



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:53 pm BST

PDB ID : 1W9Y
Title : The structure of ACC oxidase
Authors : Zhang, Z.; Ren, J.-S.; Clifton, I.J.; Schofield, C.J.
Deposited on : 2004-10-20
Resolution : 2.10 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

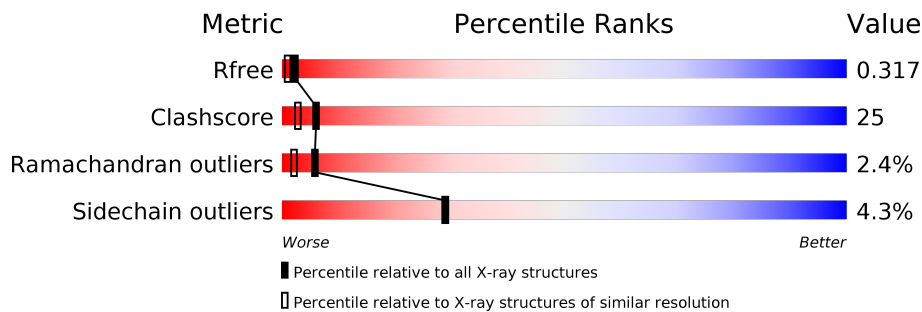
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	319	 54% 37% 6%

2 Entry composition [i](#)

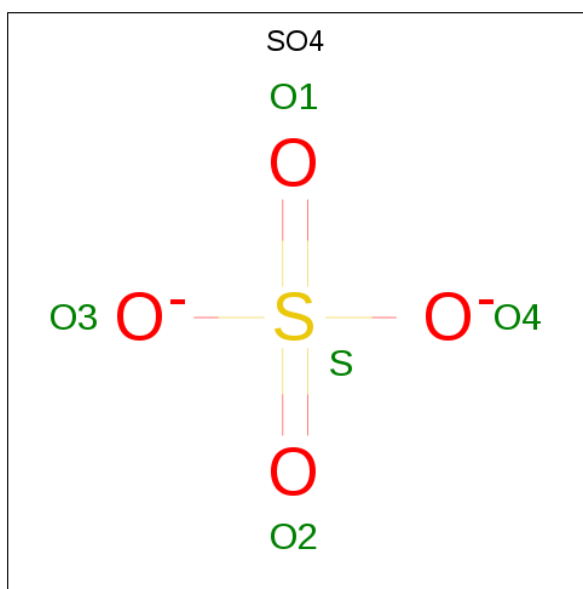
There are 3 unique types of molecules in this entry. The entry contains 2474 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 1-AMINOCYCLOPROPANE-1-CARBOXYLATE OXIDASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	N	O	S				Se
1	A	299	2374	1523	395	439	4	13	0	0	1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is water.

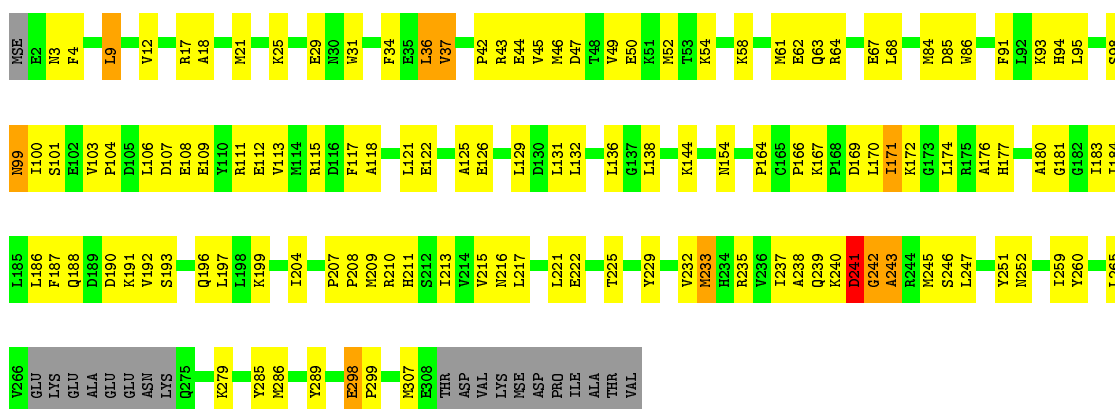
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	95	95	95	0	0

