



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:48 AM GMT

PDB ID : 2F3O
Title : Crystal Structure of a glycy radical enzyme from Archaeoglobus fulgidus
Authors : Lehtio, L.; Goldman, A.
Deposited on : 2005-11-22
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

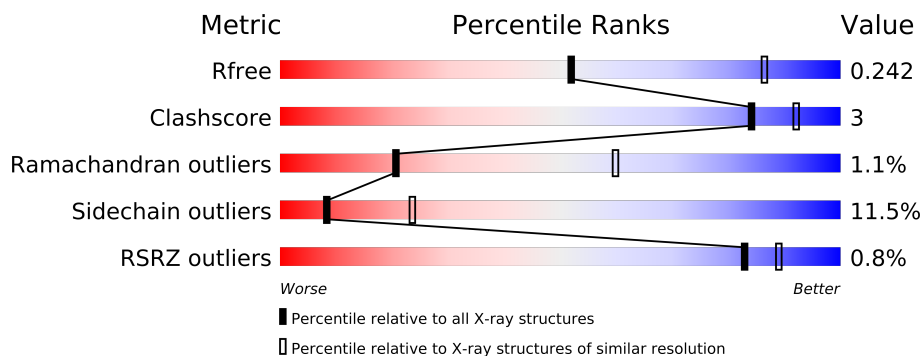
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	776	
1	B	776	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PGE	A	777	-	X
2	PGE	B	777	-	X
3	GOL	B	778	-	X

2 Entry composition i

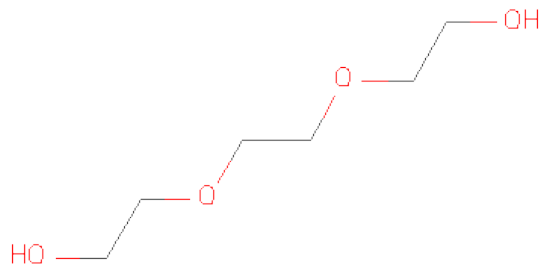
There are 4 unique types of molecules in this entry. The entry contains 12421 atoms, of which 0 are hydrogen and 0 are deuterium.

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 pyruvate formate-lyase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6111	3882	1040	1164	25			
1	B	773	Total	C	N	O	S	0	0	0
			6111	3882	1040	1164	25			

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	67	Total	O	0	0
			67	67		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.03Å 174.17Å 162.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 2.90 19.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.69-2.90) 100.0 (19.63-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.245 0.200 , 0.242	Depositor DCC
R_{free} test set	2648 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 23.1	EDS
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 52529 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12421	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.54	0/6227	0.73	2/8421 (0.0%)
1	B	0.52	1/6227 (0.0%)	0.72	1/8421 (0.0%)
All	All	0.53	1/12454 (0.0%)	0.73	3/16842 (0.0%)

