Full wwPDB X-ray Structure Validation Report (i)

Oct 13, 2022 – 01:46 am BST

PDB ID	:	7AMB
Title	:	Crystal structure of rsFolder2 in its fluorescent on-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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

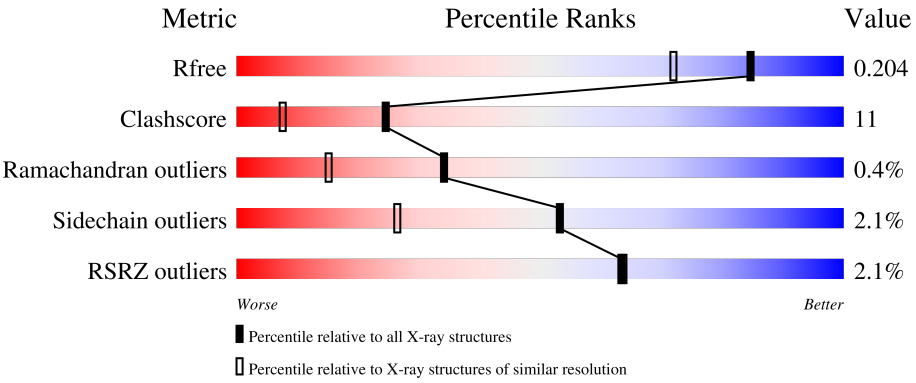
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 >=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 <=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	2% 82% 14%
1	B	236	83% 13%
1	C	236	3% 84% 12%
1	D	236	3% 86% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9302 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	24	0
			2029	1281	350	392	6			
1	B	229	Total	C	N	O	S	0	28	0
			2063	1303	355	399	6			
1	C	231	Total	C	N	O	S	0	27	0
			2057	1297	354	400	6			
1	D	230	Total	C	N	O	S	0	29	0
			2080	1309	359	406	6			

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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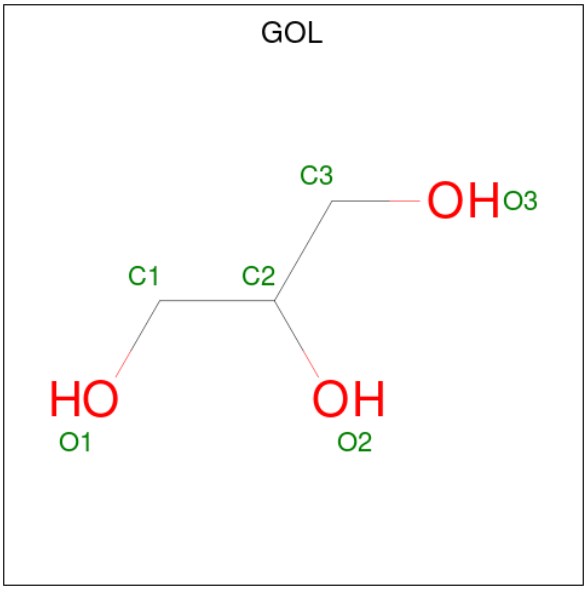
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP P42212
D	-3	HIS	-	expression tag	UNP P42212
D	-2	THR	-	expression tag	UNP P42212
D	-1	ASP	-	expression tag	UNP P42212
D	0	PRO	-	expression tag	UNP P42212
D	1	MET	-	expression tag	UNP P42212
D	2	VAL	-	expression tag	UNP P42212
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: $C_3H_8O_3$).



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

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

- Molecule 3 is water.

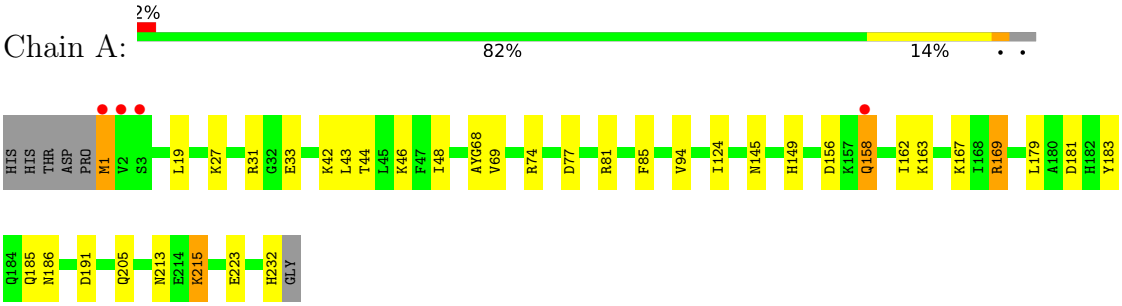
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	238	Total O 238 238	0	0
3	B	287	Total O 287 287	0	0
3	C	257	Total O 260 260	0	3
3	D	251	Total O 252 252	0	1

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.

