



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2022 – 01:45 am BST

PDB ID : 7AMF  
Title : Crystal structure of rsFolder2 in its non-fluorescent off-state  
Authors : Moreno-Chicano, T.; El Khatib, M.; Colletier, J.-P.  
Deposited on : 2020-10-08  
Resolution : 1.63 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 : 2.31.2  
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) : 2.31.2

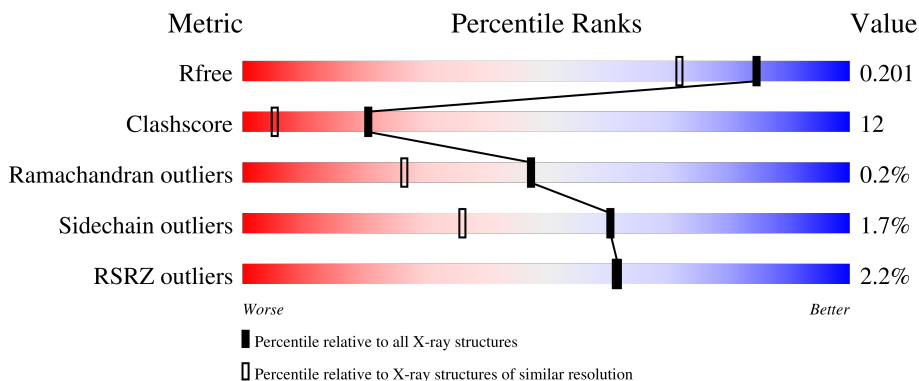
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	236	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">84% 12% ..</p>
1	B	236	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 10%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">87% 10% ..</p>
1	C	236	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 17% .</p>
1	D	236	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">81% 17% .</p>

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
1	PIA	A	68[C]	-	-	X	-
1	PIA	D	68[B]	-	-	X	-
1	PIA	D	68[C]	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9544 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	A	231	2071	1310	359	396	6	0	22	0
1	B	230	2121	1340	366	409	6	0	29	0
1	C	235	2154	1358	373	416	7	0	28	0
1	D	235	2196	1385	385	419	7	0	33	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	HIS	-	expression tag	UNP P42212
A	-3	HIS	-	expression tag	UNP P42212
A	-2	THR	-	expression tag	UNP P42212
A	-1	ASP	-	expression tag	UNP P42212
A	0	PRO	-	expression tag	UNP P42212
A	1	MET	-	expression tag	UNP P42212
A	2	VAL	-	expression tag	UNP P42212
A	31	ARG	SER	engineered mutation	UNP P42212
A	40	ASN	TYR	engineered mutation	UNP P42212
A	65	LEU	PHE	engineered mutation	UNP P42212
A	68	PIA	SER	chromophore	UNP P42212
A	68	PIA	TYR	chromophore	UNP P42212
A	68	PIA	GLY	chromophore	UNP P42212
A	70	LEU	GLN	engineered mutation	UNP P42212
A	81	ARG	GLN	engineered mutation	UNP P42212
A	100	SER	PHE	engineered mutation	UNP P42212
A	106	THR	ASN	engineered mutation	UNP P42212
A	154	THR	MET	engineered mutation	UNP P42212
A	164	SER	VAL	engineered mutation	UNP P42212
A	172	VAL	ILE	engineered mutation	UNP P42212
A	207	LYS	ALA	engineered mutation	UNP P42212

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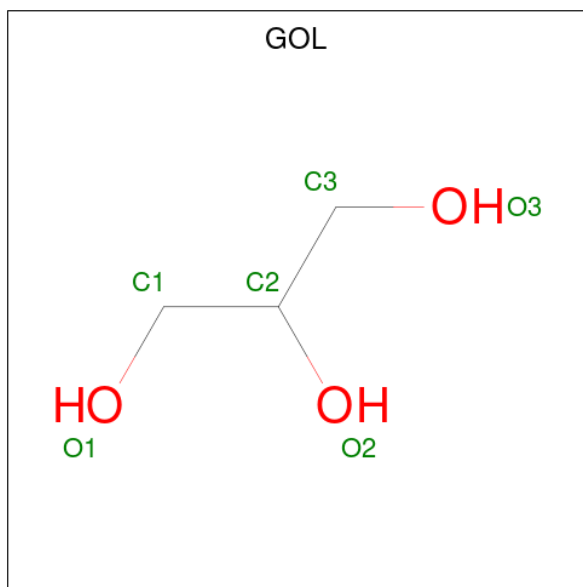
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	expression tag	UNP P42212
B	-3	HIS	-	expression tag	UNP P42212
B	-2	THR	-	expression tag	UNP P42212
B	-1	ASP	-	expression tag	UNP P42212
B	0	PRO	-	expression tag	UNP P42212
B	1	MET	-	expression tag	UNP P42212
B	2	VAL	-	expression tag	UNP P42212
B	31	ARG	SER	engineered mutation	UNP P42212
B	40	ASN	TYR	engineered mutation	UNP P42212
B	65	LEU	PHE	engineered mutation	UNP P42212
B	68	PIA	SER	chromophore	UNP P42212
B	68	PIA	TYR	chromophore	UNP P42212
B	68	PIA	GLY	chromophore	UNP P42212
B	70	LEU	GLN	engineered mutation	UNP P42212
B	81	ARG	GLN	engineered mutation	UNP P42212
B	100	SER	PHE	engineered mutation	UNP P42212
B	106	THR	ASN	engineered mutation	UNP P42212
B	154	THR	MET	engineered mutation	UNP P42212
B	164	SER	VAL	engineered mutation	UNP P42212
B	172	VAL	ILE	engineered mutation	UNP P42212
B	207	LYS	ALA	engineered mutation	UNP P42212
C	-4	HIS	-	expression tag	UNP P42212
C	-3	HIS	-	expression tag	UNP P42212
C	-2	THR	-	expression tag	UNP P42212
C	-1	ASP	-	expression tag	UNP P42212
C	0	PRO	-	expression tag	UNP P42212
C	1	MET	-	expression tag	UNP P42212
C	2	VAL	-	expression tag	UNP P42212
C	31	ARG	SER	engineered mutation	UNP P42212
C	40	ASN	TYR	engineered mutation	UNP P42212
C	65	LEU	PHE	engineered mutation	UNP P42212
C	68	PIA	SER	chromophore	UNP P42212
C	68	PIA	TYR	chromophore	UNP P42212
C	68	PIA	GLY	chromophore	UNP P42212
C	70	LEU	GLN	engineered mutation	UNP P42212
C	81	ARG	GLN	engineered mutation	UNP P42212
C	100	SER	PHE	engineered mutation	UNP P42212
C	106	THR	ASN	engineered mutation	UNP P42212
C	154	THR	MET	engineered mutation	UNP P42212
C	164	SER	VAL	engineered mutation	UNP P42212
C	172	VAL	ILE	engineered mutation	UNP P42212
C	207	LYS	ALA	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP P42212
D	-3	HIS	-	expression tag	UNP P42212
D	-2	THR	-	expression tag	UNP P42212
D	-1	ASP	-	expression tag	UNP P42212
D	0	PRO	-	expression tag	UNP P42212
D	1	MET	-	expression tag	UNP P42212
D	2	VAL	-	expression tag	UNP P42212
D	31	ARG	SER	engineered mutation	UNP P42212
D	40	ASN	TYR	engineered mutation	UNP P42212
D	65	LEU	PHE	engineered mutation	UNP P42212
D	68	PIA	SER	chromophore	UNP P42212
D	68	PIA	TYR	chromophore	UNP P42212
D	68	PIA	GLY	chromophore	UNP P42212
D	70	LEU	GLN	engineered mutation	UNP P42212
D	81	ARG	GLN	engineered mutation	UNP P42212
D	100	SER	PHE	engineered mutation	UNP P42212
D	106	THR	ASN	engineered mutation	UNP P42212
D	154	THR	MET	engineered mutation	UNP P42212
D	164	SER	VAL	engineered mutation	UNP P42212
D	172	VAL	ILE	engineered mutation	UNP P42212
D	207	LYS	ALA	engineered mutation	UNP P42212

