



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:55 AM GMT

PDB ID : 2VAO
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-
ALCOHOL OXIDASE IN COMPLEX WITH ISOEUGENOL
Authors : Mattevi, A.
Deposited on : 1997-04-10
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

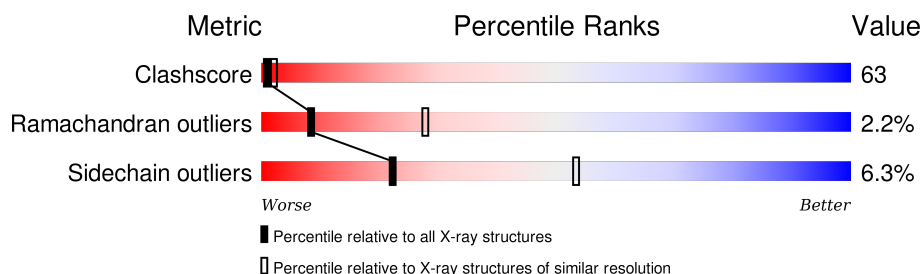
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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	560	 23% 56% 18% ..
1	B	560	 24% 55% 18% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8948 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 VANILLYL-ALCOHOL OXIDASE.

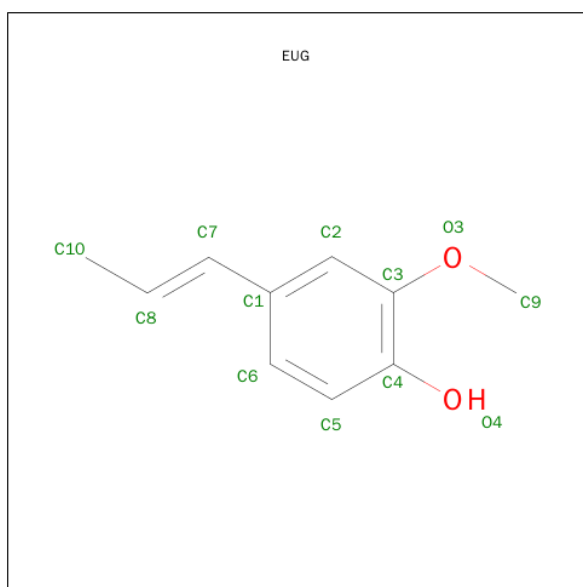
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	51	0	0
			4391	2817	751	799	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 2-METHOXY-4-VINYLPHENOL (three-letter code: EUG) (formula: $C_{10}H_{12}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

- Molecule 4 is water.

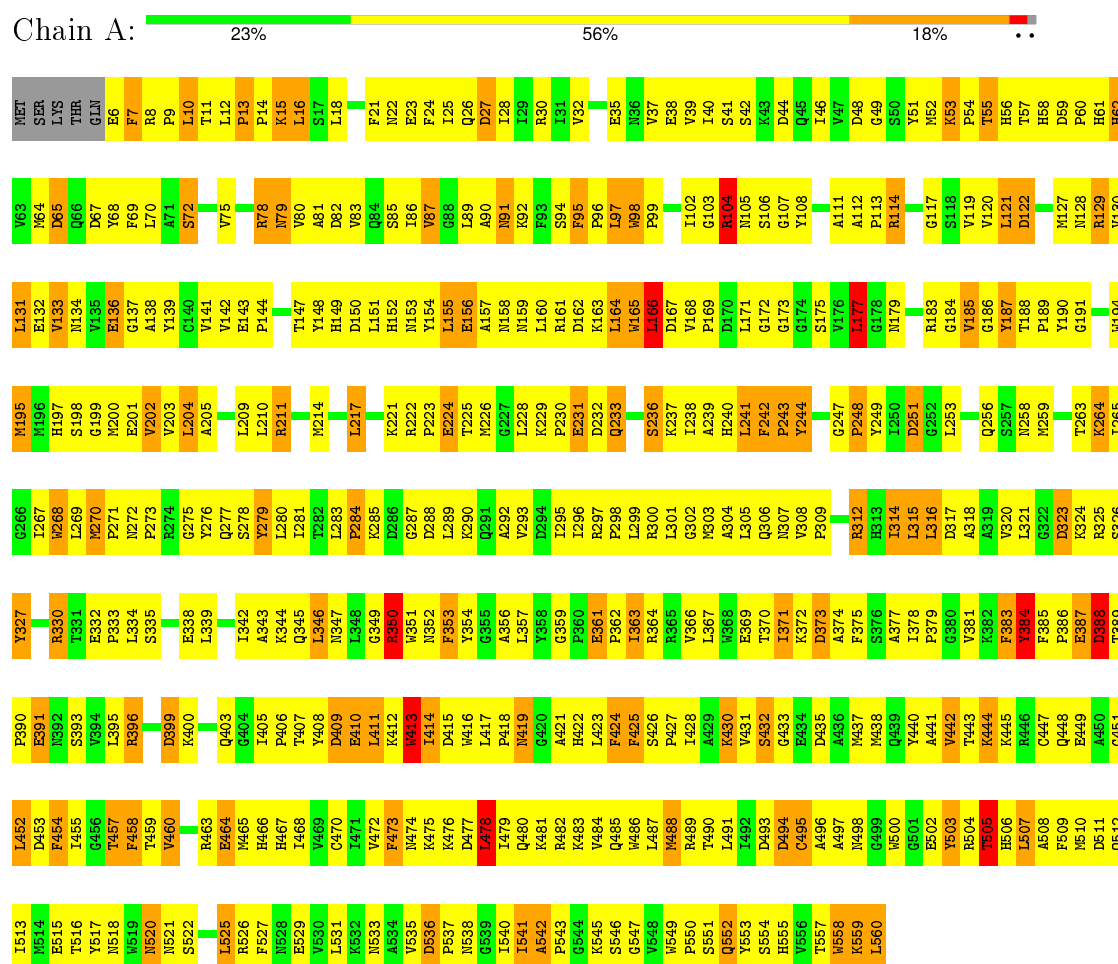
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	24	Total	O	0	0
			24	24		

