



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2026 – 09:38 PM UTC

PDB ID : 9S0T / pdb\_00009s0t  
Title : Superfolder green fluorescent protein (sfGFP) exhibiting p-(phenylazo)-L-phenylalanine (Pap) at position 39 in complex with alpha-cyclodextrin  
Authors : Eichinger, A.; Skerra, A.  
Deposited on : 2025-07-17  
Resolution : 2.05 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.

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	:	4-5-2 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

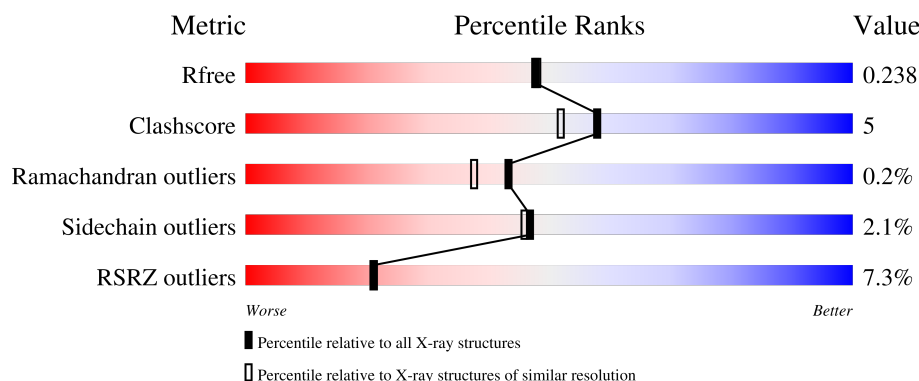
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	A	245	<div> <div>9%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	B	245	<div> <div>4%</div> <div>81%</div> <div>7%</div> <div>11%</div> </div>
2	C	6	<div> <div>33%</div> <div>67%</div> </div>
2	D	6	<div> <div>33%</div> <div>67%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3940 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	225	Total	C	N	O	S	0	2	0
			1817	1154	313	345	5			
1	B	219	Total	C	N	O	S	0	1	0
			1766	1124	302	336	4			

There are 50 discrepancies between the modelled and reference sequences:

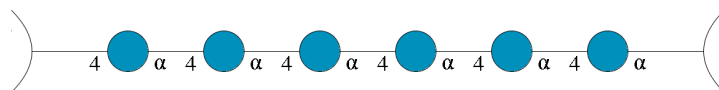
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	ARG	SER	engineered mutation	UNP P42212
A	39	OZW	TYR	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	105	THR	ASN	engineered mutation	UNP P42212
A	145	PHE	TYR	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	206	VAL	ALA	engineered mutation	UNP P42212
A	238	GLN	LYS	engineered mutation	UNP P42212
A	239	SER	-	expression tag	UNP P42212
A	240	ALA	-	expression tag	UNP P42212
A	241	TRP	-	expression tag	UNP P42212
A	242	SER	-	expression tag	UNP P42212
A	243	HIS	-	expression tag	UNP P42212
A	244	PRO	-	expression tag	UNP P42212
A	245	GLN	-	expression tag	UNP P42212
A	246	PHE	-	expression tag	UNP P42212
A	247	GLU	-	expression tag	UNP P42212
A	248	LYS	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	30	ARG	SER	engineered mutation	UNP P42212
B	39	OZW	TYR	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	105	THR	ASN	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	206	VAL	ALA	engineered mutation	UNP P42212
B	238	GLN	LYS	engineered mutation	UNP P42212
B	239	SER	-	expression tag	UNP P42212
B	240	ALA	-	expression tag	UNP P42212
B	241	TRP	-	expression tag	UNP P42212
B	242	SER	-	expression tag	UNP P42212
B	243	HIS	-	expression tag	UNP P42212
B	244	PRO	-	expression tag	UNP P42212
B	245	GLN	-	expression tag	UNP P42212
B	246	PHE	-	expression tag	UNP P42212
B	247	GLU	-	expression tag	UNP P42212
B	248	LYS	-	expression tag	UNP P42212

- Molecule 2 is an oligosaccharide called Cyclohexakis-(1-4)-( $\alpha$ -D-glucopyranose).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	6	Total	C	O	0	0	0
			66	36	30			
2	D	6	Total	C	O	0	0	0
			66	36	30			

