



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 6FVK
Title : Phosphotriesterase PTE_C23_3
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Deposited on : 2018-03-04
Resolution : 1.77 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

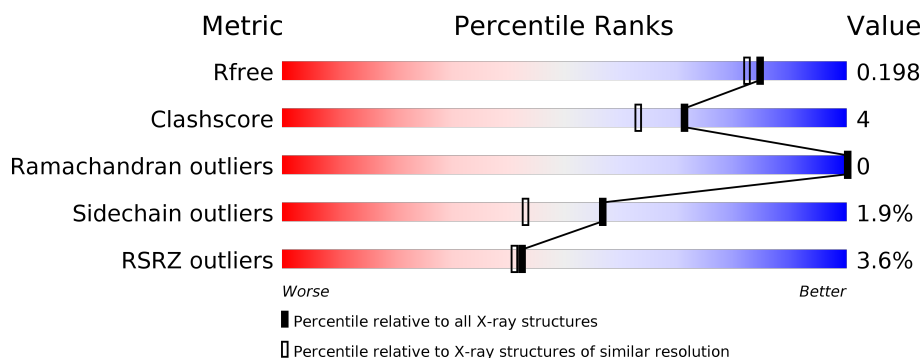
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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>4%</div> <div>87%</div> <div>11%</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
6	E8N	A	408	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 2838 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.

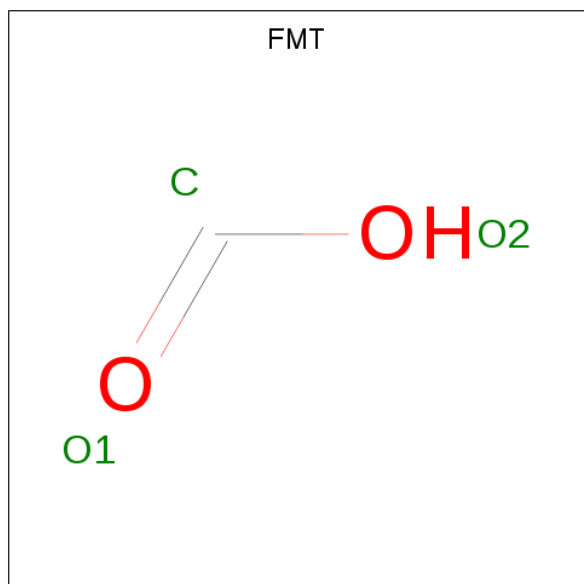
- Molecule 1 is a protein called Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2528	1591	452	478	7	0	4	0

There are 9 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	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

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

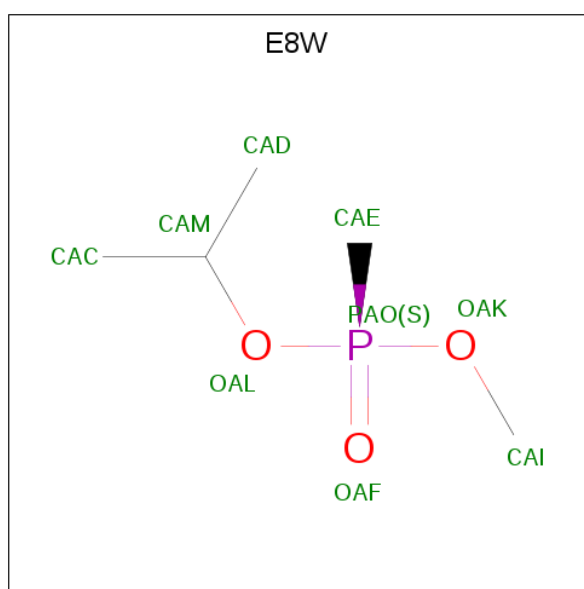


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		

- 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 2-[methoxy(methyl)phosphoryl]oxypropane (three-letter code: E8W) (formula: C₅H₁₃O₃P).



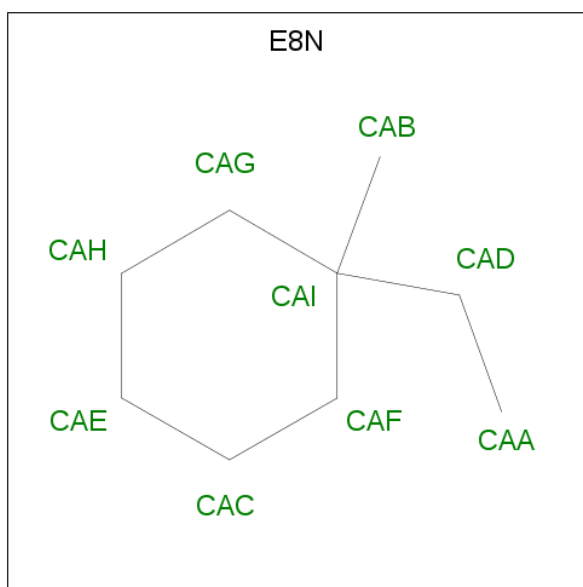
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			9	5	3	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1-ethyl-1-methyl-cyclohexane (three-letter code: E8N) (formula: C₉H₁₈).