- Molecule 2 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
			Total	C	O		
2	B	1	6	3	3	0	0

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

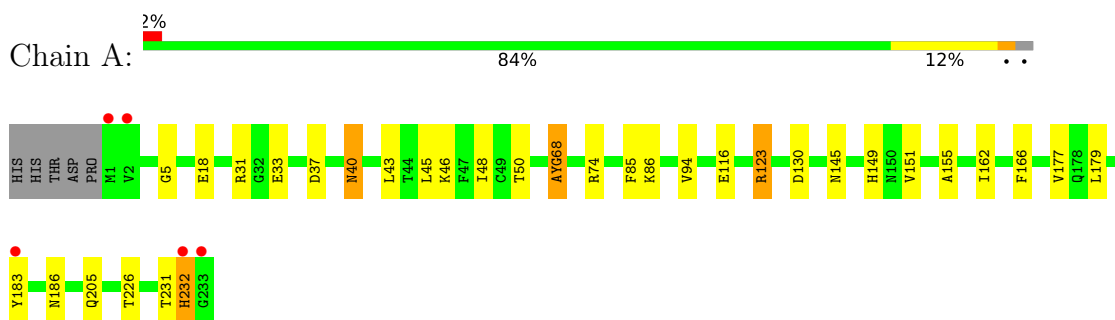
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total	O	0	1
			219	219		
3	B	277	Total	O	0	1
			278	278		
3	C	244	Total	O	0	0
			244	244		
3	D	242	Total	O	0	1
			243	243		

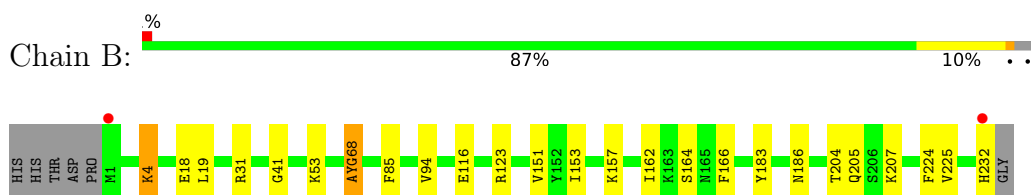
### 3 Residue-property plots [i](#)

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.

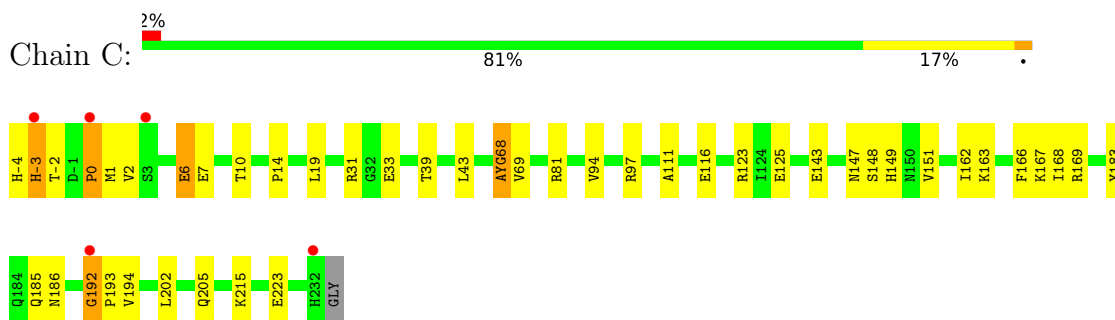
- Molecule 1: Green fluorescent protein



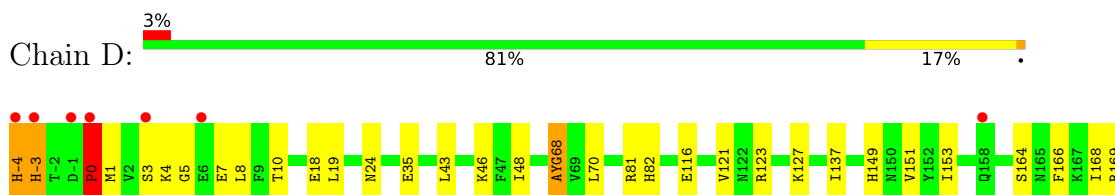
- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.30Å 134.91Å 51.66Å 90.00° 105.97° 90.00°	Depositor
Resolution (Å)	48.12 – 1.63 48.07 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.12-1.63) 99.7 (48.07-1.63)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 1.63Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.154 , 0.193 0.168 , 0.201	Depositor DCC
$R_{free}$ test set	2000 reflections (1.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtrriage
Anisotropy	0.456	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>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9544	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	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 28.04 % 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 1.9760e-03. 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: GOL, PIA

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	0.69	0/2056	0.90	0/2777
1	B	0.72	0/2106	0.90	0/2841
1	C	0.72	1/2143 (0.0%)	0.89	0/2896
1	D	0.73	0/2184	0.90	0/2948
All	All	0.72	1/8489 (0.0%)	0.90	0/11462

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	143	GLU	CD-OE1	5.01	1.31	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123[B]	ARG	Mainchain

## 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	2071	0	1992	52	0
1	B	2121	0	2038	34	0
1	C	2154	0	2053	60	0
1	D	2196	0	2108	63	0
2	B	6	0	8	0	0
2	C	6	0	8	1	0
2	D	6	0	8	1	0
3	A	219	0	0	12	0
3	B	278	0	0	15	1
3	C	244	0	0	19	1
3	D	243	0	0	14	0
All	All	9544	0	8215	209	1

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 12.

