



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 8, 2022 – 05:06 AM JST

PDB ID : 7WIR  
Title : Holo form of N381A mutant of copper amine oxidase from *Arthrobacter globiformis*  
Authors : Murakawa, T.; Okajima, T.  
Deposited on : 2022-01-04  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
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) : 2.31.2

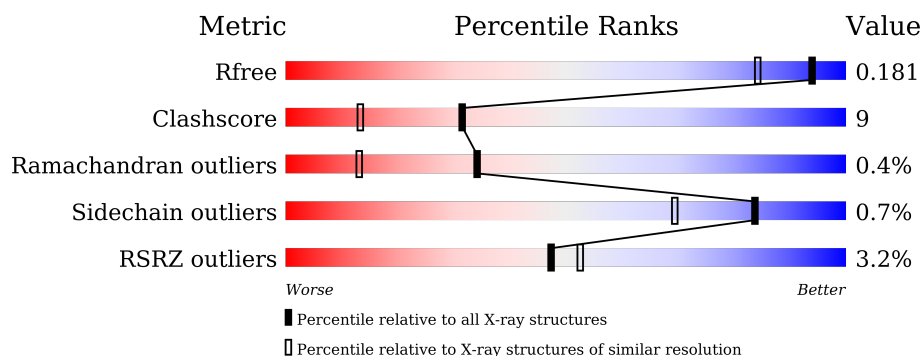
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	620	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>7%</div> <div>.</div> </div> </div>
1	B	620	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	TPQ	B	382[B]	-	-	X	-
3	GOL	A	709	-	-	X	-
3	GOL	A	711	-	-	X	-
3	GOL	A	713	-	-	X	-
3	GOL	A	714	-	-	X	-
3	GOL	B	706	-	-	X	-
3	GOL	B	709	-	-	X	-
3	GOL	B	716	-	-	X	-
3	GOL	B	718	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11725 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
1	A	620	Total	C	N	O	S	0	19	0
			5000	3172	873	946	9			
1	B	620	Total	C	N	O	S	0	22	0
			5004	3181	872	941	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	381	ALA	ASN	engineered mutation	UNP P46881
B	381	ALA	ASN	engineered mutation	UNP P46881

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

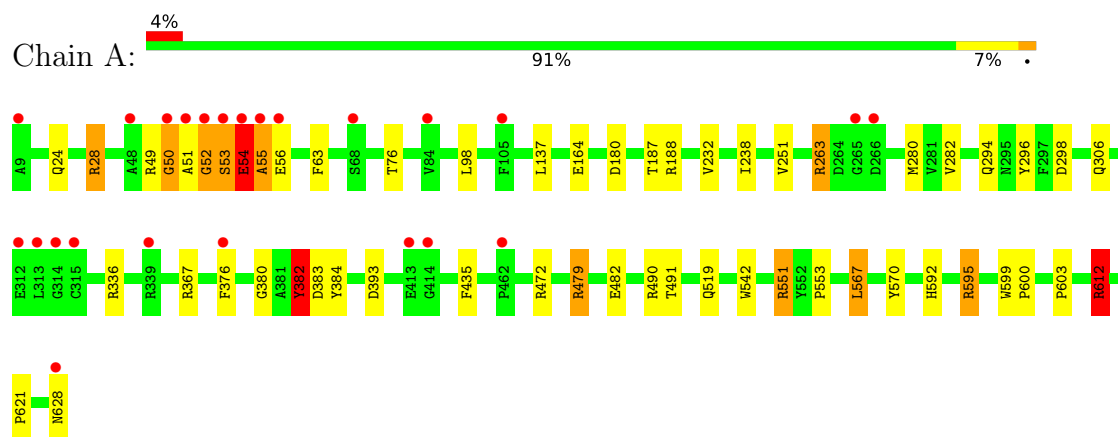
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	711	Total O 711 711	0	0
4	B	828	Total O 828 828	0	0

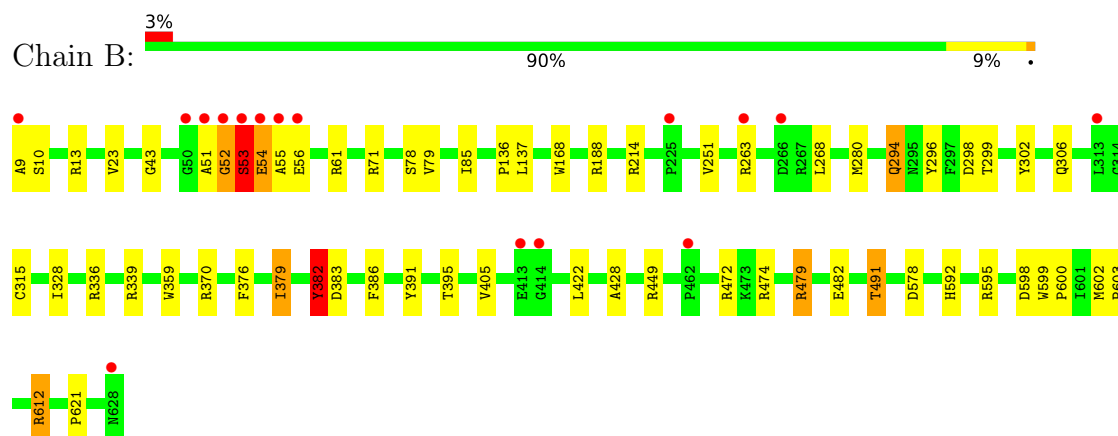
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Phenylethylamine oxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.97Å 63.02Å 158.01Å 90.00° 117.63° 90.00°	Depositor
Resolution (Å)	22.45 – 1.50 22.45 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (22.45-1.50) 99.0 (22.45-1.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.161 , 0.181 0.162 , 0.181	Depositor DCC
$R_{free}$ test set	13219 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.3	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	11725	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 61.23 % 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 1.3517e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPQ, GOL, 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	0.59	0/5154	0.78	8/7013 (0.1%)
1	B	0.62	0/5169	0.84	5/7035 (0.1%)
All	All	0.60	0/10323	0.81	13/14048 (0.1%)

