



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 03:48 am BST

PDB ID : 5Z5E
Title : Crystal structure of the Glycyl-tRNA synthetase (GlyRS) in Nanoarchaeum equitans
Authors : Noguchi, H.; Park, S.Y.; Tamura, K.
Deposited on : 2018-01-18
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

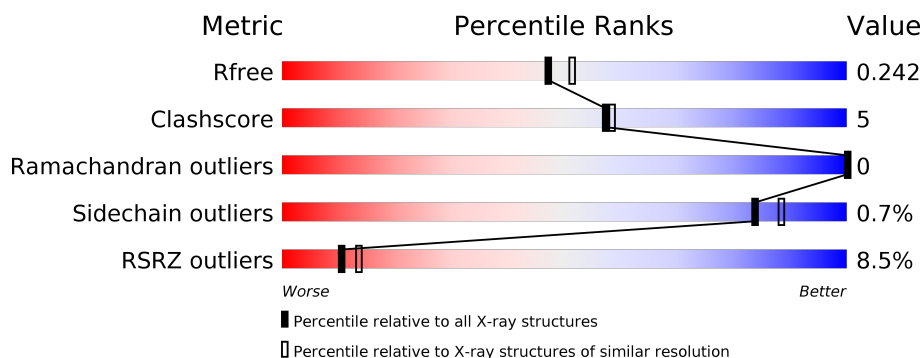
1 Overall quality at a glance

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	534	<div> <div>8%</div> <div> <div></div> <div>70%</div> <div>12%</div> <div>17%</div> </div> </div>
1	B	534	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8008 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 NEQ417.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3726	2434	616	669	7			
1	B	468	Total	C	N	O	S	0	0	0
			3923	2557	651	707	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q74N31
A	-20	GLY	-	expression tag	UNP Q74N31
A	-19	SER	-	expression tag	UNP Q74N31
A	-18	SER	-	expression tag	UNP Q74N31
A	-17	HIS	-	expression tag	UNP Q74N31
A	-16	HIS	-	expression tag	UNP Q74N31
A	-15	HIS	-	expression tag	UNP Q74N31
A	-14	HIS	-	expression tag	UNP Q74N31
A	-13	HIS	-	expression tag	UNP Q74N31
A	-12	HIS	-	expression tag	UNP Q74N31
A	-11	SER	-	expression tag	UNP Q74N31
A	-10	SER	-	expression tag	UNP Q74N31
A	-9	GLY	-	expression tag	UNP Q74N31
A	-8	LEU	-	expression tag	UNP Q74N31
A	-7	VAL	-	expression tag	UNP Q74N31
A	-6	PRO	-	expression tag	UNP Q74N31
A	-5	ARG	-	expression tag	UNP Q74N31
A	-4	GLY	-	expression tag	UNP Q74N31
A	-3	SER	-	expression tag	UNP Q74N31
A	-2	HIS	-	expression tag	UNP Q74N31
A	-1	MET	-	expression tag	UNP Q74N31
A	0	LEU	-	expression tag	UNP Q74N31
A	1	GLU	-	expression tag	UNP Q74N31
A	3	PRO	LEU	engineered mutation	UNP Q74N31
B	-21	MET	-	initiating methionine	UNP Q74N31