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



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

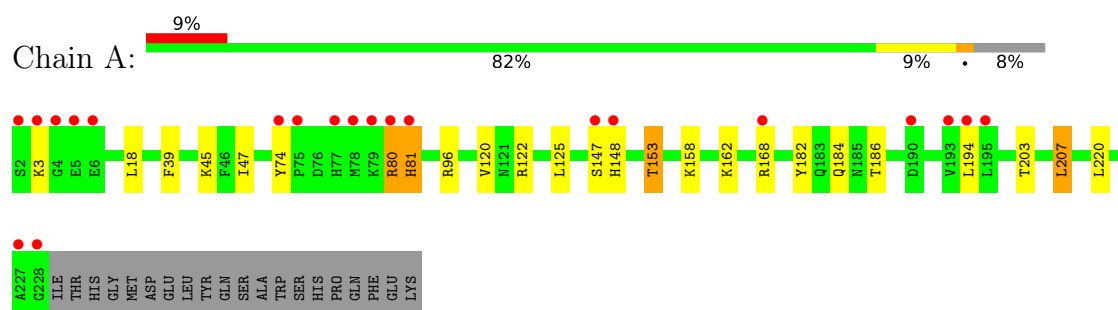
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	100	Total	O	0	0
			100	100		

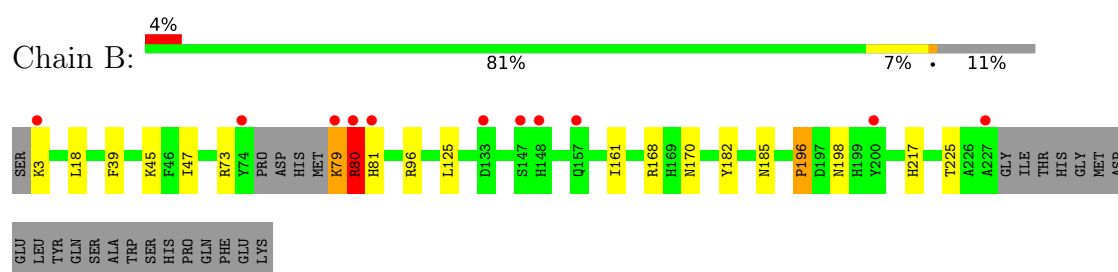
### 3 Residue-property plots [i](#)

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



- Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)



- Molecule 2: Cyclohexakis-(1-4)-(alpha-D-glucopyranose)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.27Å 69.27Å 115.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.24 – 2.05 30.24 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.24-2.05) 96.7 (30.24-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.48 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, $R_{free}$	0.188 , 0.228 0.196 , 0.238	Depositor DCC
$R_{free}$ test set	1648 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.3	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 58.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.72% 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: CRO, GOL, GLC, OZW

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	0.48	0/1819	0.81	0/2454
1	B	0.47	0/1762	0.81	0/2376
All	All	0.48	0/3581	0.81	0/4830

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	PRO	Peptide

### 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	A	1817	0	1761	21	0
1	B	1766	0	1712	15	0
2	C	66	0	54	0	0
2	D	66	0	54	0	0
3	B	6	0	8	0	0
4	A	119	0	0	4	0
4	B	100	0	0	1	0
All	All	3940	0	3589	33	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 5.

The worst 5 of 33 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:81:HIS:HB3	1:B:196:PRO:HA	1.53	0.89
1:B:198:ASN:OD1	4:B:401:HOH:O	2.12	0.67
1:B:45:LYS:HE2	1:B:47:ILE:HD11	1.77	0.65
1:B:79:LYS:O	1:B:80:ARG:O	2.19	0.60
1:A:80:ARG:HH21	1:A:81:HIS:HB2	1.67	0.60

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	221/245 (90%)	212 (96%)	9 (4%)	0	100	100
1	B	212/245 (86%)	208 (98%)	3 (1%)	1 (0%)	24	16
All	All	433/490 (88%)	420 (97%)	12 (3%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ARG

### 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	197/213 (92%)	192 (98%)	5 (2%)	42	39
1	B	191/213 (90%)	188 (98%)	3 (2%)	55	56
All	All	388/426 (91%)	380 (98%)	8 (2%)	47	46

