Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 10:38 PM GMT

PDB ID	:	5DU0
Title	:	Crystal structure of rsFolder in the non-fluorescent off-state
Authors	:	El Khatib, M.; Colletier, J.P.; Adam, V.
Deposited on	:	2015-09-18
Resolution	:	2.35 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

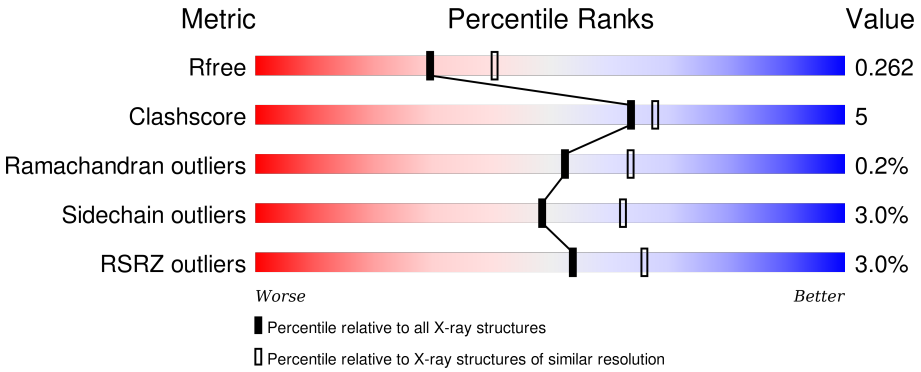
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.35 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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	264	2% 77% 9% 14%
1	B	264	% 77% 8% • 14%
1	C	264	3% 69% 16% • 14%
1	D	264	3% 74% 12% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7467 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	228	Total	C	N	O	S	0	0	0
			1820	1153	314	348	5			
1	B	226	Total	C	N	O	S	0	0	0
			1801	1141	311	344	5			
1	C	228	Total	C	N	O	S	0	0	0
			1820	1153	314	348	5			
1	D	228	Total	C	N	O	S	0	0	0
			1820	1153	314	348	5			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP P42212
A	-21	GLY	-	expression tag	UNP P42212
A	-20	SER	-	expression tag	UNP P42212
A	-19	SER	-	expression tag	UNP P42212
A	-18	HIS	-	expression tag	UNP P42212
A	-17	HIS	-	expression tag	UNP P42212
A	-16	HIS	-	expression tag	UNP P42212
A	-15	HIS	-	expression tag	UNP P42212
A	-14	HIS	-	expression tag	UNP P42212
A	-13	HIS	-	expression tag	UNP P42212
A	-12	SER	-	expression tag	UNP P42212
A	-11	SER	-	expression tag	UNP P42212
A	-10	GLY	-	expression tag	UNP P42212
A	-9	LEU	-	expression tag	UNP P42212
A	-8	VAL	-	expression tag	UNP P42212
A	-7	PRO	-	expression tag	UNP P42212
A	-6	ARG	-	expression tag	UNP P42212
A	-5	GLY	-	expression tag	UNP P42212
A	-4	SER	-	expression tag	UNP P42212
A	-3	HIS	-	expression tag	UNP P42212
A	-2	MET	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P42212
A	0	THR	-	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	conflict	UNP P42212
A	65	LEU	PHE	conflict	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	conflict	UNP P42212
A	106	THR	ASN	conflict	UNP P42212
A	146	PHE	TYR	conflict	UNP P42212
A	154	THR	MET	conflict	UNP P42212
A	164	SER	VAL	engineered mutation	UNP P42212
A	172	VAL	ILE	conflict	UNP P42212
A	207	LYS	ALA	engineered mutation	UNP P42212
A	240	GLY	-	expression tag	UNP P42212
A	241	SER	-	expression tag	UNP P42212
A	242	GLY	-	expression tag	UNP P42212
A	243	CYS	-	expression tag	UNP P42212
B	-22	MET	-	initiating methionine	UNP P42212
B	-21	GLY	-	expression tag	UNP P42212
B	-20	SER	-	expression tag	UNP P42212
B	-19	SER	-	expression tag	UNP P42212
B	-18	HIS	-	expression tag	UNP P42212
B	-17	HIS	-	expression tag	UNP P42212
B	-16	HIS	-	expression tag	UNP P42212
B	-15	HIS	-	expression tag	UNP P42212
B	-14	HIS	-	expression tag	UNP P42212
B	-13	HIS	-	expression tag	UNP P42212
B	-12	SER	-	expression tag	UNP P42212
B	-11	SER	-	expression tag	UNP P42212
B	-10	GLY	-	expression tag	UNP P42212
B	-9	LEU	-	expression tag	UNP P42212
B	-8	VAL	-	expression tag	UNP P42212
B	-7	PRO	-	expression tag	UNP P42212
B	-6	ARG	-	expression tag	UNP P42212
B	-5	GLY	-	expression tag	UNP P42212
B	-4	SER	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	UNP P42212
B	-2	MET	-	expression tag	UNP P42212
B	-1	ALA	-	expression tag	UNP P42212
B	0	THR	-	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	conflict	UNP P42212
B	65	LEU	PHE	conflict	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	conflict	UNP P42212
