



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 12, 2024 – 03:33 PM EST

PDB ID : 3OP1
Title : Crystal Structure of Macrolide-efflux Protein SP_1110 from *Streptococcus pneumoniae*
Authors : Kim, Y.; Li, H.; Cobb, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-08-31
Resolution : 2.49 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

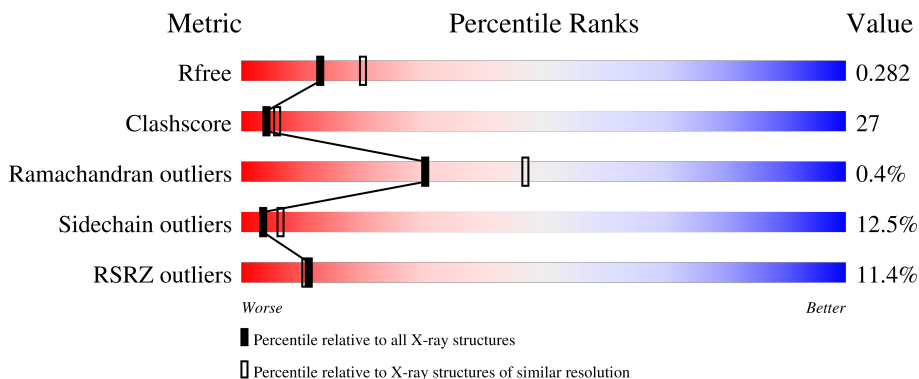
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	164625	7106 (2.50-2.46)
Clashscore	180529	7991 (2.50-2.46)
Ramachandran outliers	177936	7888 (2.50-2.46)
Sidechain outliers	177891	7890 (2.50-2.46)
RSRZ outliers	164620	7106 (2.50-2.46)

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	308	
1	B	308	
1	C	308	

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	GOL	A	315	-	-	X	-
3	GOL	A	317	-	-	X	-
4	PEG	A	319	-	-	X	-
4	PEG	B	314	-	-	X	-
5	ACY	A	316	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7247 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 Macrolide-efflux protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	297	2387	1531	399	449	8	0	1	0
1	B	304	2426	1551	411	457	7	0	0	0
1	C	260	2067	1333	346	381	7	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q97QT9
A	-1	ASN	-	expression tag	UNP Q97QT9
A	0	ALA	-	expression tag	UNP Q97QT9
B	-2	SER	-	expression tag	UNP Q97QT9
B	-1	ASN	-	expression tag	UNP Q97QT9
B	0	ALA	-	expression tag	UNP Q97QT9
C	-2	SER	-	expression tag	UNP Q97QT9
C	-1	ASN	-	expression tag	UNP Q97QT9
C	0	ALA	-	expression tag	UNP Q97QT9

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



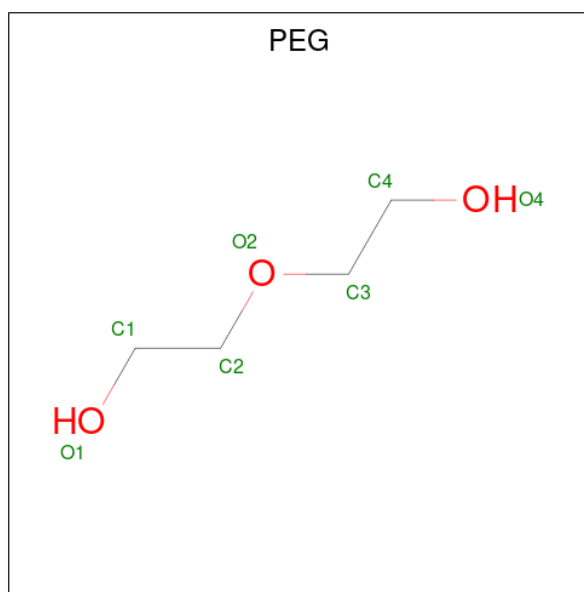
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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