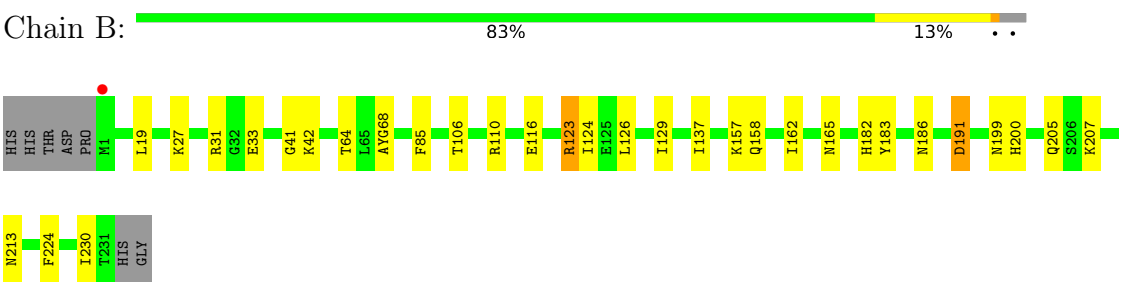
• Molecule 1: Green fluorescent protein

Chain A:



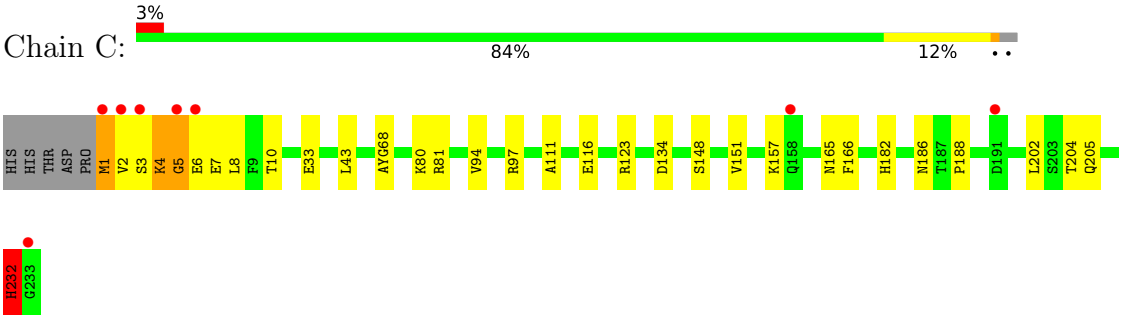
• Molecule 1: Green fluorescent protein

Chain B:



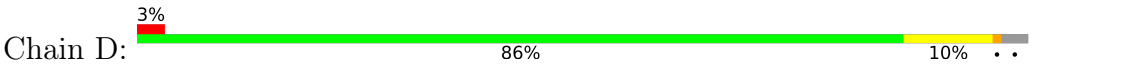
• Molecule 1: Green fluorescent protein

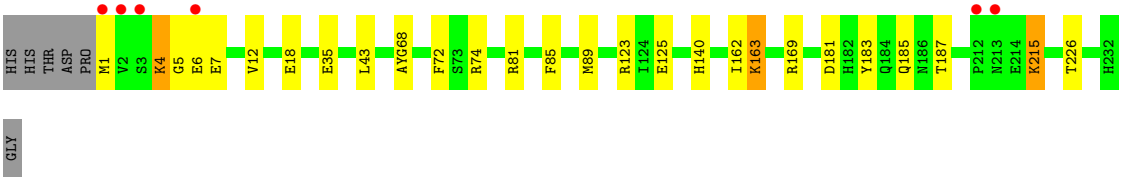
Chain C:



• Molecule 1: Green fluorescent protein

Chain D:




HIS
HIS
THR
ASP
PRO
M1
V2
S3
K4
G5
E6
E7
V12
E18
E35
L43
AYG68
F72
S73
R74
R81
F85
M89
R123
I124
E125
H140
I162
K163
R169
D181
H182
Y183
Q184
Q185
N186
T187
P212
N213
E214
K215
T226
H232
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.30Å 134.50Å 51.62Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	47.98 – 1.63 47.94 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.98-1.63) 99.7 (47.94-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.151 , 0.190 0.165 , 0.204	Depositor DCC
R_{free} test set	2000 reflections (1.73%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9302	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.74 % 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 2.9999e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.73	0/2052	0.87	2/2771 (0.1%)
1	B	0.70	0/2085	0.89	0/2812
1	C	0.71	0/2080	0.88	0/2804
1	D	0.70	0/2103	0.88	0/2839
All	All	0.71	0/8320	0.88	2/11226 (0.0%)

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	2
1	C	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169[A]	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	169[B]	ARG	NE-CZ-NH1	5.30	122.95	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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Mol	Chain	Res	Type	Group
1	C	1	MET	Mainchain

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	2029	0	1978	51	0
1	B	2063	0	2013	34	0
1	C	2057	0	2002	49	0
1	D	2080	0	2003	44	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	18	0	24	4	0
3	A	238	0	0	29	0
3	B	287	0	0	17	0
3	C	260	0	0	17	0
3	D	252	0	0	32	0
All	All	9302	0	8044	180	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 11.