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

- 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		
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

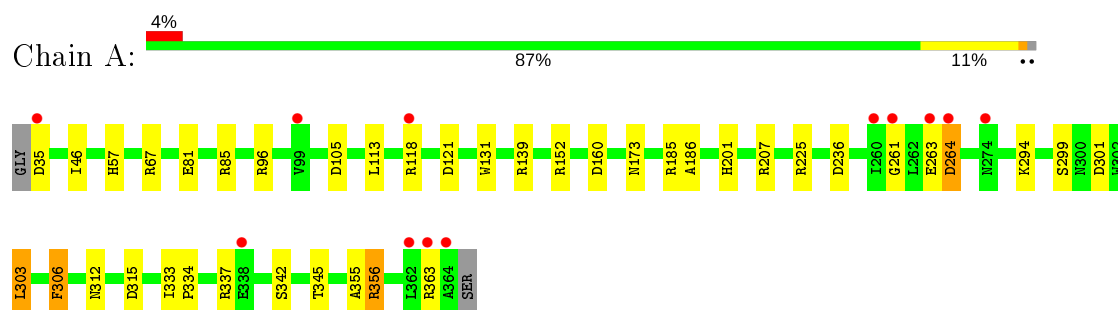
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	254	Total	O	0	0
			254	254		

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	69.56 Å 69.56 Å 186.64 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.11 – 1.77 34.78 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.11-1.77) 100.0 (34.78-1.77)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 1.77 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.157 , 0.189 0.170 , 0.198	Depositor DCC
R_{free} test set	2285 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2838	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 5.44% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, E8N, FMT, E8W, 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	1.15	4/2573 (0.2%)	1.42	31/3495 (0.9%)

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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ARG	CA-C	7.03	1.71	1.52
1	A	185	ARG	C-N	5.91	1.47	1.34
1	A	139	ARG	CZ-NH1	5.47	1.40	1.33
1	A	356	ARG	CZ-NH2	-5.04	1.26	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ARG	NE-CZ-NH1	26.20	133.40	120.30
1	A	356	ARG	NE-CZ-NH2	-23.92	108.34	120.30
1	A	185	ARG	CA-C-N	-15.15	83.88	117.20
1	A	139	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	A	96	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	A	225	ARG	NE-CZ-NH1	11.61	126.11	120.30
1	A	225	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	A	139	ARG	CG-CD-NE	8.35	129.32	111.80
1	A	152	ARG	NE-CZ-NH1	7.96	124.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	207	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	96	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	306	PHE	CB-CG-CD1	7.04	125.73	120.80
1	A	139	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	185	ARG	N-CA-C	6.48	128.50	111.00
1	A	160	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	301	ASP	CB-CG-OD1	6.17	123.86	118.30
1	A	67	ARG	CG-CD-NE	-6.16	98.87	111.80
1	A	186	ALA	N-CA-CB	5.93	118.41	110.10
1	A	121	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	236	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	356	ARG	CD-NE-CZ	5.71	131.60	123.60
1	A	301	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	356	ARG	CG-CD-NE	-5.69	99.84	111.80
1	A	105	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	A	337	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	A	315	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	35	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	264	ASP	N-CA-C	5.12	124.82	111.00
1	A	113	LEU	CB-CG-CD1	5.11	119.69	111.00
1	A	118	ARG	NE-CZ-NH1	5.09	122.85	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	261	GLY	Peptide
1	A	263	GLU	Peptide

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	2528	0	2531	17	0
2	A	3	0	0	0	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	1	0
5	A	18	0	24	2	0
6	A	9	0	0	7	0
7	A	15	0	0	0	0
8	A	254	0	0	2	0
All	All	2838	0	2555	18	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 4.

All (18) 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	6:A:408:E8N:CAE	1.80	1.29
1:A:342:SER:OG	6:A:408:E8N:CAE	2.06	1.04
1:A:173:ASN:HD21	1:A:201:HIS:HE2	1.23	0.84
6:A:408:E8N:CAC	8:A:694:HOH:O	2.33	0.75
1:A:342:SER:H	6:A:408:E8N:CAH	2.01	0.73
1:A:356:ARG:HD3	5:A:407:GOL:H12	1.70	0.73
1:A:345:THR:CB	6:A:408:E8N:CAE	2.67	0.71
1:A:81:GLU:HG2	1:A:85:ARG:NH1	2.09	0.68
1:A:342:SER:CB	6:A:408:E8N:CAE	2.82	0.57
1:A:345:THR:OG1	6:A:408:E8N:CAC	2.53	0.56
1:A:46:ILE:HG23	1:A:355:ALA:HB1	1.88	0.55
1:A:356:ARG:HD3	5:A:407:GOL:C1	2.36	0.54
1:A:173:ASN:ND2	1:A:201:HIS:HE2	1.99	0.54
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.91	0.52
1:A:57:HIS:O	1:A:303:LEU:HA	2.11	0.51
1:A:131:TRP:HE1	4:A:404:E8W:CAE	2.31	0.43
1:A:294:LYS:O	1:A:356:ARG:NH2	2.50	0.41
1:A:312:ASN:HA	8:A:695: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	332/332 (100%)	321 (97%)	11 (3%)	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	266/265 (100%)	261 (98%)	5 (2%)	57	43