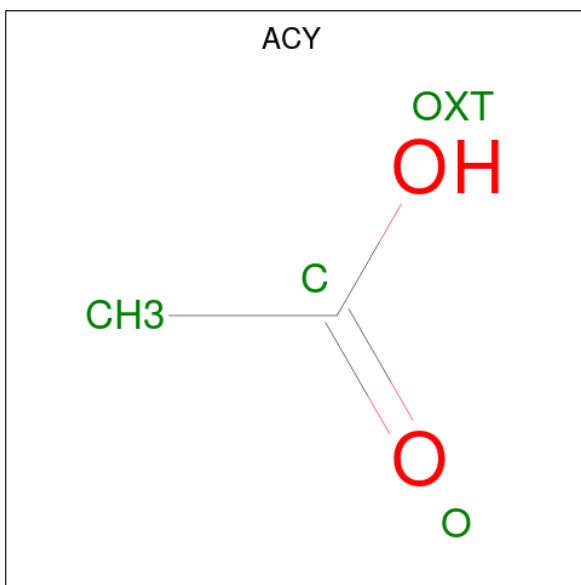
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	1
			14	8	6		

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

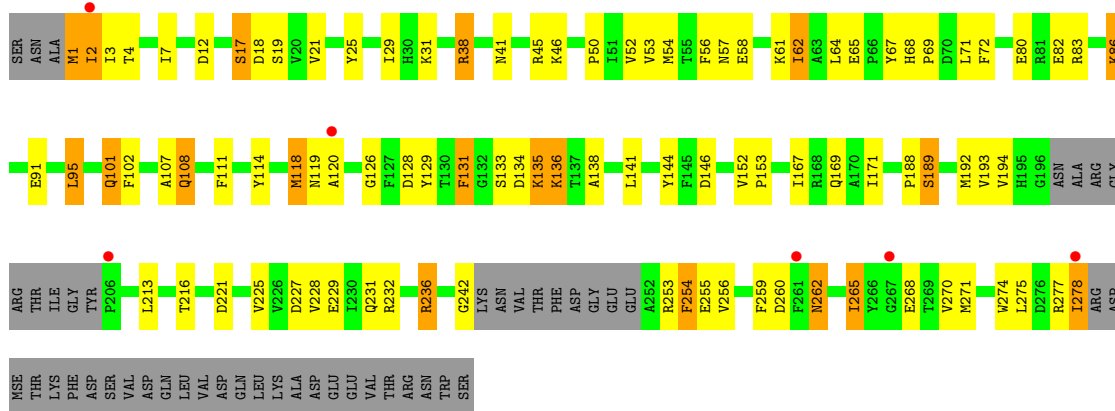
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	81	Total	O	0	0
			81	81		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	95	Total O 95 95	0	0
7	C	59	Total O 59 59	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.15Å 73.25Å 87.52Å 90.00° 112.48° 90.00°	Depositor
Resolution (Å)	35.76 – 2.49 35.76 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.76-2.49) 97.9 (35.76-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432), REFMAC 5.5	Depositor
R, R_{free}	0.198 , 0.265 0.220 , 0.282	Depositor DCC
R_{free} test set	1817 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7247	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, SO4, GOL, CL, ACY

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	0.66	0/2428	0.73	1/3271 (0.0%)
1	B	0.62	0/2468	0.69	0/3327
1	C	0.60	0/2103	0.70	0/2832
All	All	0.63	0/6999	0.71	1/9430 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	ARG	CG-CD-NE	-5.06	101.17	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2387	0	2380	110	0
1	B	2426	0	2423	177	0
1	C	2067	0	2089	100	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	1	0
3	A	24	0	32	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	24	3	0
3	C	30	0	40	2	0
4	A	14	0	20	6	0
4	B	21	0	30	9	0
5	A	4	0	3	2	0
6	B	1	0	0	0	0
7	A	81	0	0	4	0
7	B	95	0	0	10	0
7	C	59	0	0	8	0
All	All	7247	0	7041	379	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 27.

