



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:12 PM GMT

PDB ID : 5HZO
Title : GFP mutant S205G
Authors : Remington, S.J.; Trujillo, K.
Deposited on : 2016-02-02
Resolution : 2.49 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
<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

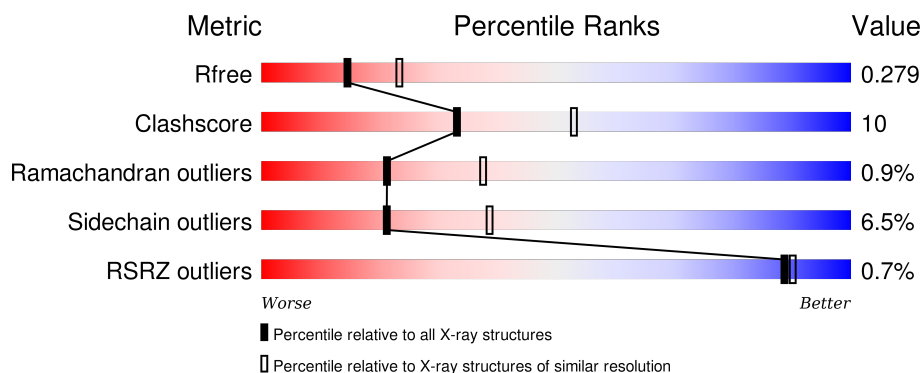
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	233	<div> <div></div> <div>73%</div> <div>23%</div> <div>..</div> </div>
1	B	233	<div> <div>%</div> <div>73%</div> <div>23%</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
2	MLT	A	301	-	-	-	X
3	UMQ	B	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3747 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.

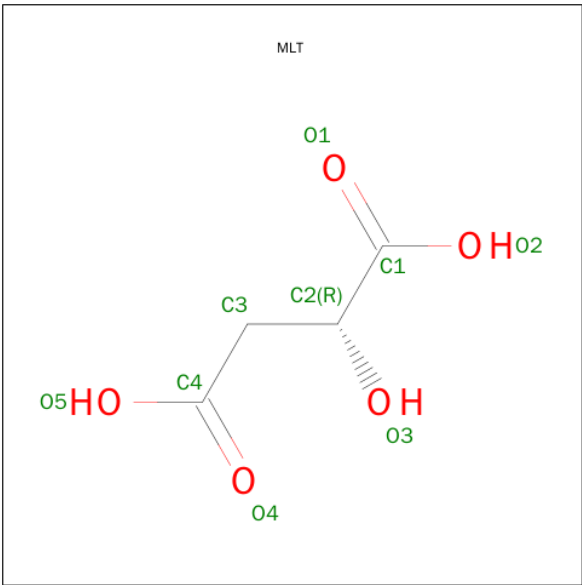
- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1781	1129	302	343	7			
1	B	230	Total	C	N	O	S	0	0	0
			1805	1150	305	343	7			

There are 10 discrepancies between the modelled and reference sequences:

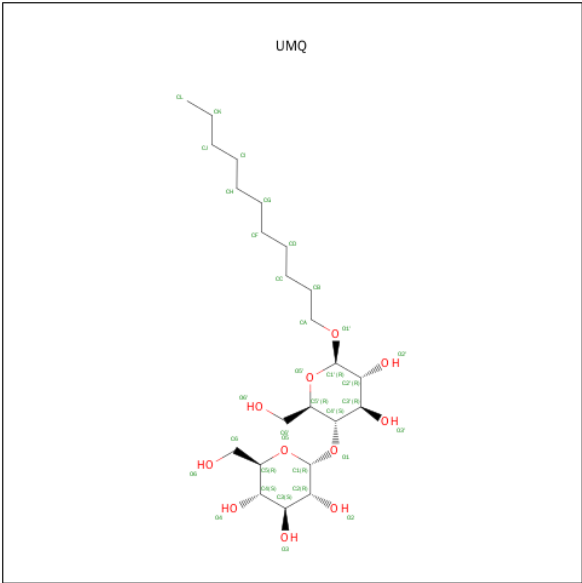
Chain	Residue	Modelled	Actual	Comment	Reference
A	66	GYS	SER	chromophore	UNP P42212
A	66	GYS	TYR	chromophore	UNP P42212
A	66	GYS	GLY	chromophore	UNP P42212
A	80	ARG	GLN	conflict	UNP P42212
A	205	GLY	SER	engineered mutation	UNP P42212
B	66	GYS	SER	chromophore	UNP P42212
B	66	GYS	TYR	chromophore	UNP P42212
B	66	GYS	GLY	chromophore	UNP P42212
B	80	ARG	GLN	conflict	UNP P42212
B	205	GLY	SER	engineered mutation	UNP P42212

