



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:34 PM UTC

PDB ID : 5Y00 / pdb_00005y00
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

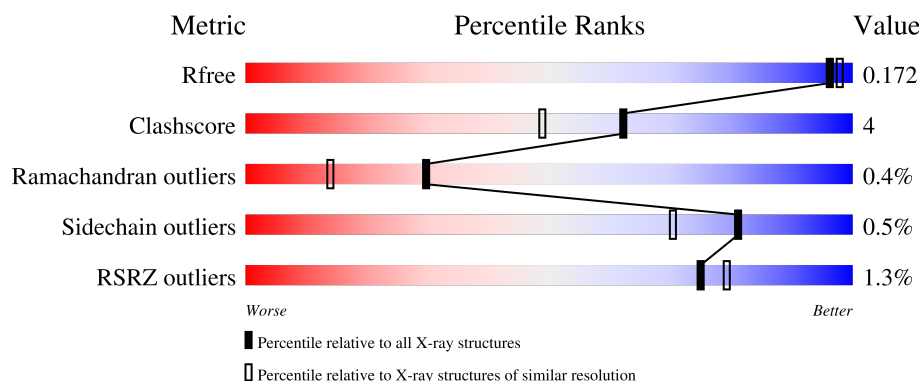
1 Overall quality at a glance

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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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 $\leq 5\%$. 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	-	-

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 (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

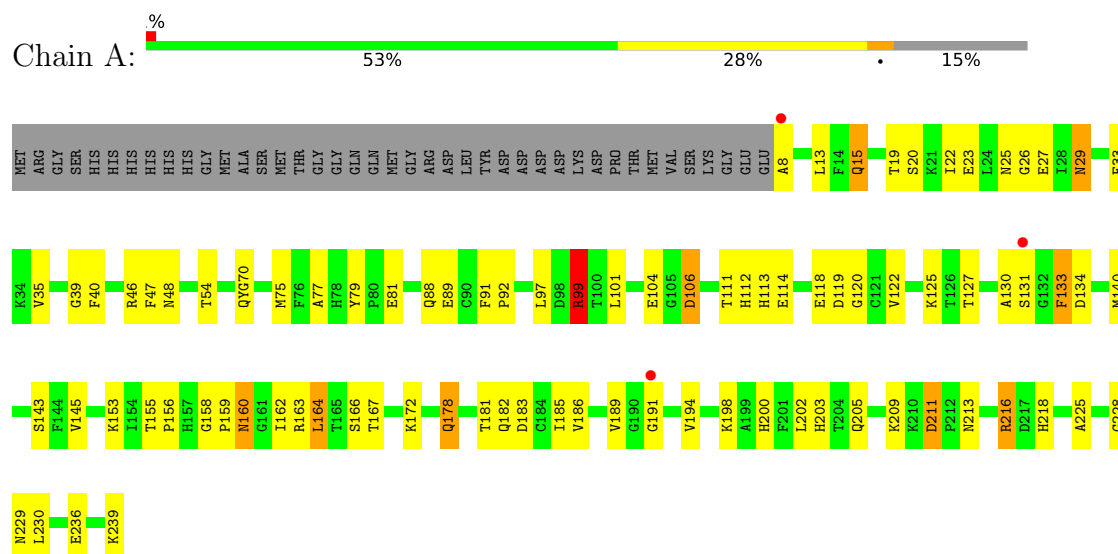
- Molecule 5 is water.