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	10
1	B	0	7
All	All	0	17

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	SER	O-C-N	-24.84	82.95	122.70
1	A	53	SER	O-C-N	-9.72	107.15	122.70
1	B	52	GLY	C-N-CA	8.50	142.94	121.70
1	A	595	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	367	ARG	CG-CD-NE	6.68	125.83	111.80
1	A	612	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	214	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	61	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	49	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	B	71	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	367	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	180	ASP	CB-CG-OD2	-5.10	113.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLY	C-N-CA	5.07	134.38	121.70

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382[A]	TPQ	Mainchain
1	A	382[B]	TPQ	Mainchain
1	A	384	TYR	Sidechain
1	A	479	ARG	Sidechain
1	A	50	GLY	Peptide
1	A	53	SER	Peptide,Mainchain
1	A	54	GLU	Peptide
1	A	551	ARG	Sidechain
1	A	612	ARG	Sidechain
1	B	294	GLN	Sidechain
1	B	382[B]	TPQ	Mainchain
1	B	386	PHE	Sidechain
1	B	479	ARG	Sidechain
1	B	52	GLY	Peptide
1	B	53	SER	Mainchain
1	B	612	ARG	Sidechain

## 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	5000	0	4858	75	0
1	B	5004	0	4902	86	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	78	0	101	32	0
3	B	102	0	134	33	0
4	A	711	0	0	22	1
4	B	828	0	0	24	1
All	All	11725	0	9995	181	2

