



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:06 pm BST

PDB ID : 6UBZ  
Title : Crystal structure of D678A GoxA bound to glycine at pH 5.5  
Authors : Yukl, E.T.  
Deposited on : 2019-09-13  
Resolution : 1.83 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 : 1.8.5 (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

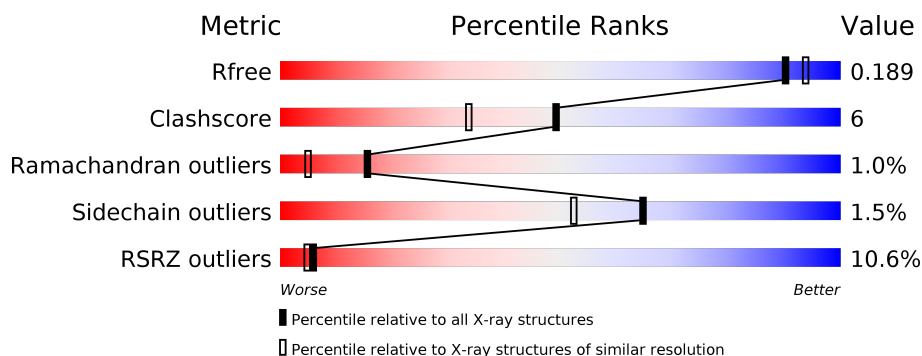
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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 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	816	<div> <div>12%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	816	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div> </div>
1	C	816	<div> <div>9%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	816	<div> <div>11%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27437 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 Uncharacterized protein GoxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	783	Total	C	N	O	S	0	7	0
			6243	3946	1061	1215	21			
1	A	791	Total	C	N	O	S	0	1	0
			6258	3954	1065	1219	20			
1	C	785	Total	C	N	O	S	0	7	0
			6264	3958	1067	1218	21			
1	D	780	Total	C	N	O	S	0	4	0
			6193	3916	1057	1199	21			

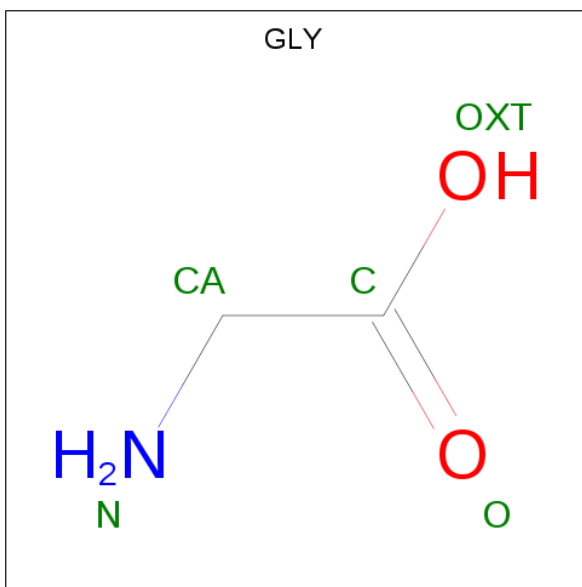
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	678	ALA	ASP	engineered mutation	UNP A0A161XU12
A	678	ALA	ASP	engineered mutation	UNP A0A161XU12
C	678	ALA	ASP	engineered mutation	UNP A0A161XU12
D	678	ALA	ASP	engineered mutation	UNP A0A161XU12

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			5	2	1	2		
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	C	1	Total	C	N	O	0	0
			5	2	1	2		
3	D	1	Total	C	N	O	0	0
			5	2	1	2		

