



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:32 pm BST

PDB ID : 2P3X
Title : Crystal structure of Grenache (*Vitis vinifera*) Polyphenol Oxidase
Authors : Reyes Grajeda, J.P.; Virador, V.M.; Blanco-Labra, A.; Mendiola-Olaya, E.;
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Deposited on : 2007-03-09
Resolution : 2.20 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

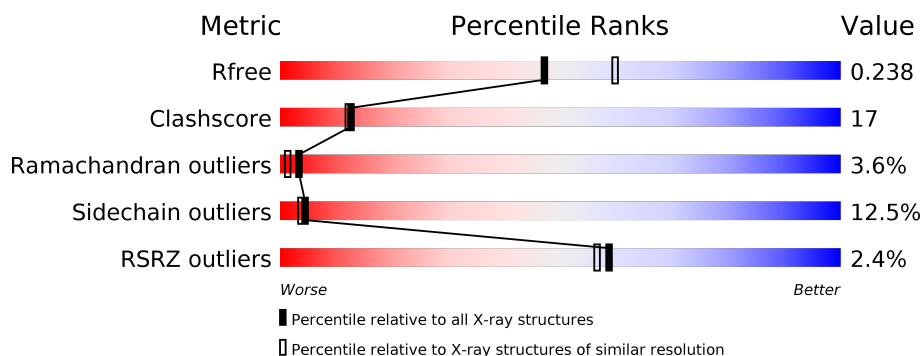
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	339	<div> <div>2%</div> <div>65%</div> <div>25%</div> <div>7%</div> <div>.</div> </div>

2 Entry composition [i](#)

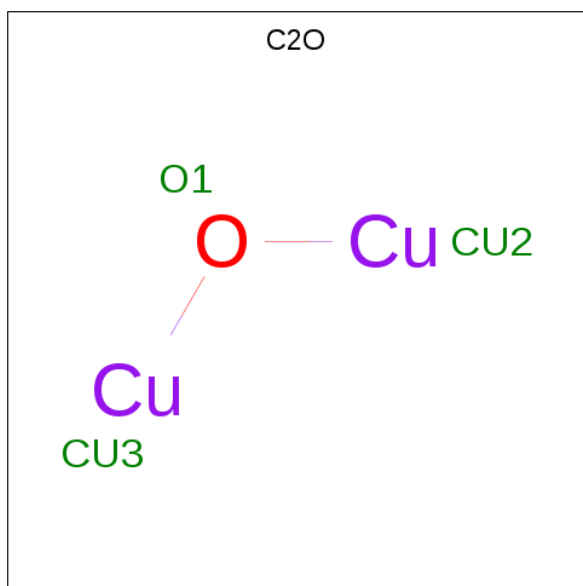
There are 3 unique types of molecules in this entry. The entry contains 2844 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polyphenol oxidase, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2713	1746	447	508	12			

- Molecule 2 is CU-O-CU LINKAGE (three-letter code: C2O) (formula: Cu₂O).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		

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: Polyphenol oxidase, chloroplast



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	60.03Å 120.77Å 140.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.06 – 2.20 37.06 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.06-2.20) 99.7 (37.06-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.252 0.193 , 0.238	Depositor DCC
R_{free} test set	2598 reflections (9.86%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2844	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: C2O

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	1.13	4/2801 (0.1%)	1.19	20/3829 (0.5%)

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	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ASP	CB-CG	5.71	1.63	1.51
1	A	151	TYR	CD2-CE2	5.71	1.48	1.39
1	A	142	TRP	CG-CD1	5.24	1.44	1.36
1	A	133	ASP	CB-CG	5.02	1.62	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	174	PRO	N-CA-C	7.54	131.69	112.10
1	A	41	SER	C-N-CA	-6.74	108.14	122.30
1	A	150	MET	CG-SD-CE	6.71	110.94	100.20
1	A	167	LYS	N-CA-C	6.58	128.75	111.00
1	A	269	PHE	CA-C-N	6.53	129.25	116.20
1	A	13	THR	N-CA-C	6.40	128.29	111.00
1	A	22	PRO	C-N-CA	6.40	137.70	121.70
1	A	23	THR	N-CA-CB	6.26	122.19	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	VAL	CG1-CB-CG2	6.11	120.68	110.90
1	A	248	LEU	CB-CG-CD1	5.78	120.83	111.00
1	A	269	PHE	N-CA-C	5.76	126.56	111.00
1	A	166	GLU	N-CA-C	5.66	126.28	111.00
1	A	291	LYS	C-N-CA	5.50	135.44	121.70
1	A	166	GLU	C-N-CA	5.47	135.38	121.70
1	A	290	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	121	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	290	ARG	C-N-CA	5.12	134.49	121.70
1	A	89	THR	N-CA-CB	-5.07	100.67	110.30
1	A	121	LEU	CB-CA-C	-5.05	100.61	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	13	THR	CA
1	A	167	LYS	CA

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	PRO	Peptide
1	A	12	GLY	Peptide
1	A	121	LEU	Peptide
1	A	125	GLU	Peptide
1	A	158	SER	Peptide
1	A	159	SER	Peptide
1	A	166	GLU	Peptide
1	A	174	PRO	Peptide
1	A	22	PRO	Peptide
1	A	250	ASP	Peptide
1	A	269	PHE	Peptide
1	A	291	LYS	Peptide
1	A	338	LEU	Peptide
1	A	99	GLY	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	2713	0	2613	89	0
2	A	3	0	0	0	0
3	A	128	0	0	9	0
All	All	2844	0	2613	89	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 17.

