



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:40 am BST

PDB ID : 2WUR
Title : Atomic resolution structure of GFP measured on a rotating anode
Authors : Palm, G.J.; Schierbeek, A.J.; Kloos, M.
Deposited on : 2009-10-07
Resolution : 0.90 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 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 : 2.11
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) : 2.11

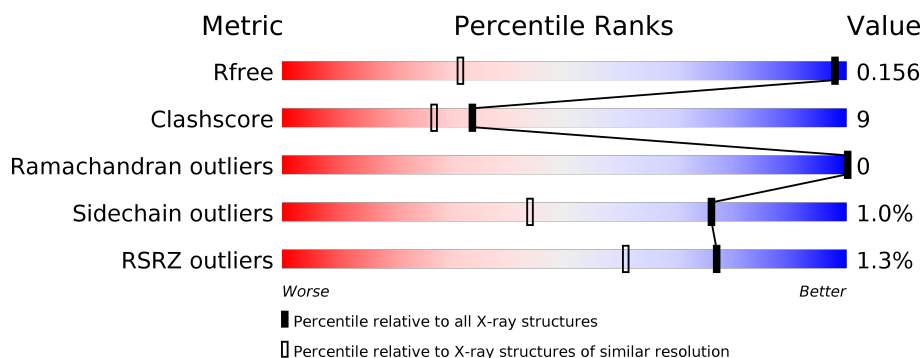
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.90 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	1061 (1.04-0.76)
Clashscore	141614	1132 (1.04-0.76)
Ramachandran outliers	138981	1055 (1.04-0.76)
Sidechain outliers	138945	1056 (1.04-0.76)
RSRZ outliers	127900	1028 (1.04-0.76)

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 on 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	236	<div> <div></div> <div>74%</div> <div>17%</div> <div>...</div> </div>

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
3	EOH	A	244	-	-	X	-
3	EOH	A	245	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4296 atoms, of which 2004 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.

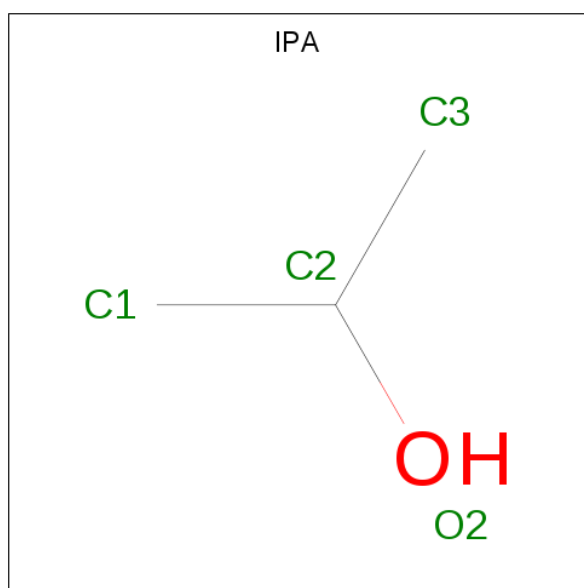
- Molecule 1 is a protein called GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	228	3885	1241	1943	328	366	7	0	22	1

There are 7 discrepancies between the modelled and reference sequences:

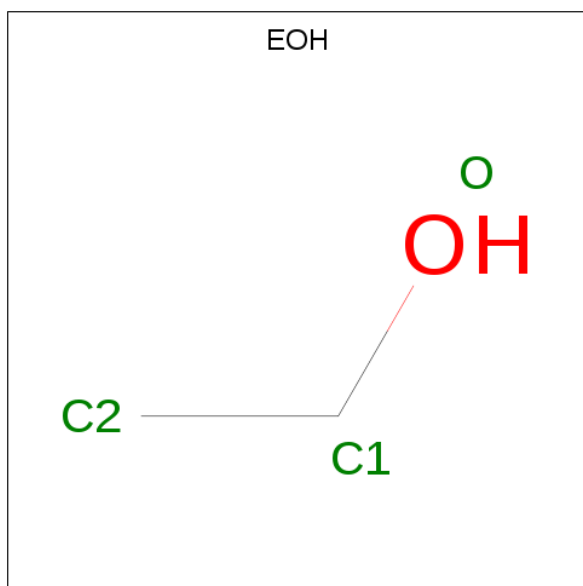
Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	167	THR	ILE	engineered mutation	UNP P42212
A	238	ASN	LYS	engineered mutation	UNP P42212

