



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 01:16 AM JST

PDB ID : 7CC8
Title : Crystal structure of White Spot Syndrome Virus Thymidylate Synthase - Apo form
Authors : Kumar, S.; Panchal, N.V.; Shaikh, N.; Vasudevan, D.
Deposited on : 2020-06-16
Resolution : 2.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

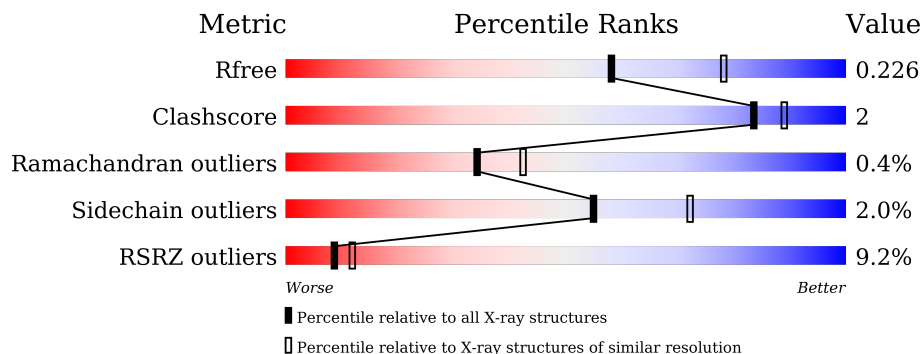
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

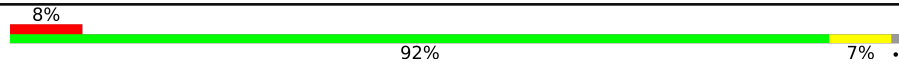

The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	297	
1	B	297	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4850 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 Thymidylate Synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2371	1514	414	426	17	0	0	0
1	B	280	2258	1444	391	408	15	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

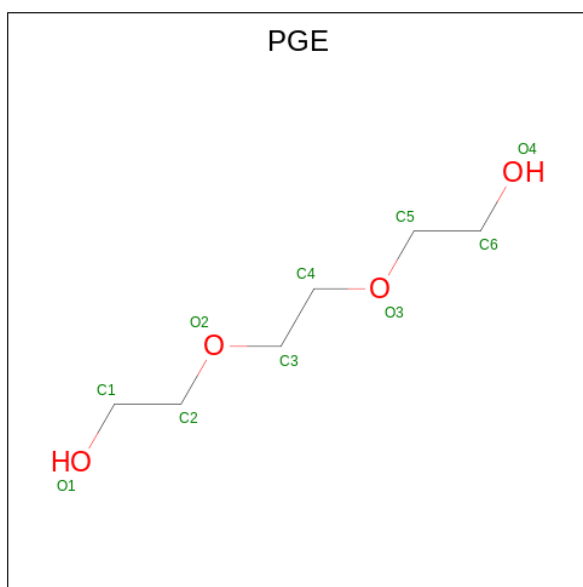
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	LEU	-	expression tag	UNP Q77J90
A	291	GLU	-	expression tag	UNP Q77J90
A	292	HIS	-	expression tag	UNP Q77J90
A	293	HIS	-	expression tag	UNP Q77J90
A	294	HIS	-	expression tag	UNP Q77J90
A	295	HIS	-	expression tag	UNP Q77J90
A	296	HIS	-	expression tag	UNP Q77J90
A	297	HIS	-	expression tag	UNP Q77J90
B	290	LEU	-	expression tag	UNP Q77J90
B	291	GLU	-	expression tag	UNP Q77J90
B	292	HIS	-	expression tag	UNP Q77J90
B	293	HIS	-	expression tag	UNP Q77J90
B	294	HIS	-	expression tag	UNP Q77J90
B	295	HIS	-	expression tag	UNP Q77J90
B	296	HIS	-	expression tag	UNP Q77J90
B	297	HIS	-	expression tag	UNP Q77J90

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 10 6 4	0	0

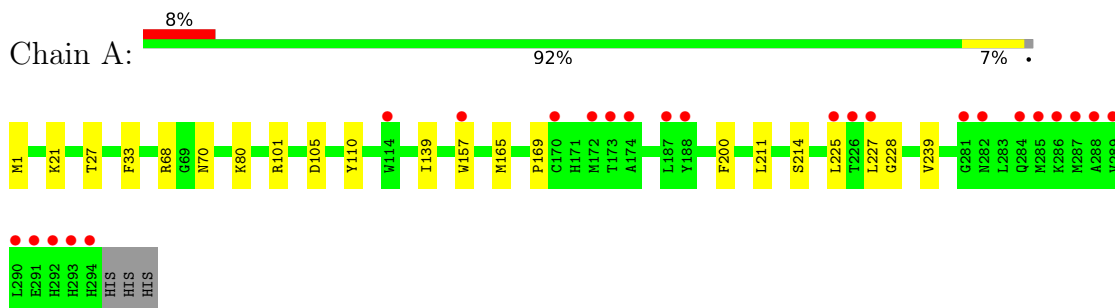
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	91	Total O 91 91	0	0
4	B	73	Total O 73 73	0	0