All (180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185[B]:GLN:HG2	3:A:519:HOH:O	1.24	1.31
1:A:213[B]:ASN:ND2	3:A:404:HOH:O	1.64	1.26
1:D:7[B]:GLU:HG3	3:D:486:HOH:O	1.25	1.25
1:D:183[B]:TYR:CD1	3:D:532:HOH:O	1.93	1.21
1:A:183[C]:TYR:CD2	3:A:525:HOH:O	1.92	1.17
1:D:123[A]:ARG:CD	3:D:413:HOH:O	1.91	1.17
1:B:183[B]:TYR:CD1	3:B:507:HOH:O	1.98	1.16
1:C:232:HIS:HB2	3:C:588:HOH:O	1.46	1.15
1:D:7[B]:GLU:CG	3:D:486:HOH:O	1.80	1.12
1:B:183[B]:TYR:CE1	3:B:507:HOH:O	1.99	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2[B]:VAL:HG23	1:C:81:ARG:HH11	1.14	1.08
1:C:134[A]:ASP:OD1	3:C:401:HOH:O	1.73	1.05
1:D:123[A]:ARG:HD3	3:D:413:HOH:O	1.51	1.03
1:C:4[B]:LYS:O	1:C:6[B]:GLU:N	1.92	1.02
1:D:226[B]:THR:HG21	3:D:530:HOH:O	1.57	1.02
1:A:205[B]:GLN:NE2	3:A:409:HOH:O	1.95	1.00
1:A:44[B]:THR:HG23	3:A:494:HOH:O	1.62	1.00
1:D:183[B]:TYR:CE1	3:D:532:HOH:O	2.06	0.99
1:A:183[C]:TYR:HD2	3:A:525:HOH:O	1.36	0.97
1:C:33[A]:GLU:OE2	3:C:402:HOH:O	1.82	0.96
1:A:31[A]:ARG:NH1	3:A:410:HOH:O	1.97	0.95
1:A:169[B]:ARG:HG2	1:A:179[B]:LEU:CD1	1.97	0.94
1:A:77[B]:ASP:OD1	3:A:406:HOH:O	1.86	0.92
1:C:33[A]:GLU:CD	3:C:402:HOH:O	2.07	0.92
1:C:10[A]:THR:HG22	3:C:622:HOH:O	1.68	0.91
1:B:106[B]:THR:HG23	3:B:504:HOH:O	1.71	0.90
1:A:181[B]:ASP:OD1	3:A:407:HOH:O	1.88	0.89
1:D:185[B]:GLN:HG3	3:D:579:HOH:O	1.72	0.89
1:D:123[A]:ARG:CG	3:D:413:HOH:O	2.11	0.88
1:D:123[A]:ARG:HG3	3:D:413:HOH:O	1.70	0.88
1:D:5[B]:GLY:HA2	3:D:472:HOH:O	1.72	0.88
1:A:33[B]:GLU:OE1	3:A:408:HOH:O	1.91	0.87
1:A:183[C]:TYR:CE2	3:A:525:HOH:O	2.19	0.87
1:C:148[B]:SER:OG	3:C:403:HOH:O	1.92	0.86
1:B:207[A]:LYS:HE2	3:B:410:HOH:O	1.75	0.83
1:C:2[B]:VAL:HG23	1:C:81:ARG:NH1	1.93	0.83
1:B:207[A]:LYS:CE	3:B:410:HOH:O	2.26	0.82
1:C:2[A]:VAL:CG2	1:C:80:LYS:HB3	2.09	0.82
1:C:151[B]:VAL:HG12	1:C:202:LEU:HB2	1.61	0.82
1:C:151[B]:VAL:HG23	1:C:166:PHE:CD1	2.14	0.81
1:D:226[B]:THR:CG2	3:D:530:HOH:O	2.19	0.81
1:C:2[B]:VAL:CG2	1:C:81:ARG:HH11	1.92	0.81
1:C:4[B]:LYS:O	1:C:5[B]:GLY:C	2.17	0.81
1:A:44[B]:THR:CG2	3:A:494:HOH:O	2.20	0.81
1:A:169[B]:ARG:HG2	1:A:179[B]:LEU:HD13	1.64	0.80
1:D:4[B]:LYS:HD2	1:D:4[B]:LYS:C	2.00	0.80
1:D:4[A]:LYS:O	1:D:7[A]:GLU:N	2.15	0.79
1:A:169[B]:ARG:HG2	1:A:179[B]:LEU:HD11	1.62	0.78
1:D:183[B]:TYR:HD1	3:D:532:HOH:O	1.43	0.77
1:B:191[A]:ASP:CG	3:B:421:HOH:O	2.22	0.77
1:C:2[B]:VAL:CG1	1:C:80:LYS:HB3	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2[A]:VAL:O	3:C:404:HOH:O	2.01	0.76
1:A:215:LYS:HD2	3:A:560:HOH:O	1.87	0.73
1:A:183[C]:TYR:OH	3:A:412:HOH:O	2.05	0.72
1:A:149:HIS:NE2	3:A:413:HOH:O	2.23	0.72
1:A:185[B]:GLN:CG	3:A:519:HOH:O	2.02	0.72
1:B:42[A]:LYS:NZ	3:B:405:HOH:O	1.97	0.72
1:B:110[B]:ARG:NH2	3:B:403:HOH:O	1.88	0.72
1:D:1:MET:N	3:D:402:HOH:O	2.23	0.70
1:C:5[B]:GLY:O	1:C:8:LEU:HB2	1.91	0.70
1:D:187[B]:THR:HG22	3:D:455:HOH:O	1.92	0.70
