



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 05:51 am GMT

PDB ID : 1N4U
Title : CHOLESTEROL OXIDASE FROM STREPTOMYCES @ pH 4.5 (STREPTOMYCES SP. SA-COO)
Authors : Vrielink, A.; Lario, P.I.
Deposited on : 2002-11-01
Resolution : 0.95 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

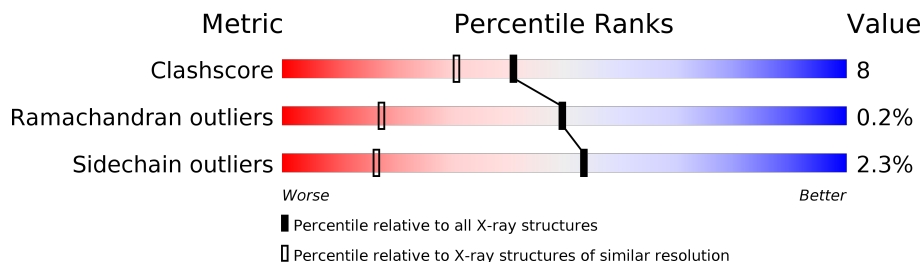
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.95 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))
Clashscore	122078	1074 (1.06-0.86)
Ramachandran outliers	120005	1152 (1.08-0.84)
Sidechain outliers	119972	1154 (1.08-0.84)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	504	

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	PO4	A	514	-	-	X	-
5	GOL	A	516	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9287 atoms, of which 4252 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 Cholesterol oxidase.

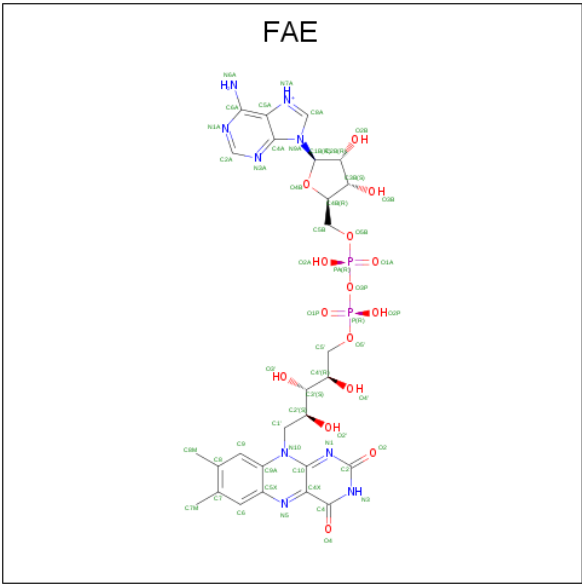
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	499	Total	C	H	N	O	S	0	84	1
			8470	2711	4220	715	799	25			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



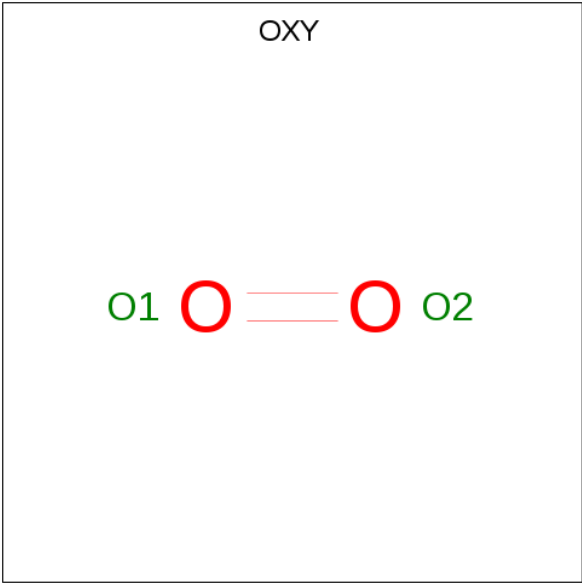
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is FLAVIN-N7 PROTONATED-ADENINE DINUCLEOTIDE (three-letter code: FAE) (formula: C₂₇H₃₄N₉O₁₅P₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

