Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 12:22 AM EST

PDB ID	:	3DZL
Title	:	Crystal structure of PhzA/B from Burkholderia cepacia R18194 in complex with (R)-3-oxocyclohexanecarboxylic acid
Authors	:	Ahuja, E.G.; Mentel, M.; Graebsch, A.; Breinbauer, R.; Blankenfeldt, W.
Deposited on	:	2008-07-30
Resolution	:	1.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

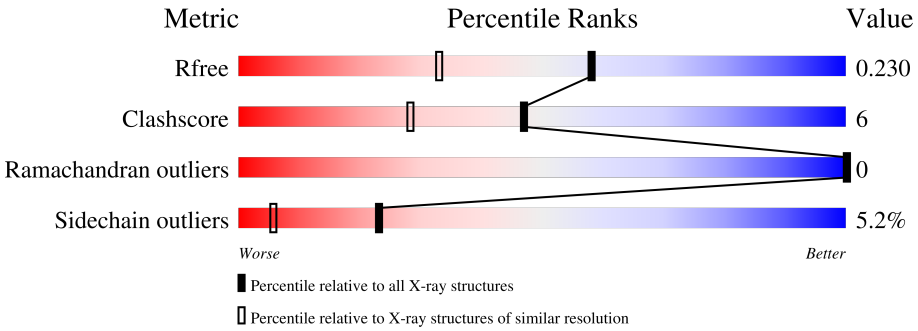
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)

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 of 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%

Mol	Chain	Length	Quality of chain
1	A	185	65% 17% • 15%
1	B	185	68% 15% • 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3051 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 Phenazine biosynthesis protein A/B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	157	Total	C	N	O	S	0	6	0
			1331	845	248	233	5			
1	B	158	Total	C	N	O	S	0	4	0
			1333	843	245	240	5			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q396C9
A	-18	GLY	-	expression tag	UNP Q396C9
A	-17	SER	-	expression tag	UNP Q396C9
A	-16	SER	-	expression tag	UNP Q396C9
A	-15	HIS	-	expression tag	UNP Q396C9
A	-14	HIS	-	expression tag	UNP Q396C9
A	-13	HIS	-	expression tag	UNP Q396C9
A	-12	HIS	-	expression tag	UNP Q396C9
A	-11	HIS	-	expression tag	UNP Q396C9
A	-10	HIS	-	expression tag	UNP Q396C9
A	-9	SER	-	expression tag	UNP Q396C9
A	-8	SER	-	expression tag	UNP Q396C9
A	-7	GLY	-	expression tag	UNP Q396C9
A	-6	LEU	-	expression tag	UNP Q396C9
A	-5	VAL	-	expression tag	UNP Q396C9
A	-4	PRO	-	expression tag	UNP Q396C9
A	-3	ARG	-	expression tag	UNP Q396C9
A	-2	GLY	-	expression tag	UNP Q396C9
A	-1	SER	-	expression tag	UNP Q396C9
A	0	HIS	-	expression tag	UNP Q396C9
B	-19	MET	-	expression tag	UNP Q396C9
B	-18	GLY	-	expression tag	UNP Q396C9
B	-17	SER	-	expression tag	UNP Q396C9
B	-16	SER	-	expression tag	UNP Q396C9
B	-15	HIS	-	expression tag	UNP Q396C9

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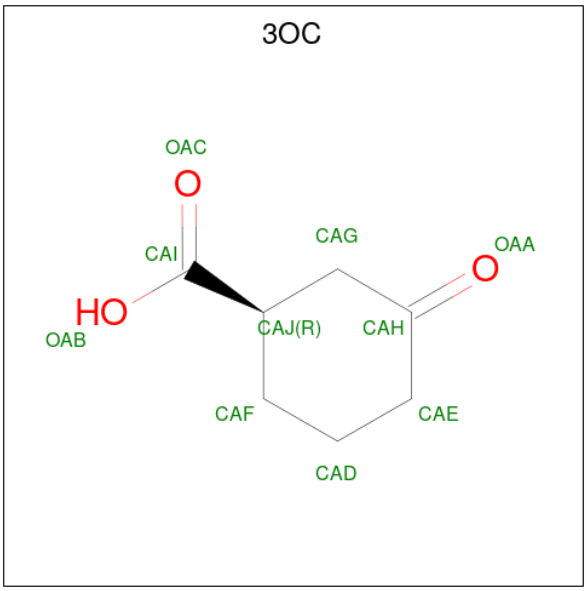
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q396C9
B	-13	HIS	-	expression tag	UNP Q396C9
B	-12	HIS	-	expression tag	UNP Q396C9
B	-11	HIS	-	expression tag	UNP Q396C9
B	-10	HIS	-	expression tag	UNP Q396C9
B	-9	SER	-	expression tag	UNP Q396C9
B	-8	SER	-	expression tag	UNP Q396C9
B	-7	GLY	-	expression tag	UNP Q396C9
B	-6	LEU	-	expression tag	UNP Q396C9
B	-5	VAL	-	expression tag	UNP Q396C9
B	-4	PRO	-	expression tag	UNP Q396C9
B	-3	ARG	-	expression tag	UNP Q396C9
B	-2	GLY	-	expression tag	UNP Q396C9
B	-1	SER	-	expression tag	UNP Q396C9
B	0	HIS	-	expression tag	UNP Q396C9

