
5	B	684	GOL	4	0
5	B	639	GOL	1	0
5	A	651	GOL	1	0
5	A	659	GOL	1	0
5	A	686	GOL	2	0
5	B	661	GOL	1	0
5	A	652	GOL	3	0
5	A	639	GOL	6	0
5	B	666	GOL	5	0
5	A	670	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	643	GOL	3	0
5	B	658	GOL	2	0
5	A	656	GOL	3	0
5	B	657	GOL	3	0
5	A	660	GOL	2	0
5	B	679	GOL	1	0
5	A	658	GOL	1	0
5	B	659	GOL	1	0
5	B	671	GOL	3	0
5	A	642	GOL	3	0
5	A	662	GOL	2	0
5	B	672	GOL	1	0
5	A	648	GOL	1	0
5	A	664	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	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%)

All (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
1	A	53	SER	8.2
1	A	50	GLY	7.0
2	B	50	GLY	6.7
1	A	51	ALA	6.1
2	B	54	GLU	6.1
1	A	54	GLU	6.0
1	A	55	ALA	5.9
2	B	225	PRO	4.7
1	A	414	GLY	4.6
2	B	266[A]	ASP	4.4
1	A	266[A]	ASP	3.8
1	A	56	GLU	3.6
1	A	70	ALA	3.5
2	B	48	ALA	3.5
1	A	145	ALA	3.3
2	B	462	PRO	3.3
2	B	163	PRO	3.1
1	A	163	PRO	3.1
2	B	414	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	463	GLY	2.8
1	A	225	PRO	2.7
1	A	143	GLU	2.7
1	A	215	THR	2.7
1	A	148	ARG	2.6
2	B	215	THR	2.6
1	A	507	ASN	2.6
2	B	415	GLY	2.5
1	A	339[A]	ARG	2.5
2	B	226	GLU	2.5
1	A	9	ALA	2.5
2	B	116[A]	GLU	2.4
2	B	9	ALA	2.4
2	B	339	ARG	2.4
2	B	413	GLU	2.3
1	A	48	ALA	2.3
1	A	461	GLY	2.3
2	B	162	PHE	2.3
1	A	462	PRO	2.3
2	B	265	GLY	2.3
2	B	87	ALA	2.3
1	A	226	GLU	2.3
1	A	413	GLU	2.2
1	A	34	GLY	2.1
1	A	234	GLY	2.1
1	A	313	LEU	2.1
1	A	463	GLY	2.1
1	A	68	SER	2.0
2	B	208	GLU	2.0
2	B	627	ALA	2.0

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 carbohydrates 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	656	6/6	0.69	0.29	74,75,75,75	0
5	GOL	B	665	6/6	0.69	0.23	61,65,66,66	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	B	687	6/6	0.74	0.38	45,56,61,62	0
5	GOL	A	667	6/6	0.74	0.27	59,60,61,61	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	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	665	6/6	0.78	0.22	54,56,57,60	0
5	GOL	A	673	6/6	0.78	0.19	45,47,51,54	0
5	GOL	B	674	6/6	0.79	0.20	62,63,63,63	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	0.31	60,63,65,67	0
5	GOL	A	680	6/6	0.80	0.15	47,52,53,56	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	A	676	6/6	0.81	0.30	60,63,63,64	0
5	GOL	B	685	6/6	0.81	0.33	56,58,58,60	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	B	680	6/6	0.82	0.23	63,64,64,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	668	6/6	0.82	0.23	61,66,66,67	0
5	GOL	B	676	6/6	0.82	0.33	55,58,59,60	0
5	GOL	B	662	6/6	0.83	0.17	65,67,67,67	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	660	6/6	0.84	0.14	32,38,42,45	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	A	678	6/6	0.84	0.24	49,53,54,58	0
5	GOL	B	672	6/6	0.84	0.19	43,50,52,54	0
5	GOL	B	675	6/6	0.84	0.18	62,63,65,65	0
5	GOL	A	661	6/6	0.85	0.23	58,62,63,63	0
5	GOL	A	647	6/6	0.85	0.25	54,57,58,59	0
5	GOL	A	686	6/6	0.85	0.17	55,57,58,59	0
5	GOL	B	655	6/6	0.85	0.22	42,45,47,47	0
5	GOL	A	658	6/6	0.86	0.20	46,50,51,51	0
5	GOL	B	649	6/6	0.86	0.19	40,49,50,51	0
5	GOL	A	657	6/6	0.86	0.17	36,41,43,48	0
5	GOL	B	646	6/6	0.86	0.16	33,43,45,50	0
5	GOL	B	681	6/6	0.87	0.34	46,53,54,58	0
5	GOL	B	670	6/6	0.87	0.26	58,60,60,60	0
5	GOL	A	685	6/6	0.87	0.23	58,59,60,61	0
5	GOL	B	667	6/6	0.87	0.19	36,46,47,48	0
5	GOL	B	661	6/6	0.88	0.17	46,47,48,51	0
5	GOL	A	651	6/6	0.88	0.16	39,41,43,44	0
5	GOL	A	655	6/6	0.88	0.16	46,48,49,52	0
5	GOL	B	684	6/6	0.88	0.18	65,66,67,67	0
5	GOL	B	666	6/6	0.88	0.22	43,50,50,53	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	A	640	6/6	0.90	0.15	34,38,40,43	0
5	GOL	A	639	6/6	0.90	0.15	34,39,41,44	0
5	GOL	B	653	6/6	0.90	0.15	31,36,39,39	0
5	GOL	B	664	6/6	0.90	0.18	43,48,49,49	0
5	GOL	A	681	6/6	0.90	0.26	44,49,51,52	0
5	GOL	A	644	6/6	0.90	0.22	40,45,46,50	0
5	GOL	A	675	6/6	0.91	0.29	61,62,63,65	0
5	GOL	B	671	6/6	0.91	0.30	54,56,58,58	0
5	GOL	A	645	6/6	0.91	0.20	36,41,44,46	0
5	GOL	B	639	6/6	0.91	0.16	28,38,40,44	0
5	GOL	B	673	6/6	0.91	0.12	52,53,54,54	0
5	GOL	A	659	6/6	0.91	0.13	32,39,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	A	648	6/6	0.91	0.15	49,51,53,54	0
5	GOL	A	643	6/6	0.91	0.15	46,49,50,51	0
5	GOL	B	644	6/6	0.91	0.29	34,42,44,48	0
5	GOL	B	654	6/6	0.92	0.14	39,44,46,47	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
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	A	641	6/6	0.93	0.29	40,51,53,55	0
5	GOL	A	662	6/6	0.93	0.21	52,54,55,56	0
5	GOL	A	649	6/6	0.93	0.14	41,46,48,49	0
5	GOL	A	656	6/6	0.93	0.13	29,36,40,43	0
5	GOL	B	648	6/6	0.93	0.19	38,44,45,45	0
5	GOL	B	642	6/6	0.94	0.14	29,36,38,38	0
5	GOL	A	674	6/6	0.94	0.14	38,46,48,49	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	651	6/6	0.94	0.09	43,45,46,46	0
5	GOL	B	659	6/6	0.94	0.16	36,37,40,45	0
5	GOL	B	641	6/6	0.94	0.12	27,29,30,30	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.