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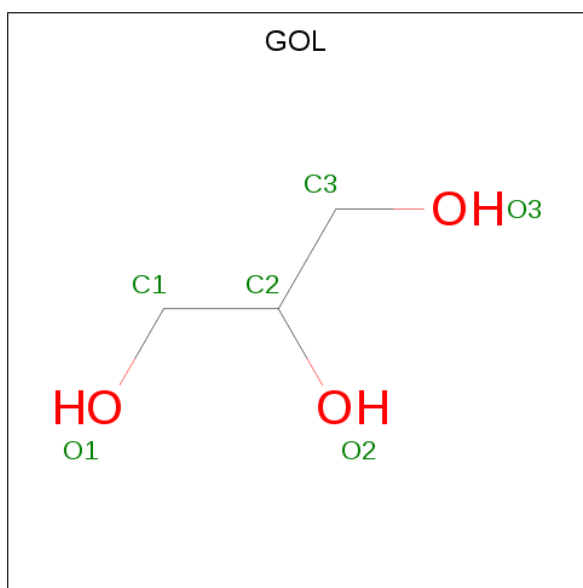
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	GLY	-	expression tag	UNP Q74N31
B	-19	SER	-	expression tag	UNP Q74N31
B	-18	SER	-	expression tag	UNP Q74N31
B	-17	HIS	-	expression tag	UNP Q74N31
B	-16	HIS	-	expression tag	UNP Q74N31
B	-15	HIS	-	expression tag	UNP Q74N31
B	-14	HIS	-	expression tag	UNP Q74N31
B	-13	HIS	-	expression tag	UNP Q74N31
B	-12	HIS	-	expression tag	UNP Q74N31
B	-11	SER	-	expression tag	UNP Q74N31
B	-10	SER	-	expression tag	UNP Q74N31
B	-9	GLY	-	expression tag	UNP Q74N31
B	-8	LEU	-	expression tag	UNP Q74N31
B	-7	VAL	-	expression tag	UNP Q74N31
B	-6	PRO	-	expression tag	UNP Q74N31
B	-5	ARG	-	expression tag	UNP Q74N31
B	-4	GLY	-	expression tag	UNP Q74N31
B	-3	SER	-	expression tag	UNP Q74N31
B	-2	HIS	-	expression tag	UNP Q74N31
B	-1	MET	-	expression tag	UNP Q74N31
B	0	LEU	-	expression tag	UNP Q74N31
B	1	GLU	-	expression tag	UNP Q74N31
B	3	PRO	LEU	engineered mutation	UNP Q74N31

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



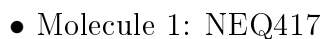
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total 157	O 157	0	0
4	B	138	Total 138	O 138	0	0

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- Molecule 1: NEQ417



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.41Å 121.10Å 133.63Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	48.20 – 2.10 48.20 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.20-2.10) 95.8 (48.20-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.201 , 0.242 0.201 , 0.242	Depositor DCC
R_{free} test set	3568 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8008	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: GOL, SO4

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	0.40	0/3822	0.53	0/5161
1	B	0.40	0/4021	0.54	0/5431
All	All	0.40	0/7843	0.53	0/10592

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3726	0	3721	47	0
1	B	3923	0	3933	34	0
2	A	15	0	0	0	0
2	B	25	0	0	0	0
3	A	6	0	8	1	0
3	B	18	0	24	2	0
4	A	157	0	0	3	0
4	B	138	0	0	2	0
All	All	8008	0	7686	76	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 5.

