



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2022 – 12:25 pm GMT

PDB ID : 6QUI  
Title : GHK tagged GFP variant at 17Kev  
Authors : Huyton, T.; Gorlich, D.  
Deposited on : 2019-02-27  
Resolution : 1.94 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

<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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.3  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

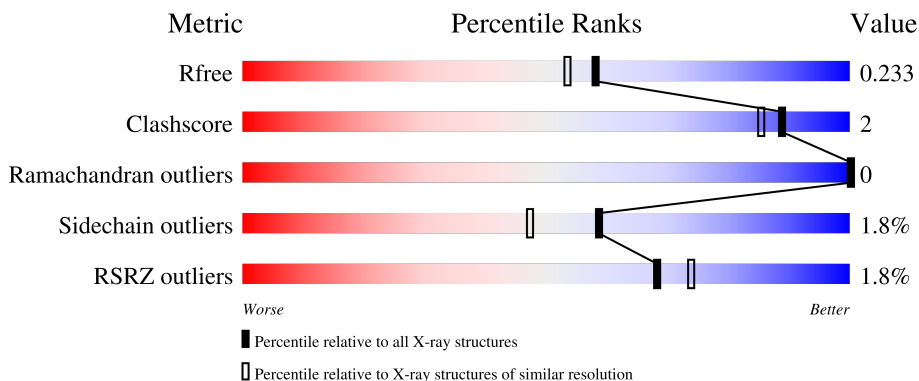
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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  $\geq 3$ , 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	B	229	 2% 92% 8%
1	E	229	 2% 94% 5%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4009 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	B	229	1857	1152	353	347	5	0	0	0
1	E	229	1864	1156	354	349	5	0	1	0

There are 82 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP P42212
B	1	HIS	SER	conflict	UNP P42212
B	3	ARG	-	insertion	UNP P42212
B	6	GLN	GLU	conflict	UNP P42212
B	26	ARG	LYS	conflict	UNP P42212
B	30	ARG	SER	conflict	UNP P42212
B	39	ASN	TYR	conflict	UNP P42212
B	41	ARG	LYS	conflict	UNP P42212
B	45	ARG	LYS	conflict	UNP P42212
B	52	ARG	LYS	conflict	UNP P42212
B	?	-	PHE	deletion	UNP P42212
B	?	-	SER	deletion	UNP P42212
B	64	LEU	TYR	conflict	UNP P42212
B	65	CRO	GLY	conflict	UNP P42212
B	77	ARG	LYS	conflict	UNP P42212
B	78	ARG	GLN	conflict	UNP P42212
B	97	SER	PHE	conflict	UNP P42212
B	99	ARG	LYS	conflict	UNP P42212
B	103	THR	ASN	conflict	UNP P42212
B	105	ARG	LYS	conflict	UNP P42212
B	109	VAL	GLU	conflict	UNP P42212
B	111	ARG	LYS	conflict	UNP P42212
B	115	ASN	ASP	conflict	UNP P42212
B	124	ARG	LYS	conflict	UNP P42212
B	126	THR	ILE	conflict	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	127	ASN	ASP	conflict	UNP P42212
B	129	ARG	LYS	conflict	UNP P42212
B	138	ARG	LYS	conflict	UNP P42212
B	151	THR	MET	conflict	UNP P42212
B	154	ARG	LYS	conflict	UNP P42212
B	156	ARG	LYS	conflict	UNP P42212
B	160	ARG	LYS	conflict	UNP P42212
B	161	ALA	VAL	conflict	UNP P42212
B	164	THR	LYS	conflict	UNP P42212
B	169	VAL	ILE	conflict	UNP P42212
B	178	ASN	ASP	conflict	UNP P42212
B	188	ASN	ASP	conflict	UNP P42212
B	196	ASP	ASN	conflict	UNP P42212
B	203	THR	SER	conflict	UNP P42212
B	207	ARG	LYS	conflict	UNP P42212
B	212	ARG	LYS	conflict	UNP P42212
E	0	GLY	-	expression tag	UNP P42212
E	1	HIS	SER	conflict	UNP P42212
E	3	ARG	-	insertion	UNP P42212
E	6	GLN	GLU	conflict	UNP P42212
E	26	ARG	LYS	conflict	UNP P42212
E	30	ARG	SER	conflict	UNP P42212
E	39	ASN	TYR	conflict	UNP P42212
E	41	ARG	LYS	conflict	UNP P42212
E	45	ARG	LYS	conflict	UNP P42212
E	52	ARG	LYS	conflict	UNP P42212
E	?	-	PHE	deletion	UNP P42212
E	?	-	SER	deletion	UNP P42212
E	64	LEU	TYR	conflict	UNP P42212
E	65	CRO	GLY	conflict	UNP P42212
E	77	ARG	LYS	conflict	UNP P42212
E	78	ARG	GLN	conflict	UNP P42212
E	97	SER	PHE	conflict	UNP P42212
E	99	ARG	LYS	conflict	UNP P42212
E	103	THR	ASN	conflict	UNP P42212
E	105	ARG	LYS	conflict	UNP P42212
E	109	VAL	GLU	conflict	UNP P42212
E	111	ARG	LYS	conflict	UNP P42212
E	115	ASN	ASP	conflict	UNP P42212
E	124	ARG	LYS	conflict	UNP P42212
E	126	THR	ILE	conflict	UNP P42212
E	127	ASN	ASP	conflict	UNP P42212