All (209) 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:D:68[C]:PIA:HE1	1:D:149[C]:HIS:CE1	1.38	1.56
1:A:68[C]:PIA:HE1	1:A:149[C]:HIS:CE1	1.49	1.47
1:D:68[C]:PIA:HE1	1:D:149[C]:HIS:NE2	1.24	1.42
1:D:68[C]:PIA:CE1	1:D:149[C]:HIS:CE1	2.04	1.38
1:A:68[B]:PIA:OH	1:A:151[B]:VAL:HG11	1.20	1.32
1:C:68[B]:PIA:OH	1:C:151[B]:VAL:HG11	1.25	1.30
1:C:10[A]:THR:HG23	3:C:519:HOH:O	1.32	1.29
1:B:68[B]:PIA:OH	1:B:151[B]:VAL:HG11	1.28	1.28
1:D:35[B]:GLU:HG3	3:D:517:HOH:O	1.29	1.28
1:D:68[C]:PIA:CZ	1:D:149[C]:HIS:HE1	1.47	1.27
1:D:183[B]:TYR:CD1	3:D:524:HOH:O	1.89	1.26
1:D:127[B]:LYS:HE3	3:D:412:HOH:O	1.24	1.26
1:D:68[C]:PIA:OH	1:D:149[C]:HIS:HE1	1.13	1.25
1:A:68[C]:PIA:HE1	1:A:149[C]:HIS:NE2	1.49	1.24
1:D:68[B]:PIA:OH	1:D:151[B]:VAL:HG11	1.09	1.24
1:B:183[B]:TYR:CE1	3:B:533:HOH:O	1.90	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183[B]:TYR:CD1	3:A:400:HOH:O	1.88	1.21
1:A:68[C]:PIA:CE1	1:A:149[C]:HIS:CE1	2.27	1.18
1:D:68[C]:PIA:OH	1:D:149[C]:HIS:CE1	1.97	1.17
1:D:68[B]:PIA:OH	1:D:151[B]:VAL:CG1	1.95	1.14
1:D:185[B]:GLN:NE2	3:D:404:HOH:O	1.79	1.14
1:B:183[B]:TYR:CD1	3:B:533:HOH:O	1.94	1.12
1:B:123[B]:ARG:HD3	3:B:418:HOH:O	1.49	1.10
1:C:-4:HIS:O	1:C:0:PRO:HD2	1.52	1.09
1:A:68[B]:PIA:OH	1:A:151[B]:VAL:CG1	1.99	1.09
1:D:127[B]:LYS:CE	3:D:412:HOH:O	1.83	1.09
1:D:-4:HIS:O	1:D:0:PRO:HD2	1.52	1.08
1:A:205[B]:GLN:NE2	3:A:304:HOH:O	1.81	1.07
1:D:183[B]:TYR:CE1	3:D:524:HOH:O	2.05	1.07
1:D:68[B]:PIA:CZ	1:D:151[B]:VAL:HG11	1.84	1.06
1:A:68[B]:PIA:CZ	1:A:151[B]:VAL:HG11	1.84	1.05
1:A:183[B]:TYR:CE1	3:A:400:HOH:O	2.03	1.04
1:B:68[B]:PIA:CZ	1:B:151[B]:VAL:HG11	1.87	1.03
1:C:68[B]:PIA:OH	1:C:151[B]:VAL:CG1	2.07	1.03
1:B:68[B]:PIA:OH	1:B:151[B]:VAL:CG1	2.07	1.02
1:D:68[C]:PIA:CE1	1:D:149[C]:HIS:NE2	2.16	1.01
1:D:4[B]:LYS:HE2	1:D:4[B]:LYS:C	1.80	1.01
1:A:48[C]:ILE:HD11	1:A:50:THR:CG2	1.91	1.00
1:A:48[C]:ILE:HD11	1:A:50:THR:HG22	1.43	0.99
1:B:207[A]:LYS:NZ	3:B:407:HOH:O	1.97	0.97
1:A:68[C]:PIA:CE1	1:A:149[C]:HIS:HE1	1.78	0.96
1:B:4[A]:LYS:NZ	3:B:405:HOH:O	1.84	0.93
1:A:68[C]:PIA:OH	1:A:149[C]:HIS:HE1	1.51	0.92
1:A:48[C]:ILE:CD1	1:A:50:THR:HG22	2.00	0.92
1:C:68[B]:PIA:CZ	1:C:151[B]:VAL:HG11	1.98	0.92
1:A:48[C]:ILE:CD1	1:A:50:THR:CG2	2.48	0.91
1:D:68[C]:PIA:CZ	1:D:149[C]:HIS:CE1	2.34	0.91
1:A:68[C]:PIA:CZ	1:A:149[C]:HIS:HE1	1.84	0.91
1:B:123[A]:ARG:CD	3:B:418:HOH:O	2.19	0.90
1:C:163[B]:LYS:HD3	3:C:564:HOH:O	1.71	0.90
1:B:205[B]:GLN:OE1	3:B:406:HOH:O	1.89	0.89
1:C:-3[A]:HIS:O	1:C:1[A]:MET:HG2	1.73	0.88
1:C:163[B]:LYS:CD	3:C:564:HOH:O	2.24	0.84
1:A:116[A]:GLU:OE1	3:A:306:HOH:O	1.91	0.83
1:A:183[B]:TYR:HD1	3:A:400:HOH:O	1.40	0.80
1:B:205[A]:GLN:NE2	3:B:406:HOH:O	2.13	0.80
1:C:148[C]:SER:OG	3:C:404:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:SER:O	1:D:7:GLU:HG3	1.82	0.79
1:C:1[A]:MET:HE3	1:C:194:VAL:HA	1.64	0.79
1:B:68[C]:PIA:HD2	1:B:68[C]:PIA:O2	1.83	0.79
1:C:205:GLN:NE2	3:C:404:HOH:O	2.12	0.78
1:D:35[B]:GLU:CG	3:D:517:HOH:O	1.99	0.78
1:D:81[B]:ARG:HG2	3:D:580[B]:HOH:O	1.86	0.76
1:D:43[A]:LEU:C	1:D:43[A]:LEU:HD12	2.05	0.76
1:D:43[A]:LEU:HD12	1:D:43[A]:LEU:O	1.87	0.76
1:B:123[A]:ARG:HD3	3:B:418:HOH:O	1.82	0.75
1:C:1[A]:MET:HE3	1:C:194:VAL:CA	2.17	0.75
1:A:48[C]:ILE:CD1	1:A:50:THR:HG23	2.17	0.75
1:B:123[A]:ARG:HG3	3:B:418:HOH:O	1.85	0.74
1:A:68[C]:PIA:OH	1:A:149[C]:HIS:CE1	2.38	0.74
1:B:123[A]:ARG:CG	3:B:418:HOH:O	2.35	0.74
1:D:-4:HIS:O	1:D:0:PRO:CD	2.35	0.74
1:A:74[B]:ARG:NH2	3:A:303:HOH:O	1.79	0.73
1:C:149[C]:HIS:HE1	1:C:166:PHE:HB2	1.54	0.73
1:A:123[B]:ARG:HG3	1:A:123[B]:ARG:NH1	2.02	0.72
1:D:205[B]:GLN:HG3	1:D:207[B]:LYS:NZ	2.04	0.72
1:A:226[B]:THR:HG23	3:A:325:HOH:O	1.89	0.71
1:A:68[C]:PIA:HD2	1:A:68[C]:PIA:O2	1.93	0.69
1:C:6[A]:GLU:O	1:C:10[A]:THR:OG1	2.09	0.69
1:D:231:THR:O	1:D:232:HIS:HB2	1.92	0.69
1:A:226[B]:THR:CG2	3:A:325:HOH:O	2.42	0.68
1:C:43[B]:LEU:CD1	1:C:223:GLU:HB3	2.23	0.67
2:C:301:GOL:C3	3:C:406:HOH:O	2.43	0.67
1:A:48[C]:ILE:HD11	1:A:50:THR:HG23	1.77	0.67
1:D:183[B]:TYR:HD1	3:D:524:HOH:O	1.43	0.66
1:C:163[B]:LYS:CG	3:C:564:HOH:O	2.42	0.66
1:D:123[B]:ARG:HD2	3:D:576:HOH:O	1.95	0.66
1:D:4[B]:LYS:HE3	1:D:8:LEU:HD12	1.78	0.65
1:A:145:ASN:HB2	3:A:466:HOH:O	1.96	0.65
1:B:205[B]:GLN:CD	3:B:406:HOH:O	2.34	0.64
1:C:-4:HIS:O	1:C:0:PRO:CD	2.38	0.63
1:C:6[A]:GLU:HG3	3:C:615:HOH:O	1.97	0.63
1:D:137[B]:ILE:HD13	1:D:137[B]:ILE:N	2.14	0.63
1:D:35[B]:GLU:CD	3:D:517:HOH:O	2.28	0.62
1:A:48[C]:ILE:HD12	1:A:50:THR:HG23	1.81	0.62
1:C:43[B]:LEU:H	1:C:43[B]:LEU:HD12	1.64	0.61
1:C:43[B]:LEU:HD12	1:C:43[B]:LEU:N	2.15	0.61
1:C:68[B]:PIA:CE1	1:C:151[B]:VAL:HG11	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68[C]:PIA:CE1	1:A:149[C]:HIS:NE2	2.45	0.60
1:A:43[B]:LEU:HD21	1:A:45:LEU:HD12	1.83	0.60
1:C:68[C]:PIA:HD2	1:C:68[C]:PIA:O2	2.01	0.59
1:D:187[B]:THR:HG22	3:D:490:HOH:O	2.02	0.58
1:D:4[B]:LYS:HE2	1:D:4[B]:LYS:O	2.02	0.58