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 (181) 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:296[B]:TYR:CD1	1:A:382[B]:TPQ:O5	1.93	1.20
3:B:706:GOL:C3	3:B:716:GOL:H11	1.69	1.18
3:A:708:GOL:O1	4:A:801:HOH:O	1.58	1.12
1:B:296[B]:TYR:HE2	1:B:382[B]:TPQ:O4	1.33	1.10
1:B:296[B]:TYR:CD2	1:B:382[B]:TPQ:O5	2.06	1.09
3:B:706:GOL:H32	3:B:716:GOL:H11	1.04	1.01
3:A:713:GOL:O2	3:A:714:GOL:H31	1.61	1.00
1:A:592[B]:HIS:CE1	3:A:709:GOL:O3	2.14	0.99
3:B:706:GOL:H32	3:B:716:GOL:C1	1.91	0.99
1:A:294[A]:GLN:HE21	1:A:296[A]:TYR:HE2	1.11	0.98
1:B:298[A]:ASP:OD1	1:B:379[A]:ILE:HG21	1.63	0.98
3:B:718:GOL:H12	4:B:867:HOH:O	1.62	0.97
1:B:296[B]:TYR:CE2	1:B:382[B]:TPQ:O5	2.18	0.96
1:B:296[B]:TYR:CE2	1:B:382[B]:TPQ:O4	2.20	0.94
3:A:709:GOL:O1	4:A:802:HOH:O	1.84	0.91
1:A:296[B]:TYR:CG	1:A:382[B]:TPQ:O5	2.24	0.90
1:A:294[A]:GLN:HG3	1:A:296[A]:TYR:CZ	2.06	0.89
1:A:612:ARG:HH12	3:B:709:GOL:H2	1.35	0.89
3:B:706:GOL:C3	3:B:716:GOL:C1	2.50	0.87
1:A:24:GLN:O	1:A:28[A]:ARG:HG2	1.77	0.84
1:B:294:GLN:HG3	1:B:296[A]:TYR:OH	1.76	0.83
1:B:56:GLU:OE1	4:B:803:HOH:O	1.96	0.82
3:A:713:GOL:O2	3:A:714:GOL:C3	2.27	0.82
1:B:379[A]:ILE:HG23	4:B:898:HOH:O	1.78	0.82
1:A:56[A]:GLU:OE1	4:A:803:HOH:O	1.99	0.81
1:B:54:GLU:HG3	1:B:55:ALA:H	1.44	0.81
1:B:592[A]:HIS:NE2	3:B:709:GOL:H11	1.98	0.78
1:A:296[B]:TYR:HD1	1:A:382[B]:TPQ:HO4	1.28	0.77
1:B:54:GLU:HG3	1:B:55:ALA:N	1.98	0.77
3:B:717:GOL:H32	4:B:822:HOH:O	1.85	0.76
3:A:713:GOL:HO2	3:A:714:GOL:H31	1.48	0.76
1:B:296[B]:TYR:HE2	1:B:382[B]:TPQ:C4	2.00	0.75
1:A:628:ASN:OXT	4:A:804:HOH:O	2.04	0.74
1:B:296[B]:TYR:HD2	1:B:382[B]:TPQ:O5	1.65	0.74
3:A:709:GOL:C3	1:B:612:ARG:HH22	2.00	0.74
1:B:592[B]:HIS:CE1	3:B:709:GOL:O1	2.41	0.73
1:B:395:THR:HG21	3:B:706:GOL:H31	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:603[B]:PRO:HG2	4:B:1109:HOH:O	1.87	0.71
1:B:592[A]:HIS:CD2	3:B:709:GOL:H31	2.25	0.71
1:B:472[B]:ARG:HH21	1:B:472[B]:ARG:HG3	1.55	0.71
3:B:718:GOL:O2	4:B:806:HOH:O	2.08	0.71
1:A:294[A]:GLN:NE2	1:A:296[A]:TYR:HE2	1.85	0.70
1:B:302:TYR:HB3	1:B:379[A]:ILE:HD11	1.75	0.69
1:B:294:GLN:HG3	1:B:296[A]:TYR:CZ	2.28	0.68
1:A:296[B]:TYR:HD1	1:A:382[B]:TPQ:O4	1.77	0.67
1:B:339:ARG:NH1	4:B:812:HOH:O	2.27	0.66
1:A:294[A]:GLN:NE2	1:A:296[A]:TYR:CE2	2.63	0.65
1:A:280:MET:HE3	1:A:298:ASP:HB2	1.78	0.65
1:B:370:ARG:HH12	3:B:715:GOL:H11	1.62	0.65
1:B:382[B]:TPQ:O2	4:B:804:HOH:O	2.06	0.64
1:A:294[A]:GLN:CG	1:A:296[A]:TYR:CZ	2.80	0.64
3:A:709:GOL:H32	1:B:612:ARG:HH22	1.62	0.64
1:A:553:PRO:HA	1:A:567[A]:LEU:HD13	1.79	0.62
1:A:603:PRO:CG	4:A:1032:HOH:O	2.46	0.62
1:B:137:LEU:HD13	1:B:296[A]:TYR:OH	1.99	0.62
1:A:376:PHE:HE2	1:A:383:ASP:HB3	1.64	0.62
1:A:490[B]:ARG:NE	4:A:814:HOH:O	2.33	0.61
4:A:1473:HOH:O	1:B:315:CYS:SG	2.56	0.61
1:B:13:ARG:NH1	1:B:56:GLU:OE2	2.30	0.61
1:B:54:GLU:CG	1:B:55:ALA:N	2.63	0.61
1:B:449[B]:ARG:HD2	1:B:578:ASP:OD1	2.01	0.61
1:A:595:ARG:HG3	3:A:709:GOL:H11	1.82	0.61
1:B:598:ASP:OD1	3:B:709:GOL:O2	2.19	0.61
1:B:376:PHE:HE2	1:B:383:ASP:HB3	1.66	0.60
1:B:599:TRP:CD2	1:B:600:PRO:HA	2.36	0.60
1:A:188:ARG:HD2	4:A:826:HOH:O	2.01	0.60
1:B:592[A]:HIS:HD2	3:B:709:GOL:H31	1.66	0.60
1:B:482:GLU:OE2	4:B:808:HOH:O	2.17	0.59
1:A:251:VAL:HG22	1:A:306:GLN:HB3	1.84	0.59
1:A:294[A]:GLN:CG	1:A:296[A]:TYR:CE2	2.85	0.59
1:A:551:ARG:NH2	4:A:812:HOH:O	2.29	0.59
1:B:592[A]:HIS:CD2	3:B:709:GOL:H11	2.38	0.59
1:B:294:GLN:HE21	1:B:296[A]:TYR:HE2	1.51	0.58
1:A:54:GLU:OE1	1:A:54:GLU:HA	2.04	0.58
1:B:595[B]:ARG:NH1	3:B:709:GOL:O2	2.37	0.57
1:A:296[B]:TYR:OH	3:A:714:GOL:O1	2.23	0.57
1:A:603:PRO:HG2	4:A:1032:HOH:O	2.05	0.56
1:A:296[B]:TYR:CD1	1:A:382[B]:TPQ:C5	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188[A]:ARG:NH2	4:B:813:HOH:O	2.29	0.56
1:A:519[B]:GLN:NE2	4:A:819:HOH:O	2.38	0.56
1:B:302:TYR:CB	1:B:379[A]:ILE:HD11	2.36	0.56
1:B:603[B]:PRO:CG	4:B:1109:HOH:O	2.51	0.55
1:A:595:ARG:NH1	4:A:806:HOH:O	2.32	0.54
1:B:296[B]:TYR:CE2	1:B:382[B]:TPQ:C5	2.90	0.53
3:B:718:GOL:H11	4:B:831:HOH:O	2.07	0.53
1:B:251:VAL:HG22	1:B:306:GLN:HB3	1.90	0.53
1:A:280:MET:SD	1:A:435:PHE:CE2	3.02	0.53