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	3
1	B	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	517	CYS	CB-SG	-5.16	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	454	LEU	CA-CB-CG	7.79	133.23	115.30
1	A	454	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	315	VAL	N-CA-C	-5.11	97.20	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	VAL	Peptide
1	A	366	GLN	Peptide
1	A	72	PRO	Peptide
1	B	242	VAL	Peptide
1	B	366	GLN	Peptide
1	B	72	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6111	0	6092	34	0
1	B	6111	0	6092	36	0
2	A	10	0	14	0	0
2	B	10	0	14	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	100	0	0	2	0
4	B	67	0	0	0	0
All	All	12421	0	12228	70	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:63:LEU:H	1:A:306:ASN:ND2	1.80	0.78
1:B:374:ASN:HB3	1:B:401:ASP:HB2	1.78	0.64
1:A:374:ASN:HB3	1:A:401:ASP:HB2	1.86	0.57
1:A:63:LEU:H	1:A:306:ASN:HD21	1.50	0.56
1:A:80:GLU:HG3	1:A:509:LYS:HD3	1.88	0.56
1:A:208:ASN:HB3	4:A:859:HOH:O	2.08	0.54
1:B:158:VAL:HG13	1:B:517:CYS:HB3	1.89	0.53
1:B:555:ILE:HD11	1:B:646:PRO:HG2	1.92	0.50
1:B:134:ASP:O	1:B:138:ILE:HG23	2.12	0.50
1:A:47:LEU:HD12	1:A:202:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:GLN:HE21	1:A:259:LEU:HG	1.77	0.49
1:A:289:ASP:HB3	1:A:295:ILE:HG12	1.93	0.49
1:A:434:ASN:HD22	1:A:434:ASN:H	1.61	0.48
1:A:731:ASP:HA	1:A:734:ARG:HB2	1.95	0.48
1:B:146:VAL:HG13	1:B:443:LEU:HB2	1.96	0.47
1:A:310:LYS:HE3	1:A:313:GLU:OE2	2.14	0.47
1:A:158:VAL:HG13	1:A:517:CYS:HB3	1.97	0.47
1:B:54:ILE:HG13	1:B:55:PRO:HD2	1.95	0.46
1:B:451:GLU:HG3	1:B:460:LEU:HB2	1.97	0.46
1:B:12:LYS:HA	1:B:12:LYS:HD3	1.82	0.46
1:B:45:LYS:HG3	1:B:201:ILE:HD13	1.97	0.46
1:B:631:PRO:HG3	1:B:657:PRO:HA	1.97	0.46
1:A:64:ILE:H	1:A:306:ASN:ND2	2.14	0.46
1:B:21:VAL:HG11	1:B:107:ASP:HB2	1.97	0.45
1:B:636:VAL:HG21	1:B:764:VAL:HG22	1.98	0.45
1:A:242:VAL:O	1:A:242:VAL:HG23	2.17	0.45
1:A:325:TYR:HB3	1:A:634:THR:HG22	1.98	0.45
1:B:24:CYS:HB2	1:B:77:ILE:HB	1.99	0.45
1:B:109:LYS:HE3	1:B:109:LYS:HB2	1.87	0.45
1:B:51:LEU:HB3	1:B:209:TYR:HB2	1.99	0.45
1:A:451:GLU:HG3	1:A:460:LEU:HB2	1.99	0.45
1:A:270:GLU:HG2	4:A:805:HOH:O	2.16	0.45
1:A:636:VAL:HG21	1:A:764:VAL:HG22	2.00	0.44
1:B:289:ASP:HB3	1:B:295:ILE:HG12	2.00	0.44
1:A:354:LEU:O	1:A:358:VAL:HG12	2.18	0.44
1:A:24:CYS:HB2	1:A:77:ILE:HB	1.99	0.44
1:A:138:ILE:HG21	1:A:138:ILE:HD13	1.68	0.43
1:B:474:LYS:HE3	1:B:474:LYS:HB2	1.63	0.43
1:A:459:ASP:HB2	1:A:464:TYR:HB2	2.00	0.43
1:B:43:GLN:HG3	1:B:510:PRO:HD2	2.00	0.43
1:B:358:VAL:HG23	1:B:362:LEU:HD22	2.00	0.43
1:B:584:LYS:HB3	1:B:584:LYS:HE2	1.84	0.43
1:B:215:LYS:HD3	1:B:215:LYS:HA	1.81	0.43
1:B:520:ASP:OD2	1:B:534:ARG:HG2	2.18	0.43
1:B:87:ILE:HD12	1:B:111:LEU:HB3	2.01	0.43
1:A:676:SER:HA	1:A:679:LYS:HD2	2.01	0.42
1:A:87:ILE:HD12	1:A:111:LEU:HB3	2.00	0.42
1:A:748:VAL:HG21	1:A:768:VAL:HG21	2.01	0.42
1:B:271:GLN:HB3	3:B:778:GOL:H32	2.02	0.42
1:B:448:LYS:HD3	1:B:448:LYS:HA	1.80	0.42
1:B:20:SER:HB2	1:B:69:LEU:HD13	2.01	0.42
1:B:68:MET:HE1	1:B:314:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:545:ILE:HD13	1:B:607:LEU:HD13	2.02	0.41
1:B:195:PHE:CD2	1:B:525:GLY:HA2	2.55	0.41
1:A:545:ILE:HD13	1:A:607:LEU:HD13	2.02	0.41
1:A:90:LEU:HA	1:A:90:LEU:HD23	1.81	0.41
1:B:246:LYS:HE3	1:B:246:LYS:HB2	1.88	0.41
1:B:746:LEU:HA	1:B:746:LEU:HD12	1.83	0.41
1:A:138:ILE:HB	1:A:466:PHE:CE1	2.56	0.41
1:A:728:LEU:HD21	1:A:748:VAL:HG23	2.03	0.41
1:B:138:ILE:HD13	1:B:138:ILE:HG21	1.80	0.41
1:A:288:LYS:O	1:A:292:GLU:HB2	2.20	0.41
1:A:278:ILE:HG21	1:A:335:VAL:HG22	2.02	0.41
1:B:282:LEU:HA	1:B:282:LEU:HD12	1.82	0.40
1:A:182:LEU:HA	1:A:182:LEU:HD23	1.77	0.40
1:B:401:ASP:O	1:B:405:VAL:HG13	2.21	0.40
1:A:555:ILE:HD11	1:A:646:PRO:HG2	2.03	0.40
1:B:742:LYS:HA	1:B:742:LYS:HD3	1.89	0.40
1:B:68:MET:HE2	1:B:310:LYS:O	2.22	0.40
1:A:166:ARG:HD3	1:A:166:ARG:HH11	1.74	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	771/776 (99%)	724 (94%)	41 (5%)	6 (1%)	27 68
1	B	771/776 (99%)	722 (94%)	38 (5%)	11 (1%)	16 52
All	All	1542/1552 (99%)	1446 (94%)	79 (5%)	17 (1%)	21 60