All (76) 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:476:ASP:OD2	1:A:497:ARG:NH2	2.21	0.73
1:A:420:VAL:HG23	1:A:449:ILE:HG23	1.72	0.72
1:A:392:GLU:HG2	1:A:405:LYS:HB3	1.71	0.71
1:A:411:ILE:HG13	1:A:412:PRO:HD2	1.71	0.69
1:A:484:THR:HG22	1:A:499:LYS:HD2	1.76	0.67
1:B:247:GLU:OE1	4:B:701:HOH:O	2.16	0.62
1:A:153:LEU:HD13	1:B:172:VAL:HG21	1.80	0.62
1:A:214:LYS:NZ	1:A:231:GLU:OE2	2.32	0.61
1:A:170:GLU:OE2	1:A:174:LYS:NZ	2.33	0.61
1:A:289:LYS:NZ	1:A:293:GLU:OE2	2.33	0.61
1:B:230:ARG:HH22	3:B:606:GOL:H31	1.66	0.59
1:B:153:LEU:HD12	1:B:168:ILE:HD11	1.83	0.59
1:B:411:ILE:HG13	1:B:412:PRO:HD2	1.84	0.58
1:B:23:ALA:HB3	3:B:606:GOL:H11	1.85	0.57
1:A:65:LYS:HG3	1:A:181:TYR:HE2	1.70	0.56
1:B:162:GLU:HA	1:B:165:ILE:HD12	1.89	0.55
1:B:312:LYS:NZ	1:B:317:LYS:O	2.41	0.53
1:A:474:THR:HB	1:A:486:THR:CG2	2.39	0.53
1:B:474:THR:HB	1:B:486:THR:HG22	1.91	0.53
1:A:145:ASP:OD1	1:A:171:ARG:NH1	2.42	0.53
1:A:434:LYS:HB3	1:A:475:ILE:HG21	1.92	0.52
1:A:474:THR:HB	1:A:486:THR:HG23	1.91	0.52
1:B:359:GLN:HE21	1:B:362:ASN:HA	1.76	0.51
1:A:149:ALA:HB2	1:A:171:ARG:HB3	1.93	0.51
1:A:230:ARG:HH12	3:A:604:GOL:H2	1.75	0.51
1:A:146:SER:HB3	1:A:175:MET:HG3	1.92	0.51
1:B:150:LEU:HD23	1:B:153:LEU:HD22	1.93	0.50
1:A:171:ARG:NH1	1:A:174:LYS:HD2	2.27	0.50
1:A:419:LYS:HA	1:A:470:PRO:HD2	1.93	0.50
1:B:360:LYS:NZ	1:B:361:ASP:OD2	2.34	0.50
1:A:141:TYR:OH	1:B:150:LEU:HD13	2.12	0.50
1:A:459:ARG:HG3	1:A:463:ARG:NH1	2.26	0.49
1:B:418:ILE:HD13	1:B:450:ILE:HG13	1.94	0.49
1:B:131:VAL:O	1:B:132:LYS:HD2	2.11	0.49
1:A:411:ILE:HG13	1:A:412:PRO:CD	2.43	0.48
1:A:439:TYR:CD1	1:A:451:TYR:HB2	2.48	0.48
1:B:301:ARG:HD2	1:B:386:LEU:HD22	1.95	0.48
1:A:150:LEU:HD23	1:A:153:LEU:HD12	1.95	0.47
1:B:419:LYS:HA	1:B:470:PRO:HD2	1.97	0.47
1:A:153:LEU:HD23	1:A:168:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLU:OE1	1:B:171:ARG:NH2	2.44	0.46
1:A:171:ARG:HH12	1:A:174:LYS:HD2	1.80	0.46
1:A:154:LYS:HE3	1:A:154:LYS:HB2	1.65	0.46
1:A:456:SER:OG	4:A:701:HOH:O	2.21	0.45
1:B:338:HIS:O	1:B:370:LEU:HD12	2.16	0.45
1:A:172:VAL:HA	1:A:175:MET:HE3	1.99	0.45
1:B:262:ASP:OD2	1:B:266:ASN:HB2	2.17	0.45
1:B:486:THR:HG23	4:B:758:HOH:O	2.18	0.44
1:A:487:ILE:HD12	1:A:498:VAL:HG21	2.00	0.44
1:A:17:GLU:OE2	1:B:196:ARG:NH2	2.45	0.44
1:A:271:LYS:HD2	1:A:273:LYS:HE2	1.99	0.44
1:B:410:LYS:HB3	1:B:410:LYS:HE2	1.74	0.43
1:B:161:SER:OG	1:B:163:GLN:HG2	2.18	0.43
1:A:327:PRO:HD3	1:A:386:LEU:HD23	2.00	0.43
