WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 05:15 pm BST

PDB ID	:	3ZWA
Title	:	CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-HEXA NOYL-COA
Authors	:	Kasaragod, P.; Schmitz, W.; Hiltunen, J.K.; Wierenga, R.K.
Deposited on	:	2011-07-28
Resolution	:	2.47 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:

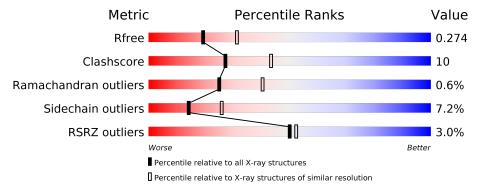|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (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 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 <=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	742	2% 78% 18% ..
1	B	742	4% 74% 20% ..

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
2	GOL	A	1722	-	-	X	-
2	GOL	B	1719	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11617 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total 5578	C 3564	N 979	O 1012	S 23	0	0	0
1	B	721	Total 5534	C 3537	N 969	O 1005	S 23	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-19	MET	-	expression tag	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896
B	-15	HIS	-	expression tag	UNP P07896

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is (S)-3-Hydroxyhexanoyl-CoA (three-letter code: 3H9) (formula: $C_{27}H_{42}N_7O_{18}P_3S$).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	0
			182	182		
5	A	1	Total	O	0	0
			1	1		
5	B	176	Total	O	0	0
			176	176		
5	B	2	Total	O	0	0
			2	2		

3 Residue-property plots ⓘ

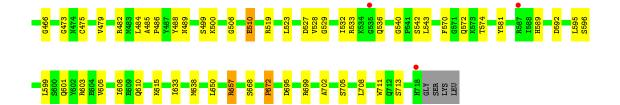These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PEROXISOMAL BIFUNCTIONAL ENZYME

- Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME

G466 G473 N474 C475 V479 R482 M483 L484 A485 P486 Y487 Y488 N489 S499 K500 G506 E510 R519 L523 D527 V528 G529 I532 K533 K534 G535 Q536 G540 P541 S542 L543 F570 G571 Q572 K573 T574 Y581 R587 I588 H589 D592 L595 S596

L599 S600 Q601 Y602 R603 E604 V605 I608 E609 Q610 K615 I633 M638 L650 R657 S668 P672 D695 R699 A702 S705 L708 W711 Q712 S713 H718 GLY SER LYS LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.35Å 125.76Å 225.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.90 – 2.47 62.77 – 2.47	Depositor EDS
% Data completeness (in resolution range)	94.9 (112.90-2.47) 94.9 (62.77-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.279 0.215 , 0.274	Depositor DCC
R_{free} test set	3247 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.2	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11617	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, SO4, 3H9

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	0.80	1/5707 (0.0%)	0.83	5/7731 (0.1%)
1	B	0.80	0/5662	0.83	7/7671 (0.1%)
All	All	0.80	1/11369 (0.0%)	0.83	12/15402 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	TYR	CD1-CE1	5.32	1.47	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	234	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	657	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	B	657	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	33	ARG	NE-CZ-NH1	6.08	123.34	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	PHE	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	5578	0	5689	105	0
1	B	5534	0	5639	126	0
2	A	6	0	8	8	0
2	B	6	0	8	4	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	56	0	42	2	0
4	B	56	0	42	4	0
5	A	183	0	0	17	1
5	B	178	0	0	31	1
All	All	11617	0	11428	229	1

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 10.

The worst 5 of 229 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:603:ARG:HG2	5:B:2112:HOH:O	1.56	1.04
1:A:3:GLU:HB2	2:A:1722:GOL:H32	1.30	1.04
1:A:0:HIS:O	2:A:1722:GOL:H31	1.58	1.02
1:A:3:GLU:HB2	2:A:1722:GOL:C3	1.91	1.00
1:B:19:PRO:HD2	5:B:2007:HOH:O	1.58	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2010:HOH:O	5:B:2051:HOH:O[2_254]	2.08	0.12

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	725/742 (98%)	687 (95%)	36 (5%)	2 (0%)	41	59
1	B	719/742 (97%)	678 (94%)	35 (5%)	6 (1%)	19	33
All	All	1444/1484 (97%)	1365 (94%)	71 (5%)	8 (1%)	25	40

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	B	284	SER
1	B	355	GLN
1	A	365	SER
1	B	356	ALA

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	596/609 (98%)	550 (92%)	46 (8%)	13	23
1	B	591/609 (97%)	551 (93%)	40 (7%)	16	28
All	All	1187/1218 (98%)	1101 (93%)	86 (7%)	14	26

5 of 86 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	VAL

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Mol	Chain	Res	Type
1	B	73	LEU
1	B	572	GLN
1	A	585	LEU
1	A	675	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	679	GLN
1	B	0	HIS
1	B	572	GLN
1	A	601	GLN
1	B	278	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