1:A:43[B]:LEU:C	1:A:43[B]:LEU:HD23	2.23	0.58
1:A:33:GLU:CD	3:A:317:HOH:O	2.41	0.57
1:C:149[C]:HIS:CD2	3:C:589:HOH:O	2.58	0.57
1:D:18:GLU:OE1	1:D:123[B]:ARG:NH2	2.38	0.57
1:D:82:HIS:HD1	1:D:198:ASP:H	1.51	0.57
1:D:205[B]:GLN:HG3	1:D:207[B]:LYS:HZ3	1.68	0.56
1:A:162[A]:ILE:HG13	1:A:186:ASN:HB2	1.87	0.56
1:A:85:PHE:CE1	1:A:162[B]:ILE:HD11	2.41	0.56
1:B:116:GLU:OE2	1:B:123[B]:ARG:NH1	2.38	0.56
1:C:68[C]:PIA:HD1	3:C:440:HOH:O	2.06	0.55
1:C:149[C]:HIS:CE1	1:C:166:PHE:HB2	2.40	0.55
1:D:68[B]:PIA:CE1	1:D:151[B]:VAL:HG11	2.34	0.55
1:B:85:PHE:CE1	1:B:162[B]:ILE:HD11	2.42	0.55
1:C:43[B]:LEU:HD13	1:C:223:GLU:HB3	1.88	0.55
1:D:153:ILE:HD13	1:D:164[B]:SER:OG	2.06	0.55
1:C:151[B]:VAL:CG1	1:C:202:LEU:HB2	2.38	0.54
1:A:18:GLU:OE2	1:A:31[B]:ARG:NH2	2.40	0.54
1:B:153:ILE:HD13	1:B:164[B]:SER:OG	2.08	0.54
1:A:37:ASP:HB3	1:A:40:ASN:HD21	1.72	0.53
1:C:-4:HIS:CE1	3:C:420:HOH:O	2.61	0.53
1:D:68[B]:PIA:HD2	1:D:68[B]:PIA:O2	2.08	0.53
1:C:151[B]:VAL:HG23	1:C:166:PHE:CD1	2.44	0.53
1:A:85:PHE:CZ	1:A:162[B]:ILE:HD11	2.45	0.52
1:D:43[A]:LEU:C	1:D:43[A]:LEU:CD1	2.77	0.52
1:C:43[B]:LEU:CD2	1:C:69:VAL:HG23	2.40	0.52
1:A:68[B]:PIA:CE1	1:A:151[B]:VAL:HG11	2.37	0.52
1:B:183[B]:TYR:HE1	3:B:533:HOH:O	1.57	0.52
1:B:207[A]:LYS:NZ	3:B:411:HOH:O	2.42	0.52
1:C:43[A]:LEU:C	1:C:43[A]:LEU:HD12	2.29	0.51
1:D:205[B]:GLN:HG3	1:D:207[B]:LYS:HZ2	1.74	0.51
1:B:151[B]:VAL:HG23	1:B:166:PHE:CD1	2.45	0.51
1:C:10[A]:THR:HG22	3:C:429:HOH:O	2.10	0.51
1:D:46:LYS:HE2	1:D:48[A]:ILE:HD11	1.91	0.51
1:C:31:ARG:NH2	1:C:33[A]:GLU:OE2	2.44	0.51
1:A:231:THR:O	1:A:232:HIS:ND1	2.41	0.51
1:C:116:GLU:OE2	1:C:123[B]:ARG:NH1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162[A]:ILE:C	1:C:162[A]:ILE:HD12	2.31	0.51
1:D:187[B]:THR:OG1	1:D:188:PRO:HD2	2.11	0.50
1:A:40:ASN:C	1:A:40:ASN:HD22	2.15	0.50
1:B:123[B]:ARG:HH11	1:B:123[B]:ARG:HG3	1.77	0.49
1:C:7:GLU:O	1:C:10[B]:THR:HG22	2.13	0.49
1:B:204[B]:THR:HG23	1:B:225:VAL:HG22	1.94	0.49
1:D:204[B]:THR:HG23	1:D:225:VAL:HG22	1.93	0.49
1:C:39[A]:THR:HG23	3:C:439:HOH:O	2.12	0.48
1:A:46:LYS:HE2	1:A:48[A]:ILE:HD11	1.96	0.48
1:D:4[B]:LYS:HE2	1:D:5:GLY:N	2.27	0.48
1:A:68[C]:PIA:CZ	1:A:149[C]:HIS:CE1	2.70	0.48
1:C:43[B]:LEU:HD12	1:C:223:GLU:O	2.14	0.47
1:C:147:ASN:ND2	1:C:169[B]:ARG:O	2.41	0.47
1:C:-4:HIS:HB3	3:C:620:HOH:O	2.13	0.47
1:C:192:GLY:N	3:C:412:HOH:O	2.45	0.47
1:B:205[B]:GLN:HG2	1:B:224:PHE:HB2	1.97	0.47
1:C:149[C]:HIS:NE2	1:C:167:LYS:O	2.48	0.47
1:A:48[C]:ILE:HD12	1:A:50:THR:CG2	2.36	0.47
1:C:1[B]:MET:HA	1:C:1[B]:MET:HE2	1.97	0.47
1:C:1[A]:MET:HE3	1:C:193:PRO:O	2.15	0.47
1:C:-2:THR:O	1:C:2:VAL:HG23	2.15	0.46
1:B:18[B]:GLU:OE1	1:B:31[B]:ARG:HG3	2.14	0.46
1:B:123[B]:ARG:NH1	1:B:123[B]:ARG:HG3	2.30	0.46
1:B:19:LEU:C	1:B:19:LEU:HD23	2.36	0.46
1:D:-3:HIS:O	1:D:1[B]:MET:HG2	2.17	0.45
1:D:151[B]:VAL:HG23	1:D:166:PHE:CD1	2.52	0.45
1:A:74[B]:ARG:HB3	1:A:226[B]:THR:HG22	1.98	0.45
1:C:39[A]:THR:HG21	3:C:593:HOH:O	2.17	0.45
1:C:68[B]:PIA:N2	1:C:223:GLU:OE2	2.50	0.45
1:C:183[B]:TYR:HD1	3:C:409:HOH:O	2.01	0.44
1:C:125[B]:GLU:HG3	3:C:604:HOH:O	2.18	0.44
1:D:68[C]:PIA:HD2	1:D:68[C]:PIA:O2	2.17	0.44
1:D:68[B]:PIA:CG2	1:D:70:LEU:HD21	2.48	0.44
1:D:153:ILE:HD13	1:D:164[B]:SER:HG	1.83	0.44
1:C:111:ALA:HA	1:C:123[B]:ARG:O	2.18	0.44
1:B:68[B]:PIA:CE1	1:B:151[B]:VAL:HG11	2.44	0.43
1:A:149[B]:HIS:HE1	1:A:166:PHE:HB2	1.83	0.43
1:C:185[B]:GLN:CD	3:C:459:HOH:O	2.56	0.43
1:D:185[A]:GLN:HG3	2:D:301:GOL:O3	2.19	0.43
1:B:116:GLU:CD	1:B:123[B]:ARG:HH12	2.21	0.43
1:A:94:VAL:O	1:A:186:ASN:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:C	1:C:19:LEU:HD23	2.39	0.43
1:C:163[B]:LYS:HB2	1:C:163[B]:LYS:HE3	1.91	0.42
1:D:7:GLU:O	1:D:10[A]:THR:HG22	2.19	0.42
1:D:116:GLU:OE1	1:D:123[B]:ARG:NH1	2.48	0.42
1:B:94:VAL:O	1:B:186:ASN:HA	2.19	0.42
1:D:1[B]:MET:HE2	3:D:408:HOH:O	2.19	0.42
1:A:177:VAL:HG12	1:A:179[A]:LEU:HD12	2.01	0.42
1:D:205[B]:GLN:CG	1:D:207[B]:LYS:NZ	2.78	0.42
1:C:149[B]:HIS:CE1	1:C:168:ILE:HD11	2.55	0.41
1:B:53:LYS:NZ	3:B:421:HOH:O	2.52	0.41
1:A:155:ALA:HA	1:A:162[B]:ILE:HG22	2.02	0.41
1:D:169[A]:ARG:HD2	3:D:554:HOH:O	2.21	0.41
1:D:68[B]:PIA:O2	1:D:68[B]:PIA:CD2	2.68	0.41
1:D:149[A]:HIS:CE1	1:D:168:ILE:HA	2.55	0.41
1:C:94:VAL:O	1:C:186:ASN:HA	2.20	0.41
1:A:5:GLY:HA3	1:A:86:LYS:O	2.20	0.41
1:A:116[B]:GLU:OE1	3:A:306:HOH:O	2.22	0.41
1:C:39[B]:THR:CG2	1:D:24:ASN:HA	2.51	0.41
1:C:68[B]:PIA:OH	1:C:151[B]:VAL:HG21	2.20	0.41
1:D:19[A]:LEU:C	1:D:19[A]:LEU:HD23	2.42	0.41
1:D:207[A]:LYS:HD2	1:D:222:LEU:HD23	2.02	0.41
1:A:130:ASP:OD2	3:A:307:HOH:O	2.22	0.40
1:B:162[A]:ILE:HG13	1:B:186:ASN:HB2	2.03	0.40
1:B:41:GLY:O	1:B:224:PHE:HA	2.21	0.40
1:D:121:VAL:HG12	1:D:123[B]:ARG:HG3	2.03	0.40
1:C:1[A]:MET:CE	1:C:194:VAL:CA	2.94	0.40
1:C:151[B]:VAL:O	1:C:151[B]:VAL:HG13	2.21	0.40
1:A:74[B]:ARG:HH11	1:A:226[B]:THR:HG21	1.86	0.40

