



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2018 – 03:48 PM EST

PDB ID : 5Y00  
Title : Acid-tolerant monomeric GFP, Gamillus, fluorescence (ON) state  
Authors : Nakashima, R.; Sakurai, K.; Shinoda, H.; Matsuda, T.; Nagai, T.  
Deposited on : 2017-07-14  
Resolution : 1.60 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

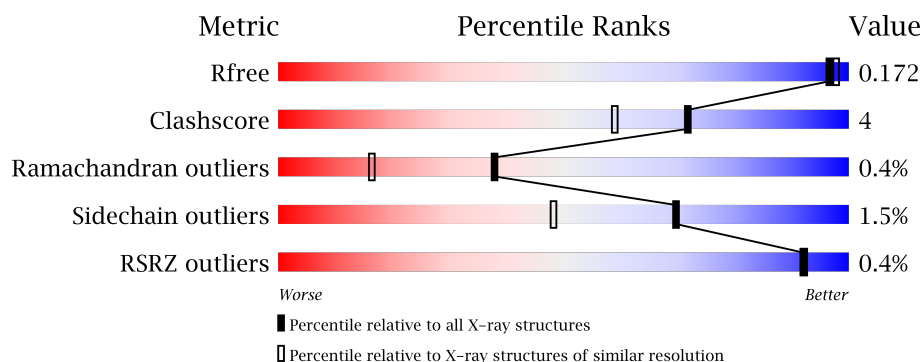
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	271	

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	A	301	-	X	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2141 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 Green fluorescent protein.

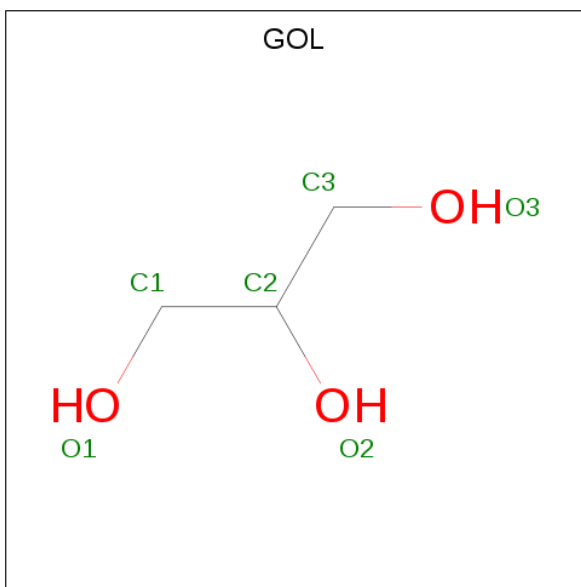
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	230	1860	1182	315	351	12	0	8	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

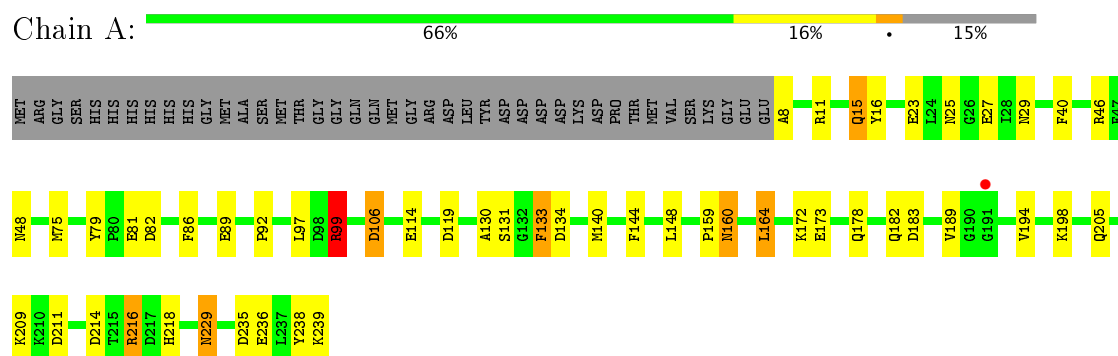
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	269	Total	O	0	0
			269	269		

### 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 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: Green fluorescent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.16Å 161.16Å 161.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.96 – 1.60 43.07 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (113.96-1.60) 99.8 (43.07-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.145 , 0.158 0.159 , 0.172	Depositor DCC
$R_{free}$ test set	4508 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	2141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, CRQ, CL

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	1.83	34/1899 (1.8%)	1.78	32/2568 (1.2%)