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			12	3	8	1		

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	1
			16	4	11	1		
3	A	1	Total	C	H	O	0	1
			18	4	12	2		
3	A	1	Total	C	H	O	0	0
			9	2	6	1		
3	A	1	Total	C	H	O	0	0
			9	2	6	1		
3	A	1	Total	C	H	O	0	0
			9	2	6	1		
3	A	1	Total	C	H	O	0	0
			9	2	6	1		

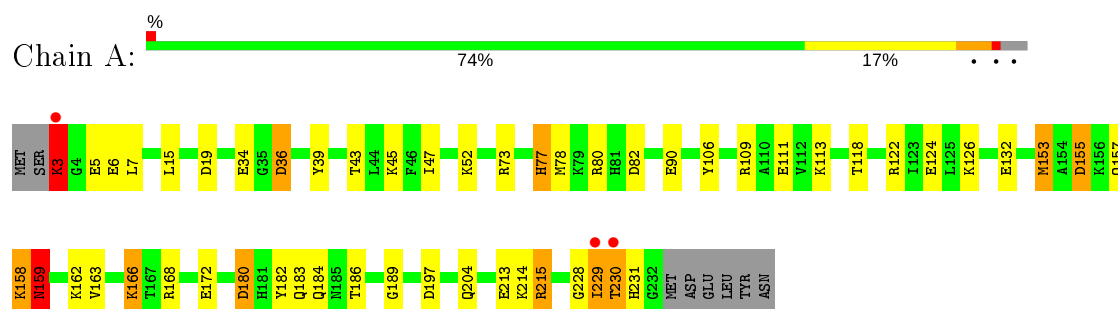
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	2
			320	320		

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	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.99Å 59.05Å 67.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 0.90 67.70 – 0.90	Depositor EDS
% Data completeness (in resolution range)	90.3 (6.00-0.90) 83.2 (67.70-0.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-1.39 (at 0.90Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.146 , 0.174 0.132 , 0.156	Depositor DCC
R_{free} test set	13553 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	6.7	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4296	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IPA, EOH, GYS