1:B:328:ILE:HG22	3:B:713:GOL:H31	1.91	0.52
3:B:711:GOL:O1	4:B:805:HOH:O	2.08	0.52
1:A:595:ARG:NE	3:A:709:GOL:O2	2.42	0.52
1:A:479:ARG:O	1:A:482[A]:GLU:HG2	2.09	0.52
1:A:187:THR:O	1:A:188:ARG:HG2	2.09	0.52
1:A:472[C]:ARG:NH2	3:A:711:GOL:O3	2.34	0.52
1:A:54:GLU:CG	1:A:55:ALA:N	2.73	0.51
1:B:391:TYR:CD2	3:B:706:GOL:H12	2.46	0.51
1:A:592[B]:HIS:CE1	3:A:709:GOL:HO3	2.26	0.51
1:B:53:SER:O	1:B:53:SER:OG	2.22	0.51
1:A:54:GLU:HG3	1:A:55:ALA:H	1.76	0.51
1:A:137:LEU:HD22	1:A:296[A]:TYR:CZ	2.46	0.51
1:A:599:TRP:CD2	1:A:600:PRO:HA	2.46	0.50
1:A:491[B]:THR:HG23	4:A:1304:HOH:O	2.10	0.50
1:B:137:LEU:HB3	1:B:296[A]:TYR:CE1	2.47	0.50
1:B:296[B]:TYR:HE2	1:B:382[B]:TPQ:C5	2.23	0.50
1:B:391:TYR:CG	3:B:706:GOL:H12	2.46	0.50
1:A:380:GLY:HA3	3:A:713:GOL:C3	2.41	0.50
1:A:294[A]:GLN:HG3	1:A:296[A]:TYR:OH	2.10	0.50
1:B:23:VAL:CG2	1:B:79[B]:VAL:CG2	2.90	0.50
1:B:595[B]:ARG:HD3	3:B:709:GOL:O2	2.11	0.50
1:A:472[C]:ARG:HG3	3:A:711:GOL:H11	1.94	0.50
1:B:379[A]:ILE:CG2	4:B:898:HOH:O	2.47	0.50
1:A:296[B]:TYR:HH	3:A:714:GOL:HO2	1.60	0.49
1:A:472[C]:ARG:HE	3:A:711:GOL:H2	1.76	0.49
3:A:713:GOL:H11	1:B:359:TRP:CZ2	2.47	0.49
1:B:43:GLY:HA2	3:B:713:GOL:H11	1.93	0.49
3:A:709:GOL:H32	1:B:612:ARG:NH2	2.28	0.49
1:A:50:GLY:O	1:A:52:GLY:HA2	2.13	0.49
1:A:595:ARG:HG3	3:A:709:GOL:C1	2.43	0.49
1:A:393:ASP:CG	4:A:823:HOH:O	2.50	0.48
1:A:592[B]:HIS:HE1	3:A:709:GOL:O3	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ARG:NH2	4:A:806:HOH:O	2.24	0.48
1:B:23:VAL:HG22	1:B:79[B]:VAL:CG2	2.44	0.48
1:B:595[A]:ARG:NE	3:B:709:GOL:O2	2.46	0.48
3:B:718:GOL:C1	4:B:867:HOH:O	2.38	0.48
1:B:251:VAL:CG2	1:B:306:GLN:HB3	2.44	0.48
1:A:542:TRP:CD2	1:A:567[A]:LEU:HD23	2.48	0.48
1:A:603:PRO:HG3	4:A:1032:HOH:O	2.13	0.48
1:B:472[B]:ARG:HH21	1:B:472[B]:ARG:CG	2.26	0.47
1:B:382[A]:TPQ:C6	1:B:382[A]:TPQ:H	2.25	0.47
1:A:592[A]:HIS:NE2	3:A:709:GOL:H2	2.30	0.47
1:B:603[A]:PRO:HG2	4:B:966:HOH:O	2.14	0.47
1:A:63:PHE:HB3	1:A:98:LEU:HD22	1.96	0.46
1:B:294:GLN:CG	1:B:296[A]:TYR:CZ	2.96	0.46
3:B:717:GOL:C3	4:B:822:HOH:O	2.55	0.46
1:B:263:ARG:HH11	1:B:268:LEU:N	2.13	0.46
1:A:232:VAL:HG22	1:A:238:ILE:HD12	1.97	0.46
1:A:567[A]:LEU:HD12	1:A:570[A]:TYR:CD1	2.50	0.46
3:A:713:GOL:O2	3:A:714:GOL:C2	2.63	0.46
1:A:380:GLY:HA3	3:A:713:GOL:H32	1.98	0.45
1:A:51:ALA:HA	1:A:52:GLY:HA3	1.74	0.45
1:B:9:ALA:HB3	4:B:830:HOH:O	2.17	0.45
1:B:10:SER:HB3	4:B:1207:HOH:O	2.17	0.44
3:B:706:GOL:C3	4:B:846:HOH:O	2.65	0.44
1:B:382[B]:TPQ:O2	1:B:382[B]:TPQ:HA	2.17	0.44
3:B:706:GOL:O3	3:B:716:GOL:H11	2.12	0.44
1:B:168:TRP:CD1	1:B:405[A]:VAL:HG21	2.53	0.44
1:B:370:ARG:HH12	3:B:715:GOL:C1	2.29	0.44
1:A:380:GLY:CA	3:A:714:GOL:H2	2.47	0.43
1:B:294:GLN:CG	1:B:296[A]:TYR:OH	2.56	0.43
1:A:595:ARG:CG	3:A:709:GOL:H11	2.48	0.43
1:A:380:GLY:HA3	3:A:714:GOL:H2	2.00	0.43
1:B:422:LEU:HD11	1:B:428:ALA:HB2	2.00	0.43
1:A:472[C]:ARG:HE	3:A:711:GOL:C2	2.32	0.43
4:A:1032:HOH:O	1:B:621:PRO:HD2	2.18	0.43
1:B:595[A]:ARG:NH2	4:B:802:HOH:O	2.26	0.43
1:A:76:THR:OG1	4:A:805:HOH:O	2.21	0.42
1:A:263[A]:ARG:HG2	4:A:1340:HOH:O	2.18	0.42
1:A:251:VAL:CG2	1:A:306:GLN:HB3	2.48	0.42
1:B:280:MET:HG2	1:B:299:THR:OG1	2.19	0.42
1:A:137:LEU:HB3	1:A:296[A]:TYR:CE1	2.55	0.42
1:A:380:GLY:HA3	3:A:713:GOL:H31	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ARG:NH1	3:B:708:GOL:O2	2.53	0.42
3:B:706:GOL:C2	4:B:811:HOH:O	2.68	0.42
1:A:164:GLU:HG3	4:A:1146:HOH:O	2.20	0.41
3:A:713:GOL:H11	1:B:359:TRP:CE2	2.56	0.41
1:A:282:VAL:HB	1:A:296[B]:TYR:HB2	2.01	0.41
1:B:78:SER:HB2	1:B:85[A]:ILE:HD11	2.03	0.41
1:B:479:ARG:O	1:B:482:GLU:HG2	2.20	0.41
1:A:137:LEU:HD13	1:A:296[A]:TYR:OH	2.20	0.41
1:A:188:ARG:CD	4:A:826:HOH:O	2.63	0.41
3:A:709:GOL:C3	1:B:612:ARG:NH2	2.78	0.41
1:A:621:PRO:HD2	4:B:1109:HOH:O	2.20	0.40
1:B:51:ALA:N	4:B:853:HOH:O	2.54	0.40
1:B:376:PHE:CE2	1:B:383:ASP:HB3	2.52	0.40
1:A:336:ARG:NH2	4:A:838:HOH:O	2.54	0.40
1:A:595:ARG:CD	3:A:709:GOL:H11	2.52	0.40
1:B:595[B]:ARG:HD3	3:B:709:GOL:C3	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:878:HOH:O	4:A:1320:HOH:O[2_555]	2.12	0.08
4:B:1051:HOH:O	4:B:1481:HOH:O[4_546]	2.13	0.07

