wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2018 – 01:55 pm GMT

PDB ID	:	3QWB
Title	:	Crystal structure of Saccharomyces cerevisiae Zeta-crystallin-like quinone oxidoreductase Zta1 complexed with NADPH
Authors	:	Guo, P.C.; Ma, X.X.; Bao, Z.Z.; Chen, Y.X.; Zhou, C.Z.
Deposited on	:	2011-02-28
Resolution	:	1.59 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

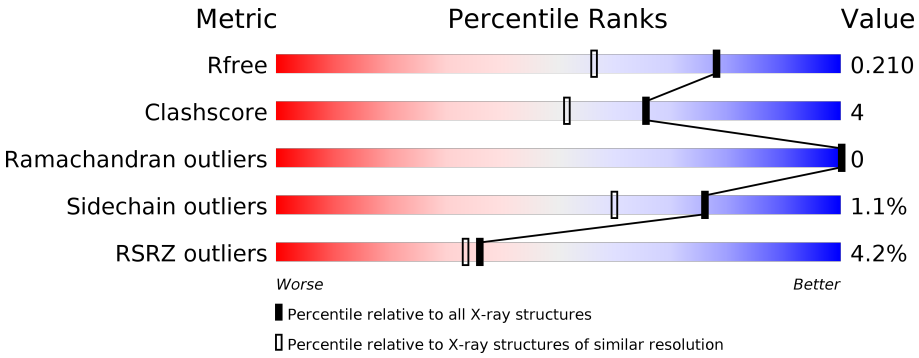
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk31020
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk31020

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 1.59 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}	111664	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (1.60-1.60)

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 <=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	334	5% 91% 7%
1	B	334	% 90% 8%
1	C	334	6% 91% 7%
1	D	334	4% 89% 9%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	336	-	-	X	-
3	GOL	B	336	-	-	X	-
3	GOL	C	336	-	-	X	-
3	GOL	D	336	-	X	X	-

2 Entry composition (i)

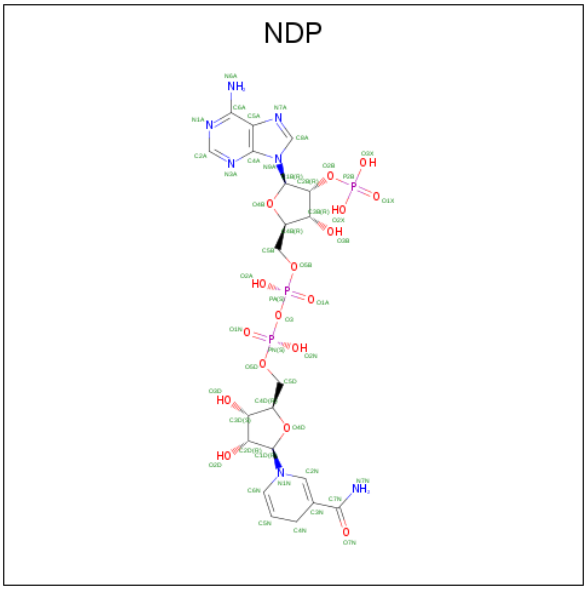
There are 4 unique types of molecules in this entry. The entry contains 12189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Probable quinone oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2585	1675	417	490	3			
1	B	330	Total	C	N	O	S	0	0	0
			2585	1675	417	490	3			
1	C	330	Total	C	N	O	S	0	0	0
			2585	1675	417	490	3			
1	D	330	Total	C	N	O	S	0	0	0
			2585	1675	417	490	3			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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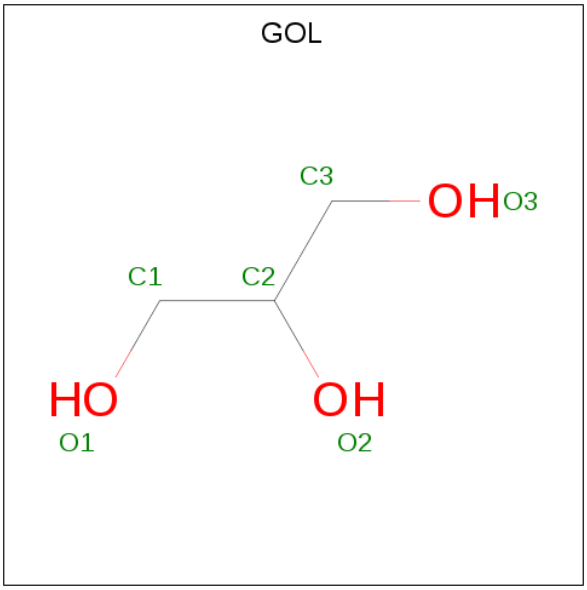
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O P 48 21 7 17 3	0	0
2	D	1	Total C N O P 48 21 7 17 3	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	439	Total O 439 439	0	0
4	B	447	Total O 447 447	0	0