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	1.62	29/2026 (1.4%)	2.54	60/2732 (2.2%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	GLU	CD-OE1	-14.38	1.09	1.25
1	A	34	GLU	CD-OE2	-10.24	1.14	1.25
1	A	182	TYR	CE2-CZ	-9.73	1.25	1.38
1	A	197	ASP	CG-OD2	-8.81	1.05	1.25
1	A	213	GLU	CD-OE1	7.86	1.34	1.25
1	A	168	ARG	NE-CZ	-7.77	1.23	1.33
1	A	34	GLU	CB-CG	-7.76	1.37	1.52
1	A	204	GLN	CG-CD	7.22	1.67	1.51
1	A	228	GLY	C-O	-6.97	1.12	1.23
1	A	231	HIS	C-N	-6.80	1.20	1.33
1	A	36	ASP	CG-OD1	6.54	1.40	1.25
1	A	172	GLU	CG-CD	6.44	1.61	1.51
1	A	3	LYS	N-CA	-6.39	1.33	1.46
1	A	5	GLU	CG-CD	6.22	1.61	1.51
1	A	111	GLU	CG-CD	-5.98	1.43	1.51
1	A	113	LYS	CD-CE	-5.94	1.36	1.51
1	A	172	GLU	CD-OE1	-5.93	1.19	1.25
1	A	204	GLN	CB-CG	-5.90	1.36	1.52
1	A	111	GLU	CD-OE1	5.79	1.32	1.25
1	A	5	GLU	CD-OE2	5.71	1.31	1.25
1	A	6	GLU	CB-CG	5.58	1.62	1.52
1	A	189	GLY	CA-C	-5.58	1.43	1.51
1	A	132	GLU	CD-OE2	5.54	1.31	1.25
1	A	77	HIS	CE1-NE2	5.41	1.45	1.32
1	A	204	GLN	CD-OE1	-5.29	1.12	1.24
1	A	182	TYR	CE1-CZ	5.27	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	GLU	CA-CB	5.21	1.65	1.53
1	A	231	HIS	CB-CG	-5.19	1.40	1.50
1	A	132	GLU	CG-CD	-5.17	1.44	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73[A]	ARG	NE-CZ-NH1	50.72	145.66	120.30
1	A	73[B]	ARG	NE-CZ-NH1	50.72	145.66	120.30
1	A	73[A]	ARG	NE-CZ-NH2	-47.74	96.43	120.30
1	A	73[B]	ARG	NE-CZ-NH2	-47.74	96.43	120.30
1	A	168	ARG	NE-CZ-NH2	21.69	131.14	120.30
1	A	168	ARG	CD-NE-CZ	16.02	146.03	123.60
1	A	168	ARG	NE-CZ-NH1	-15.74	112.43	120.30
1	A	80	ARG	NE-CZ-NH2	15.73	128.16	120.30
1	A	109	ARG	NE-CZ-NH2	-14.35	113.13	120.30
1	A	229	ILE	O-C-N	-10.81	105.40	122.70
1	A	36	ASP	CA-CB-CG	10.29	136.05	113.40
1	A	153	MET	CG-SD-CE	-10.28	83.75	100.20
1	A	36	ASP	CB-CG-OD1	10.13	127.42	118.30
1	A	204	GLN	OE1-CD-NE2	9.60	143.99	121.90
1	A	90[A]	GLU	OE1-CD-OE2	-9.47	111.94	123.30
1	A	90[B]	GLU	OE1-CD-OE2	-9.47	111.94	123.30
1	A	229	ILE	CA-C-O	9.37	139.77	120.10
1	A	166[A]	LYS	CD-CE-NZ	-8.93	91.17	111.70
1	A	166[B]	LYS	CD-CE-NZ	-8.93	91.17	111.70
1	A	182	TYR	CZ-CE2-CD2	8.71	127.64	119.80
1	A	204	GLN	CA-CB-CG	8.51	132.12	113.40
1	A	39	TYR	CB-CG-CD2	8.21	125.93	121.00
1	A	106	TYR	CB-CG-CD1	8.19	125.92	121.00
1	A	52	LYS	CB-CG-CD	7.94	132.24	111.60
1	A	230	THR	OG1-CB-CG2	7.75	127.82	110.00
1	A	3	LYS	N-CA-CB	7.71	124.48	110.60
1	A	109	ARG	NH1-CZ-NH2	7.36	127.50	119.40
1	A	36	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	204	GLN	CG-CD-OE1	-6.92	107.75	121.60
1	A	215	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	A	122[A]	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	122[B]	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	159	ASN	CB-CG-OD1	-6.53	108.54	121.60
1	A	19	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	A	122[A]	ARG	CD-NE-CZ	6.42	132.59	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122[B]	ARG	CD-NE-CZ	6.42	132.59	123.60
1	A	90[A]	GLU	CG-CD-OE2	6.28	130.87	118.30
1	A	90[B]	GLU	CG-CD-OE2	6.28	130.87	118.30
1	A	132	GLU	CB-CG-CD	6.16	130.84	114.20
1	A	19	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	124[A]	GLU	OE1-CD-OE2	6.04	130.54	123.30
1	A	124[B]	GLU	OE1-CD-OE2	6.04	130.54	123.30
1	A	180	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	A	80	ARG	NH1-CZ-NH2	-5.98	112.83	119.40
1	A	186[A]	THR	CA-CB-OG1	5.88	121.34	109.00
1	A	186[B]	THR	CA-CB-OG1	5.88	121.34	109.00
1	A	157	GLN	CG-CD-OE1	5.85	133.29	121.60
1	A	166[A]	LYS	N-CA-CB	5.75	120.95	110.60
1	A	166[B]	LYS	N-CA-CB	5.75	120.95	110.60
1	A	73[A]	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	73[B]	ARG	CD-NE-CZ	5.65	131.51	123.60
1	A	5	GLU	N-CA-CB	5.60	120.68	110.60
1	A	186[A]	THR	N-CA-CB	-5.58	99.71	110.30
1	A	186[B]	THR	N-CA-CB	-5.58	99.71	110.30
1	A	52	LYS	CD-CE-NZ	-5.52	99.01	111.70
1	A	158	LYS	CG-CD-CE	-5.42	95.64	111.90
1	A	82	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	A	155	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	197	ASP	CA-CB-CG	-5.21	101.95	113.40
1	A	7	LEU	CB-CG-CD2	5.03	119.55	111.00