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

3 Residue-property plots [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: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	161.16Å 161.16Å 161.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	113.96 – 1.60 113.96 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (113.96-1.60) 99.8 (113.96-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	4514 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: PO4, GOL, 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	2.26	79/1899 (4.2%)	1.91	41/2568 (1.6%)

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	3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	GLN	CD-NE2	-10.10	1.12	1.33
1	A	130	ALA	N-CA	10.06	1.58	1.46
1	A	8	ALA	N-CA	9.02	1.63	1.46
1	A	48	ASN	CB-CG	-8.63	1.30	1.52
1	A	229	ASN	CG-ND2	-8.56	1.15	1.33
1	A	39	GLY	CA-C	-8.09	1.44	1.52
1	A	134	ASP	CA-C	-8.05	1.42	1.52
1	A	130	ALA	CA-CB	-7.89	1.40	1.53
1	A	89	GLU	C-O	7.64	1.33	1.24
1	A	183	ASP	CG-OD2	7.57	1.39	1.25
1	A	99	ARG	CA-C	-7.53	1.43	1.52
1	A	47	PHE	CA-C	-7.43	1.43	1.52
1	A	229	ASN	CG-OD1	7.21	1.37	1.23
1	A	106[A]	ASP	N-CA	-7.09	1.37	1.46
1	A	106[B]	ASP	N-CA	-7.09	1.37	1.46
1	A	26	GLY	CA-C	-7.09	1.46	1.52
1	A	133	PHE	CA-C	-7.06	1.43	1.52
1	A	166	SER	CA-C	-6.79	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	HIS	C-N	6.68	1.43	1.33
1	A	111	THR	CA-C	-6.65	1.44	1.52
1	A	33	PHE	CA-C	-6.62	1.44	1.52
1	A	189	VAL	C-N	-6.61	1.25	1.33
1	A	106[A]	ASP	C-N	-6.60	1.25	1.33
1	A	106[B]	ASP	C-N	-6.60	1.25	1.33
1	A	164	LEU	CA-C	-6.55	1.44	1.52
1	A	54	THR	N-CA	6.44	1.54	1.46
1	A	230	LEU	CA-CB	-6.37	1.43	1.53
1	A	119	ASP	C-N	6.34	1.42	1.33
1	A	225	ALA	CA-C	-6.20	1.45	1.52
1	A	81	GLU	C-O	-6.11	1.16	1.24
1	A	13	LEU	CA-CB	-6.03	1.43	1.53
1	A	189	VAL	N-CA	6.00	1.52	1.46
1	A	156	PRO	CA-C	-5.99	1.44	1.52
1	A	92	PRO	CA-CB	5.97	1.64	1.53
1	A	228	GLY	CA-C	5.96	1.57	1.51
1	A	118	GLU	N-CA	5.87	1.53	1.46
1	A	185	ILE	C-O	5.85	1.30	1.24
1	A	202	LEU	CB-CG	-5.81	1.41	1.53
1	A	101	LEU	CA-C	-5.79	1.45	1.52
1	A	160	ASN	CG-OD1	5.74	1.34	1.23
1	A	236	GLU	C-O	5.73	1.31	1.24
1	A	153	LYS	C-N	-5.69	1.26	1.33
1	A	23	GLU	CG-CD	5.68	1.66	1.52
1	A	202	LEU	CA-C	-5.63	1.46	1.52
1	A	88	GLN	CA-CB	-5.62	1.44	1.53
1	A	20	SER	N-CA	-5.61	1.38	1.45
1	A	191	GLY	N-CA	5.60	1.53	1.45
1	A	236	GLU	CA-C	-5.60	1.45	1.52
1	A	134	ASP	C-O	5.57	1.31	1.24
1	A	19	THR	C-O	5.56	1.30	1.23
1	A	145	VAL	CA-CB	5.55	1.61	1.54
1	A	127	THR	N-CA	-5.51	1.39	1.45
1	A	92	PRO	N-CA	-5.50	1.37	1.47
1	A	113	HIS	CA-C	-5.41	1.46	1.52
1	A	160	ASN	CG-ND2	-5.41	1.21	1.33
1	A	48	ASN	CA-C	-5.38	1.46	1.52
1	A	79	TYR	CA-C	-5.36	1.45	1.52
1	A	112	HIS	N-CA	-5.35	1.39	1.46
1	A	183	ASP	CB-CG	-5.29	1.38	1.52
1	A	120	GLY	C-N	-5.27	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	VAL	CA-CB	5.27	1.60	1.54
1	A	15	GLN	CG-CD	-5.26	1.38	1.52
1	A	134	ASP	CG-OD2	5.26	1.35	1.25
1	A	213	ASN	CG-ND2	-5.22	1.22	1.33
1	A	163	ARG	CD-NE	-5.21	1.39	1.46
1	A	46	ARG	CZ-NH1	-5.18	1.25	1.32
1	A	112	HIS	C-N	-5.17	1.26	1.33
1	A	178	GLN	CA-C	-5.16	1.46	1.52
1	A	27	GLU	C-N	-5.13	1.27	1.33
1	A	163	ARG	NE-CZ	5.12	1.38	1.33
1	A	186	VAL	CA-CB	-5.12	1.48	1.54
1	A	75	MET	CG-SD	-5.12	1.68	1.80
1	A	155	THR	C-O	-5.09	1.19	1.24
1	A	22	ILE	CA-C	-5.08	1.46	1.52
1	A	23	GLU	C-N	-5.08	1.26	1.33
1	A	211	ASP	CA-C	-5.05	1.47	1.53
1	A	133	PHE	N-CA	-5.05	1.39	1.46
1	A	125[A]	LYS	C-O	5.03	1.29	1.24
1	A	125[B]	LYS	C-O	5.03	1.29	1.24

