



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 2POT / pdb_00002pot
Title : tRNA guanine transglycosylase (TGT) E235Q mutant in complex with guanine
Authors : Tidten, N.; Heine, A.; Reuter, K.; Klebe, G.
Deposited on : 2007-04-27
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

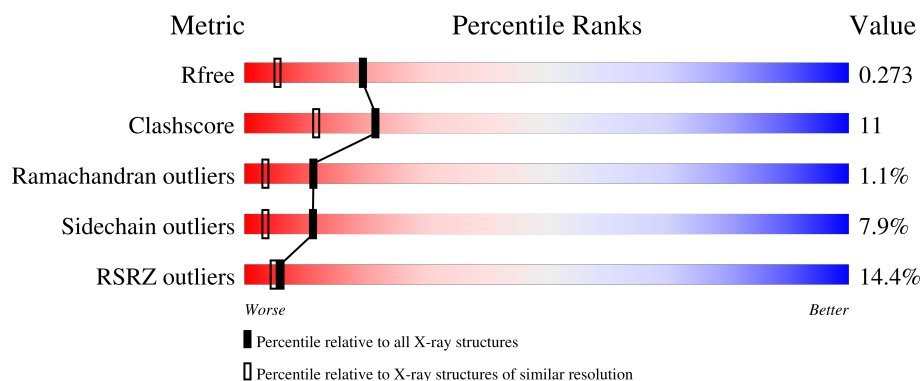
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	386	

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
3	GUN	A	600	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	706	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2836 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 Queuine tRNA-ribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2696	1697	482	498	19	0	1	0

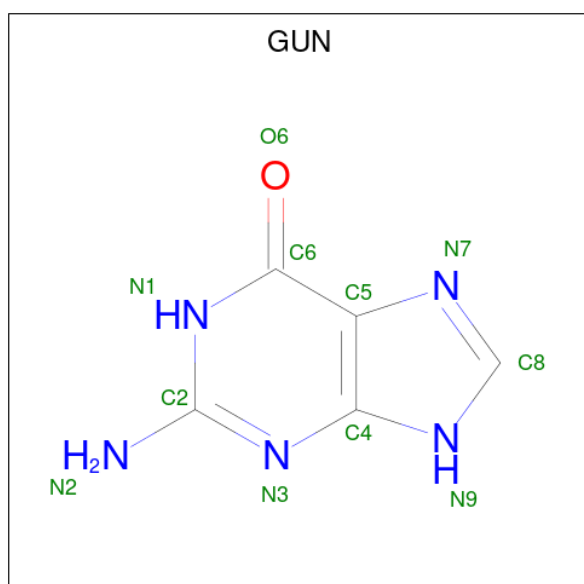
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLN	GLU	engineered mutation	UNP P28720
A	312	LYS	THR	SEE REMARK 999	UNP P28720

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

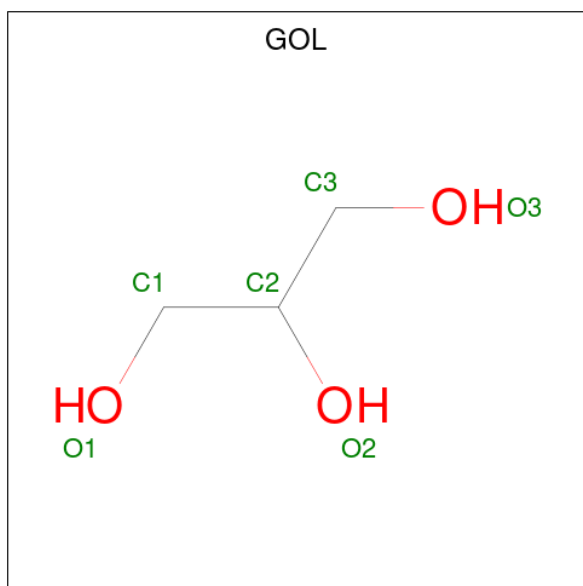
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is GUANINE (CCD ID: GUN) (formula: C₅H₅N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	5	5	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