## 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	635/620 (102%)	615 (97%)	18 (3%)	2 (0%)	41	18
1	B	639/620 (103%)	617 (97%)	19 (3%)	3 (0%)	29	9
All	All	1274/1240 (103%)	1232 (97%)	37 (3%)	5 (0%)	34	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	53	SER
1	B	54	GLU
1	A	55	ALA
1	A	54	GLU
1	B	136	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	530/512 (104%)	524 (99%)	6 (1%)	73	53
1	B	534/512 (104%)	528 (99%)	6 (1%)	73	53
All	All	1064/1024 (104%)	1052 (99%)	12 (1%)	84	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28[A]	ARG
1	A	28[B]	ARG
1	A	263[A]	ARG
1	A	263[B]	ARG
1	A	567[A]	LEU
1	A	567[B]	LEU
1	B	53	SER
1	B	336	ARG
1	B	379[A]	ILE
1	B	379[B]	ILE
1	B	491[A]	THR
1	B	491[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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	TPQ	A	382[B]	-	13,14,15	3.26	6 (46%)	15,19,21	1.43	1 (6%)
1	TPQ	A	382[A]	-	13,14,15	3.04	7 (53%)	15,19,21	1.60	3 (20%)
1	TPQ	B	382[A]	-	13,14,15	3.23	7 (53%)	15,19,21	1.15	0
1	TPQ	B	382[B]	-	13,14,15	3.09	5 (38%)	15,19,21	1.80	2 (13%)