B	106	THR	ASN	conflict	UNP P42212
B	146	PHE	TYR	conflict	UNP P42212
B	154	THR	MET	conflict	UNP P42212
B	164	SER	VAL	engineered mutation	UNP P42212
B	172	VAL	ILE	conflict	UNP P42212
B	207	LYS	ALA	engineered mutation	UNP P42212
B	240	GLY	-	expression tag	UNP P42212
B	241	SER	-	expression tag	UNP P42212
B	242	GLY	-	expression tag	UNP P42212
B	243	CYS	-	expression tag	UNP P42212
C	-22	MET	-	initiating methionine	UNP P42212
C	-21	GLY	-	expression tag	UNP P42212
C	-20	SER	-	expression tag	UNP P42212
C	-19	SER	-	expression tag	UNP P42212
C	-18	HIS	-	expression tag	UNP P42212
C	-17	HIS	-	expression tag	UNP P42212
C	-16	HIS	-	expression tag	UNP P42212
C	-15	HIS	-	expression tag	UNP P42212
C	-14	HIS	-	expression tag	UNP P42212
C	-13	HIS	-	expression tag	UNP P42212
C	-12	SER	-	expression tag	UNP P42212
C	-11	SER	-	expression tag	UNP P42212
C	-10	GLY	-	expression tag	UNP P42212
C	-9	LEU	-	expression tag	UNP P42212
C	-8	VAL	-	expression tag	UNP P42212
C	-7	PRO	-	expression tag	UNP P42212
C	-6	ARG	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	GLY	-	expression tag	UNP P42212
C	-4	SER	-	expression tag	UNP P42212
C	-3	HIS	-	expression tag	UNP P42212
C	-2	MET	-	expression tag	UNP P42212
C	-1	ALA	-	expression tag	UNP P42212
C	0	THR	-	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	conflict	UNP P42212
C	65	LEU	PHE	conflict	UNP P42212
C	68	PIA	SER	chromphore	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	conflict	UNP P42212
C	106	THR	ASN	conflict	UNP P42212
C	146	PHE	TYR	conflict	UNP P42212
C	154	THR	MET	conflict	UNP P42212
C	164	SER	VAL	engineered mutation	UNP P42212
C	172	VAL	ILE	conflict	UNP P42212
C	207	LYS	ALA	engineered mutation	UNP P42212
C	240	GLY	-	expression tag	UNP P42212
C	241	SER	-	expression tag	UNP P42212
C	242	GLY	-	expression tag	UNP P42212
C	243	CYS	-	expression tag	UNP P42212
D	-22	MET	-	initiating methionine	UNP P42212
D	-21	GLY	-	expression tag	UNP P42212
D	-20	SER	-	expression tag	UNP P42212
D	-19	SER	-	expression tag	UNP P42212
D	-18	HIS	-	expression tag	UNP P42212
D	-17	HIS	-	expression tag	UNP P42212
D	-16	HIS	-	expression tag	UNP P42212
D	-15	HIS	-	expression tag	UNP P42212
D	-14	HIS	-	expression tag	UNP P42212
D	-13	HIS	-	expression tag	UNP P42212
D	-12	SER	-	expression tag	UNP P42212
D	-11	SER	-	expression tag	UNP P42212
D	-10	GLY	-	expression tag	UNP P42212
D	-9	LEU	-	expression tag	UNP P42212
D	-8	VAL	-	expression tag	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	PRO	-	expression tag	UNP P42212
D	-6	ARG	-	expression tag	UNP P42212
D	-5	GLY	-	expression tag	UNP P42212
D	-4	SER	-	expression tag	UNP P42212
D	-3	HIS	-	expression tag	UNP P42212
D	-2	MET	-	expression tag	UNP P42212
D	-1	ALA	-	expression tag	UNP P42212
D	0	THR	-	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	conflict	UNP P42212
D	65	LEU	PHE	conflict	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	conflict	UNP P42212
D	106	THR	ASN	conflict	UNP P42212
D	146	PHE	TYR	conflict	UNP P42212
D	154	THR	MET	conflict	UNP P42212
D	164	SER	VAL	engineered mutation	UNP P42212
D	172	VAL	ILE	conflict	UNP P42212
D	207	LYS	ALA	engineered mutation	UNP P42212
D	240	GLY	-	expression tag	UNP P42212
D	241	SER	-	expression tag	UNP P42212
D	242	GLY	-	expression tag	UNP P42212
D	243	CYS	-	expression tag	UNP P42212