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	1942	1943	1930	30	1
2	A	4	8	8	0	0
3	A	26	53	52	12	0
4	A	320	0	0	16	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2292	2004	1990	34	5

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 9.

All (34) 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:229:ILE:HG23	4:A:2313:HOH:O	1.13	1.27
1:A:229:ILE:CG2	4:A:2313:HOH:O	1.65	1.25
1:A:3:LYS:HD2	4:A:2005:HOH:O	1.52	1.09
1:A:229:ILE:CA	4:A:2313:HOH:O	2.03	1.06
3:A:245:EOH:C1	4:A:2319:HOH:O	2.15	0.95
3:A:245:EOH:H11	4:A:2319:HOH:O	1.65	0.94
1:A:43[B]:THR:HG21	4:A:2076:HOH:O	1.74	0.87
1:A:230:THR:N	4:A:2313:HOH:O	2.07	0.86
3:A:245:EOH:C2	4:A:2319:HOH:O	2.35	0.75
1:A:36:ASP:OD2	4:A:2063:HOH:O	2.06	0.72
1:A:155:ASP:OD2	1:A:158:LYS:HD3	1.92	0.69
3:A:245:EOH:H21	4:A:2319:HOH:O	1.91	0.68
1:A:229:ILE:HA	4:A:2313:HOH:O	1.79	0.67
1:A:166[A]:LYS:HG2	1:A:180:ASP:OD1	1.97	0.64
1:A:126:LYS:HZ3	3:A:244:EOH:C2	2.11	0.63
1:A:15[B]:LEU:HG	1:A:118:THR:HG21	1.79	0.62
1:A:126:LYS:HD3	3:A:244:EOH:H21	1.85	0.59
1:A:126:LYS:CE	3:A:244:EOH:H21	2.35	0.56
1:A:158:LYS:HE2	1:A:184[B]:GLN:CD	2.31	0.50
1:A:3:LYS:O	4:A:2001:HOH:O	2.19	0.50
1:A:126:LYS:NZ	3:A:244:EOH:H21	2.28	0.48
1:A:126:LYS:CD	3:A:244:EOH:H21	2.42	0.48
1:A:126:LYS:HZ3	3:A:244:EOH:H21	1.76	0.48
1:A:3:LYS:HB2	4:A:2002:HOH:O	2.16	0.46
1:A:126:LYS:HD3	3:A:244:EOH:C2	2.45	0.46
1:A:214[B]:LYS:HE3	4:A:2320:HOH:O	2.15	0.45
1:A:126:LYS:NZ	3:A:244:EOH:C2	2.80	0.44
1:A:214[B]:LYS:HE2	4:A:2302:HOH:O	2.18	0.44
1:A:163:VAL:HB	1:A:183:GLN:HB3	2.00	0.44
1:A:77:HIS:CD2	1:A:78[B]:MET:HG2	2.54	0.43
1:A:45:LYS:HE2	1:A:47[B]:ILE:HD11	2.01	0.43
1:A:47[A]:ILE:HD13	1:A:215:ARG:CZ	2.51	0.41
1:A:159:ASN:HD22	1:A:159:ASN:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HB2	1:A:153:MET:HE2	1.57	0.40