All (89) 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:211:THR:HB	3:A:465:HOH:O	1.44	1.15
1:A:316:LYS:HB2	1:A:316:LYS:NZ	1.83	0.93
1:A:5:ALA:H	1:A:302:THR:HG22	1.33	0.93
1:A:213:PRO:HD3	1:A:289:ASN:HB3	1.54	0.87
1:A:249:ALA:O	1:A:250:ASP:O	1.93	0.86
1:A:213:PRO:HD3	1:A:289:ASN:CB	2.06	0.84
1:A:3:ILE:HG12	1:A:112:LEU:HD21	1.61	0.82
1:A:255:ASP:HA	1:A:261:THR:HG23	1.63	0.81
1:A:56:LYS:HE2	3:A:468:HOH:O	1.81	0.80
1:A:316:LYS:HB2	1:A:316:LYS:HZ2	1.46	0.78
1:A:250:ASP:HB3	1:A:251:LYS:CA	2.13	0.77
1:A:323:THR:HG23	1:A:328:TYR:O	1.85	0.77
1:A:316:LYS:NZ	1:A:316:LYS:CB	2.49	0.74
1:A:296:THR:HG23	3:A:370:HOH:O	1.88	0.74
1:A:250:ASP:HB3	1:A:251:LYS:HA	1.71	0.72
1:A:89:THR:HG21	3:A:428:HOH:O	1.90	0.71
1:A:76:ASP:O	1:A:82:GLN:HG3	1.90	0.70
1:A:255:ASP:O	1:A:261:THR:HG22	1.91	0.70
1:A:278:MET:HE2	1:A:281:ILE:HD12	1.72	0.70
1:A:296:THR:CG2	3:A:370:HOH:O	2.41	0.69
1:A:144:TRP:CZ3	1:A:238:PRO:HG2	2.29	0.68
1:A:250:ASP:HB3	1:A:251:LYS:C	2.14	0.68
1:A:278:MET:CE	1:A:281:ILE:HD12	2.23	0.67
1:A:316:LYS:HB2	1:A:316:LYS:HZ3	1.59	0.66
1:A:289:ASN:O	1:A:290:ARG:HG3	1.96	0.66
1:A:255:ASP:HA	1:A:261:THR:CG2	2.25	0.65
1:A:89:THR:HG23	1:A:95:TYR:CE2	2.32	0.64
1:A:274:ASN:HD21	1:A:277:ARG:HH21	1.47	0.63
1:A:5:ALA:N	1:A:302:THR:HG22	2.08	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HD3	1:A:310:LYS:HG2	1.82	0.61
1:A:212:THR:HA	1:A:289:ASN:HB2	1.83	0.61
1:A:316:LYS:HZ3	1:A:316:LYS:CB	2.11	0.60
1:A:157:ALA:CB	1:A:174:PRO:HG2	2.31	0.60
1:A:3:ILE:HD13	1:A:105:LEU:HD21	1.84	0.60
1:A:214:LYS:HD2	1:A:219:TYR:CE1	2.37	0.59
1:A:289:ASN:O	1:A:290:ARG:CB	2.49	0.59
1:A:177:VAL:HG22	1:A:194:LEU:HD13	1.84	0.58
1:A:5:ALA:H	1:A:302:THR:CG2	2.10	0.58
1:A:180:LEU:H	1:A:198:ASN:HD21	1.52	0.58
1:A:186:GLU:HG3	3:A:396:HOH:O	2.04	0.57
1:A:254:GLU:HG2	1:A:261:THR:HG21	1.86	0.56
1:A:165:ASP:OD1	1:A:167:LYS:HB2	2.05	0.56
1:A:211:THR:HG22	3:A:355:HOH:O	2.05	0.55
1:A:255:ASP:CA	1:A:261:THR:HG23	2.36	0.55
1:A:180:LEU:H	1:A:198:ASN:ND2	2.05	0.55
1:A:5:ALA:HB2	1:A:302:THR:HG23	1.88	0.54
1:A:255:ASP:O	1:A:261:THR:CG2	2.56	0.54
1:A:267:ILE:O	1:A:270:GLY:HA3	2.07	0.54
1:A:92:GLN:HE21	1:A:259:PHE:HB2	1.72	0.53
1:A:290:ARG:H	1:A:291:LYS:HB2	1.72	0.53
1:A:144:TRP:HE1	1:A:271:HIS:HD2	1.59	0.51
1:A:228:ASP:N	1:A:229:PRO:HD3	2.26	0.51
1:A:259:PHE:HD1	3:A:422:HOH:O	1.93	0.51
1:A:289:ASN:O	1:A:290:ARG:HB2	2.11	0.50
1:A:183:ASP:OD1	1:A:183:ASP:C	2.50	0.49
1:A:289:ASN:O	1:A:290:ARG:CG	2.59	0.49
1:A:288:LYS:HB3	1:A:291:LYS:CE	2.43	0.49
1:A:278:MET:HE2	1:A:278:MET:HA	1.95	0.49
1:A:44:PRO:HG2	1:A:135:PRO:HB2	1.95	0.49
1:A:109:ALA:O	1:A:229:PRO:HD2	2.13	0.48
1:A:251:LYS:HB2	1:A:252:PRO:HA	1.94	0.48
1:A:121:LEU:HD22	1:A:269:PHE:HD1	1.79	0.48
1:A:83:GLN:HE21	1:A:124:ASN:HD22	1.62	0.47
1:A:111:TRP:CD2	1:A:220:PRO:HA	2.50	0.47
1:A:207:VAL:O	1:A:290:ARG:NH2	2.47	0.47
1:A:125:GLU:HB2	1:A:139:LEU:HD22	1.98	0.46
1:A:119:TYR:CE2	1:A:315:VAL:HG13	2.51	0.46
1:A:288:LYS:HB3	1:A:291:LYS:CD	2.46	0.46
1:A:46:ARG:HB3	1:A:138:ALA:HB2	1.97	0.46
1:A:248:LEU:HB2	1:A:254:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HD2	1:A:291:LYS:NZ	2.31	0.45
1:A:121:LEU:HD22	1:A:269:PHE:CD1	2.53	0.44
1:A:134:ASP:HA	1:A:135:PRO:HD2	1.83	0.44
1:A:4:GLN:HG3	1:A:98:VAL:HB	2.00	0.44
1:A:278:MET:HE1	1:A:281:ILE:HD12	1.99	0.44
1:A:58:TYR:OH	1:A:140:PRO:HD3	2.18	0.44
1:A:189:ILE:HG13	1:A:190:PRO:HD2	2.00	0.43
1:A:48:ARG:HG2	1:A:138:ALA:HB1	1.99	0.43
1:A:323:THR:CG2	1:A:328:TYR:O	2.60	0.42
1:A:302:THR:HB	3:A:360:HOH:O	2.21	0.41
1:A:111:TRP:CD1	1:A:112:LEU:HD13	2.56	0.41
1:A:214:LYS:CD	1:A:219:TYR:CE1	3.03	0.41
1:A:288:LYS:HB3	1:A:291:LYS:HE3	2.03	0.41
1:A:100:TYR:CD2	1:A:100:TYR:N	2.89	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.87	0.41
1:A:173:LEU:HA	1:A:174:PRO:HD3	1.71	0.41
1:A:192:ASP:O	1:A:196:THR:HG23	2.21	0.41
1:A:239:HIS:CD2	1:A:271:HIS:CE1	3.09	0.40
1:A:219:TYR:N	1:A:219:TYR:CD2	2.88	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	337/339 (99%)	310 (92%)	15 (4%)	12 (4%)	3 1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	250	ASP

