wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 04:04 PM EDT

PDB ID	:	3BP1
Title	:	Crystal structure of putative 7-cyano-7-deazaguanine reductase QueF from Vibrio cholerae O1 biovar eltor
Authors	:	Kim, Y.; Zhou, M.; Moy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2007-12-18
Resolution	:	1.53 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

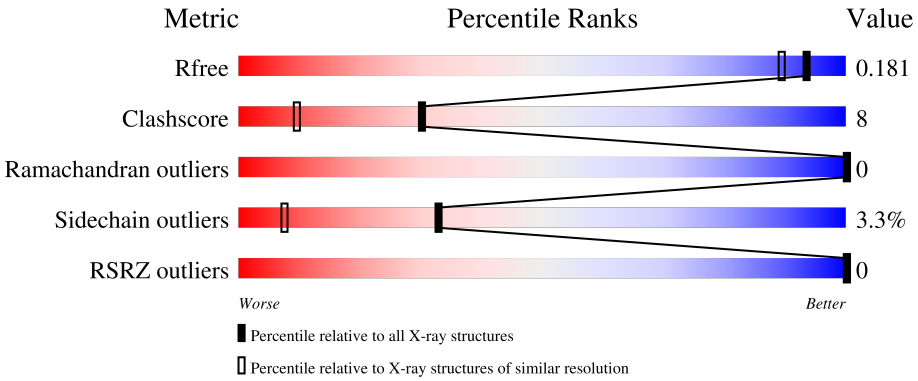
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.53 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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% 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	290	73% 14% 12%
1	B	290	77% 10% • 12%
1	C	290	75% 11% • 12%
1	D	290	73% 14% • 12%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	C	288	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10479 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.

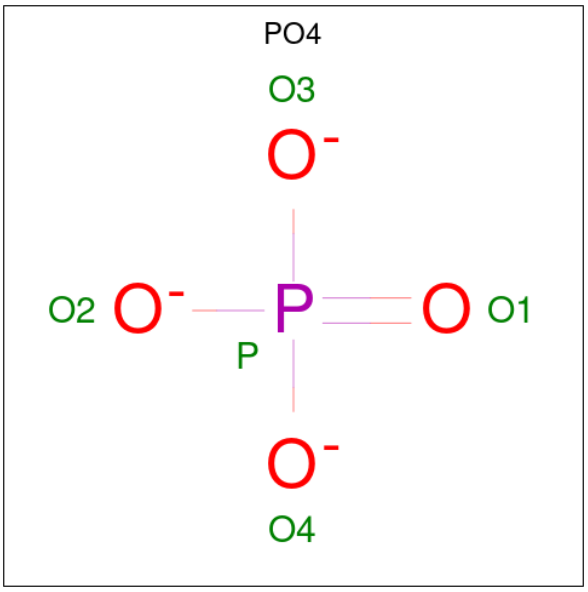
- Molecule 1 is a protein called NADPH-dependent 7-cyano-7-deazaguanine reductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	Se	0	33	0
			2330	1445	411	463	6	5			
1	B	254	Total	C	N	O	S	Se	0	25	0
			2252	1394	402	443	6	7			
1	C	254	Total	C	N	O	S	Se	0	34	0
			2326	1441	415	457	6	7			
1	D	256	Total	C	N	O	S	Se	0	29	0
			2300	1430	404	455	6	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KTK0
A	-1	ASN	-	expression tag	UNP Q9KTK0
A	0	ALA	-	expression tag	UNP Q9KTK0
B	-2	SER	-	expression tag	UNP Q9KTK0
B	-1	ASN	-	expression tag	UNP Q9KTK0
B	0	ALA	-	expression tag	UNP Q9KTK0
C	-2	SER	-	expression tag	UNP Q9KTK0
C	-1	ASN	-	expression tag	UNP Q9KTK0
C	0	ALA	-	expression tag	UNP Q9KTK0
D	-2	SER	-	expression tag	UNP Q9KTK0
D	-1	ASN	-	expression tag	UNP Q9KTK0
D	0	ALA	-	expression tag	UNP Q9KTK0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