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	0	1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLU	CG-CD	9.54	1.66	1.51
1	A	48	ASN	CB-CG	-8.94	1.30	1.51
1	A	8	ALA	N-CA	8.52	1.63	1.46
1	A	205	GLN	CD-NE2	-8.33	1.12	1.32
1	A	236	GLU	CD-OE2	7.94	1.34	1.25
1	A	114	GLU	CD-OE2	7.31	1.33	1.25
1	A	106[A]	ASP	CG-OD2	7.03	1.41	1.25
1	A	106[B]	ASP	CG-OD2	7.03	1.41	1.25
1	A	229	ASN	CG-ND2	-7.03	1.15	1.32
1	A	183	ASP	CG-OD2	6.25	1.39	1.25
1	A	131	SER	CB-OG	-6.25	1.34	1.42
1	A	183	ASP	CB-CG	-6.15	1.38	1.51
1	A	89	GLU	CD-OE1	6.06	1.32	1.25
1	A	229	ASN	CG-OD1	6.04	1.37	1.24
1	A	130	ALA	N-CA	5.93	1.58	1.46
1	A	173	GLU	CG-CD	5.84	1.60	1.51
1	A	46	ARG	CZ-NH1	-5.81	1.25	1.33
1	A	79	TYR	CE1-CZ	5.76	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	ALA	CA-CB	-5.73	1.40	1.52
1	A	27	GLU	CG-CD	5.70	1.60	1.51
1	A	89	GLU	C-O	5.54	1.33	1.23
1	A	92	PRO	N-CA	-5.50	1.37	1.47
1	A	92	PRO	CA-CB	5.47	1.64	1.53
1	A	238	TYR	CG-CD2	5.34	1.46	1.39
1	A	15	GLN	CG-CD	-5.29	1.38	1.51
1	A	81	GLU	CD-OE1	5.22	1.31	1.25
1	A	238	TYR	CE1-CZ	5.21	1.45	1.38
1	A	119	ASP	C-N	5.20	1.42	1.33
1	A	81	GLU	CG-CD	5.17	1.59	1.51
1	A	40	PHE	CB-CG	-5.12	1.42	1.51
1	A	205	GLN	CG-CD	5.10	1.62	1.51
1	A	75	MET	CG-SD	-5.07	1.68	1.81
1	A	16	TYR	CG-CD1	-5.02	1.32	1.39
1	A	189	VAL	C-O	5.01	1.32	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	CB-CG-OD1	12.74	129.76	118.30
1	A	216	ARG	NE-CZ-NH2	12.21	126.40	120.30
1	A	106[A]	ASP	CB-CG-OD1	-11.29	108.14	118.30
1	A	106[B]	ASP	CB-CG-OD1	-11.29	108.14	118.30
1	A	79	TYR	CB-CG-CD1	11.10	127.66	121.00
1	A	164	LEU	CB-CG-CD1	10.99	129.68	111.00
1	A	131	SER	N-CA-CB	-9.56	96.17	110.50
1	A	133	PHE	CB-CG-CD1	9.29	127.31	120.80
1	A	134	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	A	79	TYR	CZ-CE2-CD2	8.62	127.56	119.80
1	A	133	PHE	CB-CG-CD2	-7.98	115.22	120.80
1	A	214	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	99	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	A	114	GLU	OE1-CD-OE2	7.28	132.03	123.30
1	A	106[A]	ASP	CB-CG-OD2	7.27	124.85	118.30
1	A	106[B]	ASP	CB-CG-OD2	7.27	124.85	118.30
1	A	144	PHE	CB-CG-CD1	-6.93	115.95	120.80
1	A	216	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	239	LYS	CB-CG-CD	6.52	128.55	111.60
1	A	79	TYR	CG-CD1-CE1	6.48	126.49	121.30
1	A	86	PHE	CG-CD1-CE1	-6.17	114.01	120.80
1	A	235	ASP	CB-CG-OD2	-6.13	112.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ALA	N-CA-CB	6.12	118.66	110.10
1	A	86	PHE	CB-CG-CD1	-5.90	116.67	120.80
1	A	239	LYS	CD-CE-NZ	5.76	124.96	111.70
1	A	11	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	159	PRO	N-CD-CG	-5.47	95.00	103.20
1	A	238	TYR	CB-CG-CD1	5.41	124.25	121.00
1	A	86	PHE	CZ-CE2-CD2	-5.36	113.66	120.10
1	A	148	LEU	CB-CG-CD2	5.30	120.02	111.00
1	A	229	ASN	CB-CG-OD1	-5.16	111.28	121.60
1	A	99	ARG	NH1-CZ-NH2	-5.12	113.77	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	ARG	Sidechain

## 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	1860	0	1826	15	0
2	A	5	0	0	0	0
3	A	6	0	8	0	0
4	A	1	0	0	0	0
5	A	269	0	0	5	0
All	All	2141	0	1834	15	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.