All (5) 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:A:3:LYS:H2	1:A:162[B]:LYS:HZ2[3_645]	1.13	0.47
4:A:2198:HOH:O	4:A:2314:HOH:O[2_664]	1.77	0.43
4:A:2069:HOH:O	4:A:2271:HOH:O[3_655]	1.87	0.33
4:A:2116:HOH:O	4:A:2301:HOH:O[4_555]	2.06	0.14
4:A:2204:HOH:O	4:A:2276:HOH:O[2_664]	2.18	0.02

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	247/236 (105%)	243 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	220/206 (107%)	218 (99%)	2 (1%)	78	47

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	159	ASN

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

Mol	Chain	Res	Type
1	A	170	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	GYS	A	66	1	22,22,23	1.94	6 (27%)	27,30,32	1.27	2 (7%)

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	GYS	A	66	1	-	0/9/29/30	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CB2-CA2	5.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CA2-C2	-2.76	1.45	1.48
1	A	66	GYS	CG2-CB2	-2.68	1.41	1.46
1	A	66	GYS	CA3-N3	-2.28	1.42	1.47
1	A	66	GYS	CE1-CD1	-2.13	1.34	1.38
1	A	66	GYS	C1-N3	2.02	1.40	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GYS	CA2-C2-N3	3.01	104.80	103.37
1	A	66	GYS	O-C-CA3	-2.48	118.89	126.39

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
3	EOH	A	247	-	2,2,2	0.43	0	1,1,1	0.32	0
3	EOH	A	246	-	2,2,2	0.50	0	1,1,1	0.30	0
3	EOH	A	245	-	2,2,2	0.54	0	1,1,1	0.30	0
3	EOH	A	242[A]	-	2,2,2	0.36	0	1,1,1	0.08	0
3	EOH	A	242[B]	-	2,2,2	0.41	0	1,1,1	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EOH	A	243	-	2,2,2	0.40	0	1,1,1	0.21	0
3	EOH	A	241[A]	-	2,2,2	0.55	0	1,1,1	0.26	0
3	EOH	A	244	-	2,2,2	0.33	0	1,1,1	0.20	0
2	IPA	A	240	-	3,3,3	2.12	1 (33%)	3,3,3	1.25	1 (33%)
3	EOH	A	241[B]	-	2,2,2	0.49	0	1,1,1	0.30	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	240	IPA	C1-C2	3.37	1.71	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	240	IPA	C3-C2-C1	-2.13	97.36	113.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	245	EOH	4	0
3	A	244	EOH	8	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 [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	227/236 (96%)	-0.68	3 (1%)	77 61	4, 7, 15, 34	3 (1%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ILE	2.8
1	A	3	LYS	2.5
1	A	230	THR	2.2

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	GYS	A	66	21/22	0.99	0.05	3,4,5,8	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. 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(\AA^2)	Q<0.9
2	IPA	A	240	4/4	0.78	0.24	8,24,30,31	0
3	EOH	A	243	3/3	0.82	0.14	32,39,64,64	0
3	EOH	A	247	3/3	0.83	0.12	18,27,41,43	0
3	EOH	A	242[B]	3/3	0.91	0.15	10,16,24,29	9
3	EOH	A	242[A]	3/3	0.91	0.15	9,12,27,41	9
3	EOH	A	244	3/3	0.92	0.13	4,9,18,27	0
3	EOH	A	241[A]	3/3	0.93	0.20	1,14,30,30	7
3	EOH	A	241[B]	3/3	0.93	0.20	3,8,14,21	7
3	EOH	A	245	3/3	0.94	0.09	9,14,34,34	0
3	EOH	A	246	3/3	0.98	0.07	4,14,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.