3 Residue-property plots

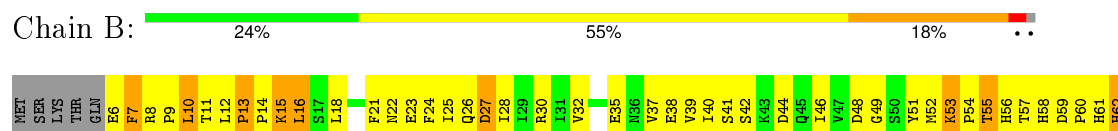
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: VANILLYL-ALCOHOL OXIDASE



• Molecule 1: VANILLYL-ALCOHOL OXIDASE



B515	F454	S393	R330	W268	H196	V130	V63
T516	I455	V394	T331	L269	H197	L131	H64
N517	G456	L395	E332	M270	S198	E132	D65
N518	T457	R396	P333	P271	G199	V133	D66
N519	F458		L334	M272	M200	N134	D67
N520	T459	D399	S335	P273	E201	V135	Y68
N521	V460	K400		R274	V202	E136	F69
S522		T401	E338	G275	V203	G137	L70
	R463	P402	L339	Y276	L204	A138	A71
L525	E464	Q403	I342	Q277	A205	Y139	S72
R526	M465	G404		S278		C140	A73
R527	H466	I405	G345	Y279	L209	V141	I74
F528	H467	P406	L346	L280	L210	V142	Y75
E529	I468	T407	L347	I281	R211	E143	
V530	V469	Y408	R347	T282		P144	
L531	C470	D409	L348	L283	M214		
N532	I471	E410	G349	R284		T147	R78
N533	V472	L411	R350	K285	L217	Y148	Y80
A534	F473	K412	R351	D286		H149	A81
V535	M474	W413	R352	Q287		D150	D82
D536	K475	I414	P353	D288	K221	H151	Y83
P537	K476	D415	Y354	L289	R222	H152	R84
N538	D477	W416	G355	K290	P223	H153	S85
G539	L478	L417	A356	Q291	T225	M154	I86
I540	L479	P418	L357	A292	T226	Y155	Y87
I541	Q480	M419	R358	V293	G227	E156	G88
A542	R481	G420	G359	D294	L228	A157	L89
	R482	A421	P360	I295	K229	M158	A90
K545	V483	H422	R361	I296	P230	N159	N91
S546	V484	L423	P362	R297	E231	L160	F93
G547	Q485	F424	I363	P298	D232	R161	S94
V548	W486	F425	R364	L299	Q233	D162	F95
W549	L487	S426	R365	R300		K163	P96
P550	M488	P427	V366	L301	S236	L164	L97
S551	R489	I428	L367	G302	K237	W165	W98
Q552	T490	A429	R368	M303	I238	L166	P99
Y553	L491	K430	R369	A304	A239		
S554	L492	V431	T370	L305	H240	L171	I102
H555	D493	S432	I371	Q306	L241	G172	G103
V556	D494	G433	K372	N307	F242	G173	R104
T557	C495	E434	D373	V308	P243	G174	N105
W558	A496	D435	A374	P309	Y244	S175	S106
K559	A497	A436	F375			W176	G107
L560	M498	M437	R376	R312	G247	L177	Y108
	G499	M438	A377	R313	P248	G178	A111
	W500	Q439	I378	I314	Y249	N179	A112
	G501	Y440	P379	L315	I250		P113
E502	E502	A441	G380	L316	D251	G183	R114
Y503	Y503	V442	V381	D317	G252	G184	
B504	B504	T443	R382	A318	L253	V185	G117
T505	T505	K444	F383	A319		G186	S118
H506	H506	K445	R384	V320	Q256	Y187	V119
L507	L507	R446	P385	L321	S257	T188	V120
A508	A508	C447	P386	G322	N258	P189	L121
F509	F509	Q448	E387	D323	N259	Y190	D122
N510	N510	E449	D388	K324		G191	
D511	D511	A450	T389	R325	K284		M127
Q512	Q512	G451	P390	S326	I265	W194	M128
I513	I513	L452	E391	Y327	G266		R129
N514	N514	D453	N392				