All (1) 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)
3:B:662:HOH:O	3:C:614:HOH:O[4_554]	2.05	0.15

## 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	249/236 (106%)	246 (99%)	3 (1%)	0	100	100
1	B	254/236 (108%)	251 (99%)	3 (1%)	0	100	100
1	C	259/236 (110%)	251 (97%)	7 (3%)	1 (0%)	34	15
1	D	263/236 (111%)	256 (97%)	6 (2%)	1 (0%)	34	15
All	All	1025/944 (109%)	1004 (98%)	19 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	192	GLY
1	D	0	PRO

### 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	224/207 (108%)	222 (99%)	2 (1%)	78	63
1	B	231/207 (112%)	227 (98%)	4 (2%)	60	36
1	C	235/207 (114%)	227 (97%)	8 (3%)	37	11
1	D	239/207 (116%)	236 (99%)	3 (1%)	69	47
All	All	929/828 (112%)	912 (98%)	17 (2%)	60	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	232	HIS
1	B	4[A]	LYS
1	B	4[B]	LYS
1	B	157	LYS
1	B	232	HIS
1	C	-3[A]	HIS
1	C	-3[B]	HIS
1	C	0	PRO
1	C	6[A]	GLU
1	C	6[B]	GLU
1	C	14	PRO
1	C	81	ARG
1	C	215	LYS
1	D	-4	HIS
1	D	-3	HIS
1	D	0	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	C	158	GLN
1	D	-3	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

12 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	PIA	B	68[B]	1	21,21,22	3.96	5 (23%)	27,29,31	4.36	9 (33%)
1	PIA	D	68[C]	1	21,21,22	3.39	5 (23%)	27,29,31	4.20	11 (40%)
1	PIA	A	68[A]	1	21,21,22	3.68	6 (28%)	27,29,31	3.93	10 (37%)
1	PIA	C	68[A]	1	21,21,22	3.61	5 (23%)	27,29,31	4.21	11 (40%)
1	PIA	C	68[C]	1	21,21,22	3.77	5 (23%)	27,29,31	4.25	10 (37%)
1	PIA	A	68[C]	1	21,21,22	4.02	5 (23%)	27,29,31	4.24	10 (37%)
1	PIA	D	68[B]	1	21,21,22	3.69	3 (14%)	27,29,31	4.15	11 (40%)
1	PIA	B	68[A]	1	21,21,22	3.63	5 (23%)	27,29,31	3.97	9 (33%)
1	PIA	B	68[C]	1	21,21,22	3.54	6 (28%)	27,29,31	4.11	9 (33%)
1	PIA	C	68[B]	1	21,21,22	3.68	4 (19%)	27,29,31	4.42	11 (40%)
1	PIA	A	68[B]	1	21,21,22	4.07	4 (19%)	27,29,31	4.48	9 (33%)
1	PIA	D	68[A]	1	21,21,22	2.88	4 (19%)	27,29,31	3.92	7 (25%)