1:C:151[B]:VAL:CG2	1:C:166:PHE:CD1	2.75	0.69
1:A:156:ASP:OD1	1:A:158:GLN:HG3	1.93	0.69
1:C:2[B]:VAL:HG21	1:C:81:ARG:CD	2.23	0.69
1:B:207[A]:LYS:NZ	3:B:410:HOH:O	2.27	0.68
1:A:169[A]:ARG:HB2	3:A:413:HOH:O	1.95	0.67
1:C:116:GLU:OE2	1:C:123[B]:ARG:NH1	2.28	0.67
1:D:5[A]:GLY:HA2	3:D:472:HOH:O	1.95	0.66
1:B:31[A]:ARG:NH1	3:B:406:HOH:O	2.01	0.66
1:A:27:LYS:HE2	3:A:620:HOH:O	1.97	0.65
1:C:2[A]:VAL:HG23	1:C:80:LYS:HB3	1.77	0.65
1:D:81:ARG:NH1	3:D:405:HOH:O	2.28	0.65
1:A:43[B]:LEU:CD1	3:A:521:HOH:O	2.44	0.65
1:D:74[B]:ARG:NH1	3:D:407:HOH:O	2.29	0.65
1:A:169[B]:ARG:NH2	3:A:416:HOH:O	2.29	0.64
1:C:6[B]:GLU:HB2	3:C:404:HOH:O	1.98	0.64
1:A:44[B]:THR:OG1	3:A:411:HOH:O	2.03	0.64
1:D:123[B]:ARG:HD2	3:D:496:HOH:O	1.98	0.64
1:A:181[B]:ASP:CG	3:A:407:HOH:O	2.35	0.63
1:C:2[B]:VAL:HG21	1:C:81:ARG:HD3	1.79	0.63
1:D:185[B]:GLN:CG	3:D:579:HOH:O	2.35	0.63
1:C:2[B]:VAL:CG2	1:C:81:ARG:HD2	2.30	0.62
1:A:19[A]:LEU:HD23	1:A:19[A]:LEU:C	2.20	0.62
1:C:2[A]:VAL:HG12	1:C:81:ARG:HH11	1.64	0.61
1:A:163[B]:LYS:HD2	3:A:510:HOH:O	2.00	0.61
1:B:183[B]:TYR:HD1	3:B:507:HOH:O	1.58	0.61
1:C:2[A]:VAL:HG21	1:C:80:LYS:HB3	1.83	0.60
1:B:116:GLU:OE2	1:B:123[B]:ARG:NH1	2.28	0.60
1:C:151[B]:VAL:HG23	1:C:166:PHE:CG	2.37	0.60
1:A:213[B]:ASN:OD1	1:A:213[B]:ASN:O	2.19	0.60
1:C:151[B]:VAL:CG1	1:C:151[B]:VAL:O	2.50	0.59
1:D:4[B]:LYS:HD2	3:D:472:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125[A]:GLU:HG3	2:D:303:GOL:H32	1.85	0.58
1:C:2[B]:VAL:O	3:C:404:HOH:O	2.17	0.57
1:C:2[A]:VAL:HG23	3:C:488:HOH:O	2.03	0.57
1:B:123[B]:ARG:NH1	1:B:123[B]:ARG:HG3	2.20	0.56
2:D:301:GOL:H2	3:D:403:HOH:O	2.04	0.56
1:B:31[B]:ARG:NH1	3:B:412:HOH:O	2.30	0.56
1:B:199:ASN:O	1:B:230[B]:ILE:HD11	2.06	0.55
1:C:2[B]:VAL:HG21	1:C:81:ARG:HD2	1.87	0.55
1:C:10[A]:THR:CG2	3:C:622:HOH:O	2.42	0.55
1:B:205[A]:GLN:NE2	3:B:404:HOH:O	1.91	0.54
1:A:19[B]:LEU:HD13	1:A:124:ILE:CG2	2.38	0.54
1:D:7[A]:GLU:OE1	3:D:401:HOH:O	2.18	0.54
1:A:1:MET:HB3	3:A:441:HOH:O	2.07	0.54
1:C:4[B]:LYS:C	1:C:6[B]:GLU:N	2.61	0.54
1:A:169[B]:ARG:CG	1:A:179[B]:LEU:CD1	2.78	0.54
1:C:232:HIS:CB	3:C:588:HOH:O	2.23	0.53
1:D:169[A]:ARG:NE	3:D:419:HOH:O	2.41	0.53
1:A:43[B]:LEU:HD11	3:A:521:HOH:O	2.06	0.53
1:B:200:HIS:HB3	1:B:230[B]:ILE:HD11	1.91	0.52
1:D:74[B]:ARG:CZ	3:D:407:HOH:O	2.57	0.52
1:C:2[B]:VAL:CG2	1:C:81:ARG:CD	2.87	0.52
1:A:43[B]:LEU:HB2	1:A:223[B]:GLU:HB3	1.92	0.52
1:C:80:LYS:HG2	3:C:419:HOH:O	2.09	0.52
1:B:183[B]:TYR:HE1	3:B:507:HOH:O	1.62	0.51
1:A:213[B]:ASN:OD1	1:A:213[B]:ASN:C	2.49	0.51
1:B:213[B]:ASN:OD1	1:B:213[B]:ASN:C	2.49	0.51
1:D:4[A]:LYS:O	1:D:5[A]:GLY:C	2.49	0.50
1:C:151[B]:VAL:O	1:C:151[B]:VAL:HG13	2.11	0.50
1:B:123[B]:ARG:HG3	1:B:123[B]:ARG:HH11	1.77	0.50
1:C:2[B]:VAL:O	1:C:6[B]:GLU:HB2	2.12	0.50
1:A:85:PHE:CE1	1:A:162[B]:ILE:HD11	2.46	0.50