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: C₄H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		
2	B	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).

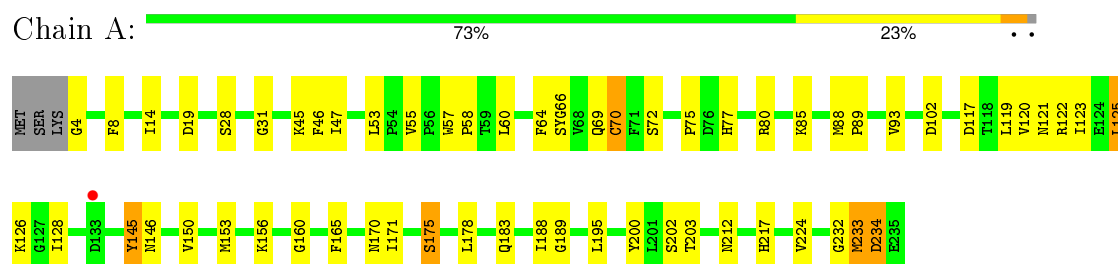


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total 48	O 48	0	0
4	B	63	Total 63	O 63	0	0

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 errors 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



- Molecule 1: Green fluorescent protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	66.03Å 96.28Å 151.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.49 9.99 – 2.49	Depositor EDS
% Data completeness (in resolution range)	75.7 (10.00-2.49) 77.1 (9.99-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.175 , 0.276 0.182 , 0.279	Depositor DCC
R_{free} test set	644 reflections (5.17%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 13112 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3747	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: UMQ, GYS, MLT

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	0.65	0/1802	0.79	0/2445
1	B	0.69	0/1826	0.85	0/2473
All	All	0.67	0/3628	0.82	0/4918

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	232	GLY	Peptide
1	B	112	VAL	Peptide

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	1781	0	1633	33	0
1	B	1805	0	1708	37	0
2	A	9	0	4	2	0
2	B	9	0	4	1	0
3	B	32	0	37	7	0
4	A	48	0	0	2	0
4	B	63	0	0	4	0
All	All	3747	0	3386	72	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 10.