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	PIA	B	68[B]	1	-	4/8/27/28	0/2/2/2
1	PIA	D	68[C]	1	-	2/8/27/28	0/2/2/2
1	PIA	A	68[A]	1	-	0/8/27/28	0/2/2/2
1	PIA	C	68[A]	1	-	0/8/27/28	0/2/2/2
1	PIA	C	68[C]	1	-	4/8/27/28	0/2/2/2
1	PIA	A	68[C]	1	-	4/8/27/28	0/2/2/2
1	PIA	D	68[B]	1	-	3/8/27/28	0/2/2/2
1	PIA	B	68[A]	1	-	0/8/27/28	0/2/2/2
1	PIA	B	68[C]	1	-	4/8/27/28	0/2/2/2
1	PIA	C	68[B]	1	-	3/8/27/28	0/2/2/2
1	PIA	A	68[B]	1	-	3/8/27/28	0/2/2/2
1	PIA	D	68[A]	1	-	0/8/27/28	0/2/2/2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68[B]	PIA	CB2-CA2	17.55	1.49	1.35
1	B	68[B]	PIA	CB2-CA2	17.18	1.49	1.35
1	A	68[C]	PIA	CB2-CA2	17.12	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68[C]	PIA	CB2-CA2	16.00	1.48	1.35
1	D	68[B]	PIA	CB2-CA2	15.95	1.48	1.35
1	C	68[B]	PIA	CB2-CA2	15.72	1.48	1.35
1	C	68[A]	PIA	CB2-CA2	15.12	1.47	1.35
1	B	68[A]	PIA	CB2-CA2	15.08	1.47	1.35
1	B	68[C]	PIA	CB2-CA2	14.73	1.47	1.35
1	A	68[A]	PIA	CB2-CA2	14.65	1.47	1.35
1	D	68[C]	PIA	CB2-CA2	14.26	1.47	1.35
1	D	68[A]	PIA	CB2-CA2	11.08	1.44	1.35
1	A	68[A]	PIA	C1-N2	4.98	1.39	1.32
1	B	68[A]	PIA	C1-N2	4.81	1.39	1.32
1	A	68[A]	PIA	CA2-C2	-3.98	1.44	1.48
1	D	68[A]	PIA	CA2-C2	-3.98	1.44	1.48
1	C	68[A]	PIA	C1-N2	3.88	1.37	1.32
1	A	68[C]	PIA	C1-N2	3.83	1.37	1.32
1	A	68[B]	PIA	C1-N2	3.55	1.37	1.32
1	C	68[C]	PIA	C1-N2	3.53	1.37	1.32
1	B	68[C]	PIA	C1-N2	3.48	1.37	1.32
1	C	68[B]	PIA	C1-N2	3.47	1.37	1.32
1	D	68[A]	PIA	C1-N2	3.46	1.37	1.32
1	C	68[A]	PIA	C2-N3	-3.31	1.32	1.39
1	B	68[B]	PIA	C1-N2	3.24	1.37	1.32
1	A	68[C]	PIA	C2-N3	-3.08	1.32	1.39
1	A	68[A]	PIA	C2-N3	-2.99	1.32	1.39
1	C	68[B]	PIA	CA2-C2	-2.98	1.45	1.48
1	D	68[C]	PIA	CA1-C1	-2.92	1.47	1.51
1	D	68[A]	PIA	C2-N3	-2.90	1.33	1.39
1	C	68[A]	PIA	CA1-C1	-2.77	1.47	1.51
1	D	68[B]	PIA	CA2-C2	-2.74	1.45	1.48
1	B	68[C]	PIA	C2-N3	-2.74	1.33	1.39
1	D	68[C]	PIA	C2-N3	-2.70	1.33	1.39
1	A	68[B]	PIA	CA1-C1	-2.67	1.47	1.51
1	B	68[A]	PIA	C2-N3	-2.61	1.33	1.39
1	B	68[C]	PIA	CA2-C2	-2.60	1.46	1.48
1	A	68[A]	PIA	CA1-C1	-2.60	1.47	1.51
1	B	68[A]	PIA	O2-C2	2.57	1.28	1.23
1	C	68[C]	PIA	C2-N3	-2.52	1.33	1.39
1	B	68[C]	PIA	CA1-C1	-2.49	1.47	1.51
1	D	68[B]	PIA	C2-N3	-2.48	1.34	1.39
1	D	68[C]	PIA	CA2-C2	-2.44	1.46	1.48
1	B	68[C]	PIA	O2-C2	2.41	1.28	1.23
1	C	68[C]	PIA	CA2-C2	-2.40	1.46	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68[B]	PIA	C2-N3	-2.39	1.34	1.39
1	A	68[C]	PIA	CA1-C1	-2.33	1.48	1.51
1	B	68[B]	PIA	CA2-C2	-2.29	1.46	1.48
1	A	68[C]	PIA	O2-C2	2.27	1.27	1.23
1	C	68[C]	PIA	O2-C2	2.24	1.27	1.23
1	B	68[B]	PIA	C2-N3	-2.19	1.34	1.39
1	B	68[A]	PIA	CA2-C2	-2.19	1.46	1.48
1	A	68[A]	PIA	O2-C2	2.17	1.27	1.23
1	B	68[B]	PIA	O2-C2	2.10	1.27	1.23
1	D	68[C]	PIA	C1-N2	2.05	1.35	1.32
1	C	68[B]	PIA	C2-N3	-2.05	1.35	1.39
1	C	68[A]	PIA	CA2-C2	-2.04	1.46	1.48