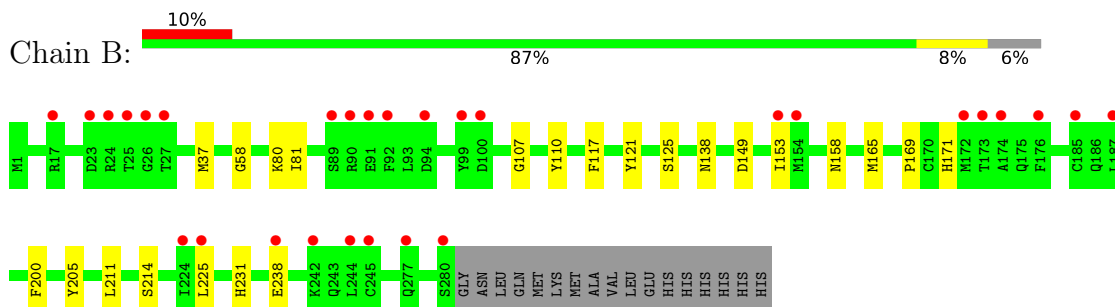
3 Residue-property plots [i](#)

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: Thymidylate Synthase



- Molecule 1: Thymidylate Synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.80Å 91.80Å 233.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.30 43.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.41-2.30) 98.8 (43.41-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8	Depositor
R, R_{free}	0.185 , 0.209 0.204 , 0.226	Depositor DCC
R_{free} test set	2277 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtrriage
Anisotropy	0.386	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4850	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: PGE, 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	1.01	0/2430	1.01	0/3283
1	B	0.96	0/2314	0.96	0/3128
All	All	0.99	0/4744	0.99	0/6411

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	2371	0	2352	11	0
1	B	2258	0	2241	13	0
2	A	25	0	0	0	0
2	B	5	0	0	0	0
3	A	7	0	9	1	0
3	B	20	0	28	2	0
4	A	91	0	0	0	0
4	B	73	0	0	1	0
All	All	4850	0	4630	22	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 2.

All (22) 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:101:ARG:HG2	1:A:101:ARG:HH11	1.57	0.70
1:B:171:HIS:HD2	1:B:205:TYR:OH	1.76	0.69
1:B:211:LEU:O	1:B:214:SER:HB2	1.99	0.63
1:B:138:ASN:HB3	3:B:302:PGE:H32	1.81	0.62
1:A:211:LEU:O	1:A:214:SER:HB2	2.00	0.61
1:A:165:MET:SD	1:A:169:PRO:HD3	2.44	0.56
1:A:101:ARG:HG2	1:A:101:ARG:NH1	2.16	0.56
1:A:68:ARG:HE	1:A:70:ASN:ND2	2.06	0.54
1:B:37:MET:CE	1:B:225:LEU:HD23	2.39	0.53
1:A:157:TRP:CZ2	1:B:153:ILE:HB	2.45	0.52
1:A:139:ILE:HG13	3:A:306:PGE:H5	1.95	0.49
1:B:149:ASP:OD2	3:B:302:PGE:H52	2.13	0.48
1:A:33:PHE:HA	1:A:228:GLY:O	2.12	0.48
1:B:165:MET:SD	1:B:169:PRO:HD3	2.54	0.48
1:B:37:MET:HE3	1:B:225:LEU:HD23	1.94	0.47
1:B:231:HIS:HE1	4:B:453:HOH:O	1.97	0.46
1:B:107:GLY:HA2	1:B:121:TYR:CE2	2.52	0.45
1:A:157:TRP:NE1	1:B:153:ILE:HG21	2.32	0.44
1:B:117:PHE:CE2	1:B:158:ASN:HB2	2.54	0.42
1:B:58:GLY:HA2	1:B:81:ILE:HD12	2.00	0.42
1:A:225:LEU:CD2	1:A:227:LEU:HG	2.49	0.42
1:A:101:ARG:HG3	1:A:105:ASP:HB3	2.01	0.41

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	292/297 (98%)	284 (97%)	7 (2%)	1 (0%)	41	50
1	B	278/297 (94%)	269 (97%)	8 (3%)	1 (0%)	34	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	570/594 (96%)	553 (97%)	15 (3%)	2 (0%)	34	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	110	TYR
1	A	110	TYR

