



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 04:25 pm BST

PDB ID : 6G3L
Title : Phosphotriesterase PTE_C23_A203L_3
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Deposited on : 2018-03-26
Resolution : 1.74 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 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

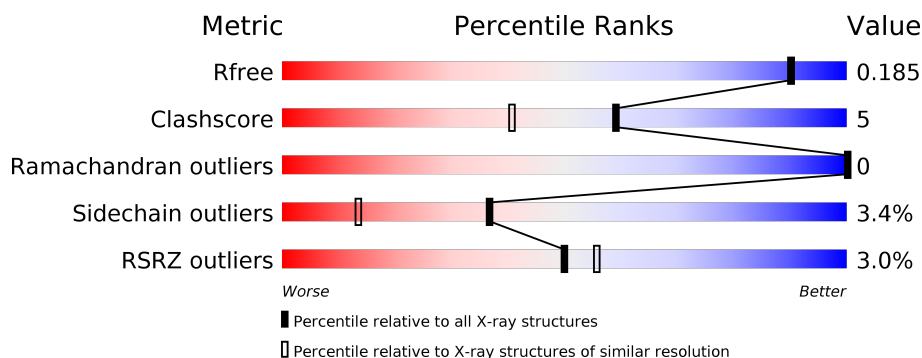
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	332	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>

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
4	E8N	A	404	-	-	X	-
5	GB	A	405	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	408	-	X	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 2875 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	4	0
			2531	1591	455	478	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ALA	LYS	conflict	UNP P0A434
A	80	VAL	ALA	conflict	UNP P0A434
A	132	GLU	PHE	conflict	UNP P0A434
A	173	ASN	THR	conflict	UNP P0A434
A	185	ARG	LYS	conflict	UNP P0A434
A	203	LEU	ALA	conflict	UNP P0A434
A	254	GLY	HIS	conflict	UNP P0A434
A	274	ASN	ILE	conflict	UNP P0A434
A	319	SER	ARG	conflict	UNP P0A434
A	342	SER	PRO	conflict	UNP P0A434
A	343	ASN	GLN	conflict	UNP P0A434
A	362	ARG	LEU	conflict	UNP P0A434
A	363	ALA	ARG	conflict	UNP P0A434
A	364	SER	ALA	conflict	UNP P0A434

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).

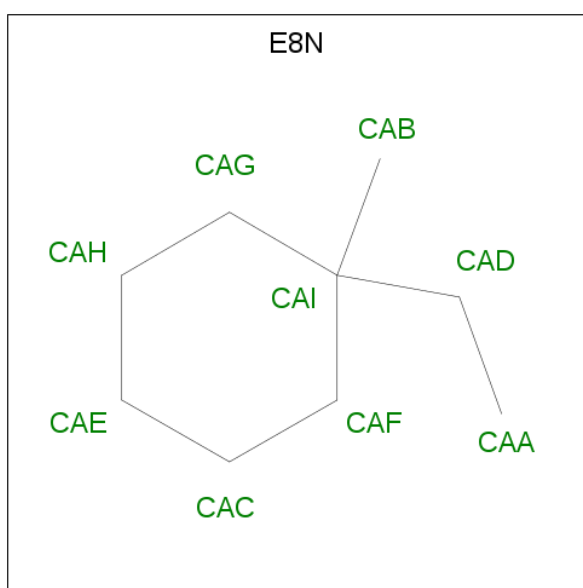


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

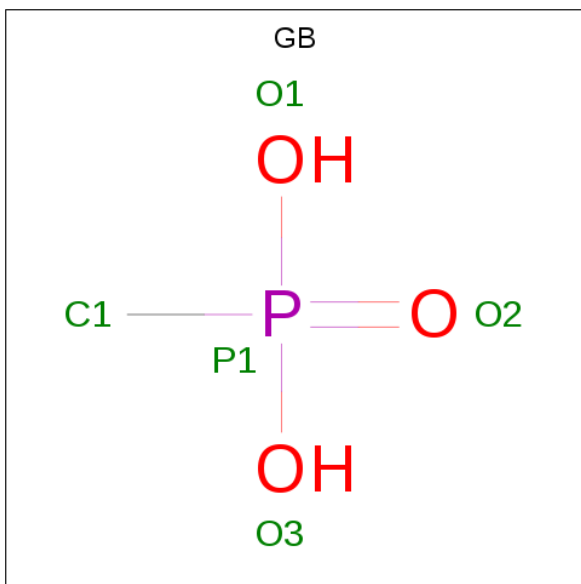
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		

- Molecule 4 is 1-ethyl-1-methyl-cyclohexane (three-letter code: E8N) (formula: C₉H₁₈).