1:A:134:PHE:CE1	1:B:144:PRO:HA	2.53	0.43
1:A:300:GLU:HG3	1:A:301:ARG:HG3	1.99	0.43
1:A:452:ASP:OD2	1:B:202:ARG:NH2	2.52	0.43
1:A:440:ASN:HA	1:A:443:LYS:HE2	2.01	0.42
1:B:223:ARG:HG2	1:B:228:ARG:HD2	2.01	0.42
1:B:313:ALA:HB3	1:B:316:ASN:ND2	2.35	0.42
1:A:198:PHE:CE2	1:A:358:VAL:HG22	2.55	0.41
1:A:349:MET:CE	1:A:366:ILE:HD11	2.50	0.41
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.94	0.41
1:A:439:TYR:CE2	1:A:443:LYS:HD3	2.55	0.41
1:B:260:PHE:CE2	1:B:262:ASP:HB3	2.56	0.41
1:B:442:LEU:HA	1:B:442:LEU:HD23	1.96	0.41
1:A:462:ARG:HG3	4:A:741:HOH:O	2.19	0.41
1:A:11:PHE:O	1:A:32:GLY:HA3	2.21	0.41
1:B:2:ASP:N	1:B:3:PRO:HD2	2.36	0.41
1:A:447:TYR:CD1	1:A:448:PRO:HA	2.56	0.40
1:B:131:VAL:C	1:B:132:LYS:HD2	2.42	0.40
1:B:505:ASN:OD1	1:B:505:ASN:N	2.55	0.40
1:B:80:PRO:HA	1:B:132:LYS:O	2.22	0.40
1:A:150:LEU:HA	1:A:153:LEU:HD12	2.03	0.40
1:A:429:PRO:HA	1:A:432:ILE:HB	2.04	0.40
1:A:488:ARG:O	4:A:702:HOH:O	2.21	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	437/534 (82%)	424 (97%)	13 (3%)	0	100	100
1	B	464/534 (87%)	457 (98%)	7 (2%)	0	100	100
All	All	901/1068 (84%)	881 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	405/487 (83%)	402 (99%)	3 (1%)	84	88
1	B	428/487 (88%)	425 (99%)	3 (1%)	84	88
All	All	833/974 (86%)	827 (99%)	6 (1%)	84	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	MET
1	A	258	LEU
1	A	486	THR
1	B	179	GLU
1	B	258	LEU
1	B	508	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	359	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](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	602	-	4,4,4	0.16	0	6,6,6	0.10	0
2	SO4	A	603	-	4,4,4	0.16	0	6,6,6	0.19	0
3	GOL	A	604	-	5,5,5	0.35	0	5,5,5	0.09	0
3	GOL	B	608	-	5,5,5	0.33	0	5,5,5	0.56	0
3	GOL	B	606	-	5,5,5	0.50	0	5,5,5	0.71	0
2	SO4	A	602	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	B	604	-	4,4,4	0.19	0	6,6,6	0.15	0
2	SO4	B	603	-	4,4,4	0.14	0	6,6,6	0.14	0
2	SO4	A	601	-	4,4,4	0.17	0	6,6,6	0.18	0
2	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.19	0
3	GOL	B	607	-	5,5,5	0.40	0	5,5,5	0.23	0
2	SO4	B	605	-	4,4,4	0.11	0	6,6,6	0.17	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	606	-	-	2/4/4/4	-
3	GOL	A	604	-	-	4/4/4/4	-
3	GOL	B	608	-	-	2/4/4/4	-
3	GOL	B	607	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	GOL	C1-C2-C3-O3
3	B	606	GOL	O1-C1-C2-O2
3	B	606	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-C3
3	B	607	GOL	O1-C1-C2-C3
3	A	604	GOL	O1-C1-C2-O2