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	ARG
1	B	79	LYS
1	A	207	LEU
1	A	184	GLN
1	B	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	A	184	GLN
1	A	212	ASN
1	B	184	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	OZW	B	39	1	19,20,21	1.22	1 (5%)	20,25,27	0.41	0
1	OZW	A	39	1	19,20,21	1.33	1 (5%)	20,25,27	0.66	0
1	CRO	B	66	1	22,23,24	0.61	0	30,32,34	0.79	0
1	CRO	A	66	1	22,23,24	0.58	0	30,32,34	0.79	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
1	OZW	B	39	1	-	6/10/11/13	0/2/2/2
1	OZW	A	39	1	-	4/10/11/13	0/2/2/2
1	CRO	B	66	1	-	0/12/31/32	0/2/2/2
1	CRO	A	66	1	-	0/12/31/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	OZW	CB-CG	-4.61	1.40	1.51
1	B	39	OZW	CB-CG	-4.12	1.41	1.51

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	39	OZW	CE1-CZ-N2-N1
1	B	39	OZW	CE1-CZ-N2-N1
1	A	39	OZW	CE2-CZ-N2-N1
1	B	39	OZW	C2-C6-N1-N2
1	B	39	OZW	CE2-CZ-N2-N1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

12 monosaccharides 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	GLC	C	1	2	11,11,12	0.66	0	15,15,17	1.34	2 (13%)
2	GLC	C	2	2	11,11,12	0.72	0	15,15,17	0.90	0
2	GLC	C	3	2	11,11,12	0.62	0	15,15,17	0.61	0
2	GLC	C	4	2	11,11,12	0.58	0	15,15,17	0.99	1 (6%)
2	GLC	C	5	2	11,11,12	1.02	1 (9%)	15,15,17	0.88	0
2	GLC	C	6	2	11,11,12	0.90	0	15,15,17	1.06	1 (6%)
2	GLC	D	1	2	11,11,12	0.79	0	15,15,17	0.85	0
2	GLC	D	2	2	11,11,12	1.14	1 (9%)	15,15,17	1.99	1 (6%)
2	GLC	D	3	2	11,11,12	1.27	2 (18%)	15,15,17	2.11	6 (40%)
2	GLC	D	4	2	11,11,12	0.74	0	15,15,17	1.15	1 (6%)
2	GLC	D	5	2	11,11,12	0.70	0	15,15,17	1.34	3 (20%)
2	GLC	D	6	2	11,11,12	0.73	0	15,15,17	0.62	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
2	GLC	C	1	2	-	2/2/19/22	0/1/1/1
2	GLC	C	2	2	-	2/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	0/2/19/22	0/1/1/1
2	GLC	C	5	2	-	2/2/19/22	0/1/1/1
2	GLC	C	6	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	GLC	D	2	2	-	1/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	GLC	D	4	2	-	0/2/19/22	0/1/1/1
2	GLC	D	5	2	-	0/2/19/22	0/1/1/1
2	GLC	D	6	2	-	1/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	GLC	O5-C5	2.51	1.48	1.43
2	D	3	GLC	O2-C2	2.38	1.48	1.43
2	C	5	GLC	O4-C4	2.18	1.48	1.43
2	D	3	GLC	O5-C5	2.18	1.47	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	GLC	C1-O5-C5	6.70	121.16	112.19
2	D	3	GLC	C1-O5-C5	5.78	119.93	112.19
2	D	4	GLC	C1-O5-C5	3.70	117.14	112.19
2	C	1	GLC	C1-O5-C5	3.44	116.80	112.19
2	C	6	GLC	C1-O5-C5	2.79	115.93	112.19

There are no chirality outliers.