1:C:165:ASN:HA	1:C:182:HIS:O	2.12	0.50
1:C:2[B]:VAL:HG13	3:C:488:HOH:O	2.11	0.50
1:C:10[B]:THR:HG22	3:C:613:HOH:O	2.11	0.49
1:A:19[B]:LEU:HD13	1:A:124:ILE:HB	1.94	0.49
1:B:33[B]:GLU:CG	3:B:533:HOH:O	2.59	0.49
1:D:1:MET:HG2	3:D:410[A]:HOH:O	2.13	0.49
1:D:140:HIS:O	2:D:302:GOL:H11	2.12	0.49
1:A:145:ASN:HB2	3:A:562:HOH:O	2.14	0.48
1:D:1:MET:CA	3:D:402:HOH:O	2.59	0.48
1:D:12:VAL:HG11	1:D:35[B]:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4[B]:LYS:HD2	1:D:4[B]:LYS:O	2.13	0.48
1:D:18:GLU:OE1	1:D:123[B]:ARG:NH1	2.46	0.48
1:A:162[A]:ILE:HD12	1:A:162[A]:ILE:C	2.34	0.47
1:B:19[B]:LEU:HD12	1:B:124:ILE:HB	1.96	0.47
1:D:215:LYS:CD	1:D:215:LYS:H	2.25	0.47
1:B:137[B]:ILE:N	1:B:137[B]:ILE:HD13	2.30	0.47
1:A:46:LYS:HE2	1:A:48[A]:ILE:HD11	1.97	0.46
1:C:205[C]:GLN:HG2	3:C:605:HOH:O	2.14	0.46
1:A:169[B]:ARG:NH1	3:C:409:HOH:O	2.40	0.46
1:B:126:LEU:C	1:B:126:LEU:HD23	2.37	0.45
3:A:617:HOH:O	1:B:129:ILE:CD1	2.64	0.45
1:B:27:LYS:NZ	3:B:426:HOH:O	2.48	0.45
1:D:43[B]:LEU:HD21	1:D:72:PHE:HB2	1.99	0.45
1:C:94:VAL:O	1:C:186:ASN:HA	2.17	0.44
1:A:169[B]:ARG:CG	1:A:179[B]:LEU:HD11	2.41	0.44
1:D:181[B]:ASP:CG	3:D:421:HOH:O	2.55	0.44
1:A:162[A]:ILE:HG13	1:A:186:ASN:HB2	1.99	0.44
1:D:4[A]:LYS:HE2	1:D:89:MET:O	2.17	0.44
2:D:301:GOL:C3	3:D:428:HOH:O	2.65	0.44
1:A:156:ASP:OD1	1:A:158:GLN:CG	2.65	0.44
1:B:41:GLY:O	1:B:224:PHE:HA	2.17	0.43
1:D:4[A]:LYS:O	1:D:7[A]:GLU:CB	2.66	0.43
1:B:85:PHE:CE1	1:B:162[B]:ILE:HD11	2.53	0.43
1:C:43[A]:LEU:C	1:C:43[A]:LEU:HD12	2.38	0.43
1:A:43[B]:LEU:HD11	1:A:69:VAL:HG23	2.01	0.43
1:C:111:ALA:HA	1:C:123[B]:ARG:O	2.19	0.43
1:A:169[B]:ARG:CG	1:A:179[B]:LEU:HD13	2.41	0.42
1:B:116:GLU:CD	1:B:123[B]:ARG:HH12	2.18	0.42
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.83	0.42
1:A:94:VAL:O	1:A:186:ASN:HA	2.20	0.42
1:B:64:THR:CG2	1:B:124:ILE:HG21	2.49	0.42
1:C:2[B]:VAL:O	1:C:6[B]:GLU:CB	2.67	0.42
1:D:85:PHE:CE1	1:D:162[B]:ILE:HD11	2.54	0.42
1:D:163:LYS:HD2	3:D:528:HOH:O	2.19	0.42
1:A:74:ARG:HD2	3:A:417:HOH:O	2.20	0.42
1:C:116:GLU:CD	1:C:123[B]:ARG:HH12	2.19	0.41
1:A:42[B]:LYS:NZ	3:A:405:HOH:O	1.67	0.41
1:D:4[A]:LYS:O	1:D:7[A]:GLU:HB3	2.21	0.41
1:A:167:LYS:HG2	1:A:181[B]:ASP:OD1	2.21	0.41
1:B:162[A]:ILE:HG13	1:B:186:ASN:HB2	2.03	0.41
1:B:42[A]:LYS:CE	3:B:405:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19[A]:LEU:C	1:B:19[A]:LEU:HD23	2.42	0.40
1:D:7[A]:GLU:CD	3:D:486:HOH:O	2.59	0.40
1:C:148[B]:SER:OG	1:C:204:THR:O	2.39	0.40
1:D:4[A]:LYS:NZ	3:D:410[A]:HOH:O	2.36	0.40
1:B:165:ASN:HA	1:B:182:HIS: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	A	249/236 (106%)	246 (99%)	3 (1%)	0	100 100
1	B	252/236 (107%)	249 (99%)	3 (1%)	0	100 100
1	C	253/236 (107%)	243 (96%)	4 (2%)	6 (2%)	6 0
1	D	255/236 (108%)	252 (99%)	3 (1%)	0	100 100
All	All	1009/944 (107%)	990 (98%)	13 (1%)	6 (1%)	34 8