- Molecule 2 is water.

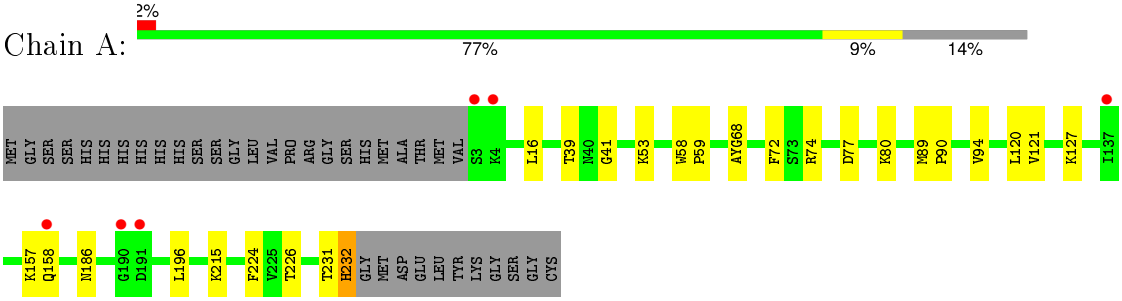
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	64	Total O 64 64	0	0
2	B	59	Total O 59 59	0	0
2	C	44	Total O 44 44	0	0
2	D	39	Total O 39 39	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

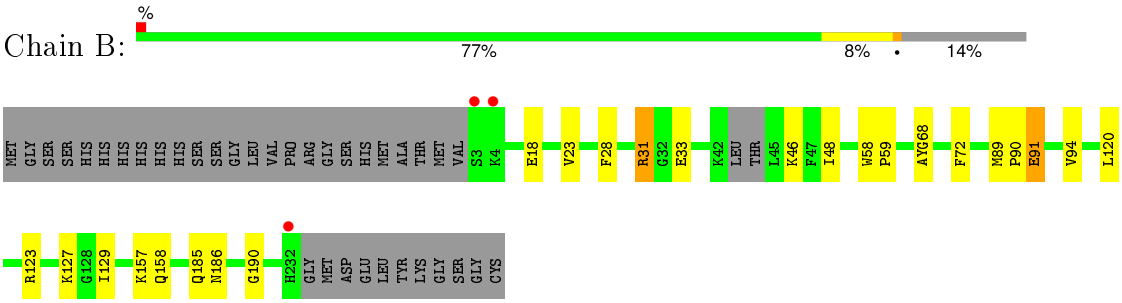
- Molecule 1: Green fluorescent protein

Chain A:



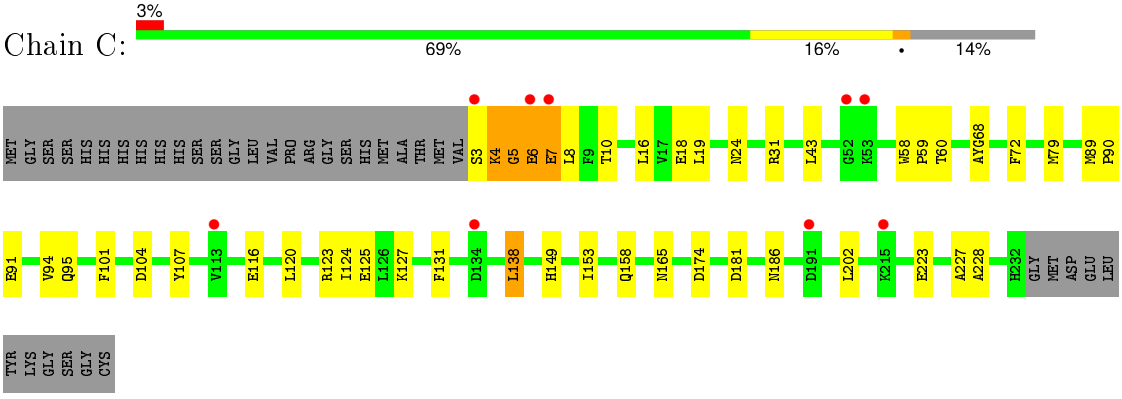
- Molecule 1: Green fluorescent protein

Chain B:



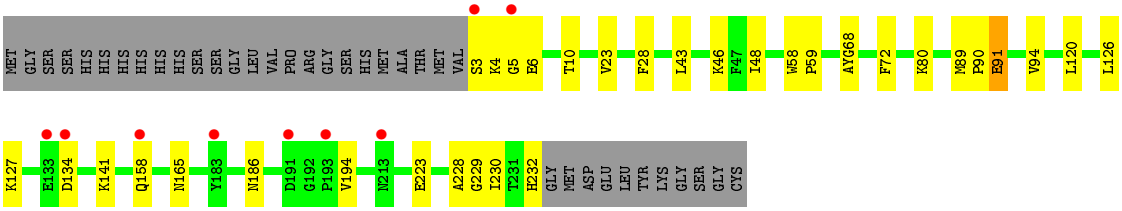
- Molecule 1: Green fluorescent protein

Chain C:



- Molecule 1: Green fluorescent protein

Chain D:


MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET ALA THR MET VAL S3 K4 G5 E6 T10 V23 F28 L43 K46 F47 I48 W58 P59 AYG68 F72 K80 M89 P90 E91 V94 L120 L126
K127 E133 D134 K141 Q158 N165 Y183 N186 D191 G192 P193 V194 M213 E223 A228 G229 I230 T231 H232 GLY MET ASP GLU LEU TYR LYS GLY SER GLY CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.29Å 134.80Å 51.05Å 90.00° 105.58° 90.00°	Depositor
Resolution (Å)	95.77 – 2.35 49.17 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.1 (95.77-2.35) 98.1 (49.17-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.208 , 0.257 0.216 , 0.262	Depositor DCC
R_{free} test set	1877 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	4 of 37525 reflections (0.011%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7467	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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 28.11 % 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 1.9530e-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, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.33	0/1839	0.50	0/2483
1	B	0.36	0/1819	0.51	1/2454 (0.0%)
1	C	0.38	0/1839	0.56	1/2483 (0.0%)
1	D	0.35	0/1839	0.50	0/2483
All	All	0.35	0/7336	0.52	2/9903 (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	C	0	1
1	D	0	2
All	All	0	3