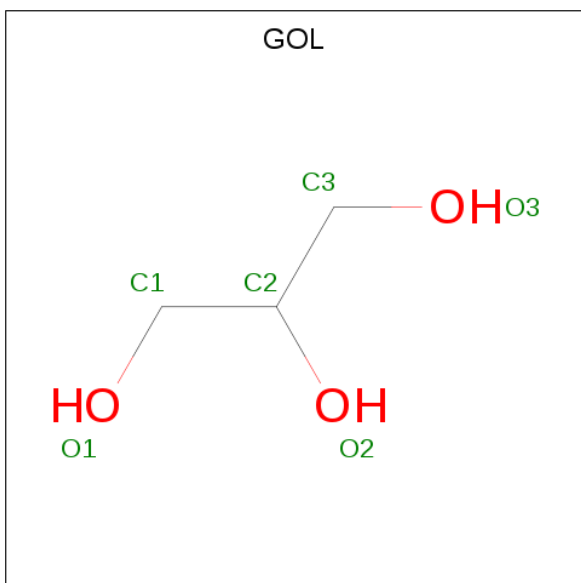
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 9 9	0	0

- Molecule 5 is METHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: GB) (formula: $\text{CH}_5\text{O}_3\text{P}$).



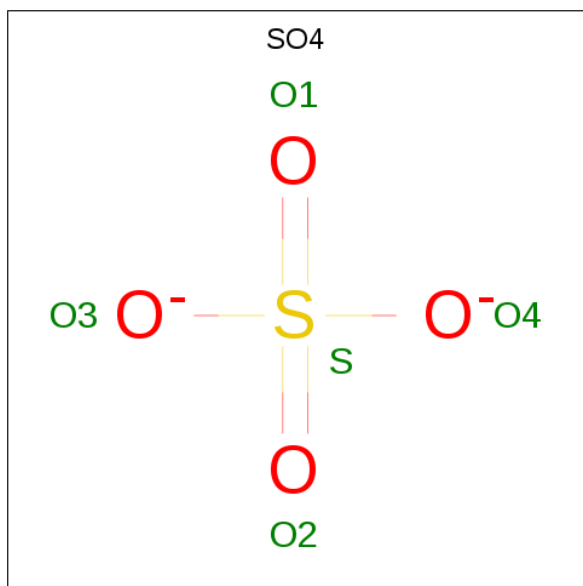
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O P 5 1 3 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

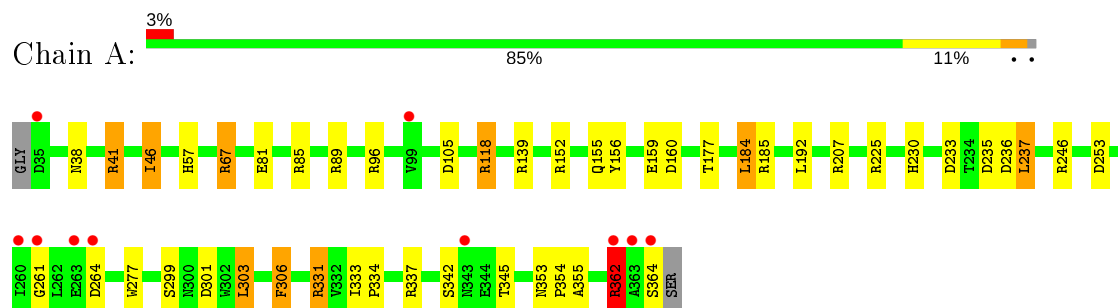
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	302	Total	O	0	0
			302	302		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Parathion hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.70 Å 69.70 Å 186.48 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.46 – 1.74 25.46 – 1.74	Depositor EDS
% Data completeness (in resolution range)	98.3 (25.46-1.74) 98.3 (25.46-1.74)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 1.74 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.157 , 0.174 0.170 , 0.185	Depositor DCC
R_{free} test set	2327 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2875	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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, ZN, E8N, FMT, SO4, GB

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	1.16	3/2576 (0.1%)	1.29	34/3499 (1.0%)

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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	156	TYR	CE1-CZ	-5.53	1.31	1.38
1	A	246	ARG	CB-CG	-5.13	1.38	1.52
1	A	277	TRP	CG-CD1	5.12	1.44	1.36