All (15) 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:ASP:H	1:A:218:HIS:HE1	1.09	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:NE2	5:A:401:HOH:O	2.07	0.88
1:A:211:ASP:H	1:A:218:HIS:CE1	1.99	0.77
1:A:29:ASN:HD21	1:A:133:PHE:H	1.34	0.73
1:A:160:ASN:HD21	1:A:194:VAL:H	1.34	0.72
1:A:25[B]:ASN:OD1	5:A:402:HOH:O	2.08	0.71
1:A:198[B]:LYS:HE2	5:A:625:HOH:O	1.97	0.64
1:A:216:ARG:O	1:A:218:HIS:HD2	1.91	0.53
1:A:140[B]:MET:CE	5:A:584:HOH:O	2.59	0.51
1:A:211:ASP:N	1:A:218:HIS:HE1	1.93	0.49
1:A:99:ARG:HH21	1:A:182:GLN:NE2	2.12	0.48
1:A:99:ARG:HD3	1:A:182:GLN:HE21	1.79	0.46
1:A:209:LYS:HE3	5:A:603:HOH:O	2.16	0.44
1:A:172:LYS:NZ	1:A:178:GLN:HE21	2.16	0.44

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	235/271 (87%)	228 (97%)	5 (2%)	2 (1%)	20 4

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106[A]	ASP
1	A	106[B]	ASP

### 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	205/231 (89%)	202 (98%)	3 (2%)	70	48

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	164	LEU
1	A	229	ASN

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

Mol	Chain	Res	Type
1	A	29	ASN
1	A	160	ASN
1	A	178	GLN
1	A	182	GLN
1	A	218	HIS
1	A	229	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue 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
1	CRQ	A	70	1	24,25,26	2.99	8 (33%)	26,34,36	3.87	11 (42%)

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
1	CRQ	A	70	1	-	0/10/32/33	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	CRQ	CA2-C2	-4.45	1.44	1.48
1	A	70	CRQ	CD2-CG2	-2.69	1.34	1.39
1	A	70	CRQ	C2-N3	-2.34	1.34	1.39
1	A	70	CRQ	O-C	2.32	1.34	1.19
1	A	70	CRQ	CA2-N2	3.02	1.45	1.38
1	A	70	CRQ	CA1-N	3.30	1.35	1.27
1	A	70	CRQ	C1-N2	4.70	1.42	1.33
1	A	70	CRQ	CB2-CA2	10.69	1.44	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	CRQ	CB2-CA2-N2	-7.63	117.24	128.79
1	A	70	CRQ	N3-C1-N2	-3.35	109.00	113.31
1	A	70	CRQ	CB1-CA1-N	-2.87	115.45	125.34
1	A	70	CRQ	CE2-CD2-CG2	-2.82	117.58	121.28
1	A	70	CRQ	O-C-CA3	-2.80	117.11	126.38
1	A	70	CRQ	CD2-CG2-CB2	-2.67	112.06	121.23
1	A	70	CRQ	C2-CA2-N2	-2.43	107.15	108.93
1	A	70	CRQ	CE1-CD1-CG2	-2.28	118.30	121.28
1	A	70	CRQ	CD2-CG2-CD1	3.61	123.06	117.63
1	A	70	CRQ	CB2-CA2-C2	10.57	135.61	122.32
1	A	70	CRQ	CA2-C2-N3	11.74	108.54	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z  > 2$
2	PO4	A	301	-	4,4,4	3.42	2 (50%)	6,6,6	1.59	3 (50%)
3	GOL	A	302	-	5,5,5	1.06	0	5,5,5	1.32	1 (20%)

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	PO4	A	301	-	-	0/0/0/0	0/0/0/0
3	GOL	A	302	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PO4	P-O2	3.68	1.67	1.54
2	A	301	PO4	P-O1	5.65	1.62	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	GOL	C3-C2-C1	-2.74	100.64	111.52
2	A	301	PO4	O2-P-O1	-2.05	102.25	110.97
2	A	301	PO4	O3-P-O2	-2.01	100.52	107.90
2	A	301	PO4	O4-P-O3	2.38	116.64	107.90

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	229/271 (84%)	-0.61	1 (0%) 92 92	9, 13, 27, 39	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	GLY	2.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRQ	A	70	24/25	0.98	0.06	-	8,10,11,12	0

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	A	301	5/5	0.96	0.12	2.39	18,23,25,31	0
3	GOL	A	302	6/6	0.98	0.04	-1.38	14,15,17,18	0
4	CL	A	303	1/1	1.00	0.03	-	17,17,17,17	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.