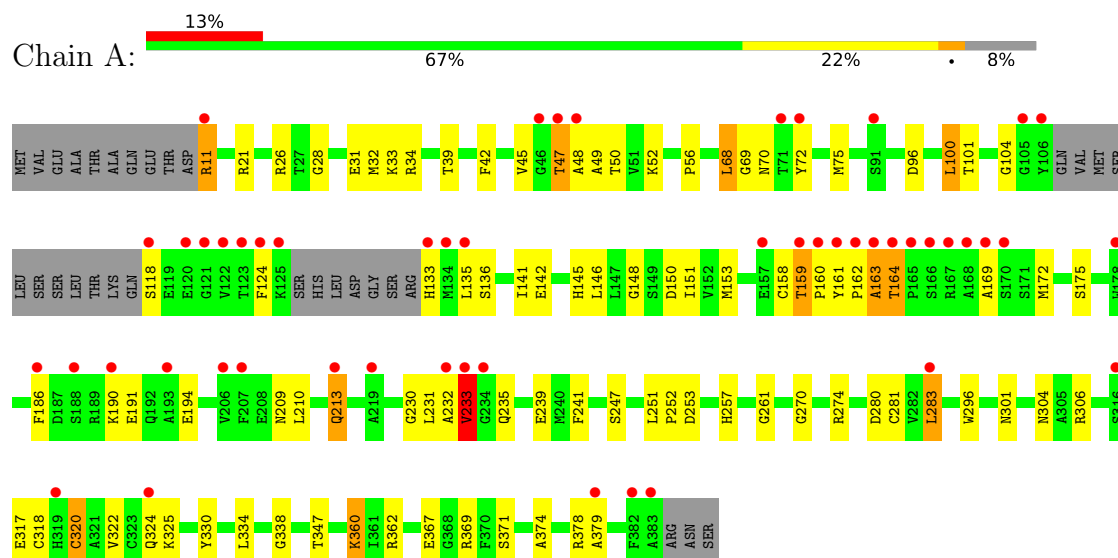
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		

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: Queuine tRNA-ribosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.14Å 63.69Å 71.10Å 90.00° 92.87° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.80) 91.8 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 1.80Å)	Xtriage
Refinement program	CNS, SHELXL-97	Depositor
R, R_{free}	0.219 , 0.286 0.220 , 0.273	Depositor DCC
R_{free} test set	3388 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2836	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, GUN, GOL

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	0.46	0/2757	1.45	20/3726 (0.5%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	GLY	CA-C-N	10.22	131.28	119.94
1	A	104	GLY	C-N-CA	10.22	131.28	119.94
1	A	162	PRO	CA-C-N	8.65	137.26	121.70
1	A	162	PRO	C-N-CA	8.65	137.26	121.70
1	A	186	PHE	CA-CB-CG	8.25	122.05	113.80
1	A	39	THR	O-C-N	8.07	129.24	121.66
1	A	39	THR	CA-C-O	-7.22	111.38	120.04
1	A	163	ALA	CA-C-N	6.98	138.82	121.80
1	A	163	ALA	C-N-CA	6.98	138.82	121.80
1	A	42	PHE	CA-CB-CG	-6.11	107.69	113.80
1	A	247	SER	CA-C-N	6.07	124.06	120.24
1	A	247	SER	C-N-CA	6.07	124.06	120.24
1	A	379	ALA	CA-C-N	5.84	128.36	120.65
1	A	379	ALA	C-N-CA	5.84	128.36	120.65
1	A	301	ASN	N-CA-CB	5.73	119.82	110.37
1	A	136	SER	CA-C-O	-5.54	115.89	120.71
1	A	230	GLY	CA-C-N	-5.39	114.19	122.60
1	A	230	GLY	C-N-CA	-5.39	114.19	122.60
1	A	70	ASN	CA-C-N	5.27	127.29	120.44
1	A	70	ASN	C-N-CA	5.27	127.29	120.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2696	0	2567	57	0
2	A	1	0	0	0	0
3	A	11	0	5	1	0
4	A	42	0	56	13	0
5	A	86	0	0	3	0
All	All	2836	0	2628	58	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 11.