- Molecule 2 is (1R)-3-oxocyclohexanecarboxylic acid (three-letter code: 3OC) (formula: $C_7H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 20 14 6	0	1
2	A	1	Total C O 10 7 3	0	0
2	B	1	Total C O 10 7 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 7 3	0	0

- Molecule 3 is water.

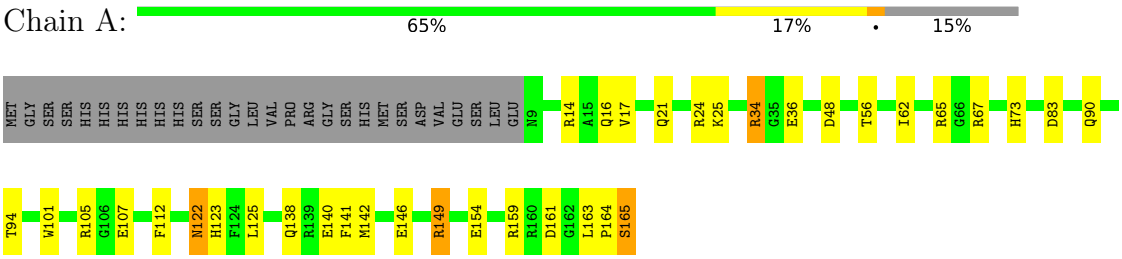
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	156	Total O 156 156	0	0
3	B	181	Total O 181 181	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

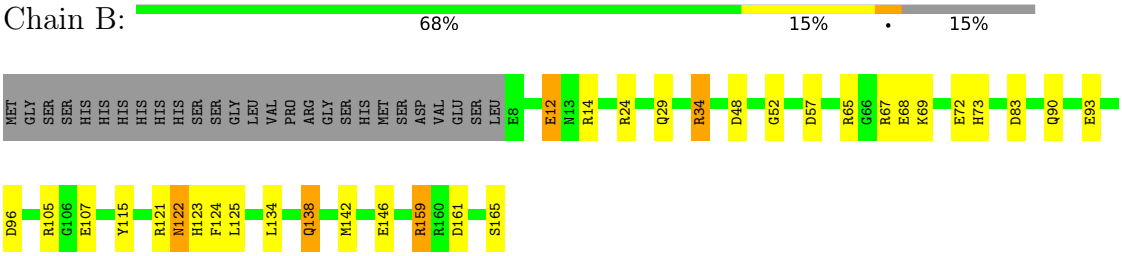
- Molecule 1: Phenazine biosynthesis protein A/B

Chain A:



- Molecule 1: Phenazine biosynthesis protein A/B

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	64.74Å 64.74Å 161.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.39 – 1.75 18.94 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.39-1.75) 99.9 (18.94-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.158 , 0.193 0.198 , 0.230	Depositor DCC
R_{free} test set	2017 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3051	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3OC