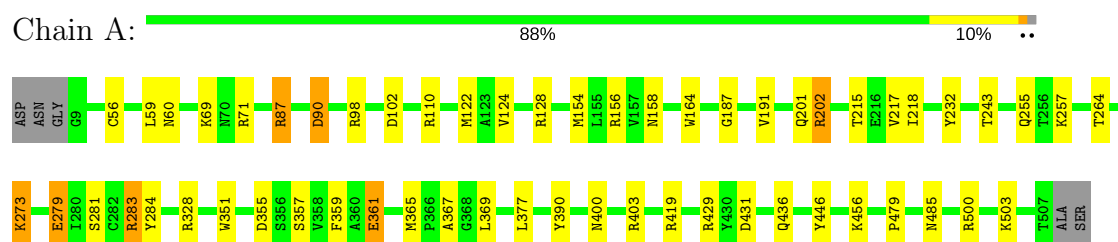
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	699	Total	O	0	0
			699	699		

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.

Note EDS was not executed.

• Molecule 1: Cholesterol oxidase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.25Å 73.28Å 63.10Å 90.00° 105.07° 90.00°	Depositor
Resolution (Å)	46.90 – 0.95	Depositor
% Data completeness (in resolution range)	94.3 (46.90-0.95)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.113 , 0.136	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9287	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, OXY, FAE

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	0.74	0/4596	1.21	36/6239 (0.6%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ARG	NE-CZ-NH2	-14.97	112.81	120.30
1	A	419	ARG	NE-CZ-NH1	-14.02	113.29	120.30
1	A	419	ARG	NE-CZ-NH2	11.22	125.91	120.30
1	A	128	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	A	87[A]	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	87[B]	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	A	500	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	A	98	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	202[A]	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	202[B]	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	202[C]	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	A	328	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	A	71	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	367	ALA	C-N-CA	-6.87	107.88	122.30
1	A	156	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	A	355	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	A	202[A]	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	202[B]	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	202[C]	ARG	CD-NE-CZ	6.72	133.01	123.60
1	A	446	TYR	CB-CG-CD1	6.61	124.96	121.00
1	A	110	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	102[A]	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	102[B]	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	436	GLN	O-C-N	-5.44	113.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	355	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	232	TYR	CB-CG-CD1	5.16	124.09	121.00
1	A	431	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	361[A]	GLU	CA-CB-CG	5.08	124.59	113.40
1	A	361[B]	GLU	CA-CB-CG	5.08	124.59	113.40
1	A	390	TYR	CB-CG-CD1	5.08	124.05	121.00
1	A	429	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	90[A]	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	90[B]	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	283[A]	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	283[B]	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	4250	4220	4178	62	0
2	A	25	0	0	3	0
3	A	53	32	32	1	0
4	A	2	0	0	0	0
5	A	6	0	8	4	0
6	A	699	0	0	55	0
All	All	5035	4252	4218	67	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 8.