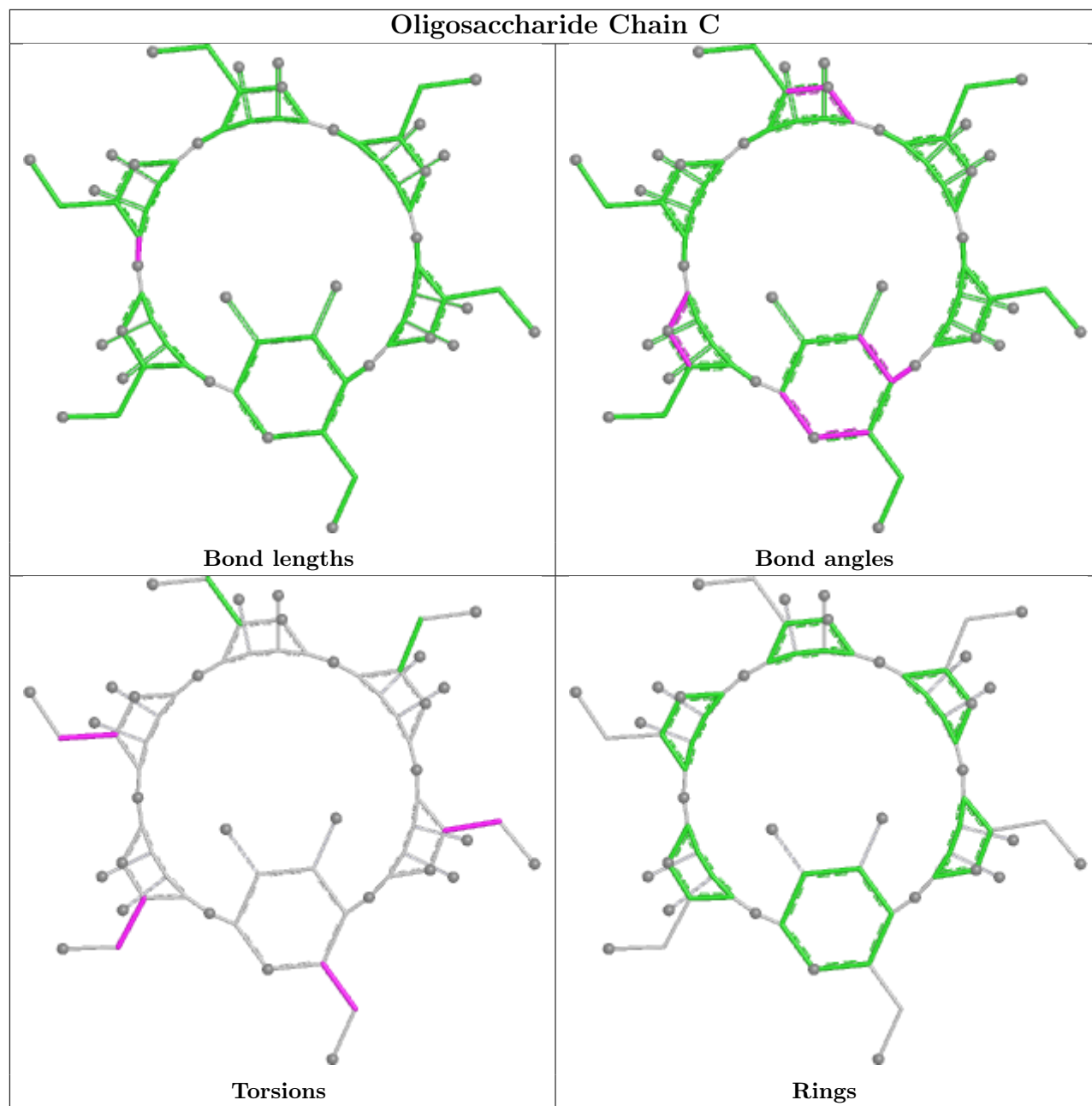
5 of 10 torsion outliers are listed below:

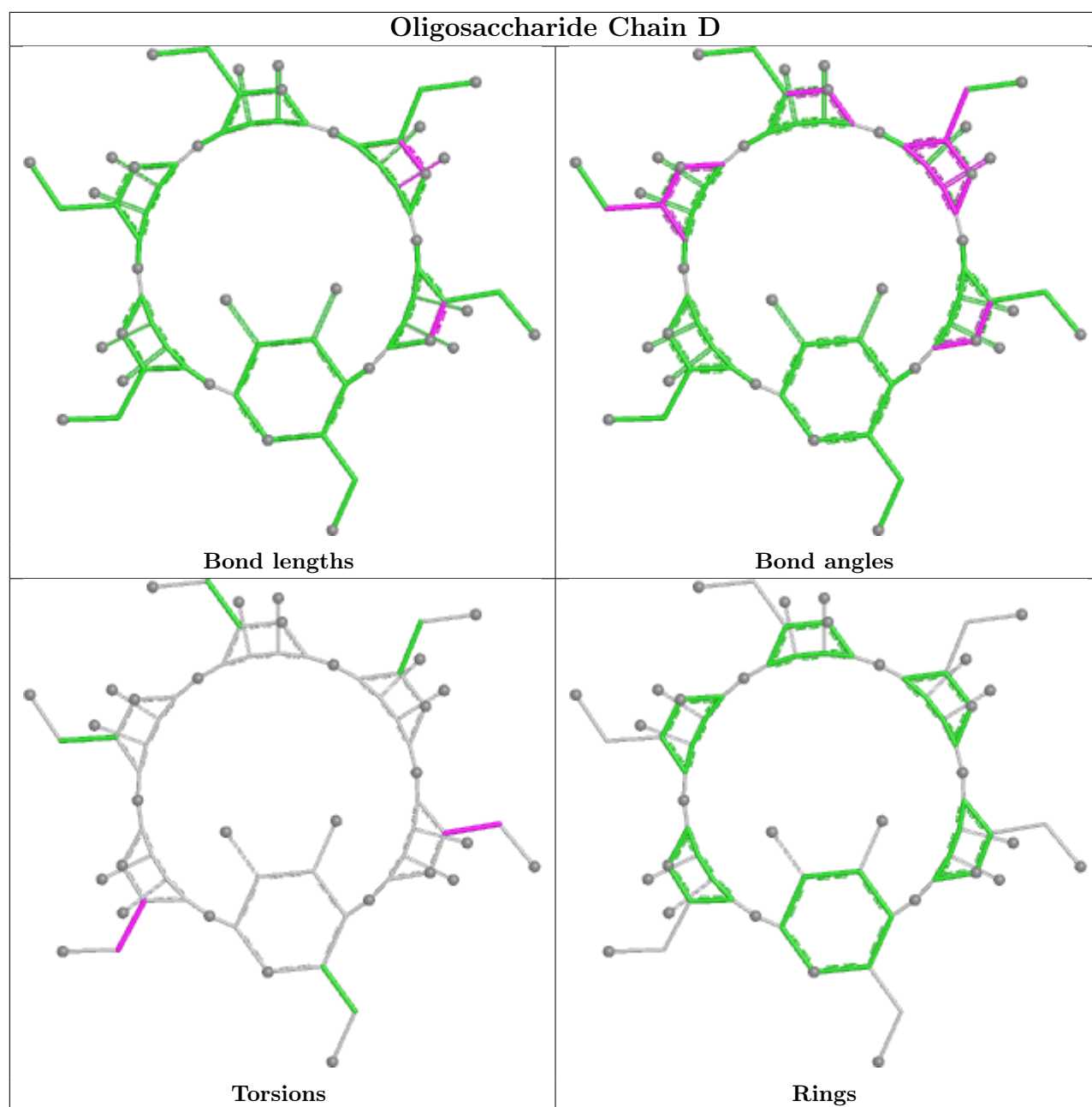
Mol	Chain	Res	Type	Atoms
2	C	1	GLC	O5-C5-C6-O6
2	C	6	GLC	C4-C5-C6-O6
2	C	1	GLC	C4-C5-C6-O6
2	C	6	GLC	O5-C5-C6-O6
2	C	2	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





## 5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z  > 2$
3	GOL	B	301	-	5,5,5	0.14	0	5,5,5	0.49	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
3	GOL	B	301	-	-	0/4/4/4	-

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 [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, 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	223/245 (91%)	0.18	21 (9%) 14 14	6, 21, 82, 167	2 (0%)
1	B	217/245 (88%)	0.06	11 (5%) 33 33	6, 23, 63, 120	1 (0%)
All	All	440/490 (89%)	0.12	32 (7%) 21 21	6, 22, 75, 167	3 (0%)

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	TYR	7.1
1	A	148	HIS	5.7
1	B	74	TYR	5.6
1	A	75	PRO	5.4
1	B	79	LYS	5.3