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	CA-C-O	9.82	129.13	119.51
1	A	134	ASP	O-C-N	-9.51	113.04	121.31
1	A	158	GLY	O-C-N	-8.86	112.91	121.77
1	A	131	SER	N-CA-CB	-8.27	96.17	111.13
1	A	216	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	A	47	PHE	CA-C-O	7.94	130.05	120.28
1	A	239	LYS	CB-CG-CD	7.50	128.55	111.30
1	A	33	PHE	O-C-N	-7.42	114.79	123.25
1	A	203	HIS	CA-C-O	-6.85	112.55	120.49
1	A	153	LYS	CA-C-O	-6.78	112.88	120.54
1	A	164	LEU	O-C-N	-6.53	115.53	123.30
1	A	164	LEU	CB-CG-CD1	6.33	129.68	110.70
1	A	111	THR	O-C-N	-6.16	116.12	123.27
1	A	205	GLN	CB-CG-CD	-6.14	102.17	112.60
1	A	114	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	127	THR	CA-C-O	-6.06	114.27	121.11
1	A	39	GLY	N-CA-C	6.05	119.94	111.10
1	A	119	ASP	CA-C-O	5.94	128.43	121.54
1	A	77	ALA	O-C-N	-5.94	115.85	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	213	ASN	CA-C-O	5.85	125.22	118.55
1	A	143	SER	CA-CB-OG	-5.83	99.45	111.10
1	A	167	THR	CA-C-O	-5.80	114.06	120.38
1	A	47	PHE	CA-CB-CG	5.74	119.54	113.80
1	A	47	PHE	O-C-N	-5.71	116.39	123.36
1	A	8	ALA	N-CA-CB	5.51	118.66	110.40
1	A	159	PRO	N-CD-CG	-5.47	95.00	103.20
1	A	189	VAL	CB-CA-C	5.42	119.78	112.36
1	A	29	ASN	O-C-N	5.40	129.48	122.40
1	A	159	PRO	CA-C-N	-5.40	112.33	121.18
1	A	159	PRO	C-N-CA	-5.40	112.33	121.18
1	A	162	ILE	O-C-N	-5.37	116.96	123.02
1	A	183	ASP	CA-C-O	-5.34	114.19	120.60
1	A	111	THR	CA-C-O	5.31	127.22	121.06
1	A	114	GLU	CA-C-O	-5.29	115.13	121.11
1	A	35	VAL	O-C-N	-5.22	117.54	123.18
1	A	153	LYS	O-C-N	5.21	129.16	123.22
1	A	181	THR	CA-C-O	-5.09	114.83	120.38
1	A	228	GLY	O-C-N	5.08	128.29	123.56
1	A	91	PHE	CA-C-O	5.07	124.91	120.19
1	A	19	THR	N-CA-C	5.03	117.05	109.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104[A]	GLU	Sidechain
1	A	104[B]	GLU	Sidechain
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	1823	15	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1831	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
1:A:15:GLN:NE2	5:A:401:HOH:O	2.07	0.88
1:A:140[B]:MET:HE1	5:A:584:HOH:O	1.83	0.77
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: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 ⓘ