The worst 5 of 379 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:B:31:LYS:HA	1:B:34:GLN:OE1	1.42	1.15
1:A:192:MSE:HE3	1:B:62:ILE:HG21	1.17	1.11
1:A:197:ASN:C	1:A:197:ASN:HD22	1.53	1.06
1:A:260:ASP:HA	3:A:315:GOL:H31	1.32	1.05
1:A:194:VAL:HG13	1:B:67:TYR:HB2	1.35	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	292/308 (95%)	283 (97%)	8 (3%)	1 (0%)	37 54
1	B	302/308 (98%)	295 (98%)	5 (2%)	2 (1%)	19 32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	254/308 (82%)	244 (96%)	10 (4%)	0	100	100
All	All	848/924 (92%)	822 (97%)	23 (3%)	3 (0%)	30	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119	ASN
1	B	135	LYS
1	A	188	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/257 (101%)	236 (91%)	23 (9%)	8	15
1	B	262/257 (102%)	220 (84%)	42 (16%)	2	3
1	C	223/257 (87%)	195 (87%)	28 (13%)	3	6
All	All	744/771 (96%)	651 (88%)	93 (12%)	3	6

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	225	VAL
1	C	62	ILE
1	B	248	ASP
1	C	1	MSE
1	C	95	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	HIS
1	B	119	ASN

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Mol	Chain	Res	Type
1	C	169	GLN
1	C	41	ASN
1	A	244	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	316	-	5,5,5	0.41	0	5,5,5	0.84	0
3	GOL	B	313	-	5,5,5	0.44	0	5,5,5	0.25	0
4	PEG	A	314	-	6,6,6	0.42	0	5,5,5	0.71	0
3	GOL	C	315	-	5,5,5	0.46	0	5,5,5	0.66	0
4	PEG	B	314	-	6,6,6	0.60	0	5,5,5	0.54	0
4	PEG	B	317[A]	-	6,6,6	0.52	0	5,5,5	0.60	0
3	GOL	B	315	-	5,5,5	0.33	0	5,5,5	0.51	0
2	SO4	C	311	-	4,4,4	0.21	0	6,6,6	0.63	0
3	GOL	A	315	-	5,5,5	0.49	0	5,5,5	0.92	0
2	SO4	B	312	-	4,4,4	0.23	0	6,6,6	0.12	0
3	GOL	C	313	-	5,5,5	0.42	0	5,5,5	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	311	-	4,4,4	0.40	0	6,6,6	0.38	0
3	GOL	A	317	-	5,5,5	0.55	0	5,5,5	0.73	0
4	PEG	B	317[B]	-	6,6,6	0.53	0	5,5,5	0.23	0
3	GOL	C	316	-	5,5,5	0.41	0	5,5,5	0.35	0
4	PEG	A	319	-	6,6,6	0.97	0	5,5,5	1.03	0
3	GOL	C	314	-	5,5,5	0.45	0	5,5,5	0.49	0
3	GOL	A	318	-	5,5,5	0.40	0	5,5,5	0.22	0
5	ACY	A	316	-	3,3,3	0.81	0	3,3,3	0.94	0
3	GOL	C	312	-	5,5,5	0.45	0	5,5,5	0.67	0
3	GOL	A	312	-	5,5,5	0.43	0	5,5,5	0.57	0
2	SO4	B	311	-	4,4,4	0.35	0	6,6,6	0.39	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	C	316	-	-	2/4/4/4	-
4	PEG	B	314	-	-	3/4/4/4	-
4	PEG	B	317[A]	-	-	1/4/4/4	-
3	GOL	A	318	-	-	2/4/4/4	-
3	GOL	B	315	-	-	2/4/4/4	-
3	GOL	B	316	-	-	3/4/4/4	-
4	PEG	A	319	-	-	4/4/4/4	-
3	GOL	B	313	-	-	4/4/4/4	-
4	PEG	A	314	-	-	3/4/4/4	-
3	GOL	A	315	-	-	2/4/4/4	-
4	PEG	B	317[B]	-	-	1/4/4/4	-
3	GOL	C	314	-	-	3/4/4/4	-
3	GOL	C	312	-	-	0/4/4/4	-
3	GOL	C	315	-	-	2/4/4/4	-
3	GOL	A	312	-	-	4/4/4/4	-
3	GOL	C	313	-	-	2/4/4/4	-
3	GOL	A	317	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	315	GOL	O1-C1-C2-C3
3	A	318	GOL	O1-C1-C2-C3
3	B	315	GOL	C1-C2-C3-O3
3	B	315	GOL	O2-C2-C3-O3
3	B	316	GOL	C1-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	316	GOL	1	0
3	B	313	GOL	1	0
4	A	314	PEG	1	0
4	B	314	PEG	4	0
4	B	317[A]	PEG	3	0
3	B	315	GOL	1	0
2	C	311	SO4	1	0
3	A	315	GOL	10	0
3	C	313	GOL	1	0
3	A	317	GOL	4	0
4	B	317[B]	PEG	2	0
4	A	319	PEG	5	0
3	C	314	GOL	1	0
5	A	316	ACY	2	0
3	A	312	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/308 (93%)	-0.15	6 (2%) 63 61	22, 45, 81, 110	1 (0%)
1	B	297/308 (96%)	1.29	84 (28%) 1 2	29, 60, 111, 141	0
1	C	253/308 (82%)	0.10	6 (2%) 59 57	31, 60, 94, 129	0
All	All	839/924 (90%)	0.44	96 (11%) 11 10	22, 54, 102, 141	1 (0%)