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	B	31	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	5	GLY	N-CA-C	-5.50	99.36	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	174	ASP	Mainchain
1	D	228	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	D	229	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1820	0	1779	16	0
1	B	1801	0	1751	13	2
1	C	1820	0	1778	34	0
1	D	1820	0	1778	14	0
2	A	64	0	0	2	0
2	B	59	0	0	2	0
2	C	44	0	0	3	0
2	D	39	0	0	0	0
All	All	7467	0	7086	74	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (74) 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:127:LYS:HE3	2:B:304:HOH:O	1.71	0.90
1:C:79:MET:HE1	1:C:228:ALA:HA	1.64	0.78
1:A:226:THR:HG22	2:A:328:HOH:O	1.85	0.76
1:D:6:GLU:OE1	1:D:80:LYS:NZ	2.13	0.75
1:C:4:LYS:HE2	1:C:89:MET:O	1.88	0.72
1:C:60:THR:HG22	1:C:107:TYR:HE2	1.56	0.70
1:D:232:HIS:O	1:D:232:HIS:CG	2.44	0.70
1:C:4:LYS:HD3	1:C:5:GLY:N	2.07	0.70
1:B:68:PIA:O2	1:B:68:PIA:HD2	1.92	0.69
1:C:116:GLU:OE1	1:C:123:ARG:NH1	2.19	0.69
1:B:18:GLU:OE1	1:B:123:ARG:NH1	2.29	0.65
1:C:60:THR:HG22	1:C:107:TYR:CE2	2.31	0.65
1:D:68:PIA:O2	1:D:68:PIA:HD2	1.97	0.64
1:A:231:THR:O	1:A:232:HIS:ND1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PIA:O2	1:A:68:PIA:HD2	1.99	0.62
1:C:227:ALA:O	2:C:301:HOH:O	2.15	0.62
1:A:39:THR:HG21	2:B:304:HOH:O	2.00	0.61
1:C:68:PIA:HD2	1:C:68:PIA:O2	2.01	0.60
1:C:4:LYS:CE	1:C:89:MET:O	2.52	0.58
1:C:7:GLU:O	1:C:10:THR:HG22	2.04	0.56
1:C:60:THR:CG2	1:C:107:TYR:CE2	2.90	0.55
1:C:19:LEU:HD13	1:C:124:ILE:HB	1.89	0.55
1:C:72:PHE:CE2	1:C:120:LEU:HD22	2.42	0.54
1:C:60:THR:HG21	1:C:107:TYR:OH	2.09	0.53
1:C:4:LYS:HD3	1:C:5:GLY:H	1.71	0.53
1:A:77:ASP:OD1	1:A:80:LYS:NZ	2.41	0.53
1:B:72:PHE:CE2	1:B:120:LEU:HD22	2.45	0.52
1:D:23:VAL:HG23	1:D:28:PHE:HE1	1.76	0.51
1:C:3:SER:OG	1:C:6:GLU:CB	2.59	0.51
1:D:58:TRP:N	1:D:59:PRO:CD	2.74	0.51
1:D:43:LEU:HB3	1:D:223:GLU:HB3	1.93	0.49
1:A:58:TRP:N	1:A:59:PRO:CD	2.75	0.49
1:C:153:ILE:HD13	1:C:202:LEU:HG	1.93	0.49
1:C:104:ASP:OD2	2:C:302:HOH:O	2.19	0.49