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	ASP
1	A	299	SER
1	A	303	LEU
1	A	306	PHE
1	A	363	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	312	ASN

5.3.3 RNA ⓘ

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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
5	GOL	A	407	-	5,5,5	0.70	0	5,5,5	1.00	0
7	SO4	A	409	-	4,4,4	0.87	0	6,6,6	0.38	0
7	SO4	A	410	-	4,4,4	0.43	0	6,6,6	1.28	1 (16%)
5	GOL	A	406	-	5,5,5	0.42	0	5,5,5	0.76	0
2	FMT	A	401	1,3	0,2,2	0.00	-	0,1,1	0.00	-
6	E8N	A	408	-	8,9,9	3.55	4 (50%)	8,12,12	2.66	4 (50%)
5	GOL	A	405	-	5,5,5	1.19	1 (20%)	5,5,5	2.19	2 (40%)
4	E8W	A	404	3	6,8,8	3.79	3 (50%)	5,11,11	1.06	0
7	SO4	A	411	-	4,4,4	0.60	0	6,6,6	1.31	1 (16%)

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	E8N	A	408	-	-	0/3/13/13	0/1/1/1
4	E8W	A	404	3	-	5/8/8/8	-
5	GOL	A	405	-	-	2/4/4/4	-
5	GOL	A	407	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	406	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	E8W	PAO-CAE	-6.75	1.59	1.77
6	A	408	E8N	CAG-CAH	-6.42	1.36	1.52
4	A	404	E8W	OAL-CAM	-5.59	1.27	1.46
6	A	408	E8N	CAH-CAE	-5.07	1.31	1.51
6	A	408	E8N	CAG-CAI	-4.24	1.43	1.53
6	A	408	E8N	CAF-CAC	-3.06	1.45	1.52
4	A	404	E8W	PAO-OAF	2.92	1.51	1.47
5	A	405	GOL	O2-C2	2.22	1.50	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	408	E8N	CAF-CAC-CAE	-5.30	103.17	111.37
6	A	408	E8N	CAA-CAD-CAI	-3.93	102.98	115.39
5	A	405	GOL	O2-C2-C3	3.63	125.10	109.12
6	A	408	E8N	CAH-CAE-CAC	2.60	119.17	111.18
5	A	405	GOL	C3-C2-C1	-2.57	101.70	111.70
7	A	410	SO4	O4-S-O2	2.44	122.06	109.31
6	A	408	E8N	CAB-CAI-CAF	2.28	112.89	109.48
7	A	411	SO4	O4-S-O1	-2.16	98.02	109.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	407	GOL	O1-C1-C2-C3
4	A	404	E8W	CAM-OAL-PAO-CAE
4	A	404	E8W	CAM-OAL-PAO-OAF
5	A	405	GOL	O1-C1-C2-C3
5	A	407	GOL	O1-C1-C2-O2
5	A	405	GOL	O1-C1-C2-O2
4	A	404	E8W	CAI-OAK-PAO-OAF
4	A	404	E8W	CAI-OAK-PAO-OAL
4	A	404	E8W	CAI-OAK-PAO-CAE

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	407	GOL	2	0
6	A	408	E8N	7	0
4	A	404	E8W	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	330/332 (99%)	0.05	12 (3%) 42 41	11, 16, 30, 61	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	264	ASP	4.7
1	A	362	LEU	4.7
1	A	363	ARG	4.4
1	A	261	GLY	3.6
1	A	263	GLU	3.6
1	A	35	ASP	2.8
1	A	260	ILE	2.7
1	A	99	VAL	2.7
1	A	364	ALA	2.6
1	A	118	ARG	2.4
1	A	274	ASN	2.3
1	A	338	GLU	2.3

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
7	SO4	A	411	5/5	0.71	0.37	59,66,78,90	0
5	GOL	A	407	6/6	0.79	0.21	32,45,47,50	0
6	E8N	A	408	9/9	0.82	0.21	15,25,28,33	0
5	GOL	A	406	6/6	0.85	0.14	32,46,48,49	0
5	GOL	A	405	6/6	0.91	0.12	21,31,36,36	0
4	E8W	A	404	9/9	0.92	0.22	9,28,35,36	9
7	SO4	A	410	5/5	0.96	0.23	42,44,52,57	0
7	SO4	A	409	5/5	0.97	0.23	26,28,38,38	0
2	FMT	A	401	3/3	0.98	0.07	12,12,12,12	0
3	ZN	A	402	1/1	1.00	0.04	14,14,14,14	0
3	ZN	A	403	1/1	1.00	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.