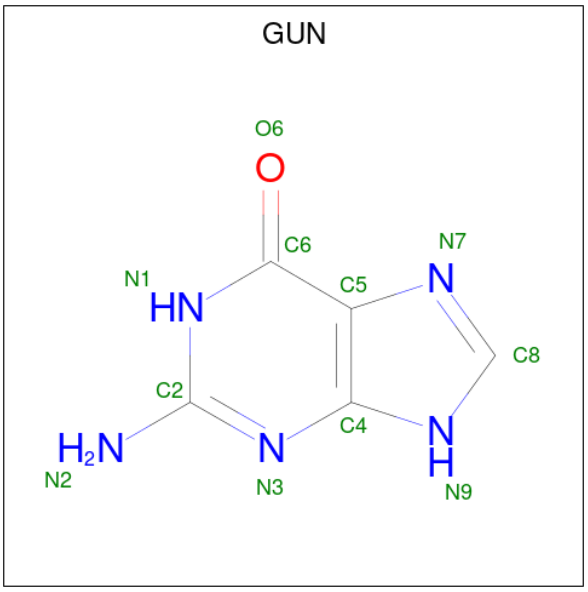


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

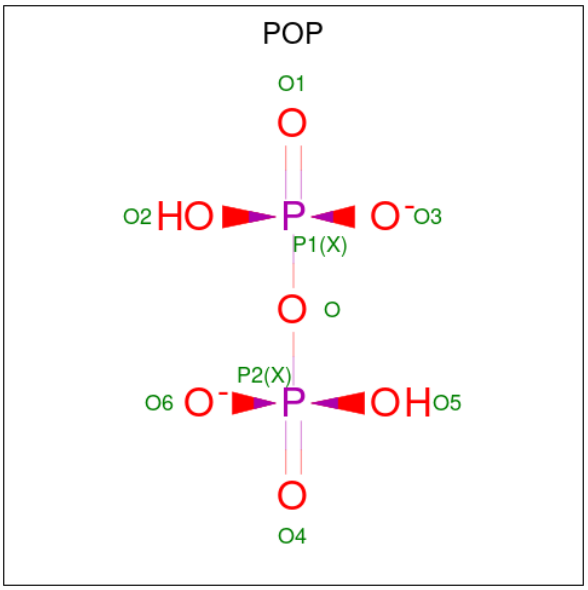
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 11 5 5 1	0	0
4	B	1	Total C N O 11 5 5 1	0	0
4	C	1	Total C N O 11 5 5 1	0	0
4	D	1	Total C N O 11 5 5 1	0	0

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 9 7 2	0	0
5	C	1	Total O P 9 7 2	0	0

- Molecule 6 is water.

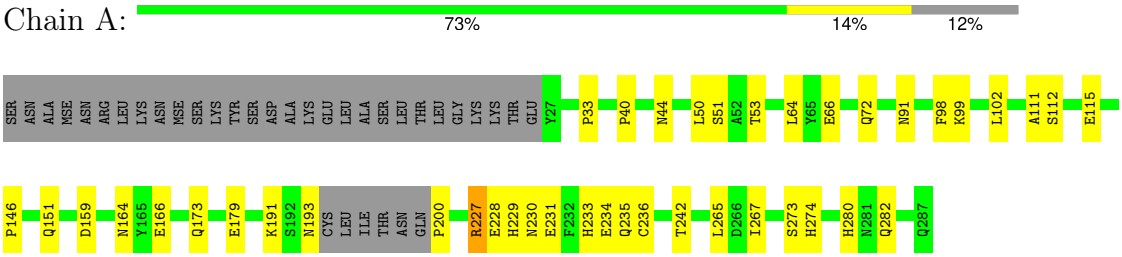
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	291	Total O 291 291	0	0
6	B	295	Total O 295 295	0	0
6	C	293	Total O 293 293	0	0
6	D	298	Total O 298 298	0	0

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 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.

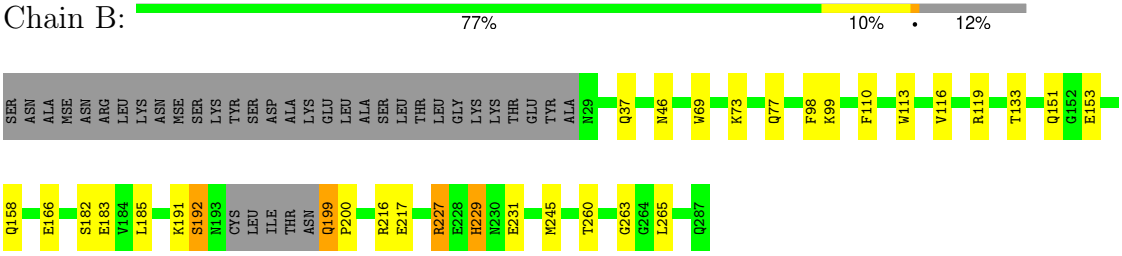
• Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase

Chain A:



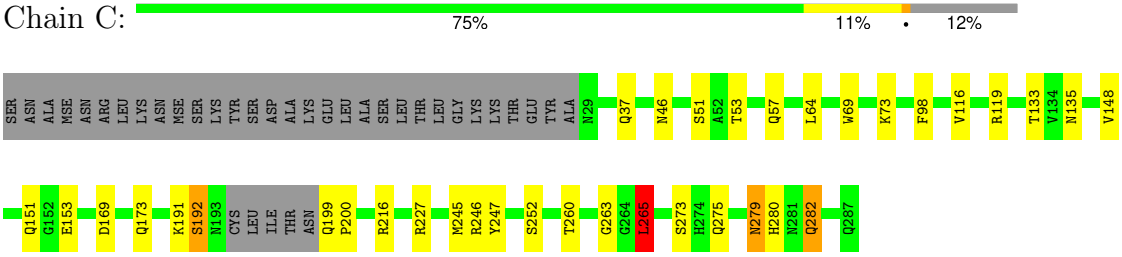
• Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase

Chain B:



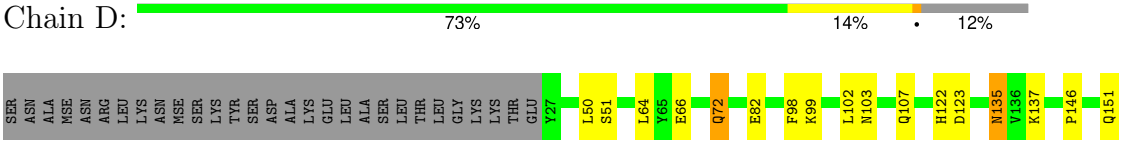
• Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase

Chain C:



• Molecule 1: NADPH-dependent 7-cyano-7-deazaguanine reductase

Chain D:




G152
E153
Q158
E161
L172
Q173
E180
V181
S182
K191
S192
N193
CYS
LEU
ILE
THR
ASN
Q199
P200
E206
H210
E217
Y222
R227
E228
H229
N230
H233
E234
T242
M245
Q249
Y259
L265
D266
I267
H274
N281
Q287

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	71.52Å 71.58Å 71.51Å 119.25° 110.18° 99.58°	Depositor
Resolution (Å)	26.16 – 1.53 26.16 – 1.53	Depositor EDS
% Data completeness (in resolution range)	93.9 (26.16-1.53) 93.7 (26.16-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.143 , 0.183 0.141 , 0.181	Depositor DCC
R_{free} test set	7527 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for l,-h-k-l,h 0.010 for k,h,-h-k-l 0.480 for -h-k-l,l,k	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	10479	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.42% 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: MG, GUN, PO4, POP

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	0.74	1/2374 (0.0%)	0.77	0/3215
1	B	0.78	1/2293 (0.0%)	0.78	0/3103
1	C	0.76	2/2368 (0.1%)	0.84	4/3204 (0.1%)
1	D	0.72	0/2344	0.77	1/3173 (0.0%)
All	All	0.75	4/9379 (0.0%)	0.79	5/12695 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	SER	CB-OG	-6.57	1.33	1.42
1	B	227	ARG	CZ-NH2	6.43	1.41	1.33
1	A	227	ARG	CZ-NH2	5.23	1.39	1.33
1	C	216	ARG	CZ-NH1	5.17	1.39	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	216	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	C	216	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	C	265[A]	LEU	CA-CB-CG	6.82	130.98	115.30
1	C	265[B]	LEU	CA-CB-CG	6.82	130.98	115.30
1	D	227	ARG	NE-CZ-NH2	5.09	122.85	120.30

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	2330	0	2179	36	0
1	B	2252	0	2129	31	1
1	C	2326	0	2202	47	0
1	D	2300	0	2163	50	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	3	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	5	0	0
4	B	11	0	5	0	0
4	C	11	0	5	0	0
4	D	11	0	5	0	0
5	B	9	0	0	1	0
5	C	9	0	0	0	0
6	A	291	0	0	6	0
6	B	295	0	0	10	0
6	C	293	0	0	16	1
6	D	298	0	0	12	0
All	All	10479	0	8693	150	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 8.

The worst 5 of 150 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:245[B]:MSE:HG2	6:C:356:HOH:O	1.44	1.15
1:C:133[A]:THR:HG22	6:C:397:HOH:O	1.50	1.10
1:B:245[B]:MSE:HG2	6:B:386:HOH:O	1.53	1.09
1:B:133[A]:THR:HG22	6:B:402:HOH:O	1.53	1.08
1:C:280:HIS:HE1	6:C:429:HOH:O	1.41	0.99

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166[B]:GLU:OE1	6:C:439:HOH:O[1_666]	2.18	0.02

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	284/290 (98%)	273 (96%)	11 (4%)	0	100	100
1	B	275/290 (95%)	272 (99%)	3 (1%)	0	100	100
1	C	283/290 (98%)	279 (99%)	4 (1%)	0	100	100
1	D	281/290 (97%)	269 (96%)	12 (4%)	0	100	100
All	All	1123/1160 (97%)	1093 (97%)	30 (3%)	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	258/250 (103%)	245 (95%)	13 (5%)	20	2
1	B	250/250 (100%)	245 (98%)	5 (2%)	50	20
1	C	259/250 (104%)	249 (96%)	10 (4%)	27	5
1	D	255/250 (102%)	243 (95%)	12 (5%)	22	2
All	All	1022/1000 (102%)	982 (96%)	40 (4%)	33	5