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	TPQ	A	382[B]	-	-	0/5/22/24	0/1/1/1
1	TPQ	A	382[A]	-	-	2/5/22/24	0/1/1/1
1	TPQ	B	382[A]	-	-	0/5/22/24	0/1/1/1
1	TPQ	B	382[B]	-	-	2/5/22/24	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382[B]	TPQ	C1-C2	-7.22	1.38	1.49
1	B	382[B]	TPQ	C1-C2	-6.87	1.38	1.49
1	B	382[A]	TPQ	C1-C2	-6.82	1.39	1.49
1	A	382[A]	TPQ	C1-C2	-6.66	1.39	1.49
1	A	382[B]	TPQ	O5-C5	5.50	1.39	1.24
1	B	382[A]	TPQ	O5-C5	5.27	1.38	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	382[B]	TPQ	O5-C5	5.22	1.38	1.24
1	B	382[A]	TPQ	O2-C2	5.06	1.38	1.24
1	A	382[A]	TPQ	O2-C2	4.94	1.37	1.24
1	A	382[B]	TPQ	O2-C2	4.91	1.37	1.24
1	B	382[B]	TPQ	O2-C2	4.76	1.37	1.24
1	A	382[A]	TPQ	O5-C5	4.56	1.36	1.24
1	B	382[B]	TPQ	C4-C5	-2.99	1.38	1.47
1	A	382[B]	TPQ	C4-C5	-2.94	1.38	1.47
1	B	382[A]	TPQ	CB-CA	-2.86	1.47	1.53
1	A	382[B]	TPQ	C3-C4	2.69	1.39	1.35
1	A	382[A]	TPQ	C4-C5	-2.53	1.39	1.47
1	B	382[A]	TPQ	C3-C4	2.46	1.39	1.35
1	B	382[A]	TPQ	C4-C5	-2.19	1.40	1.47
1	A	382[A]	TPQ	C3-C2	-2.18	1.38	1.44
1	B	382[B]	TPQ	C6-C5	-2.10	1.39	1.44
1	A	382[A]	TPQ	C3-C4	2.06	1.38	1.35
1	A	382[B]	TPQ	C6-C5	-2.04	1.39	1.44
1	A	382[A]	TPQ	C6-C5	-2.04	1.39	1.44
1	B	382[A]	TPQ	CA-N	-2.03	1.42	1.48