### 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	OZW	B	39	19/20	0.87	0.20	25,48,144,158	0
1	OZW	A	39	19/20	0.94	0.10	18,38,45,49	0
1	CRO	A	66	22/23	0.96	0.06	6,11,16,20	0
1	CRO	B	66	22/23	0.97	0.05	7,11,18,28	0

### 6.3 Carbohydrates [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,

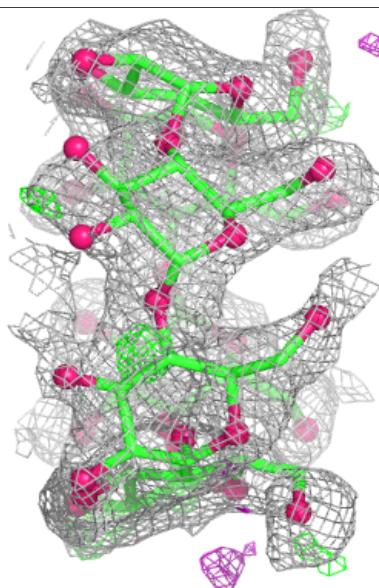
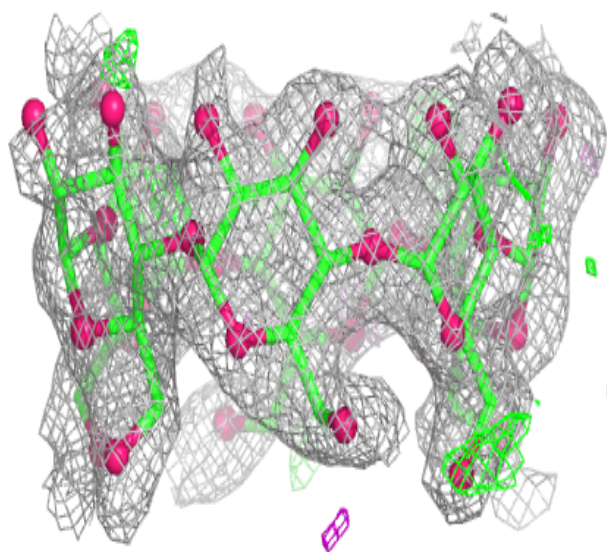
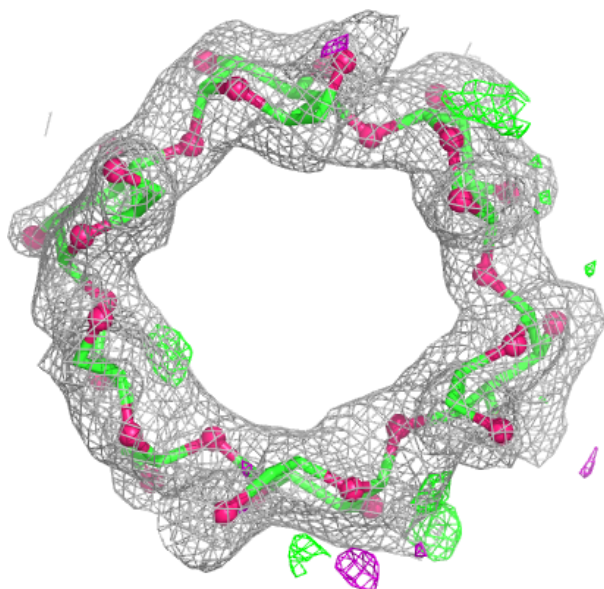
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