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	51	SER
1	D	173[B]	GLN
1	D	72[A]	GLN
1	D	135[A]	ASN
1	D	228[A]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	177	GLN
1	D	103	ASN
1	D	274	HIS
1	C	280	HIS
1	D	122	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\|>2$
5	POP	C	291	-	6,8,8	0.78	0	12,13,13	1.34	2 (16%)
2	PO4	B	288	-	4,4,4	1.05	0	6,6,6	2.45	3 (50%)
2	PO4	C	289	-	4,4,4	1.17	0	6,6,6	0.63	0
2	PO4	D	288	-	4,4,4	1.14	0	6,6,6	0.71	0
4	GUN	A	290	-	7,12,12	1.72	2 (28%)	8,17,17	2.00	4 (50%)
2	PO4	B	289	-	4,4,4	0.94	0	6,6,6	0.83	0
2	PO4	A	288	-	4,4,4	0.89	0	6,6,6	0.84	0
4	GUN	C	290	-	7,12,12	1.36	1 (14%)	8,17,17	1.44	1 (12%)
4	GUN	D	290	-	7,12,12	1.58	2 (28%)	8,17,17	1.81	3 (37%)
2	PO4	C	288	-	4,4,4	1.27	0	6,6,6	2.41	3 (50%)
4	GUN	B	290	-	7,12,12	1.41	1 (14%)	8,17,17	1.49	2 (25%)
5	POP	B	291	-	6,8,8	0.71	0	12,13,13	1.03	1 (8%)

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
5	POP	C	291	-	-	3/6/6/6	-
4	GUN	A	290	-	-	-	0/2/2/2
4	GUN	C	290	-	-	-	0/2/2/2
4	GUN	D	290	-	-	-	0/2/2/2
4	GUN	B	290	-	-	-	0/2/2/2
5	POP	B	291	-	-	2/6/6/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	290	GUN	C5-C6	-3.24	1.41	1.47
4	C	290	GUN	C5-C6	-3.10	1.41	1.47
4	D	290	GUN	C5-C6	-2.94	1.41	1.47
4	B	290	GUN	C5-C6	-2.57	1.42	1.47
4	A	290	GUN	C6-N1	2.32	1.41	1.37

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	288	PO4	O4-P-O3	-4.47	93.99	107.91
2	C	288	PO4	O4-P-O1	-4.26	95.89	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	290	GUN	C8-N7-C5	3.15	107.91	102.55
4	D	290	GUN	C8-N7-C5	3.12	107.86	102.55
4	D	290	GUN	C2-N1-C6	-2.88	119.84	125.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	291	POP	P1-O-P2-O5
5	C	291	POP	P2-O-P1-O2
5	C	291	POP	P2-O-P1-O3
5	B	291	POP	P1-O-P2-O4
5	C	291	POP	P2-O-P1-O1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	288	PO4	3	0
5	B	291	POP	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

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	251/290 (86%)	-1.21	0	100	100	6, 17, 34, 51	32 (12%)
1	B	250/290 (86%)	-1.24	0	100	100	6, 15, 33, 42	22 (8%)
1	C	250/290 (86%)	-1.24	0	100	100	5, 15, 29, 42	31 (12%)
1	D	252/290 (86%)	-1.20	0	100	100	5, 17, 37, 47	28 (11%)
All	All	1003/1160 (86%)	-1.22	0	100	100	5, 16, 34, 51	113 (11%)

There are no RSRZ outliers to report.

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 monosaccharides 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
2	PO4	B	288	5/5	0.98	0.07	17,20,27,30	1
2	PO4	C	288	5/5	0.98	0.06	17,21,27,29	1
5	POP	B	291	9/9	0.98	0.06	37,38,39,40	9
5	POP	C	291	9/9	0.98	0.06	34,35,37,37	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	289	1/1	0.99	0.10	35,35,35,35	0
3	MG	D	289	1/1	0.99	0.15	37,37,37,37	0
4	GUN	A	290	11/11	0.99	0.03	18,20,22,22	0
4	GUN	B	290	11/11	0.99	0.03	15,18,19,20	0
4	GUN	C	290	11/11	0.99	0.02	15,17,19,21	0
4	GUN	D	290	11/11	0.99	0.03	17,19,21,22	0
2	PO4	B	289	5/5	0.99	0.04	24,24,32,33	1
2	PO4	C	289	5/5	0.99	0.04	23,24,32,32	1
2	PO4	A	288	5/5	1.00	0.02	18,19,25,25	0
2	PO4	D	288	5/5	1.00	0.04	18,19,23,24	0

6.5 Other polymers (i)

There are no such residues in this entry.