5.3.1 Protein backbone ⓘ

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	233/271 (86%)	227 (97%)	4 (2%)	2 (1%)	14 3

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 ⓘ

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%)	204 (100%)	1 (0%)	81 70

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) 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	205	GLN
1	A	208	GLN
1	A	218	HIS
1	A	221	GLN
1	A	229	ASN
1	A	232	HIS

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	25,25,26	3.02	10 (40%)	28,34,36	3.30	10 (35%)

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	-	2/10/32/33	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	70	CRQ	CB2-CA2	9.82	1.44	1.35
1	A	70	CRQ	C1-CA1	5.49	1.56	1.48
1	A	70	CRQ	C1-N2	4.29	1.42	1.33
1	A	70	CRQ	CA2-C2	-4.14	1.44	1.48
1	A	70	CRQ	CA1-N1	3.70	1.35	1.27
1	A	70	CRQ	CA2-N2	3.04	1.45	1.38
1	A	70	CRQ	CD2-CG2	-2.59	1.34	1.39
1	A	70	CRQ	C2-N3	-2.57	1.34	1.40
1	A	70	CRQ	O3-C3	2.47	1.34	1.20
1	A	70	CRQ	O2-C2	2.12	1.27	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	CRQ	CB2-CA2-C2	10.94	135.61	122.36
1	A	70	CRQ	CB2-CA2-N2	-8.49	117.24	128.76
1	A	70	CRQ	CA2-C2-N3	6.00	108.54	103.50
1	A	70	CRQ	CD2-CG2-CD1	3.64	123.06	117.65
1	A	70	CRQ	N3-C1-N2	-3.05	109.00	112.62
1	A	70	CRQ	CE2-CD2-CG2	-2.82	117.58	121.22
1	A	70	CRQ	CD2-CG2-CB2	-2.67	112.06	121.22
1	A	70	CRQ	C2-CA2-N2	-2.51	107.15	108.95
1	A	70	CRQ	CE1-CD1-CG2	-2.27	118.30	121.22
1	A	70	CRQ	CA3-N3-C1	-2.02	124.41	128.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	70	CRQ	C2-CA2-CB2-CG2
1	A	70	CRQ	N2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	3.47	2 (50%)	6,6,6	1.89	3 (50%)
3	GOL	A	302	-	5,5,5	1.07	0	5,5,5	1.48	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
3	GOL	A	302	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	PO4	P-O1	5.22	1.62	1.50
2	A	301	PO4	P-O2	4.37	1.67	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	GOL	C3-C2-C1	-3.04	100.64	111.80
2	A	301	PO4	O4-P-O3	2.81	116.64	107.91
2	A	301	PO4	O2-P-O1	-2.46	102.25	110.95
2	A	301	PO4	O3-P-O2	-2.38	100.52	107.91

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	229/271 (84%)	-0.41	3 (1%) 75 79	7, 13, 27, 39	8 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	4.4
1	A	131	SER	3.1
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. 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(Å ²)	Q<0.9
1	CRQ	A	70	24/25	0.98	0.04	8,10,11,12	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	A	301	5/5	0.96	0.17	18,23,25,31	0
3	GOL	A	302	6/6	0.98	0.06	14,15,17,18	0
4	CL	A	303	1/1	1.00	0.06	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.