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382[B]	TPQ	CB-CA-C	-4.32	103.37	111.47
1	A	382[B]	TPQ	CA-CB-C1	3.97	121.10	113.51
1	B	382[B]	TPQ	CA-CB-C1	3.80	120.77	113.51
1	A	382[A]	TPQ	C3-C4-C5	-2.73	118.43	121.26
1	A	382[A]	TPQ	CA-CB-C1	2.18	117.69	113.51
1	A	382[A]	TPQ	C6-C5-C4	2.08	120.57	117.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	382[A]	TPQ	C2-C1-CB-CA
1	B	382[B]	TPQ	C2-C1-CB-CA
1	A	382[A]	TPQ	C6-C1-CB-CA
1	B	382[B]	TPQ	C6-C1-CB-CA

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	382[B]	TPQ	5	0
1	B	382[A]	TPQ	2	0
1	B	382[B]	TPQ	10	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 2 are monoatomic - leaving 30 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	$\# Z  > 2$
3	GOL	B	714	-	5,5,5	0.30	0	5,5,5	0.26	0
3	GOL	A	707	-	5,5,5	0.39	0	5,5,5	0.87	0
3	GOL	A	709	-	5,5,5	0.44	0	5,5,5	0.50	0
3	GOL	A	711	-	5,5,5	0.45	0	5,5,5	0.26	0
3	GOL	A	706	-	5,5,5	0.26	0	5,5,5	0.23	0
3	GOL	B	716	-	5,5,5	0.14	0	5,5,5	0.82	0
3	GOL	B	709	-	5,5,5	0.34	0	5,5,5	0.33	0
3	GOL	A	714	-	5,5,5	0.31	0	5,5,5	0.61	0
3	GOL	B	711	-	5,5,5	0.34	0	5,5,5	0.16	0
3	GOL	A	708	-	5,5,5	0.31	0	5,5,5	0.46	0
3	GOL	B	704	-	5,5,5	0.16	0	5,5,5	0.18	0
3	GOL	B	710	-	5,5,5	0.34	0	5,5,5	0.27	0
3	GOL	B	712	-	5,5,5	0.35	0	5,5,5	0.49	0
3	GOL	A	702	-	5,5,5	0.23	0	5,5,5	0.26	0
3	GOL	B	715	-	5,5,5	0.34	0	5,5,5	0.23	0
3	GOL	B	707	-	5,5,5	0.39	0	5,5,5	0.13	0
3	GOL	B	718	-	5,5,5	0.34	0	5,5,5	0.31	0
3	GOL	B	702	-	5,5,5	0.25	0	5,5,5	0.31	0
3	GOL	A	710	-	5,5,5	0.43	0	5,5,5	0.35	0
3	GOL	A	705	-	5,5,5	0.23	0	5,5,5	0.34	0
3	GOL	B	703	-	5,5,5	0.43	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	704	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	B	717	-	5,5,5	0.21	0	5,5,5	0.59	0
3	GOL	B	706	-	5,5,5	0.13	0	5,5,5	0.52	0
3	GOL	A	712	-	5,5,5	0.36	0	5,5,5	0.24	0
3	GOL	B	705	-	5,5,5	0.30	0	5,5,5	0.29	0
3	GOL	A	713	-	5,5,5	0.20	0	5,5,5	0.30	0
3	GOL	A	703	-	5,5,5	0.36	0	5,5,5	1.02	0
3	GOL	B	713	-	5,5,5	0.32	0	5,5,5	0.54	0
3	GOL	B	708	-	5,5,5	0.47	0	5,5,5	0.26	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
3	GOL	B	714	-	-	2/4/4/4	-
3	GOL	A	707	-	-	0/4/4/4	-
3	GOL	A	709	-	-	4/4/4/4	-
3	GOL	A	711	-	-	1/4/4/4	-
3	GOL	A	706	-	-	2/4/4/4	-
3	GOL	B	716	-	-	0/4/4/4	-
3	GOL	B	709	-	-	4/4/4/4	-
3	GOL	A	714	-	-	4/4/4/4	-
3	GOL	B	711	-	-	0/4/4/4	-
3	GOL	A	708	-	-	2/4/4/4	-
3	GOL	B	704	-	-	0/4/4/4	-
3	GOL	B	710	-	-	0/4/4/4	-
3	GOL	B	712	-	-	4/4/4/4	-
3	GOL	A	702	-	-	4/4/4/4	-
3	GOL	B	715	-	-	4/4/4/4	-
3	GOL	B	707	-	-	0/4/4/4	-
3	GOL	B	718	-	-	4/4/4/4	-
3	GOL	B	702	-	-	1/4/4/4	-
3	GOL	A	710	-	-	4/4/4/4	-
3	GOL	A	705	-	-	2/4/4/4	-
3	GOL	B	703	-	-	0/4/4/4	-
3	GOL	A	704	-	-	0/4/4/4	-
3	GOL	B	717	-	-	2/4/4/4	-
3	GOL	B	706	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	712	-	-	4/4/4/4	-
3	GOL	B	705	-	-	0/4/4/4	-
3	GOL	A	713	-	-	4/4/4/4	-
3	GOL	A	703	-	-	4/4/4/4	-
3	GOL	B	713	-	-	2/4/4/4	-
3	GOL	B	708	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GOL	O1-C1-C2-C3
3	A	702	GOL	C1-C2-C3-O3
3	A	703	GOL	C1-C2-C3-O3
3	A	705	GOL	C1-C2-C3-O3
3	A	706	GOL	O1-C1-C2-C3
3	A	708	GOL	O1-C1-C2-C3
3	A	709	GOL	O1-C1-C2-O2
3	A	709	GOL	O1-C1-C2-C3
3	A	709	GOL	C1-C2-C3-O3
3	A	712	GOL	O1-C1-C2-C3
3	A	712	GOL	C1-C2-C3-O3
3	A	713	GOL	C1-C2-C3-O3
3	A	714	GOL	O1-C1-C2-C3
3	A	714	GOL	C1-C2-C3-O3
3	B	708	GOL	O1-C1-C2-C3
3	B	708	GOL	C1-C2-C3-O3
3	B	709	GOL	C1-C2-C3-O3
3	B	712	GOL	O1-C1-C2-C3
3	B	712	GOL	C1-C2-C3-O3
3	B	715	GOL	O1-C1-C2-C3
3	B	717	GOL	O1-C1-C2-C3
3	B	718	GOL	C1-C2-C3-O3
3	A	713	GOL	O2-C2-C3-O3
3	B	709	GOL	O2-C2-C3-O3
3	B	715	GOL	O2-C2-C3-O3
3	A	710	GOL	O1-C1-C2-C3
3	A	710	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	713	GOL	O1-C1-C2-C3
3	B	709	GOL	O1-C1-C2-C3
3	B	713	GOL	C1-C2-C3-O3
3	B	715	GOL	C1-C2-C3-O3
3	B	718	GOL	O1-C1-C2-C3
3	A	702	GOL	O1-C1-C2-O2
3	A	706	GOL	O1-C1-C2-O2
3	A	709	GOL	O2-C2-C3-O3
3	A	710	GOL	O1-C1-C2-O2
3	A	710	GOL	O2-C2-C3-O3
3	A	714	GOL	O2-C2-C3-O3
3	B	708	GOL	O1-C1-C2-O2
3	B	709	GOL	O1-C1-C2-O2
3	B	712	GOL	O2-C2-C3-O3
3	B	713	GOL	O2-C2-C3-O3
3	B	717	GOL	O1-C1-C2-O2
3	B	718	GOL	O2-C2-C3-O3
3	A	702	GOL	O2-C2-C3-O3
3	A	703	GOL	O2-C2-C3-O3
3	A	705	GOL	O2-C2-C3-O3
3	A	712	GOL	O1-C1-C2-O2
3	A	712	GOL	O2-C2-C3-O3
3	A	713	GOL	O1-C1-C2-O2
3	A	714	GOL	O1-C1-C2-O2
3	B	708	GOL	O2-C2-C3-O3
3	B	712	GOL	O1-C1-C2-O2
3	B	715	GOL	O1-C1-C2-O2
3	A	703	GOL	O1-C1-C2-O2
3	B	714	GOL	O1-C1-C2-O2
3	B	718	GOL	O1-C1-C2-O2
3	A	708	GOL	O1-C1-C2-O2
3	B	714	GOL	O1-C1-C2-C3
3	A	703	GOL	O1-C1-C2-C3
3	A	711	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	709	GOL	14	0
3	A	711	GOL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	716	GOL	5	0
3	B	709	GOL	11	0
3	A	714	GOL	8	0
3	B	711	GOL	1	0
3	A	708	GOL	1	0
3	B	715	GOL	2	0
3	B	718	GOL	4	0
3	B	717	GOL	2	0
3	B	706	GOL	10	0
3	A	713	GOL	9	0
3	B	713	GOL	2	0
3	B	708	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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	619/620 (99%)	-0.18	24 (3%)	39 44	9, 21, 40, 116	0
1	B	619/620 (99%)	-0.38	16 (2%)	56 61	8, 17, 31, 115	0
All	All	1238/1240 (99%)	-0.28	40 (3%)	47 52	8, 19, 38, 116	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	52	GLY	16.4
1	B	53	SER	10.5
1	A	53	SER	10.1
1	A	55	ALA	9.0
1	B	52	GLY	8.7
1	B	54	GLU	8.5
1	B	51	ALA	7.3
1	A	51	ALA	7.0
1	A	50	GLY	6.4
1	A	54	GLU	5.6
1	A	313	LEU	5.6
1	A	266	ASP	4.9
1	A	105	PHE	4.8
1	A	9	ALA	4.2
1	B	266	ASP	4.0
1	B	313	LEU	3.8
1	A	413	GLU	3.7
1	B	225	PRO	3.5
1	B	55	ALA	3.4
1	B	50	GLY	3.3
1	A	56[A]	GLU	3.2
1	A	414	GLY	2.8
1	A	48	ALA	2.8
1	B	9	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	628	ASN	2.6
1	B	414	GLY	2.5
1	A	312	GLU	2.5
1	B	628	ASN	2.4
1	A	315	CYS	2.3
1	A	84	VAL	2.3
1	B	56	GLU	2.3
1	A	68	SER	2.2
1	A	314	GLY	2.2
1	A	462	PRO	2.2
1	B	413	GLU	2.1
1	A	339	ARG	2.1
1	B	263	ARG	2.1
1	A	376	PHE	2.1
1	B	462	PRO	2.0
1	A	265	GLY	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	TPQ	A	382[A]	14/15	0.93	0.13	16,19,21,22	11
1	TPQ	A	382[B]	14/15	0.93	0.13	16,19,21,21	11
1	TPQ	B	382[A]	14/15	0.95	0.12	14,19,21,22	11
1	TPQ	B	382[B]	14/15	0.95	0.12	14,18,20,22	11