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. 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. 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: 1-AMINOCYCLOPROPANE-1-CARBOXYLATE OXIDASE 1

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	70.30Å 107.93Å 108.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 24.53 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.8 (25.00-2.10) 99.4 (24.53-2.12)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.11Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.292 0.275 , 0.317	Depositor DCC
R_{free} test set	1141 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.007 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2474	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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: 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	0.40	0/2413	0.64	0/3231

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 [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	2374	0	2372	118	0
2	A	5	0	0	0	0
3	A	95	0	0	5	0
All	All	2474	0	2372	118	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 25.

All (118) 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:171:ILE:HG23	1:A:174:LEU:HD12	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:THR:HA	1:A:265:LEU:HD23	1.44	0.98
1:A:191:LYS:HG2	1:A:208:PRO:HB2	1.47	0.96
1:A:101:SER:HB3	1:A:115:ARG:HH22	1.33	0.94
1:A:180:ALA:HB1	1:A:286:MSE:HE1	1.60	0.82
1:A:167:LYS:HE3	1:A:169:ASP:HB3	1.64	0.80
1:A:21:MSE:HE1	1:A:131:LEU:HD13	1.64	0.79
1:A:109:GLU:O	1:A:113:VAL:HG23	1.85	0.77
1:A:115:ARG:HD2	3:A:2043:HOH:O	1.84	0.77
1:A:101:SER:CB	1:A:115:ARG:HH22	1.99	0.76
1:A:42:PRO:HB2	1:A:45:VAL:HG23	1.66	0.75
1:A:64:ARG:HG2	1:A:84:MSE:HE1	1.69	0.73
1:A:166:PRO:HG2	1:A:170:LEU:CD1	2.18	0.73
1:A:68:LEU:HD22	1:A:84:MSE:HE3	1.70	0.73
1:A:199:LYS:HB3	1:A:204:ILE:HD12	1.72	0.72
1:A:52:MSE:SE	1:A:113:VAL:HG21	2.41	0.70
1:A:52:MSE:HE1	1:A:109:GLU:HG3	1.74	0.69
1:A:285:TYR:HD2	1:A:286:MSE:CE	2.05	0.68
1:A:190:ASP:CG	1:A:191:LYS:H	1.96	0.68
1:A:99:ASN:HD22	1:A:99:ASN:C	1.96	0.68
1:A:138:LEU:HD21	1:A:265:LEU:HD13	1.77	0.67
1:A:199:LYS:HB3	1:A:204:ILE:CD1	2.25	0.66
1:A:136:LEU:HD21	1:A:225:THR:HG22	1.79	0.65
1:A:63:GLN:O	1:A:67:GLU:HG3	1.97	0.65
1:A:196:GLN:HE22	1:A:235:ARG:HH21	1.46	0.63
1:A:136:LEU:HD13	1:A:229:TYR:CZ	2.34	0.62