3	A	604	GOL	O2-C2-C3-O3
3	B	608	GOL	O2-C2-C3-O3
3	B	607	GOL	O1-C1-C2-O2
3	B	608	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	GOL	1	0
3	B	606	GOL	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	443/534 (82%)	0.42	43 (9%) 7 10	13, 30, 63, 87	0
1	B	468/534 (87%)	0.40	34 (7%) 15 19	15, 32, 62, 75	0
All	All	911/1068 (85%)	0.41	77 (8%) 10 13	13, 31, 63, 87	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	LEU	8.7
1	A	393	TYR	6.7
1	B	156	LEU	5.0
1	A	430	GLU	4.9
1	B	168	ILE	4.8
1	A	153	LEU	4.8
1	A	405	LYS	4.5
1	A	156	LEU	4.3
1	A	428	LYS	4.3
1	B	154	LYS	4.2
1	A	403	LYS	4.0
1	A	431	LEU	4.0
1	A	496	VAL	3.9
1	B	362	ASN	3.8
1	B	125	ASN	3.7
1	A	158	GLU	3.7
1	A	445	TYR	3.6
1	B	2	ASP	3.5
1	B	314	PHE	3.5
1	A	314	PHE	3.4
1	B	508	THR	3.3
1	A	425	LEU	3.2
1	A	404	GLU	3.2
1	B	150	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	509	LEU	3.2
1	A	480	LEU	3.1
1	A	429	PRO	3.1
1	A	246	ASN	3.0
1	A	501	GLU	3.0
1	B	172	VAL	3.0
1	A	426	LEU	3.0
1	A	133	TRP	2.9
1	A	482	ASP	2.9
1	B	164	TYR	2.9
1	B	160	VAL	2.8
1	A	161	SER	2.8
1	B	171	ARG	2.8
1	A	483	ASN	2.8
1	B	155	ASN	2.7
1	B	430	GLU	2.7
1	A	437	GLU	2.7
1	B	167	ASP	2.6
1	A	361	ASP	2.6
1	B	507	LEU	2.6
1	A	160	VAL	2.6
1	B	426	LEU	2.6
1	A	481	GLU	2.5
1	B	158	GLU	2.5
1	A	159	ASN	2.5
1	A	497	ARG	2.5
1	B	165	ILE	2.4
1	A	151	ASN	2.4
1	A	211	VAL	2.4
1	A	475	ILE	2.4
1	B	264	GLU	2.4
1	B	363	LYS	2.4
1	A	392	GLU	2.3
1	B	151	ASN	2.3
1	A	441	MET	2.3
1	B	501	GLU	2.3
1	B	128	LEU	2.2
1	A	476	ASP	2.2
1	A	503	LEU	2.1
1	B	361	ASP	2.1
1	A	457	ILE	2.1
1	A	499	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	159	ASN	2.1
1	A	456	SER	2.1
1	A	459	ARG	2.1
1	B	244	GLU	2.1
1	A	477	TYR	2.1
1	A	391	GLU	2.0
1	B	61	ILE	2.0
1	A	157	LYS	2.0
1	B	174	LYS	2.0
1	B	360	LYS	2.0
1	B	82	VAL	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 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
3	GOL	B	608	6/6	0.68	0.18	46,46,52,53	0
3	GOL	B	607	6/6	0.83	0.16	43,44,49,50	0
3	GOL	B	606	6/6	0.85	0.14	29,41,48,51	0
3	GOL	A	604	6/6	0.86	0.18	35,43,45,49	0
2	SO4	B	603	5/5	0.93	0.19	63,66,69,76	0
2	SO4	B	604	5/5	0.93	0.14	49,52,66,67	0
2	SO4	B	601	5/5	0.94	0.29	55,56,62,66	0
2	SO4	A	603	5/5	0.94	0.24	47,53,61,68	0
2	SO4	A	602	5/5	0.96	0.10	51,56,62,66	0
2	SO4	B	605	5/5	0.96	0.09	45,53,58,65	0
2	SO4	B	602	5/5	0.97	0.10	39,47,50,55	0
2	SO4	A	601	5/5	0.99	0.09	38,40,41,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.