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	128.38Å 128.38Å 130.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	90.6 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.214 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8948	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: EUG, FAD

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	0.81	3/4511 (0.1%)	1.88	127/6131 (2.1%)
1	B	0.81	2/4511 (0.0%)	1.88	128/6131 (2.1%)
All	All	0.81	5/9022 (0.1%)	1.88	255/12262 (2.1%)

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	2	0
1	B	2	0
All	All	4	0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	TRP	CB-CG	-5.99	1.39	1.50
1	B	156	GLU	CG-CD	5.97	1.60	1.51
1	B	268	TRP	CB-CG	-5.95	1.39	1.50
1	A	156	GLU	CG-CD	5.94	1.60	1.51
1	A	244	TYR	CB-CG	-5.03	1.44	1.51

The worst 5 of 255 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	LEU	CB-CG-CD2	-12.85	89.15	111.00
1	A	560	LEU	CB-CG-CD2	-12.83	89.19	111.00
1	B	16	LEU	CA-CB-CG	-11.58	88.66	115.30
1	A	16	LEU	CA-CB-CG	-11.56	88.70	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	495	CYS	CA-CB-SG	-11.13	93.97	114.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	363	ILE	CA
1	A	410	GLU	CA
1	B	363	ILE	CA
1	B	410	GLU	CA

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	4391	0	4330	550	0
1	B	4391	0	4330	552	0
2	A	53	0	31	17	0
2	B	53	0	31	18	0
3	A	11	0	7	4	0
3	B	11	0	7	5	0
4	A	14	0	0	2	0
4	B	24	0	0	0	0
All	All	8948	0	8736	1088	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 63.

The worst 5 of 1088 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:422:HIS:NE2	2:B:600:FAD:HM81	1.45	1.12
1:A:422:HIS:NE2	2:A:600:FAD:HM82	1.42	1.10
2:B:600:FAD:H8A	2:B:600:FAD:H51A	1.27	1.08
1:A:422:HIS:NE2	2:A:600:FAD:HM81	1.45	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.27	1.08

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	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	8	28
1	B	553/560 (99%)	472 (85%)	69 (12%)	12 (2%)	8	28
All	All	1106/1120 (99%)	944 (85%)	138 (12%)	24 (2%)	8	28

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	559	LYS
1	B	46	ILE
1	B	559	LYS
1	A	157	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	475/482 (98%)	445 (94%)	30 (6%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	475/482 (98%)	445 (94%)	30 (6%)	22	53
All	All	950/964 (98%)	890 (94%)	60 (6%)	22	53

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	THR
1	B	78	ARG
1	B	488	MET
1	B	27	ASP
1	B	91	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	533	ASN
1	B	91	ASN
1	B	528	ASN
1	A	552	GLN
1	B	152	HIS

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](#)

4 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
2	FAD	A	600	1	48,58,58	0.94	3 (6%)	54,89,89	1.59	5 (9%)
3	EUG	A	601	-	11,11,12	0.46	0	14,14,15	1.59	2 (14%)
2	FAD	B	600	1	48,58,58	0.94	3 (6%)	54,89,89	1.59	5 (9%)
3	EUG	B	601	-	11,11,12	0.47	0	14,14,15	1.60	2 (14%)

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
2	FAD	A	600	1	-	0/30/50/50	0/6/6/6
3	EUG	A	601	-	-	0/4/4/5	0/1/1/1
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
3	EUG	B	601	-	-	0/4/4/5	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C10-N10	-2.28	1.36	1.39
2	B	600	FAD	O5B-C5B	-2.27	1.35	1.44
2	A	600	FAD	O5B-C5B	-2.25	1.35	1.44
2	A	600	FAD	C10-N10	-2.24	1.36	1.39
2	B	600	FAD	C4-N3	3.38	1.39	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4X-C4-N3	-5.64	115.87	123.59
2	B	600	FAD	C4X-C4-N3	-5.63	115.90	123.59
2	A	600	FAD	C2B-C1B-N9A	-2.87	109.91	114.29
2	B	600	FAD	C2B-C1B-N9A	-2.84	109.95	114.29
2	B	600	FAD	C6-C5X-N5	-2.26	116.05	118.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	17	0
3	A	601	EUG	4	0
2	B	600	FAD	18	0
3	B	601	EUG	5	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.