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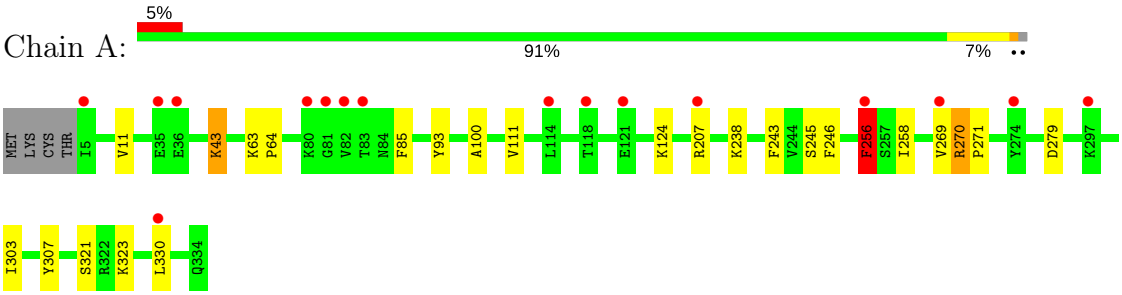
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	406	Total O 406 406	0	0
4	D	335	Total O 335 335	0	0

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 geometryand 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.

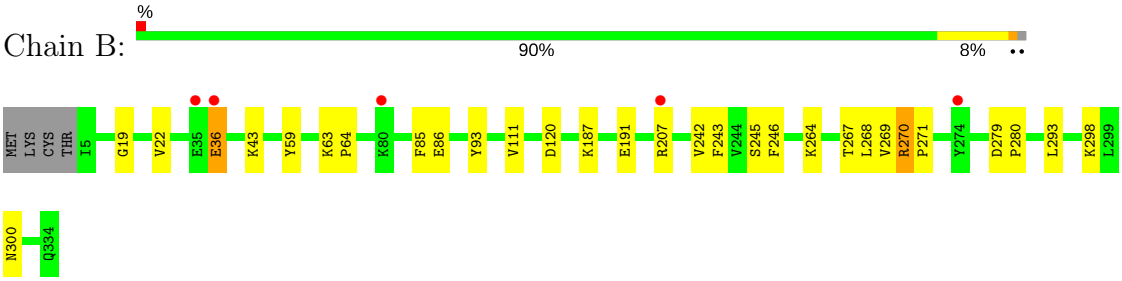
• Molecule 1: Probable quinone oxidoreductase

Chain A:



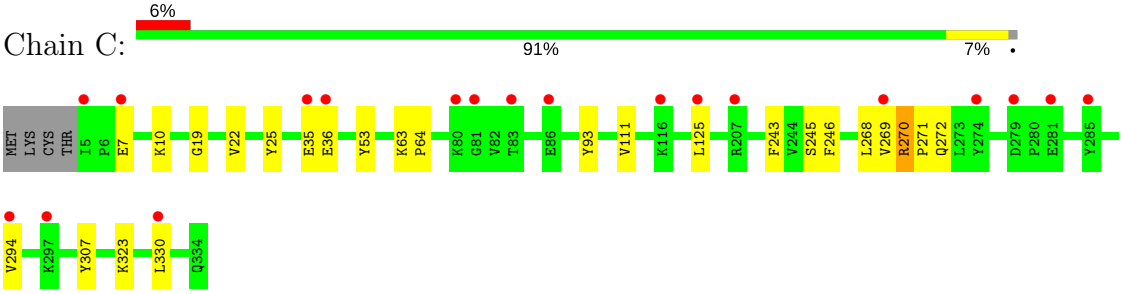
• Molecule 1: Probable quinone oxidoreductase

Chain B:



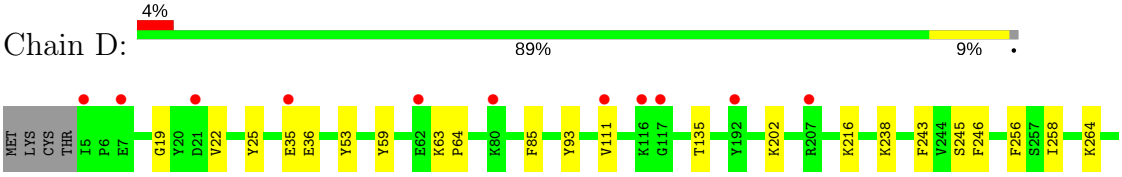
• Molecule 1: Probable quinone oxidoreductase

Chain C:



• Molecule 1: Probable quinone oxidoreductase

Chain D:



V269
R270
P271
Y274
D279
P280
E281
K302
T303
Y304
Y307
R313
V325
L330
Q334

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.96Å 75.36Å 182.83Å 90.00° 92.11° 90.00°	Depositor
Resolution (Å)	35.50 – 1.59 35.50 – 1.59	Depositor EDS
% Data completeness (in resolution range)	97.3 (35.50-1.59) 97.3 (35.50-1.59)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 1.59Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.188 , 0.211 0.186 , 0.210	Depositor DCC
R_{free} test set	9636 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12189	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: GOL, NDP

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	0.63	1/2637 (0.0%)	0.60	1/3563 (0.0%)
1	B	0.73	2/2637 (0.1%)	0.62	0/3563
1	C	0.50	0/2637	0.54	0/3563
1	D	0.65	2/2637 (0.1%)	0.59	2/3563 (0.1%)
All	All	0.63	5/10548 (0.0%)	0.59	3/14252 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25	TYR	CD1-CE1	-5.77	1.30	1.39
1	A	256	PHE	CG-CD2	-5.26	1.30	1.38
1	B	264	LYS	CD-CE	-5.16	1.38	1.51
1	B	86	GLU	CD-OE2	-5.08	1.20	1.25
1	D	264	LYS	CD-CE	-5.03	1.38	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	256	PHE	N-CA-CB	-5.26	101.14	110.60
1	D	202	LYS	CD-CE-NZ	5.09	123.40	111.70
1	A	279	ASP	CB-CA-C	-5.03	100.34	110.40

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	2585	0	2640	19	0
1	B	2585	0	2640	22	0
1	C	2585	0	2640	18	0
1	D	2585	0	2640	23	0
2	A	48	0	26	4	0
2	B	48	0	26	4	0
2	C	48	0	26	3	0
2	D	48	0	26	5	0
3	A	12	0	14	5	0
3	B	6	0	6	6	0
3	C	6	0	6	5	0
3	D	6	0	5	10	0
4	A	439	0	0	7	0
4	B	447	0	0	4	0
4	C	406	0	0	3	0
4	D	335	0	0	2	0
All	All	12189	0	10695	93	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 4.

The worst 5 of 93 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:C:7:GLU:HG2	4:C:1551:HOH:O	1.31	1.29
2:B:335:NDP:C2N	3:B:336:GOL:H12	1.82	1.09
2:A:335:NDP:C2N	3:A:336:GOL:H31	1.85	1.06
1:D:216:LYS:HE2	4:D:1570:HOH:O	1.56	1.04
2:D:335:NDP:C2N	3:D:336:GOL:H12	1.88	1.01

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	328/334 (98%)	325 (99%)	3 (1%)	0	100	100
1	B	328/334 (98%)	325 (99%)	3 (1%)	0	100	100
1	C	328/334 (98%)	325 (99%)	3 (1%)	0	100	100
1	D	328/334 (98%)	325 (99%)	3 (1%)	0	100	100
All	All	1312/1336 (98%)	1300 (99%)	12 (1%)	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	278/282 (99%)	274 (99%)	4 (1%)	69	50
1	B	278/282 (99%)	275 (99%)	3 (1%)	76	60
1	C	278/282 (99%)	276 (99%)	2 (1%)	85	75
1	D	278/282 (99%)	275 (99%)	3 (1%)	76	60
All	All	1112/1128 (99%)	1100 (99%)	12 (1%)	76	60

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	243	PHE
1	B	270	ARG
1	D	238	LYS
1	B	36	GLU
1	C	270	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	272	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)