All (72) 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:19:ASP:OD1	1:A:28:SER:OG	2.02	0.76
1:B:145:TYR:HA	2:B:302:MLT:H2	1.72	0.71
1:A:146:ASN:HD21	1:A:170:ASN:HD21	1.36	0.69
1:B:1:MET:HB3	1:B:86:SER:HA	1.74	0.68
1:A:203:THR:HG22	1:A:224:VAL:HG22	1.76	0.67
3:B:301:UMQ:O5	4:B:401:HOH:O	2.13	0.66
1:B:171:ILE:HD12	1:B:175:SER:HB3	1.78	0.65
1:A:70:CYS:SG	1:A:119:LEU:HD11	2.38	0.64
1:B:81:HIS:CE1	3:B:301:UMQ:H61	2.33	0.63
3:B:301:UMQ:O5'	3:B:301:UMQ:HC1	1.98	0.63
1:A:233:MET:O	1:A:234:ASP:HB2	1.98	0.62
1:A:53:LEU:HD21	1:A:60:LEU:HD12	1.80	0.62
1:B:80:ARG:HB3	3:B:301:UMQ:H41	1.81	0.62
1:B:1:MET:HE2	1:B:79:LYS:O	2.01	0.61
1:B:54:PRO:HG3	4:B:437:HOH:O	2.01	0.60
1:A:14:ILE:HA	1:A:119:LEU:O	2.02	0.58
1:A:145:TYR:HA	2:A:301:MLT:H2	1.86	0.57
1:A:66:GYS:OH	2:A:301:MLT:O5	2.22	0.57
1:B:126:LYS:HE3	1:B:128:ILE:HG23	1.87	0.56
1:A:121:ASN:ND2	1:A:123:ILE:HD11	2.21	0.55
1:A:31:GLY:HA2	1:A:45:LYS:O	2.09	0.53
1:B:134:GLY:O	1:B:136:ILE:N	2.42	0.52
3:B:301:UMQ:C5'	3:B:301:UMQ:HC1	2.39	0.52
1:B:42:LEU:HD21	1:B:71:PHE:CB	2.42	0.49
1:B:150:VAL:O	1:B:200:TYR:HA	2.12	0.49
1:B:17:GLU:OE2	1:B:122:ARG:NH1	2.45	0.49
1:A:46:PHE:O	1:A:217:HIS:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:ILE:HG22	1:B:15:LEU:N	2.28	0.48
1:B:164:ASN:HA	1:B:181:HIS:O	2.13	0.48
1:B:145:TYR:CD1	1:B:146:ASN:N	2.82	0.48
1:B:149:ASN:HA	1:B:201:LEU:O	2.13	0.48
1:B:42:LEU:HD21	1:B:71:PHE:HB2	1.95	0.48
1:B:105:ASN:O	1:B:127:GLY:HA2	2.14	0.48
1:A:53:LEU:HD23	1:A:55:VAL:O	2.14	0.47
3:B:301:UMQ:C1	4:B:401:HOH:O	2.62	0.47
1:A:93:VAL:HG23	1:A:188:ILE:HG13	1.97	0.46
1:A:53:LEU:HD21	1:A:60:LEU:CD1	2.44	0.46
1:A:8:PHE:CZ	1:A:70:CYS:HB2	2.51	0.46
1:B:57:TRP:N	1:B:58:PRO:CD	2.79	0.46
1:B:220:LEU:HD21	1:B:222:GLU:OE1	2.16	0.45
1:B:56:PRO:CB	1:B:58:PRO:HD2	2.46	0.45
1:B:80:ARG:CB	3:B:301:UMQ:H41	2.45	0.45
1:B:119:LEU:HG	1:B:120:VAL:N	2.30	0.45
1:A:75:PRO:HB2	1:A:77:HIS:CE1	2.51	0.45
1:B:6:GLU:HG2	4:B:446:HOH:O	2.17	0.44
1:A:150:VAL:O	1:A:200:TYR:HA	2.17	0.44
1:A:117:ASP:HA	1:B:192:PRO:HD2	1.99	0.44
1:A:125:LEU:HD23	1:A:125:LEU:C	2.38	0.44
1:B:62:THR:O	1:B:66:GYS:C2	2.66	0.44
1:A:69:GLN:HE22	1:A:183:GLN:HE22	1.66	0.43
1:A:171:ILE:HD12	1:A:175:SER:HB3	2.01	0.43
1:A:212:ASN:HB2	4:A:441:HOH:O	2.18	0.43
1:B:7:LEU:HD12	1:B:88:MET:HB3	2.00	0.43
1:B:147:SER:HA	1:B:203:THR:O	2.19	0.42
1:B:155:ASP:HB2	1:B:162:LYS:HD3	2.01	0.42
1:B:145:TYR:HD1	1:B:146:ASN:N	2.17	0.42
1:A:60:LEU:HB3	1:A:64:PHE:CE2	2.55	0.42
1:B:71:PHE:HE2	1:B:119:LEU:HD22	1.83	0.42
1:A:160:GLY:O	1:A:195:LEU:HD22	2.19	0.42
1:A:117:ASP:HB3	1:B:191:GLY:HA3	2.02	0.42
1:A:156:LYS:N	4:A:406:HOH:O	2.53	0.42
1:A:233:MET:O	1:A:234:ASP:CB	2.66	0.41
1:B:57:TRP:HB3	1:B:218:MET:SD	2.60	0.41
1:A:88:MET:HB3	1:A:89:PRO:HA	2.02	0.41
1:B:56:PRO:HD3	1:B:136:ILE:O	2.20	0.41
1:A:120:VAL:HG12	1:A:122:ARG:HG3	2.03	0.41
1:A:4:GLY:HA3	1:A:85:LYS:O	2.20	0.41
1:B:135:ASN:HA	1:B:140:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:N	1:A:58:PRO:HD2	2.35	0.41
1:B:53:LEU:HA	1:B:54:PRO:HD3	1.89	0.40
1:A:66:GYS:HD2	1:A:165:PHE:CZ	2.56	0.40
1:B:108:THR:CG2	1:B:125:LEU:HD12	2.52	0.40