1:A:245:MSE:HE3	1:A:247:LEU:CD1	2.31	0.61
1:A:25:LYS:O	1:A:29:GLU:HG3	2.01	0.60
1:A:101:SER:HB3	1:A:115:ARG:NH2	2.11	0.60
1:A:84:MSE:HE2	1:A:84:MSE:HA	1.83	0.60
1:A:166:PRO:HG2	1:A:170:LEU:HD12	1.83	0.60
1:A:99:ASN:C	1:A:99:ASN:ND2	2.56	0.59
1:A:107:ASP:O	1:A:111:ARG:HG3	2.03	0.59
1:A:180:ALA:CB	1:A:286:MSE:HE1	2.31	0.59
1:A:164:PRO:HA	1:A:238:ALA:HB1	1.86	0.58
1:A:43:ARG:HH11	1:A:43:ARG:HB2	1.69	0.58
1:A:239:GLN:HB3	1:A:241:ASP:HB3	1.85	0.58
1:A:99:ASN:HD22	1:A:100:ILE:N	2.02	0.58
1:A:196:GLN:HE21	1:A:235:ARG:HE	1.52	0.58
1:A:196:GLN:NE2	1:A:235:ARG:HE	2.02	0.58
1:A:93:LYS:NZ	1:A:154:ASN:HB3	2.19	0.57
1:A:241:ASP:OD1	1:A:242:GLY:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HB	1:A:216:ASN:OD1	2.05	0.56
1:A:43:ARG:NH1	1:A:43:ARG:HB2	2.20	0.56
1:A:122:GLU:O	1:A:126:GLU:HG3	2.06	0.56
1:A:298:GLU:CB	1:A:299:PRO:HD3	2.37	0.55
1:A:298:GLU:OE1	1:A:298:GLU:HA	2.07	0.55
1:A:181:GLY:HA3	1:A:252:ASN:OD1	2.06	0.55
1:A:117:PHE:CE2	1:A:121:LEU:HD11	2.42	0.55
1:A:61:MSE:HE2	1:A:86:TRP:CE3	2.43	0.54
1:A:171:ILE:HG21	1:A:237:ILE:CD1	2.38	0.54
1:A:192:VAL:HB	1:A:241:ASP:OD1	2.07	0.54
1:A:43:ARG:HH11	1:A:43:ARG:CB	2.21	0.54
1:A:52:MSE:HE3	1:A:109:GLU:OE2	2.06	0.54
1:A:221:LEU:O	1:A:225:THR:HG23	2.07	0.53
1:A:50:GLU:O	1:A:54:LYS:HG3	2.09	0.53
1:A:285:TYR:CD2	1:A:286:MSE:CE	2.91	0.52
1:A:259:ILE:O	1:A:279:LYS:HA	2.09	0.52
1:A:183:ILE:HG22	1:A:251:TYR:HB3	1.90	0.52
1:A:18:ALA:HB3	3:A:2006:HOH:O	2.08	0.52
1:A:93:LYS:O	1:A:98:SER:HA	2.10	0.52
1:A:177:HIS:O	1:A:233:MSE:HA	2.10	0.52
1:A:239:GLN:C	1:A:241:ASP:N	2.63	0.52
1:A:171:ILE:HA	1:A:174:LEU:HG	1.92	0.52
1:A:176:ALA:HB3	1:A:233:MSE:CE	2.41	0.51
1:A:99:ASN:O	1:A:103:VAL:HG23	2.11	0.51
1:A:61:MSE:HE1	1:A:85:ASP:O	2.11	0.51
1:A:84:MSE:HE2	3:A:2032:HOH:O	2.11	0.51
1:A:242:GLY:O	1:A:243:ALA:C	2.49	0.51
1:A:46:MSE:HE2	1:A:187:PHE:CD1	2.45	0.50
1:A:93:LYS:HZ1	1:A:154:ASN:HB3	1.77	0.50
1:A:132:LEU:O	1:A:136:LEU:HB2	2.12	0.49
1:A:176:ALA:HB3	1:A:233:MSE:HE3	1.94	0.49
1:A:184:ILE:N	1:A:184:ILE:HD12	2.27	0.49
1:A:171:ILE:HG22	1:A:171:ILE:O	2.13	0.49
1:A:94:HIS:CE1	1:A:100:ILE:HD11	2.47	0.49
1:A:68:LEU:HD22	1:A:84:MSE:CE	2.42	0.49
1:A:109:GLU:HA	1:A:112:GLU:OE1	2.13	0.49
1:A:138:LEU:HD21	1:A:265:LEU:CD1	2.41	0.49
1:A:34:PHE:CE1	1:A:36:LEU:HD13	2.48	0.48
1:A:260:TYR:HB3	1:A:279:LYS:HG3	1.95	0.48
1:A:109:GLU:O	1:A:112:GLU:HG2	2.13	0.48