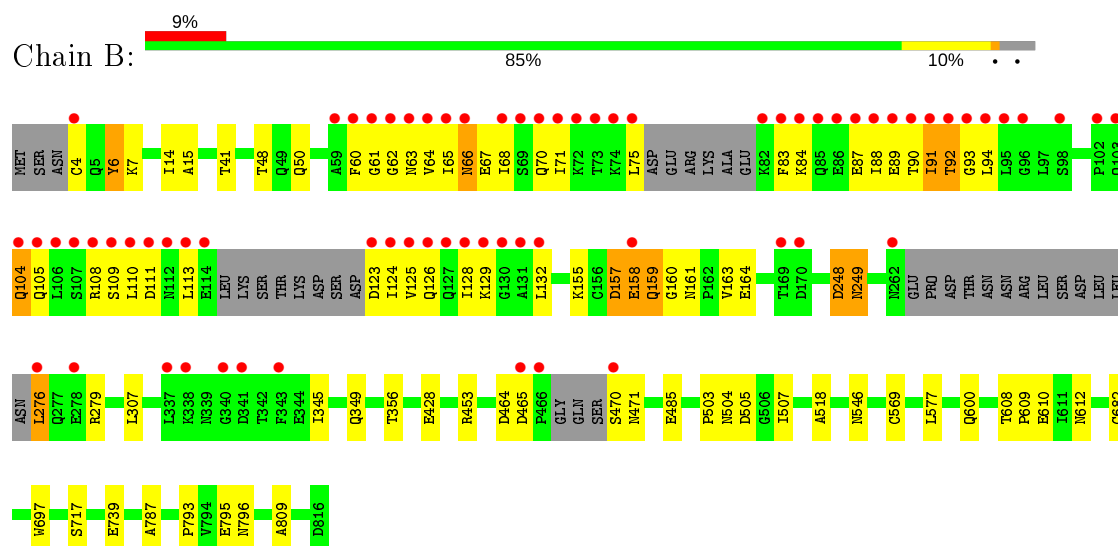
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	672	Total	O	0	1
			673	673		
4	A	554	Total	O	0	0
			554	554		
4	C	650	Total	O	0	0
			650	650		
4	D	578	Total	O	0	0
			578	578		

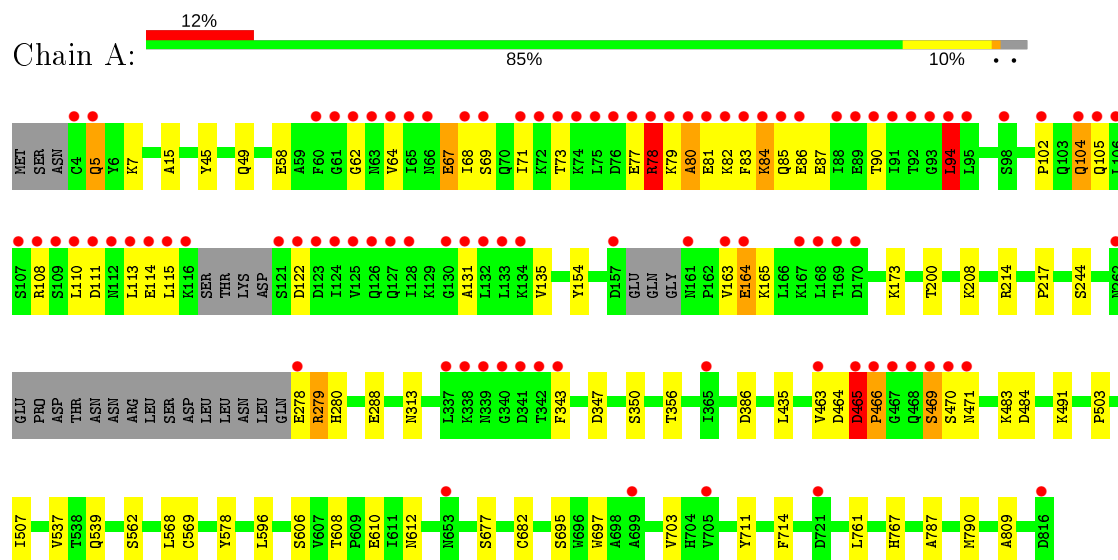
### 3 Residue-property plots [i](#)

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.