All (58) 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:318:CYS:SG	1:A:320:CYS:HB3	2.23	0.78
1:A:28:GLY:HA2	4:A:701:GOL:H12	1.68	0.74
1:A:362:ARG:HD2	4:A:701:GOL:H31	1.74	0.69
1:A:190:LYS:O	1:A:194:GLU:HG3	1.93	0.67
1:A:304:ASN:OD1	1:A:306:ARG:HG2	1.94	0.66
1:A:320:CYS:O	1:A:324:GLN:HG2	1.97	0.64
1:A:317:GLU:OE1	4:A:706:GOL:H32	1.99	0.62
1:A:100:LEU:HD11	1:A:153:MET:SD	2.40	0.62
1:A:296:TRP:CG	4:A:706:GOL:HO3	2.20	0.59
1:A:232:ALA:O	1:A:233:VAL:HG23	2.03	0.59
1:A:161:TYR:CE2	1:A:235:GLN:HG3	2.37	0.59
1:A:34:ARG:HD2	1:A:150:ASP:OD2	2.06	0.56
1:A:11:ARG:HD3	1:A:33:LYS:O	2.05	0.56
1:A:100:LEU:HD22	1:A:151:ILE:HG21	1.87	0.55
1:A:172:MET:HE1	1:A:213:GLN:NE2	2.21	0.55
1:A:252:PRO:O	1:A:257:HIS:HE1	1.90	0.55
1:A:320:CYS:SG	1:A:322:VAL:HB	2.46	0.55
1:A:158:CYS:O	1:A:160:PRO:HD3	2.08	0.54
1:A:28:GLY:CA	4:A:701:GOL:H12	2.35	0.53
1:A:360:LYS:HE3	4:A:706:GOL:C1	2.38	0.52
1:A:360:LYS:HE3	4:A:706:GOL:H12	1.90	0.52
1:A:281:CYS:SG	1:A:283:LEU:HB2	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:O	4:A:717:GOL:H32	2.10	0.51
1:A:96:ASP:OD1	4:A:702:GOL:H12	2.10	0.51
1:A:261:GLY:HA2	4:A:703:GOL:H31	1.91	0.50
1:A:172:MET:HE1	1:A:213:GLN:CD	2.36	0.50
1:A:100:LEU:HD22	1:A:151:ILE:CG2	2.43	0.48
1:A:52:LYS:O	1:A:347:THR:HG21	2.15	0.47
1:A:69:GLY:O	1:A:101:THR:HA	2.15	0.46
1:A:11:ARG:O	1:A:33:LYS:HE3	2.16	0.46
1:A:148:GLY:HA2	4:A:705:GOL:H12	1.98	0.46
1:A:47:THR:O	1:A:48:ALA:HB3	2.17	0.46
1:A:374:ALA:O	1:A:378:ARG:HG3	2.15	0.45
1:A:169:ALA:HB2	1:A:210:LEU:HD13	1.98	0.45
1:A:31:GLU:HG3	5:A:721:HOH:O	2.16	0.45
1:A:191:GLU:H	1:A:191:GLU:CD	2.25	0.45
1:A:367:GLU:OE1	1:A:369:ARG:NH2	2.50	0.45
1:A:124:PHE:O	1:A:133:HIS:N	2.50	0.44
1:A:21[B]:ARG:NH1	1:A:253:ASP:OD1	2.50	0.44
1:A:233:VAL:O	1:A:233:VAL:HG12	2.16	0.44
1:A:280:ASP:O	1:A:281:CYS:HB2	2.17	0.44
1:A:169:ALA:HB2	1:A:210:LEU:CD1	2.47	0.43
1:A:330:TYR:CE2	1:A:334:LEU:HD11	2.53	0.43
1:A:338:GLY:HA2	5:A:773:HOH:O	2.18	0.43
1:A:320:CYS:O	1:A:324:GLN:NE2	2.50	0.43
3:A:600:GUN:HN9	4:A:703:GOL:H11	1.83	0.43
1:A:72:TYR:O	1:A:75:MET:HG2	2.19	0.42
1:A:45:VAL:HG13	1:A:68:LEU:CD2	2.49	0.42
1:A:161:TYR:CZ	1:A:235:GLN:HG3	2.54	0.42
1:A:48:ALA:O	1:A:49:ALA:HB3	2.20	0.42
1:A:270:GLY:O	1:A:274:ARG:HG3	2.20	0.42
1:A:142:GLU:O	1:A:146:LEU:HG	2.20	0.42
1:A:11:ARG:NH1	1:A:32:MET:O	2.50	0.42
1:A:56:PRO:HD2	5:A:724:HOH:O	2.20	0.41
1:A:191:GLU:OE1	1:A:191:GLU:N	2.50	0.41
1:A:241:PHE:CZ	1:A:270:GLY:HA3	2.55	0.41
1:A:145:HIS:CE1	4:A:705:GOL:HO1	2.36	0.40
1:A:209:ASN:ND2	1:A:210:LEU:HD23	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	350/386 (91%)	336 (96%)	10 (3%)	4 (1%)	11 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	ALA
1	A	164	THR
1	A	159	THR
1	A	233	VAL