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	1.39	10/1387 (0.7%)	1.24	12/1874 (0.6%)
1	B	1.29	7/1383 (0.5%)	1.18	10/1869 (0.5%)
All	All	1.34	17/2770 (0.6%)	1.21	22/3743 (0.6%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	GLU	CB-CG	-10.62	1.31	1.52
1	A	140	GLU	CD-OE1	7.65	1.34	1.25
1	B	107[A]	GLU	CG-CD	6.46	1.61	1.51
1	B	107[B]	GLU	CG-CD	6.46	1.61	1.51
1	A	140	GLU	CB-CG	-6.45	1.39	1.52
1	B	72	GLU	CG-CD	6.45	1.61	1.51
1	A	141	PHE	CD2-CE2	6.35	1.51	1.39
1	B	72	GLU	CD-OE1	6.27	1.32	1.25
1	A	34	ARG	CB-CG	-6.10	1.36	1.52
1	A	25	LYS	CE-NZ	5.65	1.63	1.49
1	A	146	GLU	CD-OE1	-5.56	1.19	1.25
1	A	105	ARG	CG-CD	-5.53	1.38	1.51
1	A	146	GLU	CG-CD	5.50	1.60	1.51
1	B	12	GLU	CB-CG	5.44	1.62	1.52
1	A	25	LYS	CD-CE	5.43	1.64	1.51
1	B	115	TYR	CD2-CE2	5.35	1.47	1.39
1	B	34	ARG	CB-CG	-5.08	1.38	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	NE-CZ-NH2	-13.89	113.36	120.30
1	B	24	ARG	NE-CZ-NH2	-7.57	116.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	83	ASP	CB-CG-OD1	7.54	125.08	118.30
1	A	146	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	A	149	ARG	CG-CD-NE	-6.58	97.98	111.80
1	B	14	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	24	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	A	105	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	48	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	146	GLU	OE1-CD-OE2	-5.76	116.38	123.30
1	A	48	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	121	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	65	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	140	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	B	83	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	65	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	67	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	161	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	140	GLU	OE1-CD-OE2	5.24	129.58	123.30
1	B	96	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	105	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	112	PHE	CB-CG-CD2	5.05	124.34	120.80

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	1331	0	1280	20	0
1	B	1333	0	1269	22	1
2	A	30	0	27	1	0
2	B	20	0	18	1	0
3	A	156	0	0	3	1
3	B	181	0	0	7	0
All	All	3051	0	2594	33	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 6.

All (33) 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:73:HIS:HD2	3:B:685:HOH:O	1.54	0.89
1:A:90:GLN:OE1	3:A:748:HOH:O	1.92	0.88
1:A:125[A]:LEU:HD12	1:B:125[A]:LEU:HD12	1.61	0.82
1:B:90:GLN:NE2	3:B:728:HOH:O	2.11	0.78
1:B:73:HIS:CD2	3:B:685:HOH:O	2.34	0.75
1:B:29:GLN:NE2	3:B:763:HOH:O	2.12	0.70
1:B:134:LEU:HD23	3:B:759:HOH:O	1.95	0.67
1:B:68:GLU:OE2	3:B:772:HOH:O	2.17	0.57
1:A:16[B]:GLN:NE2	1:A:16[B]:GLN:HA	2.19	0.57
1:B:12:GLU:OE2	3:B:664:HOH:O	2.18	0.57
1:A:36:GLU:OE1	3:A:650:HOH:O	2.18	0.56
1:B:122:ASN:HD22	1:B:123:HIS:H	1.53	0.56
1:A:122:ASN:HD22	1:A:123:HIS:H	1.55	0.55
1:A:125[A]:LEU:CD1	1:B:125[A]:LEU:HD12	2.35	0.55
1:A:125[A]:LEU:HD12	1:B:125[A]:LEU:CD1	2.34	0.54
1:A:17:VAL:O	1:A:21:GLN:HG3	2.09	0.53
1:A:125[A]:LEU:CD1	1:B:125[A]:LEU:CD1	2.88	0.52
1:A:163:LEU:HD12	1:A:164:PRO:HD2	1.94	0.48
1:A:163:LEU:HD12	1:A:164:PRO:CD	2.43	0.48
1:B:124:PHE:O	1:B:125[B]:LEU:HD22	2.14	0.48
1:A:56:THR:HG21	1:A:62:ILE:HG13	1.95	0.47
1:B:52:GLY:H	1:B:138:GLN:HE22	1.61	0.47
1:A:165:SER:OXT	1:B:69:LYS:HE3	2.15	0.47
1:B:159:ARG:H	1:B:159:ARG:HG2	1.47	0.46
1:A:34:ARG:NH1	3:A:606:HOH:O	2.37	0.46
1:A:149:ARG:NH2	1:B:57:ASP:O	2.44	0.45
1:B:73:HIS:HE1	2:B:600:3OC:HAD	1.82	0.45
1:A:73:HIS:CE1	2:A:600:3OC:HAE	2.52	0.44
1:A:125[A]:LEU:HD13	1:B:125[A]:LEU:HD13	1.98	0.44
1:A:94:THR:HA	1:B:93:GLU:O	2.18	0.43
1:A:16[B]:GLN:NE2	1:A:16[B]:GLN:CA	2.82	0.43
1:A:101:TRP:CH2	1:B:125[B]:LEU:HD11	2.54	0.43
1:B:122:ASN:HB3	1:B:124:PHE:CE1	2.54	0.43

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)
1:B:34:ARG:NH1	3:A:649:HOH:O[4_656]	2.12	0.08