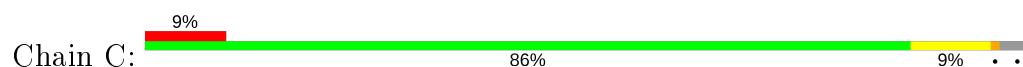
#### • Molecule 1: Uncharacterized protein GoxA

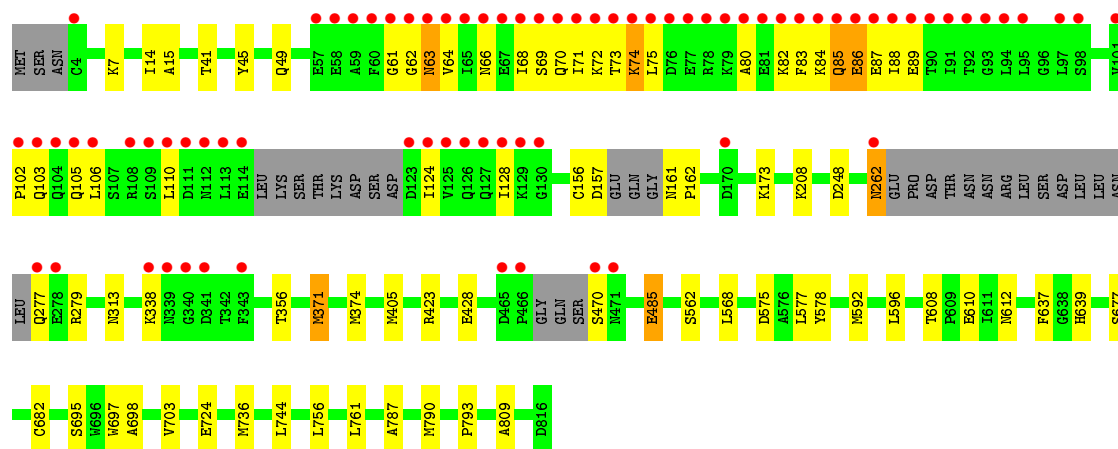


#### • Molecule 1: Uncharacterized protein GoxA

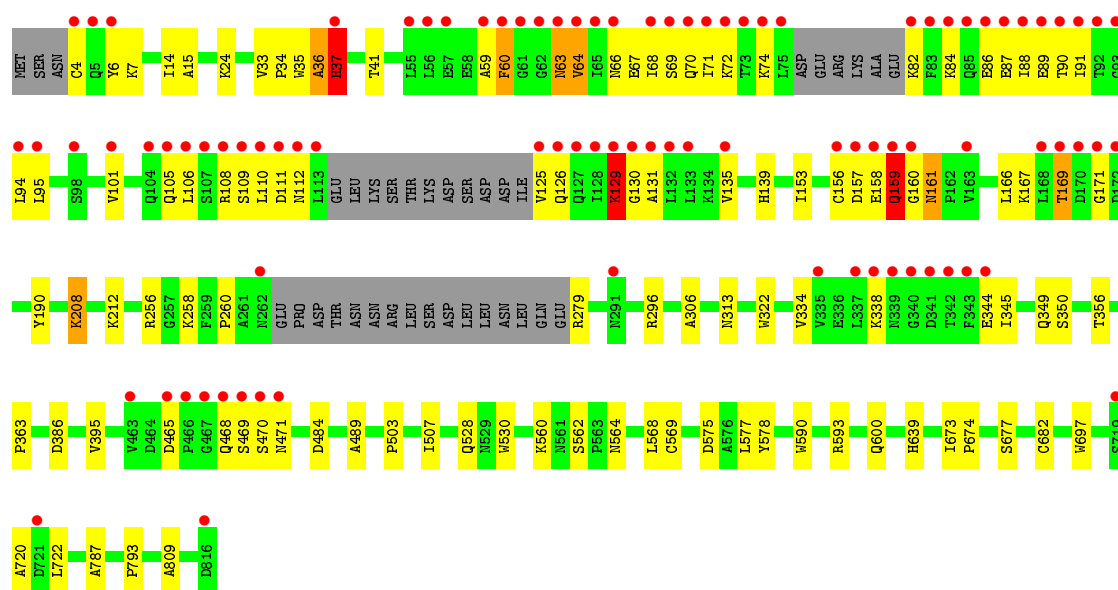
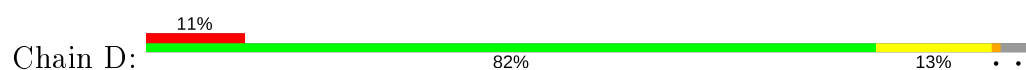