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	267/315 (85%)	246 (92%)	21 (8%)	11 3

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	26	ARG
1	A	47	THR
1	A	50	THR
1	A	68	LEU
1	A	100	LEU
1	A	118	SER

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Mol	Chain	Res	Type
1	A	135	LEU
1	A	141	ILE
1	A	159	THR
1	A	164	THR
1	A	175	SER
1	A	213	GLN
1	A	231	LEU
1	A	233	VAL
1	A	239	GLU
1	A	283	LEU
1	A	320	CYS
1	A	325	LYS
1	A	360	LYS
1	A	371	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	ASN
1	A	213	GLN
1	A	257	HIS
1	A	375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
4	GOL	A	705	-	5,5,5	0.32	0	5,5,5	0.32	0
4	GOL	A	717	-	5,5,5	0.27	0	5,5,5	0.31	0
4	GOL	A	703	-	5,5,5	0.32	0	5,5,5	0.26	0
4	GOL	A	706	-	5,5,5	0.30	0	5,5,5	0.36	0
4	GOL	A	702	-	5,5,5	0.38	0	5,5,5	0.41	0
4	GOL	A	701	-	5,5,5	0.26	0	5,5,5	0.30	0
3	GUN	A	600	-	12,12,12	2.62	8 (66%)	15,17,17	3.16	8 (53%)
4	GOL	A	700	-	5,5,5	0.26	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	705	-	-	4/4/4/4	-
4	GOL	A	717	-	-	4/4/4/4	-
4	GOL	A	703	-	-	4/4/4/4	-
4	GOL	A	706	-	-	2/4/4/4	-
4	GOL	A	702	-	-	4/4/4/4	-
4	GOL	A	701	-	-	4/4/4/4	-
3	GUN	A	600	-	-	-	0/2/2/2
4	GOL	A	700	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	GUN	C4-N3	5.17	1.44	1.36
3	A	600	GUN	C6-N1	-3.72	1.31	1.38
3	A	600	GUN	C8-N7	-2.84	1.26	1.33
3	A	600	GUN	C5-N7	2.55	1.44	1.39
3	A	600	GUN	C4-N9	-2.45	1.31	1.36
3	A	600	GUN	C8-N9	-2.44	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	600	GUN	C5-C4	-2.26	1.33	1.39
3	A	600	GUN	C2-N1	-2.02	1.32	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	GUN	C4-C5-N7	-5.82	101.06	110.17
3	A	600	GUN	C6-C5-N7	5.33	139.99	130.29
3	A	600	GUN	C2-N3-C4	4.54	121.37	113.36
3	A	600	GUN	C5-C4-N9	4.29	112.30	106.17
3	A	600	GUN	N9-C4-N3	3.42	130.15	125.99
3	A	600	GUN	C8-N7-C5	3.39	108.96	104.38
3	A	600	GUN	O6-C6-C5	-2.98	118.66	126.53
3	A	600	GUN	N9-C8-N7	-2.19	110.44	112.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	GOL	C1-C2-C3-O3
4	A	703	GOL	O1-C1-C2-C3
4	A	701	GOL	O2-C2-C3-O3
4	A	705	GOL	O1-C1-C2-C3
4	A	717	GOL	C1-C2-C3-O3