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	139	ARG	NE-CZ-NH1	14.63	127.61	120.30
1	A	96	ARG	NE-CZ-NH1	10.75	125.67	120.30
1	A	362	ARG	NE-CZ-NH2	10.01	125.31	120.30
1	A	225	ARG	NE-CZ-NH2	9.44	125.02	120.30
1	A	96	ARG	NE-CZ-NH2	-8.46	116.07	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide

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	2531	0	2536	21	0
2	A	3	0	0	0	0
3	A	2	0	0	0	0
4	A	9	0	0	7	0
5	A	5	0	3	2	0
6	A	18	0	21	2	0
7	A	5	0	0	1	0
8	A	302	0	0	4	0
All	All	2875	0	2560	24	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.

The worst 5 of 24 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:345:THR:OG1	4:A:404:E8N:CAE	1.80	1.30
1:A:342:SER:OG	4:A:404:E8N:CAE	2.14	0.96
5:A:405:GB:H3	8:A:761:HOH:O	1.82	0.79
1:A:342:SER:H	4:A:404:E8N:CAH	1.97	0.78
1:A:345:THR:CB	4:A:404:E8N:CAE	2.63	0.76

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	332/332 (100%)	322 (97%)	10 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	267/266 (100%)	258 (97%)	9 (3%)	37	13

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	299	SER
1	A	364	SER
1	A	306	PHE
1	A	237	LEU
1	A	303	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	155	GLN
1	A	212	GLN
1	A	230	HIS
1	A	295	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](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
6	GOL	A	406	-	5,5,5	0.69	0	5,5,5	1.80	1 (20%)
4	E8N	A	404	-	8,9,9	2.66	4 (50%)	8,12,12	3.11	4 (50%)
2	FMT	A	401	1,3	0,2,2	0.00	-	0,1,1	0.00	-
6	GOL	A	407	-	5,5,5	0.98	0	5,5,5	0.89	0
7	SO4	A	409	-	4,4,4	0.41	0	6,6,6	1.80	2 (33%)
5	GB	A	405	3	4,4,4	8.93	3 (75%)	6,6,6	1.33	1 (16%)
6	GOL	A	408	-	5,5,5	2.36	2 (40%)	5,5,5	2.37	3 (60%)

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
6	GOL	A	408	-	-	4/4/4/4	-
6	GOL	A	406	-	-	4/4/4/4	-
4	E8N	A	404	-	-	0/3/13/13	0/1/1/1
6	GOL	A	407	-	-	2/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	GB	P1-O1	14.66	1.81	1.54
5	A	405	GB	P1-C1	-8.91	1.54	1.77
4	A	404	E8N	CAH-CAE	-5.13	1.31	1.51
5	A	405	GB	P1-O2	4.93	1.58	1.50
6	A	408	GOL	O2-C2	-4.45	1.30	1.43

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	404	E8N	CAA-CAD-CAI	-5.69	97.42	115.39
4	A	404	E8N	CAF-CAC-CAE	-4.49	104.42	111.37
4	A	404	E8N	CAG-CAI-CAF	3.87	115.10	109.06
7	A	409	SO4	O4-S-O2	3.37	126.91	109.31
6	A	406	GOL	O1-C1-C2	-3.12	95.23	110.20

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	406	GOL	C1-C2-C3-O3
6	A	408	GOL	O1-C1-C2-C3
6	A	408	GOL	C1-C2-C3-O3
6	A	408	GOL	O2-C2-C3-O3
6	A	407	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	E8N	7	0
6	A	407	GOL	1	0
7	A	409	SO4	1	0
5	A	405	GB	2	0
6	A	408	GOL	1	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 [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	330/332 (99%)	0.07	10 (3%) 50 56	12, 17, 31, 63	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.9
1	A	364	SER	4.7
1	A	264	ASP	4.7
1	A	362	ARG	3.9
1	A	261	GLY	3.9

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
4	E8N	A	404	9/9	0.80	0.22	17,26,30,30	0
6	GOL	A	407	6/6	0.89	0.16	24,34,39,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	A	408	6/6	0.91	0.15	20,27,32,32	0
6	GOL	A	406	6/6	0.93	0.13	18,30,35,43	0
7	SO4	A	409	5/5	0.96	0.20	42,44,51,63	0
5	GB	A	405	5/5	0.98	0.08	11,12,14,20	0
2	FMT	A	401	3/3	0.99	0.05	11,11,11,12	0
3	ZN	A	403	1/1	1.00	0.03	13,13,13,13	0
3	ZN	A	402	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.