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	PRO
1	B	73	PRO

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Mol	Chain	Res	Type
1	B	223	SER
1	A	751	ALA
1	B	226	GLY
1	B	332	ASN
1	B	731	ASP
1	A	243	PRO
1	A	332	ASN
1	B	72	PRO
1	B	376	GLY
1	A	367	PRO
1	B	243	PRO
1	B	367	PRO
1	A	72	PRO
1	B	631	PRO
1	B	654	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	656/660 (99%)	579 (88%)	77 (12%)	8	22
1	B	656/660 (99%)	582 (89%)	74 (11%)	9	25
All	All	1312/1320 (99%)	1161 (88%)	151 (12%)	8	23

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	7	GLU
1	A	13	VAL
1	A	21	VAL
1	A	47	LEU
1	A	50	VAL
1	A	69	LEU
1	A	82	VAL
1	A	95	ASN
1	A	103	VAL

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Mol	Chain	Res	Type
1	A	105	GLU
1	A	110	VAL
1	A	125	GLU
1	A	138	ILE
1	A	146	VAL
1	A	147	LEU
1	A	166	ARG
1	A	191	GLU
1	A	202	VAL
1	A	206	VAL
1	A	215	LYS
1	A	216	LEU
1	A	257	VAL
1	A	260	VAL
1	A	269	TYR
1	A	270	GLU
1	A	282	LEU
1	A	294	ARG
1	A	307	LEU
1	A	308	TRP
1	A	315	VAL
1	A	327	SER
1	A	335	VAL
1	A	356	LEU
1	A	358	VAL
1	A	362	LEU
1	A	369	VAL
1	A	380	SER
1	A	395	ASN
1	A	396	LEU
1	A	414	ASP
1	A	416	ARG
1	A	419	LEU
1	A	434	ASN
1	A	454	LEU
1	A	460	LEU
1	A	474	LYS
1	A	493	LEU
1	A	494	VAL
1	A	501	LEU
1	A	502	SER
1	A	508	VAL