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	227/233 (97%)	207 (91%)	18 (8%)	2 (1%)	21	37
1	B	227/233 (97%)	210 (92%)	15 (7%)	2 (1%)	21	37
All	All	454/466 (97%)	417 (92%)	33 (7%)	4 (1%)	21	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASP
1	B	135	ASN
1	B	172	GLU
1	A	189	GLY

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	181/202 (90%)	167 (92%)	14 (8%)	16	30
1	B	188/202 (93%)	178 (95%)	10 (5%)	28	50
All	All	369/404 (91%)	345 (94%)	24 (6%)	21	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ILE
1	A	70	CYS
1	A	72	SER
1	A	80	ARG
1	A	102	ASP
1	A	125	LEU
1	A	126	LYS
1	A	128	ILE
1	A	145	TYR
1	A	153	MET
1	A	175	SER
1	A	178	LEU
1	A	202	SER
1	A	233	MET
1	B	3	LYS
1	B	5	GLU
1	B	6	GLU
1	B	26	LYS
1	B	79	LYS
1	B	105	ASN
1	B	113	LYS
1	B	118	THR
1	B	147	SER
1	B	162	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	146	ASN
1	A	164	ASN
1	B	135	ASN
1	B	146	ASN
1	B	149	ASN

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Mol	Chain	Res	Type
1	B	231	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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$
1	GYS	A	66	1	22,22,23	3.73	5 (22%)	29,30,32	4.00	10 (34%)
1	GYS	B	66	1	22,22,23	3.88	4 (18%)	29,30,32	3.93	7 (24%)