#### • Molecule 1: Uncharacterized protein GoxA





● Molecule 1: Uncharacterized protein GoxA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.33Å 93.40Å 187.99Å 90.00° 95.20° 90.00°	Depositor
Resolution (Å)	47.35 – 1.83 47.35 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.35-1.83) 99.2 (47.35-1.83)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.162 , 0.189 0.163 , 0.189	Depositor DCC
$R_{free}$ test set	16599 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	27437	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: TRQ, MG

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	0.39	2/6390 (0.0%)	0.58	3/8695 (0.0%)
1	B	1.08	6/6374 (0.1%)	1.03	13/8675 (0.1%)
1	C	0.40	0/6395	0.59	2/8702 (0.0%)
1	D	0.37	0/6326	0.58	1/8610 (0.0%)
All	All	0.63	8/25485 (0.0%)	0.72	19/34682 (0.1%)

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	4
1	B	0	1
1	D	0	3
All	All	0	8

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	6	TYR	CD1-CE1	49.48	2.13	1.39
1	B	6	TYR	CD2-CE2	49.36	2.13	1.39
1	B	6	TYR	CE1-CZ	-20.20	1.12	1.38
1	B	6	TYR	CE2-CZ	-20.04	1.12	1.38
1	B	6	TYR	CG-CD2	-17.77	1.16	1.39

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	TYR	CE1-CZ-CE2	-35.52	62.96	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	TYR	CG-CD2-CE2	-30.20	97.14	121.30
1	B	6	TYR	CG-CD1-CE1	-30.12	97.21	121.30
1	B	6	TYR	CD1-CG-CD2	-29.50	85.45	117.90
1	B	6	TYR	CB-CG-CD2	26.18	136.71	121.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ASP	Peptide
1	A	469	SER	Peptide
1	A	80	ALA	Peptide
1	A	94	LEU	Peptide
1	B	91	ILE	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	6258	0	6028	64	1
1	B	6243	0	6005	80	1
1	C	6264	0	6032	59	0
1	D	6193	0	5966	86	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	2	2	0
3	B	5	0	2	3	0
3	C	5	0	2	1	0
3	D	5	0	2	1	0
4	A	554	0	0	9	0
4	B	673	0	0	12	1
4	C	650	0	0	6	0
4	D	578	0	0	9	0
All	All	27437	0	24039	291	2

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 6.

The worst 5 of 291 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:C:82:LYS:NZ	1:C:83:PHE:O	1.61	1.31
1:C:86:GLU:HB3	1:C:89:GLU:HB2	1.41	1.01
1:D:157:ASP:OD2	1:D:160:GLY:N	1.93	1.01
1:D:86:GLU:HA	1:D:89:GLU:HG2	1.47	0.94
1:D:36:ALA:HA	1:D:560:LYS:HZ1	1.33	0.93

All (2) 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)
4:B:1006:HOH:O	4:B:1105:HOH:O[2_558]	2.02	0.18
1:B:62:GLY:N	1:A:67:GLU:OE2[1_455]	2.08	0.12

## 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	783/816 (96%)	747 (95%)	27 (3%)	9 (1%)	14	4
1	B	779/816 (96%)	744 (96%)	29 (4%)	6 (1%)	19	7
1	C	781/816 (96%)	757 (97%)	19 (2%)	5 (1%)	25	12
1	D	775/816 (95%)	736 (95%)	28 (4%)	11 (1%)	11	3
All	All	3118/3264 (96%)	2984 (96%)	103 (3%)	31 (1%)	15	5