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	5[A]	GLY
1	C	5[B]	GLY
1	C	4[A]	LYS
1	C	4[B]	LYS
1	C	7	GLU
1	C	232	HIS

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	225/207 (109%)	220 (98%)	5 (2%)	52	25
1	B	229/207 (111%)	225 (98%)	4 (2%)	60	36
1	C	228/207 (110%)	222 (97%)	6 (3%)	46	19
1	D	228/207 (110%)	222 (97%)	6 (3%)	46	19
All	All	910/828 (110%)	889 (98%)	21 (2%)	53	23

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	158	GLN
1	A	191	ASP
1	A	215	LYS
1	A	232	HIS
1	B	157	LYS
1	B	158	GLN
1	B	191[A]	ASP
1	B	191[B]	ASP
1	C	1	MET
1	C	3[A]	SER
1	C	3[B]	SER
1	C	157	LYS
1	C	188	PRO
1	C	232	HIS
1	D	4[A]	LYS
1	D	4[B]	LYS
1	D	6[A]	GLU
1	D	6[B]	GLU
1	D	163	LYS
1	D	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	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	PIA	C	68	1	21,21,22	3.58	5 (23%)	27,29,31	3.38	8 (29%)
1	PIA	D	68	1	21,21,22	2.79	6 (28%)	27,29,31	2.80	11 (40%)
1	PIA	B	68	1	21,21,22	2.90	7 (33%)	27,29,31	3.48	13 (48%)
1	PIA	A	68	1	21,21,22	3.12	7 (33%)	27,29,31	3.19	12 (44%)