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68[A]	PIA	CA2-C2-N3	15.88	110.88	103.37
1	C	68[B]	PIA	CA2-C2-N3	14.00	109.99	103.37
1	D	68[A]	PIA	O2-C2-CA2	-13.85	123.18	130.96
1	A	68[C]	PIA	CA2-C2-N3	13.66	109.83	103.37
1	A	68[A]	PIA	CA2-C2-N3	13.30	109.66	103.37
1	B	68[A]	PIA	O2-C2-CA2	-13.23	123.53	130.96
1	C	68[C]	PIA	CA2-C2-N3	12.86	109.45	103.37
1	D	68[C]	PIA	CB2-CA2-C2	12.56	137.27	122.28
1	B	68[A]	PIA	CA2-C2-N3	12.39	109.23	103.37
1	B	68[B]	PIA	CB2-CA2-C2	12.39	137.06	122.28
1	A	68[B]	PIA	CB2-CA2-C2	12.26	136.91	122.28
1	A	68[B]	PIA	CA2-C2-N3	12.11	109.10	103.37
1	A	68[A]	PIA	O2-C2-CA2	-12.09	124.17	130.96
1	B	68[C]	PIA	CA2-C2-N3	11.86	108.98	103.37
1	D	68[A]	PIA	CA2-C2-N3	11.47	108.80	103.37
1	A	68[C]	PIA	CB2-CA2-C2	11.14	135.57	122.28
1	D	68[C]	PIA	CA2-C2-N3	11.03	108.59	103.37
1	D	68[B]	PIA	CB2-CA2-C2	11.03	135.44	122.28
1	B	68[C]	PIA	CB2-CA2-C2	10.72	135.07	122.28
1	C	68[C]	PIA	CB2-CA2-C2	10.70	135.05	122.28
1	B	68[B]	PIA	CA2-C2-N3	10.52	108.35	103.37
1	D	68[B]	PIA	CA2-C2-N3	10.31	108.25	103.37
1	C	68[B]	PIA	CB2-CA2-C2	9.31	133.39	122.28
1	C	68[C]	PIA	O2-C2-CA2	-8.68	126.09	130.96
1	C	68[A]	PIA	O2-C2-CA2	-8.63	126.11	130.96
1	B	68[B]	PIA	CG2-CB2-CA2	-8.61	119.39	129.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	68[C]	PIA	CB2-CA2-N2	-8.57	116.94	128.83
1	B	68[B]	PIA	CB2-CA2-N2	-8.52	117.01	128.83
1	D	68[B]	PIA	CG2-CB2-CA2	-8.15	119.96	129.94
1	B	68[C]	PIA	O2-C2-CA2	-7.95	126.50	130.96
1	A	68[B]	PIA	CB2-CA2-N2	-7.74	118.09	128.83
1	C	68[B]	PIA	C2-CA2-N2	-7.70	103.54	108.93
1	B	68[C]	PIA	CB2-CA2-N2	-7.43	118.52	128.83
1	A	68[B]	PIA	CG2-CB2-CA2	-7.31	120.99	129.94
1	D	68[B]	PIA	CB2-CA2-N2	-7.23	118.80	128.83
1	C	68[B]	PIA	O2-C2-CA2	-7.00	127.03	130.96
1	A	68[C]	PIA	CB2-CA2-N2	-6.81	119.38	128.83
1	C	68[C]	PIA	CB2-CA2-N2	-6.59	119.69	128.83
1	C	68[B]	PIA	CG2-CB2-CA2	-6.48	122.00	129.94
1	A	68[B]	PIA	C2-CA2-N2	-6.09	104.67	108.93
1	C	68[A]	PIA	C2-CA2-N2	-6.01	104.72	108.93
1	A	68[B]	PIA	O2-C2-CA2	-5.80	127.70	130.96
1	C	68[A]	PIA	C2-N3-C1	-5.78	105.04	107.97
1	B	68[B]	PIA	O3-C3-CA3	-5.61	109.45	126.39
1	A	68[C]	PIA	C2-CA2-N2	-5.56	105.04	108.93
1	D	68[B]	PIA	O2-C2-CA2	-5.55	127.85	130.96
1	D	68[A]	PIA	C2-N3-C1	-5.40	105.23	107.97
1	B	68[B]	PIA	C2-CA2-N2	-5.31	105.21	108.93
1	C	68[C]	PIA	C2-CA2-N2	-5.27	105.24	108.93
1	D	68[B]	PIA	C2-CA2-N2	-5.26	105.25	108.93
1	A	68[C]	PIA	O2-C2-CA2	-5.15	128.07	130.96
1	C	68[A]	PIA	O3-C3-CA3	-5.00	111.29	126.39
1	B	68[A]	PIA	C2-N3-C1	-4.94	105.47	107.97
1	A	68[A]	PIA	C2-N3-C1	-4.92	105.48	107.97
1	C	68[B]	PIA	CA2-N2-C1	4.83	109.33	105.77
1	D	68[C]	PIA	O3-C3-CA3	-4.72	112.13	126.39
1	D	68[C]	PIA	C2-CA2-N2	-4.60	105.71	108.93
1	D	68[C]	PIA	O2-C2-CA2	-4.58	128.39	130.96
1	B	68[C]	PIA	C2-N3-C1	-4.40	105.74	107.97
1	A	68[B]	PIA	O3-C3-CA3	-4.39	113.13	126.39
1	C	68[B]	PIA	CB2-CA2-N2	-4.30	122.86	128.83
1	B	68[C]	PIA	O3-C3-CA3	-4.26	113.54	126.39
1	A	68[C]	PIA	O3-C3-CA3	-4.23	113.60	126.39
1	B	68[A]	PIA	O3-C3-CA3	-4.19	113.74	126.39
1	D	68[B]	PIA	O3-C3-CA3	-4.10	114.01	126.39
1	D	68[C]	PIA	C2-N3-C1	-4.01	105.93	107.97
1	A	68[C]	PIA	CA3-N3-C1	3.93	131.88	127.16
1	C	68[C]	PIA	C2-N3-C1	-3.87	106.00	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68[C]	PIA	C2-N3-C1	-3.76	106.06	107.97
1	A	68[A]	PIA	O3-C3-CA3	-3.72	115.14	126.39
1	D	68[A]	PIA	O3-C3-CA3	-3.72	115.15	126.39
1	C	68[C]	PIA	O3-C3-CA3	-3.72	115.15	126.39
1	A	68[B]	PIA	CA2-N2-C1	3.67	108.48	105.77
1	B	68[C]	PIA	C2-CA2-N2	-3.62	106.39	108.93
1	C	68[B]	PIA	O3-C3-CA3	-3.57	115.62	126.39
1	B	68[B]	PIA	CA2-N2-C1	3.34	108.24	105.77
1	A	68[B]	PIA	C2-N3-C1	-3.34	106.27	107.97
1	D	68[B]	PIA	CA2-N2-C1	3.31	108.21	105.77
1	C	68[A]	PIA	CB2-CA2-C2	3.16	126.05	122.28
1	B	68[C]	PIA	CG2-CB2-CA2	-3.13	126.11	129.94
1	A	68[A]	PIA	CA1-C1-N3	-3.10	121.03	124.75
1	C	68[C]	PIA	CA2-N2-C1	3.09	108.05	105.77
1	C	68[A]	PIA	CG2-CB2-CA2	3.03	133.66	129.94
1	B	68[A]	PIA	CA1-C1-N3	-3.00	121.15	124.75
1	C	68[A]	PIA	N3-C1-N2	2.89	113.45	111.45
1	D	68[A]	PIA	CA1-C1-N3	-2.87	121.31	124.75
1	D	68[A]	PIA	CD2-CG2-CD1	2.85	121.86	117.64
1	D	68[C]	PIA	C1-CA1-N1	-2.84	100.96	109.24
1	A	68[A]	PIA	CD2-CG2-CD1	2.83	121.83	117.64
1	B	68[A]	PIA	C2-CA2-N2	-2.79	106.98	108.93
1	B	68[B]	PIA	CA1-C1-N3	-2.78	121.42	124.75
1	C	68[B]	PIA	CA1-C1-N2	2.74	127.55	124.05
1	C	68[A]	PIA	C1-CA1-N1	-2.71	101.36	109.24
1	D	68[C]	PIA	CD1-CG2-CB2	-2.67	112.14	121.22
1	A	68[C]	PIA	CG2-CB2-CA2	-2.64	126.71	129.94
1	B	68[B]	PIA	CA1-C1-N2	2.59	127.36	124.05
1	B	68[A]	PIA	CD2-CG2-CD1	2.54	121.39	117.64
1	C	68[B]	PIA	C2-N3-C1	-2.52	106.69	107.97
1	C	68[A]	PIA	CD2-CG2-CB2	-2.52	112.66	121.22
1	C	68[B]	PIA	CA1-C1-N3	-2.50	121.75	124.75
1	A	68[C]	PIA	CA2-N2-C1	2.47	107.59	105.77
1	B	68[C]	PIA	CA3-N3-C1	2.39	130.03	127.16
1	D	68[A]	PIA	CD2-CG2-CB2	-2.34	113.27	121.22
1	D	68[B]	PIA	CA1-C1-N3	-2.31	121.97	124.75
1	D	68[C]	PIA	CA2-N2-C1	2.30	107.47	105.77
1	A	68[A]	PIA	CA3-N3-C1	2.30	129.92	127.16
1	A	68[A]	PIA	CD2-CG2-CB2	-2.27	113.49	121.22
1	B	68[A]	PIA	CE1-CD1-CG2	-2.26	118.30	121.25
1	D	68[B]	PIA	C2-N3-C1	-2.25	106.83	107.97
1	A	68[A]	PIA	C2-CA2-N2	-2.22	107.38	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68[C]	PIA	CA3-N3-C1	2.21	129.82	127.16
1	C	68[A]	PIA	CA1-C1-N3	-2.21	122.09	124.75
1	C	68[C]	PIA	CD1-CG2-CB2	-2.15	113.91	121.22
1	D	68[B]	PIA	C1-CA1-N1	-2.13	103.05	109.24
1	D	68[C]	PIA	CD2-CG2-CD1	2.10	120.74	117.64
1	A	68[A]	PIA	CE1-CD1-CG2	-2.09	118.52	121.25
1	B	68[A]	PIA	CD2-CG2-CB2	-2.07	114.19	121.22