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	-	0/8/29/30	0/2/2/2
1	GYS	B	66	1	-	0/8/29/30	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	C2-N3	-3.49	1.31	1.39
1	A	66	GYS	CA2-C2	-2.62	1.45	1.48
1	B	66	GYS	C2-N3	-2.49	1.33	1.39
1	A	66	GYS	O2-C2	2.36	1.28	1.23
1	B	66	GYS	O2-C2	2.78	1.29	1.23
1	B	66	GYS	C1-N2	3.74	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	C1-N2	3.99	1.38	1.32
1	A	66	GYS	CB2-CA2	15.99	1.49	1.35
1	B	66	GYS	CB2-CA2	16.99	1.50	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GYS	O2-C2-CA2	-11.90	124.13	130.97
1	B	66	GYS	O2-C2-CA2	-10.30	125.05	130.97
1	B	66	GYS	C2-CA2-N2	-6.15	104.35	109.03
1	A	66	GYS	C2-CA2-N2	-4.15	105.87	109.03
1	A	66	GYS	OG1-CB1-CA1	-2.93	104.89	111.27
1	B	66	GYS	CG2-CB2-CA2	-2.34	127.31	130.27
1	A	66	GYS	C2-N3-C1	-2.05	104.45	108.28
1	A	66	GYS	CA1-C1-N3	-2.04	122.50	124.98
1	A	66	GYS	CA3-N3-C1	2.08	129.67	127.38
1	A	66	GYS	CB2-CA2-C2	2.08	125.17	122.24
1	A	66	GYS	N3-C1-N2	2.13	113.11	111.53
1	B	66	GYS	CA3-N3-C1	3.12	130.82	127.38
1	A	66	GYS	C-CA3-N3	3.64	120.49	112.97
1	B	66	GYS	CA2-N2-C1	3.68	108.63	105.54
1	B	66	GYS	CB2-CA2-C2	5.80	130.40	122.24
1	B	66	GYS	CA2-C2-N3	14.75	110.67	103.37
1	A	66	GYS	CA2-C2-N3	15.59	111.09	103.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	GYS	2	0
1	B	66	GYS	1	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 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	MLT	A	301	-	1,8,8	0.69	0	2,10,10	3.87	1 (50%)
3	UMQ	B	301	-	33,33,35	1.93	7 (21%)	44,44,46	1.70	8 (18%)
2	MLT	B	302	-	1,8,8	1.53	0	2,10,10	3.13	1 (50%)

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	MLT	A	301	-	-	0/2/8/8	0/0/0/0
3	UMQ	B	301	-	-	0/18/58/60	0/2/2/2
2	MLT	B	302	-	-	0/2/8/8	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	301	UMQ	C3'-C4'	2.17	1.58	1.52
3	B	301	UMQ	C3-C4	2.68	1.59	1.52
3	B	301	UMQ	O4-C4	2.93	1.49	1.43
3	B	301	UMQ	O5-C1	3.22	1.50	1.41
3	B	301	UMQ	O1-C4'	3.49	1.52	1.43
3	B	301	UMQ	O1'-C1'	4.84	1.49	1.40
3	B	301	UMQ	O1-C1	5.59	1.56	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MLT	C4-C3-C2	-5.35	108.66	114.33
2	B	302	MLT	C4-C3-C2	-4.17	109.90	114.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	UMQ	C3'-C4'-C5'	-3.61	102.61	110.85
3	B	301	UMQ	O6'-C6'-C5'	-3.59	99.31	111.30
3	B	301	UMQ	O5'-C1'-O1'	-2.22	104.66	109.99
3	B	301	UMQ	O5-C1-C2	-2.21	105.68	110.28
3	B	301	UMQ	O4-C4-C3	2.57	116.16	110.36
3	B	301	UMQ	O1-C1-C2	3.56	116.97	108.12
3	B	301	UMQ	O1-C4'-C3'	4.10	117.88	107.18
3	B	301	UMQ	O1'-C1'-C2'	5.41	114.66	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	MLT	2	0
3	B	301	UMQ	7	0
2	B	302	MLT	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 [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	229/233 (98%)	-0.54	1 (0%) 93 93	26, 39, 61, 83	0
1	B	229/233 (98%)	-0.50	2 (0%) 85 88	25, 36, 52, 79	0
All	All	458/466 (98%)	-0.52	3 (0%) 89 90	25, 38, 57, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	ASP	3.2
1	B	1	MET	2.7
1	B	174	GLY	2.7

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, 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	LLDF	B-factors(Å ²)	Q<0.9
1	GYS	A	66	21/22	0.96	0.10	-	27,31,36,38	0
1	GYS	B	66	21/22	0.95	0.10	-	29,37,38,41	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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	UMQ	B	301	32/34	0.73	0.23	3.58	53,65,82,84	0
2	MLT	A	301	9/9	0.90	0.20	3.42	49,55,64,79	0
2	MLT	B	302	9/9	0.95	0.14	0.48	30,43,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.