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Mol	Chain	Res	Type
1	A	516	LEU
1	A	526	VAL
1	A	543	VAL
1	A	560	ASN
1	A	566	ASP
1	A	569	VAL
1	A	581	LYS
1	A	585	LEU
1	A	618	ARG
1	A	649	ARG
1	A	651	SER
1	A	670	VAL
1	A	676	SER
1	A	703	LYS
1	A	707	VAL
1	A	708	ILE
1	A	720	VAL
1	A	734	ARG
1	A	735	LYS
1	A	739	GLU
1	A	741	GLU
1	A	747	LEU
1	A	748	VAL
1	A	768	VAL
1	A	776	ILE
1	B	8	LYS
1	B	13	VAL
1	B	14	SER
1	B	35	GLU
1	B	47	LEU
1	B	48	LYS
1	B	50	VAL
1	B	69	LEU
1	B	82	VAL
1	B	84	LEU
1	B	86	ILE
1	B	95	ASN
1	B	103	VAL
1	B	109	LYS
1	B	110	VAL
1	B	112	ARG
1	B	138	ILE

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Mol	Chain	Res	Type
1	B	143	SER
1	B	146	VAL
1	B	147	LEU
1	B	150	ILE
1	B	166	ARG
1	B	202	VAL
1	B	216	LEU
1	B	222	GLU
1	B	229	ARG
1	B	257	VAL
1	B	269	TYR
1	B	270	GLU
1	B	282	LEU
1	B	298	GLU
1	B	306	ASN
1	B	307	LEU
1	B	308	TRP
1	B	327	SER
1	B	352	THR
1	B	356	LEU
1	B	358	VAL
1	B	362	LEU
1	B	365	ARG
1	B	369	VAL
1	B	384	ARG
1	B	396	LEU
1	B	402	ASP
1	B	419	LEU
1	B	434	ASN
1	B	454	LEU
1	B	460	LEU
1	B	461	GLN
1	B	469	LYS
1	B	493	LEU
1	B	501	LEU
1	B	502	SER
1	B	526	VAL
1	B	534	ARG
1	B	543	VAL
1	B	548	VAL
1	B	553	VAL
1	B	568	ILE

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Mol	Chain	Res	Type
1	B	580	GLU
1	B	649	ARG
1	B	681	SER
1	B	697	SER
1	B	714	SER
1	B	717	GLU
1	B	720	VAL
1	B	727	ILE
1	B	734	ARG
1	B	741	GLU
1	B	745	TRP
1	B	748	VAL
1	B	768	VAL
1	B	773	SER
1	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	71	ASN
1	A	261	GLN
1	A	306	ASN
1	A	333	GLN
1	A	395	ASN
1	A	434	ASN
1	A	455	ASN
1	A	461	GLN
1	B	43	GLN
1	B	88	ASN
1	B	434	ASN
1	B	455	ASN
1	B	461	GLN
1	B	656	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 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	PGE	A	777	-	9,9,9	0.56	0	8,8,8	0.23	0
3	GOL	A	778	-	5,5,5	0.37	0	5,5,5	0.91	0
2	PGE	B	777	-	9,9,9	0.58	0	8,8,8	0.18	0
3	GOL	B	778	-	5,5,5	0.31	0	5,5,5	0.85	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
2	PGE	A	777	-	-	0/7/7/7	0/0/0/0
3	GOL	A	778	-	-	0/4/4/4	0/0/0/0
2	PGE	B	777	-	-	0/7/7/7	0/0/0/0
3	GOL	B	778	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	773/776 (99%)	-0.40	6 (0%) 83 89	33, 53, 75, 85	0
1	B	773/776 (99%)	-0.29	6 (0%) 83 89	42, 60, 82, 91	0
All	All	1546/1552 (99%)	-0.34	12 (0%) 83 89	33, 56, 80, 91	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	703	LYS	3.2
1	A	578	GLY	3.1
1	B	95	ASN	2.6
1	B	12	LYS	2.5
1	B	225	ASP	2.4
1	A	702	GLU	2.4
1	A	222	GLU	2.3
1	A	667	ARG	2.2
1	B	222	GLU	2.2
1	A	12	LYS	2.1
1	B	469	LYS	2.1
1	B	177	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	B	778	6/6	0.26	6.27	56,58,58,59	0
2	PGE	A	777	10/10	0.22	3.65	57,61,64,64	0
2	PGE	B	777	10/10	0.21	2.00	73,76,76,76	0
3	GOL	A	778	6/6	0.17	1.78	39,41,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.