8 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
3	SO4	A	1726	-	4,4,4	0.39	0	6,6,6	0.82	0
4	3H9	A	1725	-	49,58,58	1.57	8 (16%)	60,85,85	1.47	9 (15%)
3	SO4	A	1724	-	4,4,4	0.30	0	6,6,6	0.37	0
3	SO4	A	1723	-	4,4,4	0.36	0	6,6,6	0.52	0
2	GOL	A	1722	-	5,5,5	0.80	0	5,5,5	1.59	1 (20%)
2	GOL	B	1719	-	5,5,5	0.35	0	5,5,5	0.45	0
3	SO4	B	1721	-	4,4,4	0.25	0	6,6,6	0.34	0
4	3H9	B	1720	-	49,58,58	1.10	4 (8%)	60,85,85	1.48	10 (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
4	3H9	A	1725	-	-	14/54/74/74	0/3/3/3
2	GOL	B	1719	-	-	2/4/4/4	-
2	GOL	A	1722	-	-	4/4/4/4	-
4	3H9	B	1720	-	-	10/54/74/74	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1725	3H9	P3B-O8A	4.94	1.66	1.50
4	A	1725	3H9	P3B-O3B	4.80	1.68	1.59
4	A	1725	3H9	O4B-C1B	4.21	1.47	1.41
4	B	1720	3H9	O4B-C1B	3.71	1.46	1.41
4	B	1720	3H9	P3B-O9A	-3.01	1.43	1.54

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1725	3H9	N3A-C2A-N1A	-4.85	121.10	128.68
4	B	1720	3H9	N3A-C2A-N1A	-4.68	121.36	128.68
4	B	1720	3H9	C2-C1-S1P	3.75	118.27	113.63
4	B	1720	3H9	O9A-P3B-O7A	3.69	121.76	107.64
4	A	1725	3H9	P2A-O3A-P1A	-3.31	121.45	132.83

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1725	3H9	C1-C2-C3-O3
4	A	1725	3H9	C1-C2-C3-C4
4	A	1725	3H9	P1A-O3A-P2A-O6A
4	A	1725	3H9	CCP-O6A-P2A-O4A
4	A	1725	3H9	CCP-O6A-P2A-O5A

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1725	3H9	2	0
2	A	1722	GOL	8	0
2	B	1719	GOL	4	0
4	B	1720	3H9	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 3H9 A 1725

Bond lengths

Bond angles

Torsions

Rings

Ligand 3H9 B 1720

Bond lengths

Bond angles

Torsions

Rings

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	727/742 (97%)	0.15	17 (2%)	60	62	9, 33, 72, 112	0
1	B	721/742 (97%)	-0.00	27 (3%)	41	44	11, 34, 72, 112	0
All	All	1448/1484 (97%)	0.07	44 (3%)	50	52	9, 34, 73, 112	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	GLN	4.9
1	A	356	ALA	4.8
1	A	411	ALA	4.8
1	B	354	GLY	4.7
1	A	357	SER	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)
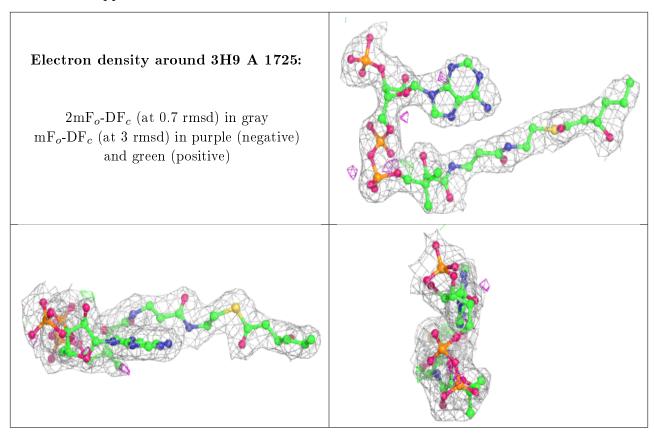
There are no carbohydrates in this entry.

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.
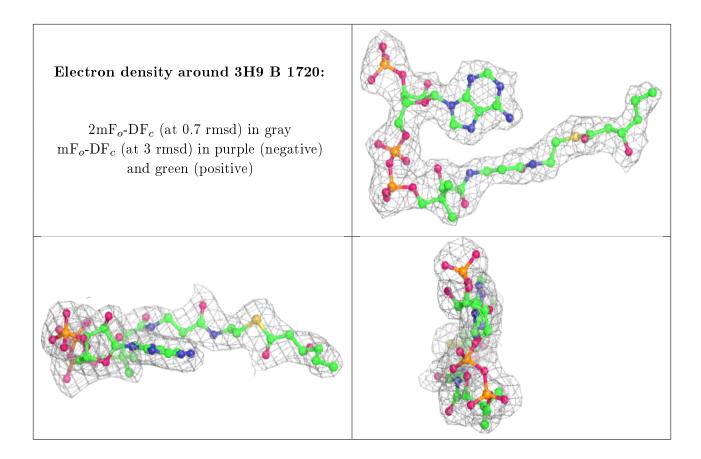
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	A	1722	6/6	0.83	0.39	36,37,38,39	0
2	GOL	B	1719	6/6	0.88	0.23	51,52,54,56	0
3	SO4	A	1724	5/5	0.90	0.14	71,73,74,74	0
3	SO4	A	1723	5/5	0.91	0.19	50,54,56,57	0
4	3H9	A	1725	56/56	0.94	0.13	21,50,55,59	0
3	SO4	B	1721	5/5	0.96	0.11	59,61,63,63	0
4	3H9	B	1720	56/56	0.98	0.12	21,31,38,40	0
3	SO4	A	1726	5/5	0.99	0.10	29,29,32,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3H9 A 1725:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 3H9 B 1720:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.