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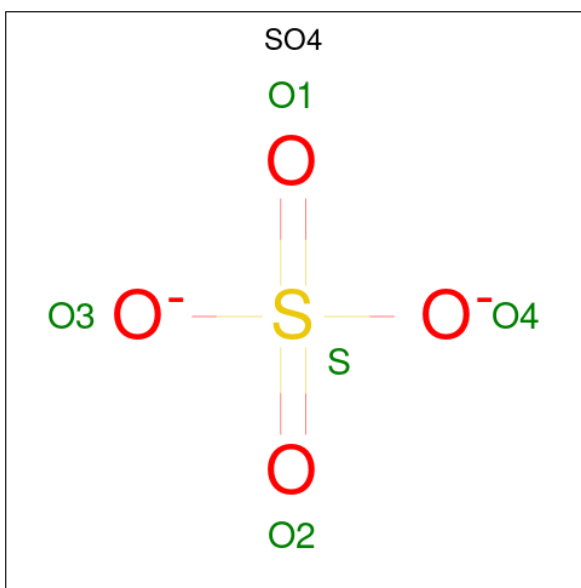
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Chain	Residue	Modelled	Actual	Comment	Reference
E	129	ARG	LYS	conflict	UNP P42212
E	138	ARG	LYS	conflict	UNP P42212
E	151	THR	MET	conflict	UNP P42212
E	154	ARG	LYS	conflict	UNP P42212
E	156	ARG	LYS	conflict	UNP P42212
E	160	ARG	LYS	conflict	UNP P42212
E	161	ALA	VAL	conflict	UNP P42212
E	164	THR	LYS	conflict	UNP P42212
E	169	VAL	ILE	conflict	UNP P42212
E	178	ASN	ASP	conflict	UNP P42212
E	188	ASN	ASP	conflict	UNP P42212
E	196	ASP	ASN	conflict	UNP P42212
E	203	THR	SER	conflict	UNP P42212
E	207	ARG	LYS	conflict	UNP P42212
E	212	ARG	LYS	conflict	UNP P42212

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

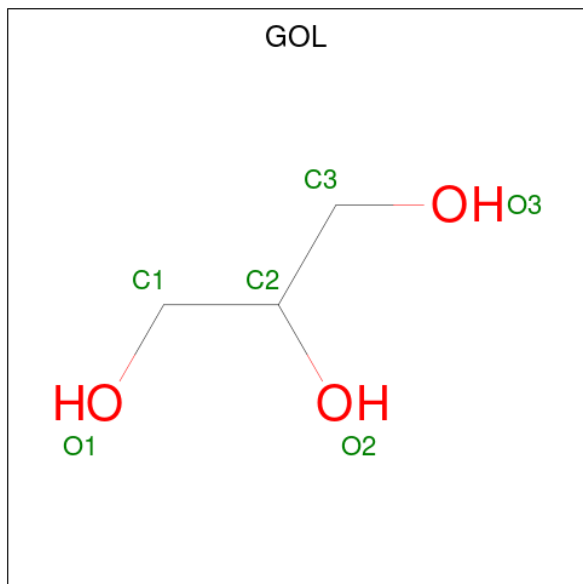
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Cu 1 1	0	0
2	E	1	Total Cu 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 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
4	E	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0

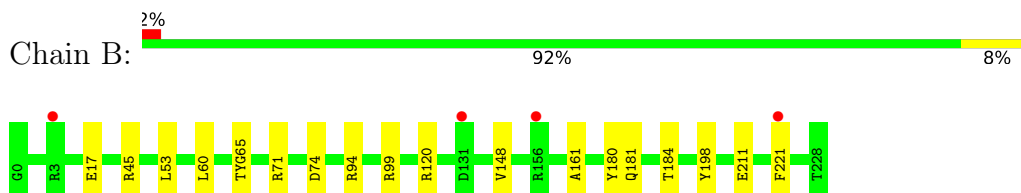
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	142	Total O 142 142	0	0
5	E	117	Total O 117 117	0	0