1:A:144:LYS:HB2	3:A:2046:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:O	1:A:12:VAL:HG22	2.15	0.47
1:A:193:SER:HA	1:A:243:ALA:CB	2.44	0.47
1:A:37:VAL:HG11	1:A:209:MSE:HE2	1.96	0.47
1:A:94:HIS:HD1	1:A:100:ILE:HD11	1.80	0.47
1:A:94:HIS:C	1:A:95:LEU:HD12	2.35	0.47
1:A:190:ASP:CG	1:A:191:LYS:N	2.67	0.46
1:A:42:PRO:C	1:A:44:GLU:N	2.66	0.46
1:A:94:HIS:ND1	1:A:100:ILE:HD11	2.29	0.46
1:A:210:ARG:HG2	1:A:211:HIS:ND1	2.30	0.46
1:A:68:LEU:CD2	1:A:84:MSE:HE3	2.43	0.46
1:A:285:TYR:HD2	1:A:286:MSE:HE3	1.80	0.46
1:A:104:PRO:O	1:A:106:LEU:HG	2.16	0.46
1:A:217:LEU:HD22	1:A:221:LEU:CD1	2.45	0.46
1:A:186:LEU:HD11	1:A:246:SER:OG	2.17	0.46
1:A:94:HIS:CE1	1:A:118:ALA:HB2	2.52	0.45
1:A:225:THR:HA	1:A:265:LEU:CD2	2.31	0.45
1:A:125:ALA:O	1:A:129:LEU:HG	2.17	0.44
1:A:188:GLN:OE1	1:A:193:SER:CB	2.66	0.44
1:A:49:VAL:HG22	1:A:113:VAL:HG12	2.00	0.44
1:A:12:VAL:O	1:A:17:ARG:HD2	2.18	0.44
1:A:45:VAL:O	1:A:49:VAL:HG23	2.18	0.44
1:A:46:MSE:HE3	1:A:213:ILE:HD11	2.00	0.43
1:A:4:PHE:CD2	1:A:207:PRO:HD2	2.54	0.42
1:A:31:TRP:O	1:A:232:VAL:HG21	2.20	0.42
1:A:240:LYS:HB3	1:A:240:LYS:HE2	1.77	0.42
1:A:222:GLU:HA	1:A:229:TYR:O	2.20	0.42
1:A:36:LEU:HD22	1:A:215:VAL:HG21	2.02	0.42
1:A:188:GLN:OE1	1:A:193:SER:HB3	2.20	0.41
1:A:93:LYS:H	1:A:99:ASN:ND2	2.18	0.41
1:A:91:PHE:HB3	3:A:2038:HOH:O	2.20	0.41
1:A:58:LYS:O	1:A:62:GLU:HG3	2.19	0.41
1:A:106:LEU:HB2	1:A:111:ARG:CZ	2.50	0.41
1:A:136:LEU:CD1	1:A:229:TYR:CZ	3.03	0.41
1:A:34:PHE:CD1	1:A:36:LEU:HD13	2.56	0.41
1:A:298:GLU:HB2	1:A:299:PRO:HD3	2.03	0.40

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	295/319 (92%)	276 (94%)	12 (4%)	7 (2%)	6 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	A	307	MSE
1	A	3	ASN
1	A	243	ALA
1	A	241	ASP
1	A	171	ILE
1	A	242	GLY

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	257/261 (98%)	246 (96%)	11 (4%)	29 29

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	36	LEU
1	A	37	VAL
1	A	47	ASP

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Mol	Chain	Res	Type
1	A	99	ASN
1	A	108	GLU
1	A	197	LEU
1	A	233	MSE
1	A	241	ASP
1	A	289	TYR
1	A	298	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	63	GLN
1	A	99	ASN
1	A	196	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](#)

1 ligand is 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	A	901	-	4,4,4	0.53	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.