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	255/258 (99%)	249 (98%)	6 (2%)	49	66
1	B	243/258 (94%)	239 (98%)	4 (2%)	62	78
All	All	498/516 (96%)	488 (98%)	10 (2%)	55	72

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	21	LYS
1	A	27	THR
1	A	80	LYS
1	A	200	PHE
1	A	239	VAL
1	B	80	LYS
1	B	125	SER
1	B	200	PHE
1	B	238	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN

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Mol	Chain	Res	Type
1	B	171	HIS
1	B	279	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	301	-	4,4,4	0.78	0	6,6,6	0.31	0
3	PGE	B	302	-	9,9,9	0.40	0	8,8,8	0.37	0
2	SO4	A	301	-	4,4,4	0.62	0	6,6,6	0.15	0
2	SO4	A	303	-	4,4,4	0.33	0	6,6,6	0.17	0
3	PGE	B	303	-	9,9,9	0.31	0	8,8,8	0.16	0
2	SO4	A	304	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	A	302	-	4,4,4	0.30	0	6,6,6	0.11	0
2	SO4	A	305	-	4,4,4	0.31	0	6,6,6	0.22	0
3	PGE	A	306	-	6,6,9	0.42	0	5,5,8	0.44	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	PGE	B	303	-	-	4/7/7/7	-
3	PGE	B	302	-	-	5/7/7/7	-
3	PGE	A	306	-	-	1/4/4/7	-

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	B	302	PGE	O2-C3-C4-O3
3	B	302	PGE	O1-C1-C2-O2
3	B	302	PGE	O3-C5-C6-O4
3	B	303	PGE	O1-C1-C2-O2
3	B	303	PGE	O3-C5-C6-O4
3	B	303	PGE	O2-C3-C4-O3
3	B	302	PGE	C6-C5-O3-C4
3	B	303	PGE	C6-C5-O3-C4
3	A	306	PGE	O2-C3-C4-O3
3	B	302	PGE	C3-C4-O3-C5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	PGE	2	0
3	A	306	PGE	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	294/297 (98%)	0.17	24 (8%) 11 15	23, 29, 56, 82	0
1	B	280/297 (94%)	0.33	29 (10%) 6 9	22, 31, 49, 93	0
All	All	574/594 (96%)	0.25	53 (9%) 9 12	22, 30, 55, 93	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	HIS	6.7
1	A	289	VAL	6.1
1	A	285	MET	5.9
1	A	293	HIS	5.7
1	A	288	ALA	4.9
1	B	25	THR	4.6
1	B	24	ARG	4.0
1	A	294	HIS	3.7
1	A	287	MET	3.6
1	B	23	ASP	3.6
1	B	245	CYS	3.3
1	B	174	ALA	3.3
1	B	187	LEU	3.2
1	B	26	GLY	3.1
1	A	227	LEU	3.1
1	A	187	LEU	3.0
1	B	224	ILE	3.0
1	A	282	ASN	2.9
1	A	291	GLU	2.9
1	A	286	LYS	2.9
1	A	290	LEU	2.9
1	A	226	THR	2.8
1	B	27	THR	2.8
1	A	172	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	17	ARG	2.8
1	A	157	TRP	2.7
1	B	99	TYR	2.7
1	B	153	ILE	2.7
1	A	284	GLN	2.6
1	B	173	THR	2.6
1	A	188	TYR	2.5
1	B	91	GLU	2.4
1	B	94	ASP	2.4
1	B	277	GLN	2.4
1	A	114	TRP	2.3
1	B	100	ASP	2.3
1	B	154	MET	2.3
1	B	90	ARG	2.3
1	B	185	CYS	2.2
1	B	238	GLU	2.2
1	B	225	LEU	2.2
1	A	225	LEU	2.2
1	A	170	CYS	2.1
1	B	242	LYS	2.1
1	B	244	LEU	2.1
1	A	281	GLY	2.1
1	A	174	ALA	2.1
1	B	176	PHE	2.1
1	A	173	THR	2.1
1	B	89	SER	2.1
1	B	172	MET	2.1
1	B	280	SER	2.1
1	B	92	PHE	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 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(Å ²)	Q<0.9
3	PGE	A	306	7/10	0.75	0.29	40,49,58,64	0
2	SO4	A	304	5/5	0.88	0.30	90,102,111,115	0
3	PGE	B	302	10/10	0.88	0.32	45,60,70,77	0
3	PGE	B	303	10/10	0.88	0.21	64,69,72,74	0
2	SO4	A	302	5/5	0.92	0.21	81,83,94,103	0
2	SO4	A	305	5/5	0.93	0.42	80,108,120,127	0
2	SO4	A	303	5/5	0.94	0.27	103,105,121,125	0
2	SO4	A	301	5/5	0.98	0.15	54,56,63,71	0
2	SO4	B	301	5/5	0.99	0.20	45,51,56,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.