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	711	6/6	0.66	0.27	34,42,43,44	6
3	GOL	B	708	6/6	0.67	0.27	38,45,50,53	0
3	GOL	B	714	6/6	0.69	0.16	58,60,60,61	0
3	GOL	A	712	6/6	0.70	0.24	37,45,49,53	0
3	GOL	A	709	6/6	0.71	0.34	36,39,44,49	0
3	GOL	B	716	6/6	0.72	0.28	29,35,39,42	6
3	GOL	B	709	6/6	0.74	0.38	49,55,58,59	0
3	GOL	A	714	6/6	0.75	0.19	28,32,36,39	6
3	GOL	B	710	6/6	0.75	0.20	62,64,65,65	0
3	GOL	A	713	6/6	0.77	0.25	30,31,32,33	6
3	GOL	A	708	6/6	0.79	0.17	33,42,46,48	0
3	GOL	A	710	6/6	0.82	0.14	28,42,46,47	0
3	GOL	A	706	6/6	0.82	0.15	50,54,56,58	0
3	GOL	B	702	6/6	0.83	0.17	32,41,42,48	0
3	GOL	A	704	6/6	0.83	0.15	29,40,42,42	0
3	GOL	B	715	6/6	0.85	0.16	27,41,43,43	0
3	GOL	A	702	6/6	0.86	0.15	44,47,48,50	0
3	GOL	A	705	6/6	0.87	0.12	29,39,40,45	0
3	GOL	B	706	6/6	0.88	0.17	25,37,38,41	6
3	GOL	B	711	6/6	0.89	0.14	23,40,46,47	0
3	GOL	B	705	6/6	0.89	0.10	28,31,32,35	0
3	GOL	B	712	6/6	0.90	0.13	21,29,30,33	0
3	GOL	B	717	6/6	0.90	0.24	32,39,43,47	0
3	GOL	B	718	6/6	0.91	0.20	37,46,48,49	0
3	GOL	B	713	6/6	0.92	0.13	17,30,35,40	0
3	GOL	B	707	6/6	0.92	0.10	22,26,30,33	0
3	GOL	B	704	6/6	0.92	0.09	29,29,30,30	0
3	GOL	A	707	6/6	0.93	0.13	20,27,29,30	0
3	GOL	A	703	6/6	0.95	0.10	28,30,31,31	0
3	GOL	B	703	6/6	0.98	0.06	12,13,14,15	0
2	CU	B	701	1/1	0.99	0.03	14,14,14,14	0
2	CU	A	701	1/1	1.00	0.03	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.