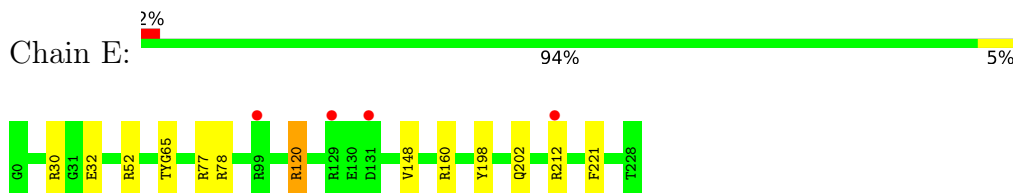
### 3 Residue-property plots [i](#)

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: Green fluorescent protein



- Molecule 1: Green fluorescent protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.25Å 86.25Å 269.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.96 – 1.94 44.92 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.96-1.94) 100.0 (44.92-1.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.201 , 0.224 0.209 , 0.233	Depositor DCC
$R_{free}$ test set	2261 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.1	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1986e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, SO4, GOL, CRO

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	B	0.72	0/1874	0.82	0/2538
1	E	0.71	0/1881	0.83	1/2548 (0.0%)
All	All	0.72	0/3755	0.82	1/5086 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	120	ARG	NE-CZ-NH1	-5.46	117.57	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	B	1857	0	1786	9	0
1	E	1864	0	1792	7	0
2	B	1	0	0	0	0
2	E	1	0	0	0	0
3	B	15	0	0	1	0
4	E	12	0	16	0	0
5	B	142	0	0	0	0
5	E	117	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4009	0	3594	14	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 2.

All (14) 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:B:17:GLU:OE1	1:B:120:ARG:NH1	2.38	0.56
1:B:221:PHE:HD2	1:E:221:PHE:HD2	1.54	0.55
1:E:30:ARG:NH1	1:E:32:GLU:OE2	2.41	0.53
1:E:78:ARG:NH2	5:E:402:HOH:O	2.45	0.49
1:E:120:ARG:NH1	1:E:120:ARG:HG3	2.28	0.48
1:B:184:THR:OG1	3:B:303:SO4:O2	2.24	0.46
1:B:221:PHE:CD1	1:E:202:GLN:HB3	2.54	0.43
1:B:45:ARG:NH2	1:B:211:GLU:OE1	2.47	0.42
1:B:53:LEU:HD21	1:B:60:LEU:HD12	2.01	0.42
1:E:148:VAL:O	1:E:198:TYR:HA	2.20	0.42
1:B:161:ALA:HB3	1:B:181:GLN:HB3	2.01	0.41
1:B:148:VAL:O	1:B:198:TYR:HA	2.21	0.41
1:E:120:ARG:HG3	1:E:120:ARG:HH11	1.85	0.41
1:B:94:ARG:HA	1:B:180:TYR:O	2.22	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	B	224/229 (98%)	222 (99%)	2 (1%)	0	100	100
1	E	225/229 (98%)	223 (99%)	2 (1%)	0	100	100
All	All	449/458 (98%)	445 (99%)	4 (1%)	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	B	198/198 (100%)	195 (98%)	3 (2%)	65	56
1	E	199/198 (100%)	195 (98%)	4 (2%)	55	42
All	All	397/396 (100%)	390 (98%)	7 (2%)	59	47

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	71	ARG
1	B	74	ASP
1	B	99	ARG
1	E	52	ARG
1	E	77	ARG
1	E	160	ARG
1	E	212	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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	CRO	E	65	1	23,23,24	3.03	8 (34%)	30,32,34	2.34	9 (30%)
1	CRO	B	65	1	23,23,24	2.37	7 (30%)	30,32,34	2.34	13 (43%)