9 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	NDP	A	335	-	45,52,52	1.26	5 (11%)	54,80,80	1.54	2 (3%)
3	GOL	A	336	-	5,5,5	2.74	2 (40%)	5,5,5	1.77	1 (20%)
3	GOL	A	337	-	5,5,5	1.15	1 (20%)	5,5,5	1.04	0
2	NDP	B	335	-	45,52,52	1.30	5 (11%)	54,80,80	1.58	2 (3%)
3	GOL	B	336	-	5,5,5	2.34	2 (40%)	5,5,5	1.97	2 (40%)
2	NDP	C	335	-	45,52,52	1.26	5 (11%)	54,80,80	1.57	1 (1%)
3	GOL	C	336	-	5,5,5	2.04	2 (40%)	5,5,5	1.72	1 (20%)
2	NDP	D	335	-	45,52,52	1.30	5 (11%)	54,80,80	1.60	3 (5%)
3	GOL	D	336	-	5,5,5	2.75	4 (80%)	5,5,5	2.64	2 (40%)

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	NDP	A	335	-	-	0/30/77/77	0/5/5/5
3	GOL	A	336	-	-	0/4/4/4	0/0/0/0
3	GOL	A	337	-	-	0/4/4/4	0/0/0/0
2	NDP	B	335	-	-	0/30/77/77	0/5/5/5
3	GOL	B	336	-	-	0/4/4/4	0/0/0/0
2	NDP	C	335	-	-	0/30/77/77	0/5/5/5
3	GOL	C	336	-	-	0/4/4/4	0/0/0/0
2	NDP	D	335	-	-	0/30/77/77	0/5/5/5
3	GOL	D	336	-	-	0/4/4/4	0/0/0/0

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	336	GOL	O3-C3	-4.51	1.23	1.42
3	D	336	GOL	O2-C2	-4.13	1.31	1.43
3	A	336	GOL	O2-C2	-3.87	1.32	1.43
3	B	336	GOL	O2-C2	-3.73	1.32	1.43
3	B	336	GOL	O1-C1	-3.12	1.29	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	335	NDP	N3A-C2A-N1A	-10.31	120.04	128.86
2	B	335	NDP	N3A-C2A-N1A	-10.16	120.17	128.86
2	C	335	NDP	N3A-C2A-N1A	-10.06	120.25	128.86
2	A	335	NDP	N3A-C2A-N1A	-9.77	120.50	128.86
3	D	336	GOL	O3-C3-C2	-4.55	88.03	110.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	335	NDP	4	0
3	A	336	GOL	5	0
2	B	335	NDP	4	0
3	B	336	GOL	6	0
2	C	335	NDP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	336	GOL	5	0
2	D	335	NDP	5	0
3	D	336	GOL	10	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

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, 95^{th} 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	330/334 (98%)	0.22	16 (4%)	30	28	6, 12, 27, 34	3 (0%)
1	B	330/334 (98%)	0.03	5 (1%)	73	74	6, 11, 19, 24	3 (0%)
1	C	330/334 (98%)	0.19	19 (5%)	23	21	9, 15, 28, 33	3 (0%)
1	D	330/334 (98%)	0.20	15 (4%)	33	30	9, 16, 27, 34	3 (0%)
All	All	1320/1336 (98%)	0.16	55 (4%)	36	33	6, 14, 27, 34	12 (0%)

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	7	GLU	4.9
1	C	274	TYR	4.7
1	A	83	THR	4.4
1	C	80	LYS	4.4
1	A	269	VAL	4.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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(Å^2)	Q<0.9
3	GOL	A	336	6/6	0.71	0.20	21,21,21,21	0
3	GOL	B	336	6/6	0.78	0.18	20,20,20,21	0
3	GOL	C	336	6/6	0.78	0.16	21,21,22,22	0
3	GOL	D	336	6/6	0.85	0.19	21,21,21,21	0
3	GOL	A	337	6/6	0.91	0.12	22,22,23,23	0
2	NDP	D	335	48/48	0.98	0.07	7,10,14,16	0
2	NDP	A	335	48/48	0.98	0.08	4,6,10,14	0
2	NDP	B	335	48/48	0.98	0.06	4,6,10,12	0
2	NDP	C	335	48/48	0.98	0.07	7,10,15,17	0

6.5 Other polymers (i)

There are no such residues in this entry.