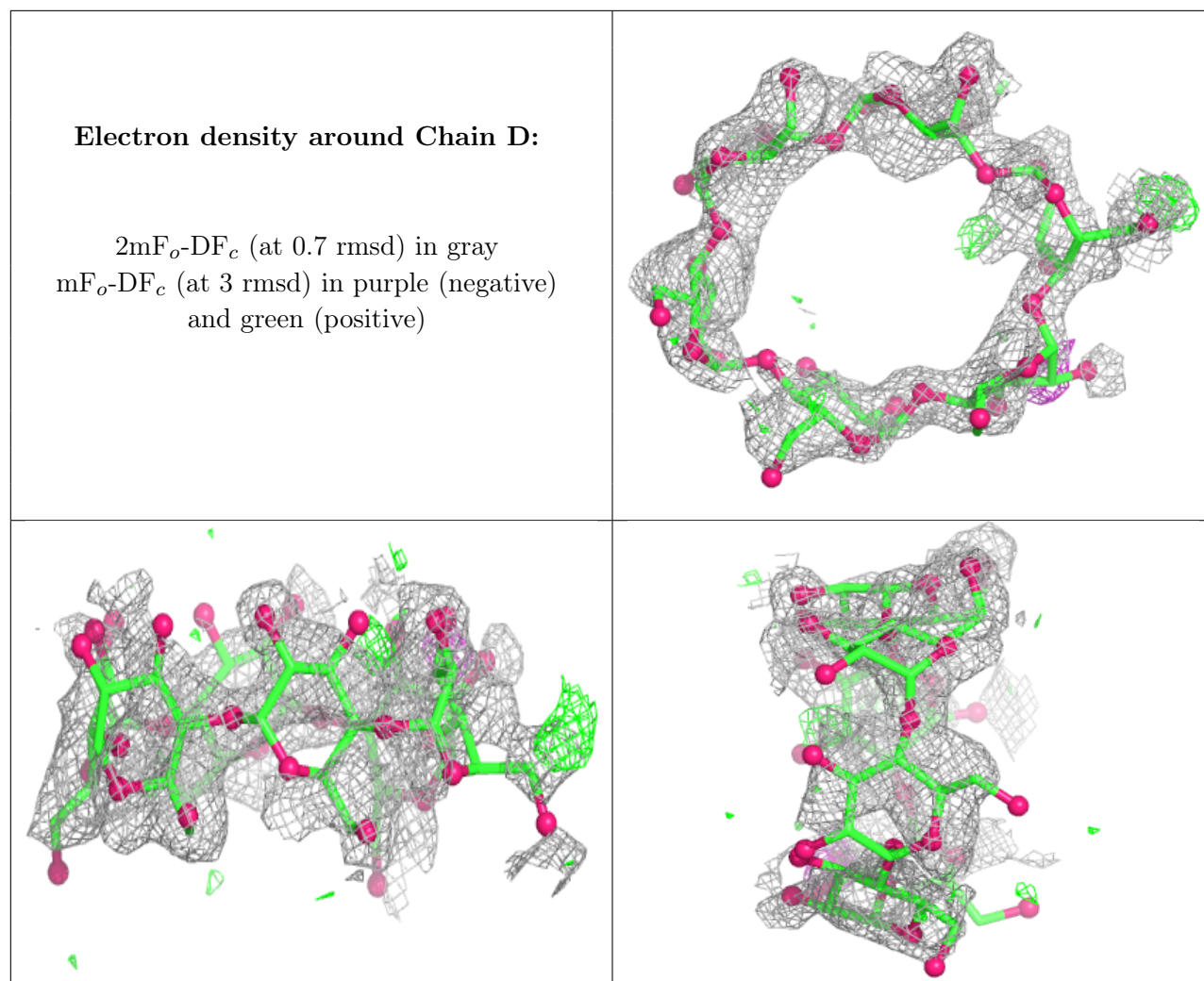
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	GLC	D	1	11/12	0.72	0.20	47,100,122,155	0
2	GLC	D	4	11/12	0.72	0.20	63,78,144,220	0
2	GLC	D	2	11/12	0.75	0.23	37,100,143,147	0
2	GLC	D	3	11/12	0.76	0.23	44,82,183,194	0
2	GLC	D	5	11/12	0.77	0.20	41,73,141,222	0
2	GLC	C	1	11/12	0.85	0.14	34,50,79,90	0
2	GLC	D	6	11/12	0.85	0.16	37,88,145,156	0
2	GLC	C	6	11/12	0.86	0.15	31,42,64,90	0
2	GLC	C	3	11/12	0.88	0.11	23,33,41,56	0
2	GLC	C	2	11/12	0.89	0.12	28,40,72,89	0
2	GLC	C	5	11/12	0.91	0.09	25,33,41,43	0
2	GLC	C	4	11/12	0.91	0.09	18,28,37,38	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around Chain C:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 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	GOL	B	301	6/6	0.92	0.19	18,27,68,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.