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	ASP
1	B	249	ASN
1	A	78	ARG
1	A	94	LEU
1	C	62	GLY

### 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	687/710 (97%)	676 (98%)	11 (2%)	62	49
1	B	686/710 (97%)	679 (99%)	7 (1%)	76	68
1	C	688/710 (97%)	677 (98%)	11 (2%)	62	49
1	D	679/710 (96%)	667 (98%)	12 (2%)	59	44
All	All	2740/2840 (96%)	2699 (98%)	41 (2%)	65	52

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	GLN
1	C	208	LYS
1	D	208	LYS
1	C	72	LYS
1	C	74	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	142	HIS
1	D	142	HIS
1	A	105	GLN
1	A	112	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	TRQ	C	697	1	13,17,18	1.69	2 (15%)	14,24,26	1.76	3 (21%)
1	TRQ	A	697	1	13,17,18	1.90	3 (23%)	14,24,26	1.87	5 (35%)
1	TRQ	D	697	1	13,17,18	1.79	2 (15%)	14,24,26	1.97	4 (28%)
1	TRQ	B	697	1	13,17,18	1.74	3 (23%)	14,24,26	1.79	3 (21%)

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	TRQ	C	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	D	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CE2-CZ2	-4.24	1.44	1.50
1	D	697	TRQ	CE2-CZ2	-4.18	1.44	1.50
1	B	697	TRQ	CE2-CZ2	-4.05	1.44	1.50
1	C	697	TRQ	CE2-CZ2	-3.96	1.44	1.50
1	A	697	TRQ	CB-CG	-3.03	1.47	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	TRQ	CZ2-CE2-NE1	4.41	126.98	119.94
1	C	697	TRQ	CZ2-CE2-NE1	4.39	126.96	119.94
1	D	697	TRQ	CZ2-CE2-NE1	4.01	126.35	119.94
1	D	697	TRQ	CB-CG-CD1	-3.75	123.34	127.97
1	A	697	TRQ	CZ2-CE2-NE1	3.45	125.45	119.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	697	TRQ	2	0
1	A	697	TRQ	3	0
1	D	697	TRQ	3	0
1	B	697	TRQ	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

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	790/816 (96%)	0.35	94 (11%) 4 3	15, 30, 86, 122	0
1	B	782/816 (95%)	0.21	70 (8%) 9 8	12, 22, 81, 117	0
1	C	784/816 (96%)	0.24	76 (9%) 7 6	12, 24, 79, 116	0
1	D	779/816 (95%)	0.34	92 (11%) 4 4	14, 28, 87, 123	0
All	All	3135/3264 (96%)	0.28	332 (10%) 6 5	12, 26, 83, 123	0

The worst 5 of 332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	10.8
1	D	68	ILE	9.7
1	C	61	GLY	9.3
1	C	62	GLY	9.2
1	B	83	PHE	9.2

### 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, 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	TRQ	B	697	16/17	0.96	0.12	13,15,27,30	0
1	TRQ	A	697	16/17	0.97	0.14	16,18,29,29	0
1	TRQ	D	697	16/17	0.97	0.11	15,18,28,29	0
1	TRQ	C	697	16/17	0.97	0.12	10,15,24,25	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, 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( $\text{\AA}^2$ )	Q<0.9
3	GLY	B	902	5/5	0.85	0.19	29,31,34,35	0
3	GLY	D	902	5/5	0.93	0.14	34,36,41,44	0
3	GLY	C	902	5/5	0.94	0.12	29,34,36,39	0
3	GLY	A	902	5/5	0.96	0.14	35,39,43,46	0
2	MG	D	901	1/1	0.99	0.06	22,22,22,22	0
2	MG	A	901	1/1	0.99	0.09	22,22,22,22	0
2	MG	B	901	1/1	1.00	0.07	16,16,16,16	0
2	MG	C	901	1/1	1.00	0.07	16,16,16,16	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.