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	C	68	1	-	1/8/27/28	0/2/2/2
1	PIA	D	68	1	-	0/8/27/28	0/2/2/2
1	PIA	B	68	1	-	0/8/27/28	0/2/2/2
1	PIA	A	68	1	-	0/8/27/28	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	PIA	CB2-CA2	14.96	1.47	1.35
1	A	68	PIA	CB2-CA2	11.13	1.44	1.35
1	B	68	PIA	CB2-CA2	10.88	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	68	PIA	CB2-CA2	10.14	1.43	1.35
1	A	68	PIA	CA2-C2	-4.84	1.43	1.48
1	D	68	PIA	CA2-C2	-4.25	1.44	1.48
1	A	68	PIA	C1-N2	4.06	1.38	1.32
1	C	68	PIA	CA2-C2	-4.00	1.44	1.48
1	B	68	PIA	C1-N2	3.59	1.37	1.32
1	A	68	PIA	O2-C2	3.28	1.30	1.23
1	A	68	PIA	CA1-C1	-3.25	1.46	1.51
1	D	68	PIA	CA1-C1	-3.08	1.47	1.51
1	D	68	PIA	C2-N3	-3.06	1.32	1.39
1	A	68	PIA	C2-N3	-2.96	1.32	1.39
1	B	68	PIA	CA1-C1	-2.95	1.47	1.51
1	C	68	PIA	C2-N3	-2.94	1.32	1.39
1	B	68	PIA	C2-N3	-2.89	1.33	1.39
1	D	68	PIA	C1-N2	2.74	1.36	1.32
1	C	68	PIA	C1-N2	2.62	1.36	1.32
1	D	68	PIA	O2-C2	2.58	1.28	1.23
1	B	68	PIA	O2-C2	2.53	1.28	1.23
1	C	68	PIA	CA1-C1	-2.49	1.47	1.51
1	B	68	PIA	CA2-C2	-2.18	1.46	1.48
1	B	68	PIA	CA3-N3	-2.05	1.43	1.47
1	A	68	PIA	CG2-CB2	-2.01	1.43	1.46

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	PIA	CA2-C2-N3	13.41	109.71	103.37
1	A	68	PIA	CA2-C2-N3	10.26	108.22	103.37
1	D	68	PIA	CA2-C2-N3	8.85	107.56	103.37
1	A	68	PIA	O2-C2-CA2	-8.76	126.04	130.96
1	B	68	PIA	CA2-C2-N3	8.60	107.44	103.37
1	B	68	PIA	O2-C2-CA2	-8.14	126.39	130.96
1	D	68	PIA	O2-C2-CA2	-6.89	127.09	130.96
1	B	68	PIA	C2-N3-C1	-6.83	104.51	107.97
1	B	68	PIA	CA1-C1-N3	-4.88	118.90	124.75
1	B	68	PIA	N3-C1-N2	4.79	114.77	111.45
1	C	68	PIA	O2-C2-CA2	-4.78	128.28	130.96
1	B	68	PIA	CA2-N2-C1	-4.49	102.46	105.77
1	A	68	PIA	O3-C3-CA3	-4.41	113.08	126.39
1	D	68	PIA	CA1-C1-N3	-4.40	119.47	124.75
1	C	68	PIA	C2-CA2-N2	-4.37	105.87	108.93
1	C	68	PIA	O3-C3-CA3	-4.21	113.67	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	68	PIA	C2-N3-C1	-4.16	105.86	107.97
1	B	68	PIA	O3-C3-CA3	-3.93	114.53	126.39
1	C	68	PIA	CA1-C1-N3	-3.91	120.05	124.75
1	A	68	PIA	CE1-CD1-CG2	-3.61	116.54	121.25
1	D	68	PIA	C2-N3-C1	-3.55	106.17	107.97
1	D	68	PIA	O3-C3-CA3	-3.22	116.66	126.39
1	B	68	PIA	CD2-CG2-CB2	-2.84	111.56	121.22
1	A	68	PIA	CD2-CG2-CD1	2.79	121.77	117.64
1	A	68	PIA	CA3-N3-C1	2.76	130.48	127.16
1	A	68	PIA	C2-N3-C1	-2.72	106.59	107.97
1	A	68	PIA	CA2-N2-C1	-2.70	103.79	105.77
1	C	68	PIA	CA3-N3-C1	2.69	130.39	127.16
1	B	68	PIA	CD2-CG2-CD1	2.57	121.44	117.64
1	A	68	PIA	CG2-CB2-CA2	-2.56	126.81	129.94
1	D	68	PIA	N3-C1-N2	2.47	113.17	111.45
1	D	68	PIA	CA2-N2-C1	-2.47	103.96	105.77
1	D	68	PIA	CA1-C1-N2	2.41	127.14	124.05
1	D	68	PIA	CE1-CD1-CG2	-2.39	118.13	121.25
1	A	68	PIA	N3-C1-N2	2.38	113.10	111.45
1	B	68	PIA	OH-CZ-CE1	-2.33	113.39	120.02
1	B	68	PIA	C2-CA2-N2	2.30	110.54	108.93
1	B	68	PIA	CB2-CA2-N2	-2.26	125.69	128.83
1	D	68	PIA	CD2-CG2-CD1	2.26	120.98	117.64
1	A	68	PIA	CD2-CG2-CB2	-2.25	113.56	121.22
1	C	68	PIA	CA1-C1-N2	2.20	126.87	124.05
1	B	68	PIA	CA3-N3-C1	2.09	129.68	127.16
1	D	68	PIA	C1-CA1-N1	-2.06	103.24	109.24
1	A	68	PIA	CD1-CE1-CZ	2.03	122.10	119.88