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	VAL	5.4
1	B	50	PRO	5.3
1	B	20	VAL	5.1
1	B	44	ALA	4.8
1	B	41	ASN	4.7

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 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, 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(\AA^2)	Q<0.9
2	SO4	B	311	5/5	0.58	0.20	95,96,99,102	0
3	GOL	C	315	6/6	0.75	0.19	75,92,95,95	0
2	SO4	B	312	5/5	0.77	0.15	142,143,144,144	0
3	GOL	A	312	6/6	0.78	0.25	70,75,86,86	0
5	ACY	A	316	4/4	0.78	0.21	74,75,79,79	0
3	GOL	B	316	6/6	0.79	0.14	77,81,84,85	0
3	GOL	C	314	6/6	0.82	0.14	70,71,74,74	0
3	GOL	A	315	6/6	0.83	0.17	61,68,110,114	0
3	GOL	C	316	6/6	0.84	0.15	76,83,87,92	0
4	PEG	B	317[A]	7/7	0.84	0.26	48,64,72,73	7
4	PEG	B	317[B]	7/7	0.84	0.26	71,72,74,76	7
3	GOL	A	317	6/6	0.84	0.21	69,76,80,81	0
3	GOL	B	313	6/6	0.86	0.18	80,86,91,94	0
3	GOL	C	313	6/6	0.87	0.14	61,66,69,69	0
6	CL	B	306	1/1	0.87	0.12	85,85,85,85	0
3	GOL	B	315	6/6	0.88	0.12	76,80,81,85	0
3	GOL	A	318	6/6	0.91	0.16	76,79,87,93	0
4	PEG	A	319	7/7	0.91	0.12	43,46,53,57	0
4	PEG	A	314	7/7	0.92	0.12	42,48,55,61	0
2	SO4	C	311	5/5	0.92	0.15	72,74,80,88	0
4	PEG	B	314	7/7	0.93	0.08	42,50,57,58	0
2	SO4	A	311	5/5	0.94	0.10	60,62,70,71	0
3	GOL	C	312	6/6	0.95	0.08	42,48,49,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.