4	A	703	GOL	O2-C2-C3-O3
4	A	702	GOL	O1-C1-C2-C3
4	A	703	GOL	C1-C2-C3-O3
4	A	701	GOL	O1-C1-C2-C3
4	A	701	GOL	C1-C2-C3-O3
4	A	705	GOL	C1-C2-C3-O3
4	A	706	GOL	C1-C2-C3-O3
4	A	717	GOL	O1-C1-C2-C3
4	A	702	GOL	O2-C2-C3-O3
4	A	703	GOL	O1-C1-C2-O2
4	A	705	GOL	O1-C1-C2-O2
4	A	717	GOL	O2-C2-C3-O3
4	A	702	GOL	O1-C1-C2-O2
4	A	705	GOL	O2-C2-C3-O3
4	A	701	GOL	O1-C1-C2-O2
4	A	706	GOL	O2-C2-C3-O3
4	A	717	GOL	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	GOL	2	0
4	A	717	GOL	1	0
4	A	703	GOL	2	0
4	A	706	GOL	4	0
4	A	702	GOL	1	0
4	A	701	GOL	3	0
3	A	600	GUN	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, 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	355/386 (91%)	0.90	51 (14%) 6 5	18, 36, 61, 92	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	PHE	5.6
1	A	163	ALA	5.5
1	A	47	THR	4.7
1	A	382	PHE	4.6
1	A	134	MET	4.2
1	A	161	TYR	4.0
1	A	106	TYR	3.9
1	A	169	ALA	3.8
1	A	159	THR	3.8
1	A	125	LYS	3.8
1	A	383	ALA	3.7
1	A	162	PRO	3.7
1	A	121	GLY	3.6
1	A	157	GLU	3.4
1	A	168	ALA	3.4
1	A	166	SER	3.4
1	A	316	SER	3.3
1	A	160	PRO	3.3
1	A	232	ALA	3.3
1	A	233	VAL	3.3
1	A	72	TYR	3.2
1	A	170	SER	3.2
1	A	120	GLU	3.1
1	A	164	THR	3.1
1	A	165	PRO	3.1
1	A	206	VAL	3.0
1	A	122	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	213	GLN	2.8
1	A	193	ALA	2.7
1	A	133	HIS	2.7
1	A	124	PHE	2.7
1	A	11	ARG	2.6
1	A	123	THR	2.6
1	A	46	GLY	2.6
1	A	118	SER	2.6
1	A	190	LYS	2.5
1	A	379	ALA	2.4
1	A	178	TRP	2.4
1	A	283	LEU	2.4
1	A	135	LEU	2.4
1	A	71	THR	2.3
1	A	219	ALA	2.3
1	A	324	GLN	2.3
1	A	167	ARG	2.2
1	A	105	GLY	2.2
1	A	186	PHE	2.2
1	A	319	HIS	2.1
1	A	234	GLY	2.1
1	A	48	ALA	2.1
1	A	91	SER	2.0
1	A	188	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	705	6/6	0.68	0.23	59,63,66,76	0
4	GOL	A	703	6/6	0.78	0.17	41,67,81,82	0
4	GOL	A	706	6/6	0.78	0.21	66,70,76,89	0
4	GOL	A	700	6/6	0.79	0.15	50,52,63,65	0
4	GOL	A	701	6/6	0.81	0.17	41,54,63,64	0
4	GOL	A	717	6/6	0.81	0.18	49,69,76,78	0
3	GUN	A	600	11/11	0.83	0.12	44,53,56,59	11
4	GOL	A	702	6/6	0.88	0.16	38,46,52,64	0
2	ZN	A	500	1/1	0.99	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.