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	68	PIA	N3-C1-CA1-CB1

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)

6 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	D	301	-	5,5,5	0.09	0	5,5,5	0.32	0
2	GOL	C	301	-	5,5,5	0.16	0	5,5,5	0.46	0
2	GOL	A	301	-	5,5,5	0.12	0	5,5,5	0.30	0
2	GOL	D	302	-	5,5,5	0.13	0	5,5,5	0.54	0
2	GOL	D	303	-	5,5,5	0.12	0	5,5,5	0.27	0
2	GOL	B	301	-	5,5,5	0.14	0	5,5,5	0.38	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	D	301	-	-	2/4/4/4	-
2	GOL	C	301	-	-	2/4/4/4	-
2	GOL	A	301	-	-	3/4/4/4	-
2	GOL	D	302	-	-	4/4/4/4	-
2	GOL	D	303	-	-	2/4/4/4	-
2	GOL	B	301	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	D	302	GOL	O1-C1-C2-O2
2	D	302	GOL	O1-C1-C2-C3
2	D	302	GOL	C1-C2-C3-O3
2	D	303	GOL	C1-C2-C3-O3
2	C	301	GOL	O2-C2-C3-O3
2	D	302	GOL	O2-C2-C3-O3
2	B	301	GOL	C1-C2-C3-O3
2	D	303	GOL	O2-C2-C3-O3
2	D	301	GOL	O1-C1-C2-C3
2	D	301	GOL	O1-C1-C2-O2
2	A	301	GOL	C1-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	GOL	2	0
2	D	302	GOL	1	0
2	D	303	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

6.1 Protein, DNA and RNA chains

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	229/236 (97%)	-0.40	4 (1%)	70	71	16, 24, 45, 77	0
1	B	228/236 (96%)	-0.50	1 (0%)	92	92	13, 20, 37, 60	0
1	C	230/236 (97%)	-0.34	8 (3%)	44	42	14, 21, 49, 82	0
1	D	229/236 (97%)	-0.36	6 (2%)	56	55	15, 24, 46, 71	0
All	All	916/944 (97%)	-0.40	19 (2%)	63	64	13, 22, 45, 82	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	233	GLY	6.6
1	A	1	MET	4.7
1	C	2[A]	VAL	4.5
1	C	3[A]	SER	4.4
1	D	6[A]	GLU	3.5
1	C	1	MET	3.0
1	D	3	SER	2.7
1	B	1	MET	2.6
1	D	2	VAL	2.5
1	A	3	SER	2.5
1	C	191	ASP	2.5
1	D	212	PRO	2.4
1	C	6[A]	GLU	2.4
1	C	158	GLN	2.3
1	A	2	VAL	2.2
1	C	5[A]	GLY	2.2
1	D	1	MET	2.2
1	D	213	ASN	2.2
1	A	158	GLN	2.2

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^{th} 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^2)	Q<0.9
1	PIA	A	68	20/21	0.97	0.06	14,16,19,20	0
1	PIA	B	68	20/21	0.98	0.05	13,14,15,16	0
1	PIA	C	68	20/21	0.98	0.05	14,16,18,18	0
1	PIA	D	68	20/21	0.98	0.06	15,16,19,21	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^{th} 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^2)	Q<0.9
2	GOL	D	302	6/6	0.70	0.24	51,59,62,65	0
2	GOL	A	301	6/6	0.73	0.24	59,62,76,82	0
2	GOL	D	301	6/6	0.74	0.27	60,63,64,67	0
2	GOL	C	301	6/6	0.80	0.12	54,56,57,61	0
2	GOL	B	301	6/6	0.82	0.14	60,63,66,67	0
2	GOL	D	303	6/6	0.88	0.33	59,63,65,71	0

6.5 Other polymers (i)

There are no such residues in this entry.