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	161/185 (87%)	158 (98%)	3 (2%)	0	100	100
1	B	160/185 (86%)	158 (99%)	2 (1%)	0	100	100
All	All	321/370 (87%)	316 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	139/161 (86%)	131 (94%)	8 (6%)	20	4
1	B	140/161 (87%)	134 (96%)	6 (4%)	29	9
All	All	279/322 (87%)	265 (95%)	14 (5%)	23	6

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	67	ARG
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	138	GLN
1	A	142	MET
1	A	154	GLU
1	A	159	ARG
1	A	165	SER
1	B	122	ASN
1	B	138	GLN
1	B	142	MET
1	B	159	ARG
1	B	161	ASP
1	B	165	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	138	GLN
1	B	29	GLN
1	B	119	GLN
1	B	122	ASN
1	B	138	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	3OC	B	500	-	10,10,10	1.96	2 (20%)	12,13,13	1.91	5 (41%)
2	3OC	A	500[A]	-	10,10,10	1.05	1 (10%)	12,13,13	2.31	4 (33%)
2	3OC	A	600	-	10,10,10	2.22	3 (30%)	12,13,13	2.12	5 (41%)
2	3OC	B	600	-	10,10,10	2.10	5 (50%)	12,13,13	1.18	1 (8%)
2	3OC	A	500[B]	-	10,10,10	0.90	1 (10%)	12,13,13	2.14	3 (25%)

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	3OC	B	500	-	-	0/4/14/14	0/1/1/1
2	3OC	A	500[A]	-	-	2/4/14/14	0/1/1/1
2	3OC	A	600	-	-	1/4/14/14	0/1/1/1
2	3OC	B	600	-	-	2/4/14/14	0/1/1/1
2	3OC	A	500[B]	-	-	1/4/14/14	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	3OC	CAE-CAH	-4.49	1.40	1.50
2	A	600	3OC	CAG-CAH	4.01	1.57	1.50
2	A	600	3OC	OAA-CAH	3.65	1.27	1.21
2	B	500	3OC	OAB-CAI	-3.46	1.19	1.30
2	B	600	3OC	CAG-CAJ	3.23	1.61	1.53
2	A	600	3OC	CAE-CAH	3.14	1.57	1.50
2	B	600	3OC	OAB-CAI	-3.12	1.20	1.30
2	B	600	3OC	CAE-CAH	3.01	1.56	1.50
2	A	500[A]	3OC	OAB-CAI	-2.54	1.22	1.30
2	B	600	3OC	OAA-CAH	2.36	1.25	1.21
2	A	500[B]	3OC	OAB-CAI	-2.21	1.23	1.30
2	B	600	3OC	CAD-CAE	2.05	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500[A]	3OC	CAE-CAH-CAG	4.89	123.18	115.89
2	A	500[A]	3OC	OAA-CAH-CAG	-4.83	115.83	121.96
2	A	600	3OC	OAC-CAI-CAJ	-4.70	111.42	122.93
2	A	500[B]	3OC	CAE-CAH-CAG	4.42	122.47	115.89
2	A	500[B]	3OC	OAA-CAH-CAG	-4.00	116.89	121.96
2	A	600	3OC	CAF-CAJ-CAG	3.26	115.06	109.79
2	A	500[B]	3OC	OAC-CAI-CAJ	-3.17	115.16	122.93
2	B	500	3OC	OAA-CAH-CAE	-3.08	116.78	122.05
2	B	500	3OC	CAF-CAJ-CAI	3.07	117.29	111.32
2	B	600	3OC	CAD-CAE-CAH	-2.52	105.02	111.90
2	B	500	3OC	CAD-CAF-CAJ	-2.50	106.59	111.33
2	A	600	3OC	CAE-CAH-CAG	-2.26	112.52	115.89
2	B	500	3OC	CAE-CAH-CAG	2.21	119.19	115.89
2	A	500[A]	3OC	CAF-CAJ-CAI	-2.19	107.05	111.32
2	A	500[A]	3OC	CAG-CAJ-CAI	-2.19	104.19	110.74
2	A	600	3OC	OAB-CAI-OAC	2.12	128.91	124.09
2	B	500	3OC	OAC-CAI-CAJ	-2.05	117.91	122.93
2	A	600	3OC	OAB-CAI-CAJ	2.04	119.56	114.21

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500[A]	3OC	OAB-CAI-CAJ-CAF
2	B	600	3OC	OAC-CAI-CAJ-CAG
2	B	600	3OC	OAB-CAI-CAJ-CAG
2	A	500[B]	3OC	OAB-CAI-CAJ-CAG
2	A	500[A]	3OC	OAC-CAI-CAJ-CAF
2	A	600	3OC	OAB-CAI-CAJ-CAG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	3OC	1	0
2	B	600	3OC	1	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

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.