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	CRO	E	65	1	-	0/12/31/32	0/2/2/2
1	CRO	B	65	1	-	1/12/31/32	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	65	CRO	CB2-CA2	-7.45	1.28	1.35
1	E	65	CRO	CA2-C2	7.14	1.55	1.48
1	B	65	CRO	CB2-CA2	-6.97	1.29	1.35
1	E	65	CRO	C1-N3	6.77	1.48	1.37
1	B	65	CRO	C1-N2	4.93	1.39	1.32
1	E	65	CRO	C1-N2	4.47	1.38	1.32
1	B	65	CRO	C1-N3	4.26	1.44	1.37
1	B	65	CRO	CA2-C2	3.29	1.51	1.48
1	E	65	CRO	C2-N3	3.11	1.47	1.39
1	E	65	CRO	CA2-N2	2.76	1.44	1.38
1	E	65	CRO	CG2-CB2	2.61	1.51	1.46
1	B	65	CRO	C2-N3	2.36	1.45	1.39
1	B	65	CRO	CA2-N2	2.34	1.43	1.38
1	B	65	CRO	CG2-CB2	2.08	1.50	1.46
1	E	65	CRO	CA1-C1	-2.03	1.48	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	CRO	CA2-C2-N3	6.63	106.51	103.37
1	E	65	CRO	CA2-C2-N3	5.25	105.85	103.37
1	E	65	CRO	O2-C2-CA2	-5.17	128.06	130.96
1	E	65	CRO	O3-C3-CA3	-5.17	110.78	126.39
1	B	65	CRO	O3-C3-CA3	-5.14	110.88	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	CRO	C2-N3-C1	-4.25	105.81	107.97
1	E	65	CRO	CA2-N2-C1	4.11	108.80	105.77
1	B	65	CRO	CA2-N2-C1	4.08	108.78	105.77
1	B	65	CRO	C2-CA2-N2	-3.22	106.68	108.93
1	E	65	CRO	C1-CA1-N1	-3.01	105.08	109.96
1	B	65	CRO	CG2-CB2-CA2	-2.98	126.29	129.94
1	B	65	CRO	CA1-C1-N3	-2.67	121.54	124.75
1	B	65	CRO	C2-N3-C1	-2.55	106.67	107.97
1	E	65	CRO	CG1-CB1-CA1	-2.50	106.28	112.16
1	E	65	CRO	C2-CA2-N2	-2.44	107.23	108.93
1	B	65	CRO	C1-CA1-N1	-2.39	106.08	109.96
1	B	65	CRO	CA1-C1-N2	2.27	127.06	123.89
1	B	65	CRO	O2-C2-CA2	-2.19	129.73	130.96
1	B	65	CRO	CD2-CG2-CD1	2.12	120.77	117.64
1	B	65	CRO	CE1-CD1-CG2	-2.10	118.50	121.25
1	B	65	CRO	CB2-CA2-N2	2.09	131.73	128.83
1	E	65	CRO	CA1-C1-N3	-2.03	122.31	124.75

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	65	CRO	N2-CA2-CB2-CG2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
3	SO4	B	303	-	4,4,4	0.45	0	6,6,6	0.09	0
3	SO4	B	304	-	4,4,4	0.39	0	6,6,6	0.11	0
4	GOL	E	301	-	5,5,5	0.13	0	5,5,5	0.48	0
3	SO4	B	302	-	4,4,4	0.41	0	6,6,6	0.05	0
4	GOL	E	302	-	5,5,5	0.13	0	5,5,5	0.41	0

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
4	GOL	E	302	-	-	1/4/4/4	-
4	GOL	E	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	GOL	O1-C1-C2-C3
4	E	301	GOL	O1-C1-C2-O2
4	E	301	GOL	C1-C2-C3-O3
4	E	302	GOL	C1-C2-C3-O3
4	E	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	SO4	1	0

## 5.7 Other polymers [\(i\)](#)

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	B	228/229 (99%)	0.21	4 (1%) 68 74	25, 36, 55, 68	1 (0%)
1	E	228/229 (99%)	0.26	4 (1%) 68 74	28, 39, 60, 71	3 (1%)
All	All	456/458 (99%)	0.24	8 (1%) 68 74	25, 38, 59, 71	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	131	ASP	3.8
1	E	212	ARG	3.6
1	B	221	PHE	3.6
1	B	3	ARG	2.9
1	B	156	ARG	2.7
1	B	131	ASP	2.7
1	E	129	ARG	2.5
1	E	99	ARG	2.3

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	CRO	E	65	22/23	0.96	0.10	28,29,31,31	0
1	CRO	B	65	22/23	0.97	0.11	26,27,28,28	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	E	301	6/6	0.64	0.16	72,75,75,76	0
4	GOL	E	302	6/6	0.64	0.23	59,61,62,63	0
3	SO4	B	303	5/5	0.85	0.63	48,50,51,51	5
3	SO4	B	304	5/5	0.92	0.23	49,50,51,53	1
2	CU	E	303	1/1	0.94	0.07	40,40,40,40	0
3	SO4	B	302	5/5	0.95	0.10	61,61,62,64	1
2	CU	B	301	1/1	0.96	0.06	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.