All (67) 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)
5:A:516:GOL:C1	6:A:883:HOH:O	1.72	1.35
1:A:87[A]:ARG:NE	6:A:1077:HOH:O	1.57	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122[B]:MET:SD	6:A:1208:HOH:O	1.91	1.24
1:A:359[A]:PHE:CZ	6:A:1210:HOH:O	1.92	1.23
1:A:359[A]:PHE:CE2	6:A:1215:HOH:O	2.04	1.10
1:A:503[B]:LYS:HD3	6:A:1168:HOH:O	1.64	0.96
1:A:361[B]:GLU:OE2	6:A:1212:HOH:O	1.83	0.96
1:A:359[A]:PHE:HZ	6:A:1210:HOH:O	1.29	0.94
5:A:516:GOL:H32	6:A:1087:HOH:O	1.69	0.92
1:A:479[A]:PRO:HG2	6:A:1061:HOH:O	1.71	0.90
1:A:187[A]:GLY:O	6:A:1108:HOH:O	1.87	0.89
1:A:215[B]:THR:HG21	6:A:1086:HOH:O	1.73	0.88
1:A:400[B]:ASN:ND2	6:A:1060:HOH:O	2.06	0.88
1:A:90[B]:ASP:OD2	6:A:1147:HOH:O	1.92	0.86
1:A:257[A]:LYS:N	2:A:514:PO4:O3	2.10	0.85
1:A:377[A]:LEU:CD1	6:A:1213:HOH:O	2.25	0.83
1:A:359[A]:PHE:CE2	6:A:1210:HOH:O	2.24	0.80
1:A:257[A]:LYS:H	2:A:514:PO4:P	2.04	0.79
1:A:485[B]:ASN:OD1	6:A:1208:HOH:O	2.01	0.78
1:A:377[A]:LEU:HD12	6:A:1213:HOH:O	1.83	0.77
1:A:87[A]:ARG:CG	6:A:1077:HOH:O	2.30	0.77
1:A:359[A]:PHE:HE2	6:A:1215:HOH:O	1.54	0.74
1:A:479[A]:PRO:O	6:A:1061:HOH:O	2.00	0.72
1:A:215[B]:THR:CG2	6:A:1086:HOH:O	2.35	0.72
1:A:377[A]:LEU:HD12	6:A:1214:HOH:O	1.89	0.72
1:A:154[B]:MET:HG2	6:A:1055:HOH:O	1.89	0.71
1:A:485[A]:ASN:ND2	6:A:1208:HOH:O	2.24	0.70
1:A:218[A]:ILE:CG2	6:A:1087:HOH:O	2.40	0.69
1:A:122[B]:MET:CE	6:A:1208:HOH:O	2.33	0.69
1:A:191[A]:VAL:HG22	6:A:907:HOH:O	1.94	0.68
1:A:264:THR:HG22	1:A:279[B]:GLU:OE2	1.96	0.65
1:A:503[B]:LYS:HE2	6:A:1168:HOH:O	1.97	0.63
1:A:218[A]:ILE:HG23	6:A:1087:HOH:O	1.99	0.63
1:A:87[A]:ARG:HG3	6:A:1077:HOH:O	1.94	0.62
1:A:154[C]:MET:HE2	6:A:1056:HOH:O	1.99	0.61
1:A:122[B]:MET:HE3	6:A:1208:HOH:O	2.00	0.57
1:A:218[A]:ILE:HG22	6:A:544:HOH:O	2.04	0.57
1:A:377[A]:LEU:HD13	6:A:1213:HOH:O	1.99	0.57
1:A:485[A]:ASN:OD1	6:A:1215:HOH:O	2.15	0.56
5:A:516:GOL:O1	6:A:883:HOH:O	1.54	0.56
1:A:154[B]:MET:HE2	6:A:1055:HOH:O	2.06	0.55
1:A:187[A]:GLY:C	6:A:1108:HOH:O	2.35	0.54
1:A:283[B]:ARG:HD3	1:A:284:TYR:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243[B]:THR:HG21	6:A:921:HOH:O	2.08	0.52
1:A:503[B]:LYS:CE	6:A:1168:HOH:O	2.55	0.52
5:A:516:GOL:H12	6:A:883:HOH:O	1.72	0.51
1:A:154[B]:MET:CE	6:A:1056:HOH:O	0.82	0.51
1:A:456[B]:LYS:HE2	6:A:864:HOH:O	2.10	0.51
1:A:273[A]:LYS:NZ	6:A:837:HOH:O	2.44	0.50
1:A:479[A]:PRO:C	6:A:1061:HOH:O	2.47	0.50
1:A:69[B]:LYS:HE2	6:A:668:HOH:O	2.10	0.49
1:A:124[A]:VAL:CG2	1:A:191[A]:VAL:HG13	2.42	0.48
1:A:202[B]:ARG:NE	6:A:972:HOH:O	2.42	0.48
1:A:154[B]:MET:HE2	6:A:1056:HOH:O	0.75	0.48
1:A:122[A]:MET:HE2	1:A:191[A]:VAL:HG11	1.96	0.48
1:A:283[B]:ARG:HD3	1:A:284:TYR:CZ	2.52	0.45
2:A:512:PO4:P	6:A:1111:HOH:O	2.74	0.45
1:A:124[A]:VAL:HG22	1:A:191[A]:VAL:HG13	2.00	0.44
1:A:503[B]:LYS:CD	6:A:1168:HOH:O	2.39	0.43
1:A:485[A]:ASN:HB3	3:A:510:FAE:C2	2.48	0.43
1:A:283[A]:ARG:NE	6:A:900:HOH:O	2.50	0.43
1:A:154[B]:MET:CE	6:A:1055:HOH:O	2.63	0.43
1:A:60[B]:ASN:ND2	6:A:1076:HOH:O	2.53	0.42
1:A:164:TRP:CD1	1:A:201[B]:GLN:HG3	2.55	0.41
1:A:122[A]:MET:CE	1:A:191[A]:VAL:HG11	2.50	0.41
1:A:273[A]:LYS:HD2	6:A:1018:HOH:O	2.21	0.41
1:A:351:TRP:CD2	1:A:357:SER:HB3	2.56	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	583/504 (116%)	563 (97%)	19 (3%)	1 (0%)	49 17