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68[B]	PIA	C2-CA2-CB2-CG2
1	A	68[C]	PIA	C3-CA3-N3-C1
1	A	68[C]	PIA	C3-CA3-N3-C2
1	B	68[B]	PIA	C2-CA2-CB2-CG2
1	B	68[C]	PIA	C3-CA3-N3-C1
1	B	68[C]	PIA	C3-CA3-N3-C2
1	C	68[B]	PIA	C2-CA2-CB2-CG2
1	C	68[C]	PIA	C3-CA3-N3-C1
1	C	68[C]	PIA	C3-CA3-N3-C2
1	D	68[B]	PIA	C2-CA2-CB2-CG2
1	A	68[C]	PIA	C2-CA2-CB2-CG2
1	B	68[C]	PIA	C2-CA2-CB2-CG2
1	C	68[C]	PIA	C2-CA2-CB2-CG2
1	D	68[C]	PIA	C2-CA2-CB2-CG2
1	A	68[B]	PIA	N2-CA2-CB2-CG2
1	A	68[C]	PIA	N2-CA2-CB2-CG2
1	B	68[B]	PIA	N2-CA2-CB2-CG2
1	B	68[C]	PIA	N2-CA2-CB2-CG2
1	C	68[B]	PIA	N2-CA2-CB2-CG2
1	C	68[C]	PIA	N2-CA2-CB2-CG2
1	D	68[B]	PIA	N2-CA2-CB2-CG2
1	D	68[C]	PIA	N2-CA2-CB2-CG2
1	B	68[B]	PIA	CA2-CB2-CG2-CD1
1	A	68[B]	PIA	CA2-CB2-CG2-CD1
1	B	68[B]	PIA	N3-C1-CA1-CB1
1	C	68[B]	PIA	N3-C1-CA1-CB1
1	D	68[B]	PIA	N3-C1-CA1-CB1

There are no ring outliers.

8 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	68[B]	PIA	4	0
1	D	68[C]	PIA	9	0
1	C	68[C]	PIA	2	0
1	A	68[C]	PIA	10	0
1	D	68[B]	PIA	7	0
1	B	68[C]	PIA	1	0
1	C	68[B]	PIA	6	0
1	A	68[B]	PIA	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	GOL	B	301	-	5,5,5	0.12	0	5,5,5	0.34	0
2	GOL	D	301	-	5,5,5	0.10	0	5,5,5	0.28	0
2	GOL	C	301	-	5,5,5	0.11	0	5,5,5	0.27	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	GOL	B	301	-	-	2/4/4/4	-
2	GOL	D	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	GOL	O1-C1-C2-C3
2	D	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O2-C2-C3-O3
2	B	301	GOL	O1-C1-C2-C3
2	C	301	GOL	C1-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-O2
2	D	301	GOL	O1-C1-C2-O2
2	B	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GOL	1	0
2	C	301	GOL	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, 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	230/236 (97%)	-0.35	5 (2%) 62 61	17, 25, 47, 75	0
1	B	229/236 (97%)	-0.48	2 (0%) 84 85	13, 20, 37, 76	0
1	C	234/236 (99%)	-0.32	5 (2%) 63 64	15, 23, 47, 86	0
1	D	234/236 (99%)	-0.31	8 (3%) 45 43	14, 22, 47, 70	0
All	All	927/944 (98%)	-0.36	20 (2%) 62 61	13, 23, 45, 86	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	-3[A]	HIS	4.9
1	A	1	MET	3.6
1	D	-3	HIS	3.5
1	D	0	PRO	3.4
1	D	3	SER	3.3
1	A	233	GLY	3.2
1	B	1	MET	3.1
1	C	232	HIS	3.0
1	C	0	PRO	3.0
1	D	-4	HIS	2.9
1	D	-1	ASP	2.6
1	B	232	HIS	2.5
1	D	158[A]	GLN	2.5
1	C	3[A]	SER	2.5
1	A	2	VAL	2.4
1	D	6	GLU	2.4
1	A	232	HIS	2.3
1	A	183[A]	TYR	2.2
1	C	192	GLY	2.1
1	D	183[A]	TYR	2.0

## 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	PIA	A	68[A]	20/21	0.97	0.12	16,22,32,32	20
1	PIA	A	68[B]	20/21	0.97	0.12	12,12,13,14	20
1	PIA	A	68[C]	20/21	0.97	0.12	10,13,14,15	20
1	PIA	B	68[A]	20/21	0.98	0.10	13,16,22,23	20
1	PIA	B	68[B]	20/21	0.98	0.10	10,11,13,13	20
1	PIA	B	68[C]	20/21	0.98	0.10	7,10,12,12	20
1	PIA	C	68[A]	20/21	0.98	0.12	13,15,25,27	20
1	PIA	C	68[B]	20/21	0.98	0.12	11,13,15,17	20
1	PIA	C	68[C]	20/21	0.98	0.12	9,12,14,14	20
1	PIA	D	68[A]	20/21	0.98	0.11	13,16,22,23	20
1	PIA	D	68[B]	20/21	0.98	0.11	12,13,14,15	20
1	PIA	D	68[C]	20/21	0.98	0.11	10,11,12,13	20

## 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
2	GOL	D	301	6/6	0.72	0.18	71,73,77,77	0
2	GOL	C	301	6/6	0.89	0.15	69,72,74,76	0
2	GOL	B	301	6/6	0.91	0.14	49,62,62,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.