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Mol	Chain	Res	Type
1	A	290	ARG
1	A	291	LYS
1	A	292	ASP
1	A	167	LYS
1	A	174	PRO
1	A	122	TYR
1	A	116	PHE
1	A	160	PRO
1	A	126	ARG
1	A	318	SER

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	295/295 (100%)	258 (88%)	37 (12%)	4 4

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	13	THR
1	A	23	THR
1	A	46	ARG
1	A	64	LYS
1	A	68	LEU
1	A	74	ASP
1	A	89	THR
1	A	103	LEU
1	A	105	LEU
1	A	107	VAL
1	A	111	TRP
1	A	112	LEU
1	A	121	LEU
1	A	139	LEU
1	A	159	SER

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Mol	Chain	Res	Type
1	A	177	VAL
1	A	186	GLU
1	A	188	THR
1	A	193	GLU
1	A	194	LEU
1	A	248	LEU
1	A	251	LYS
1	A	261	THR
1	A	280	ASN
1	A	288	LYS
1	A	291	LYS
1	A	296	THR
1	A	302	THR
1	A	304	VAL
1	A	311	GLN
1	A	312	LEU
1	A	315	VAL
1	A	318	SER
1	A	323	THR
1	A	324	SER
1	A	326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN
1	A	92	GLN
1	A	124	ASN
1	A	198	ASN
1	A	240	ASN
1	A	258	ASN
1	A	271	HIS
1	A	274	ASN
1	A	280	ASN
1	A	309	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](#)

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	C2O	A	340	1	0,2,2	0.00	-	-		

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 [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	339/339 (100%)	-0.10	8 (2%) 59 56	22, 38, 59, 68	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	THR	3.4
1	A	102	ASP	3.1
1	A	18	ASP	2.9
1	A	339	PRO	2.8
1	A	185	THR	2.8
1	A	287	GLY	2.7
1	A	188	THR	2.6
1	A	250	ASP	2.4

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(\AA^2)	Q<0.9
2	C2O	A	340	3/3	0.96	0.10	20,20,49,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.