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	VAL

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	474/401 (118%)	458 (97%)	16 (3%)	40 8

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56[A]	CYS
1	A	56[B]	CYS
1	A	59[A]	LEU
1	A	59[B]	LEU
1	A	158	ASN
1	A	255[A]	GLN
1	A	255[B]	GLN
1	A	273[A]	LYS
1	A	273[B]	LYS
1	A	279[A]	GLU
1	A	279[B]	GLU
1	A	281[A]	SER
1	A	281[B]	SER
1	A	365[A]	MET
1	A	365[B]	MET
1	A	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	FAE	A	510	-	48,58,58	1.37	6 (12%)	55,89,89	1.01	2 (3%)
2	PO4	A	511	-	4,4,4	1.99	1 (25%)	6,6,6	0.87	0
2	PO4	A	512	-	4,4,4	1.60	0	6,6,6	0.98	0
2	PO4	A	513	-	4,4,4	1.24	0	6,6,6	0.74	0
2	PO4	A	514	-	4,4,4	1.28	0	6,6,6	1.11	0
2	PO4	A	515	-	4,4,4	1.74	1 (25%)	6,6,6	1.36	1 (16%)
5	GOL	A	516	-	5,5,5	0.44	0	5,5,5	0.82	0
4	OXY	A	517[B]	-	1,1,1	0.17	0	0,0,0	0.00	-

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	FAE	A	510	-	-	0/28/50/50	0/6/6/6
2	PO4	A	511	-	-	0/0/0/0	0/0/0/0
2	PO4	A	512	-	-	0/0/0/0	0/0/0/0
2	PO4	A	513	-	-	0/0/0/0	0/0/0/0
2	PO4	A	514	-	-	0/0/0/0	0/0/0/0
2	PO4	A	515	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	516	-	-	0/4/4/4	0/0/0/0
4	OXY	A	517[B]	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	511	PO4	P-O1	-3.13	1.42	1.50
2	A	515	PO4	P-O4	-2.79	1.44	1.54
3	A	510	FAE	C2-N1	-2.45	1.33	1.38
3	A	510	FAE	C9-C9A	-2.01	1.36	1.40
3	A	510	FAE	O4B-C1B	2.61	1.44	1.41
3	A	510	FAE	C5X-N5	3.39	1.40	1.35
3	A	510	FAE	C9A-N10	4.19	1.43	1.38
3	A	510	FAE	C4X-N5	4.73	1.40	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	515	PO4	O4-P-O3	-2.03	100.53	107.94
3	A	510	FAE	C1'-N10-C9A	2.89	120.88	118.31
3	A	510	FAE	C2-N1-C10	3.42	118.19	114.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	510	FAE	1	0
2	A	512	PO4	1	0
2	A	514	PO4	2	0
5	A	516	GOL	4	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.