1:C:60:THR:HG23	1:C:101:PHE:CZ	2.48	0.48
1:C:58:TRP:N	1:C:59:PRO:CD	2.76	0.48
1:A:72:PHE:CE2	1:A:120:LEU:HD22	2.49	0.48
1:C:8:LEU:HD23	1:C:8:LEU:HA	1.75	0.48
1:D:134:ASP:O	1:D:141:LYS:NZ	2.39	0.47
1:B:58:TRP:N	1:B:59:PRO:CD	2.77	0.47
1:A:53:LYS:HG2	2:A:304:HOH:O	2.15	0.46
1:B:91:GLU:HG3	1:B:190:GLY:HA3	1.98	0.46
1:D:72:PHE:CE2	1:D:120:LEU:HD22	2.51	0.45
1:A:94:VAL:O	1:A:186:ASN:HA	2.17	0.45
1:A:74:ARG:NH1	1:B:129:ILE:HD12	2.32	0.45
1:C:24:ASN:ND2	1:C:131:PHE:O	2.45	0.45
1:B:23:VAL:HG23	1:B:28:PHE:HE1	1.81	0.45
1:C:16:LEU:HD11	1:C:31:ARG:CZ	2.46	0.45
1:A:231:THR:HG21	1:C:149:HIS:HA	1.98	0.45
1:C:3:SER:OG	1:C:6:GLU:HB3	2.18	0.44
1:A:16:LEU:O	1:A:121:VAL:HA	2.17	0.44
1:D:91:GLU:H	1:D:91:GLU:HG2	1.41	0.44
1:B:31:ARG:NH1	1:B:31:ARG:HG3	2.31	0.44
1:C:138:LEU:HD12	1:C:138:LEU:HA	1.84	0.43
1:B:89:MET:HB3	1:B:90:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:VAL:O	1:D:186:ASN:HA	2.19	0.43
1:C:94:VAL:O	1:C:186:ASN:HA	2.18	0.43
1:B:94:VAL:O	1:B:186:ASN:HA	2.19	0.43
1:D:46:LYS:HE2	1:D:48:ILE:HD11	2.00	0.42
1:C:43:LEU:HB3	1:C:223:GLU:HB3	2.00	0.42
1:A:157:LYS:HG2	1:A:158:GLN:N	2.35	0.42
1:D:4:LYS:O	1:D:6:GLU:N	2.52	0.42
1:C:89:MET:HB3	1:C:90:PRO:HA	2.01	0.42
1:C:18:GLU:HG3	1:C:123:ARG:HG2	2.02	0.42
1:C:125:GLU:HG2	2:C:339:HOH:O	2.20	0.41
1:D:89:MET:HB3	1:D:90:PRO:HA	2.01	0.41
1:B:46:LYS:HE2	1:B:48:ILE:HD11	2.03	0.41
1:D:126:LEU:C	1:D:126:LEU:HD23	2.41	0.41
1:A:89:MET:HB3	1:A:90:PRO:HA	2.03	0.41
1:A:39:THR:HG21	1:B:127:LYS:HE3	2.03	0.41
1:C:68:PIA:HA32	1:C:95:GLN:HE22	1.86	0.41
1:C:5:GLY:O	1:C:6:GLU:CB	2.69	0.41
1:A:41:GLY:O	1:A:224:PHE:HA	2.21	0.40
1:C:5:GLY:HA2	1:C:8:LEU:HB2	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:CZ	1:B:31:ARG:NH2[2_554]	1.38	0.82
1:B:33:GLU:OE1	1:B:33:GLU:OE1[2_554]	2.13	0.07

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	223/264 (84%)	221 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	219/264 (83%)	216 (99%)	3 (1%)	0	100 100
1	C	223/264 (84%)	217 (97%)	5 (2%)	1 (0%)	39 46
1	D	223/264 (84%)	215 (96%)	7 (3%)	1 (0%)	39 46
All	All	888/1056 (84%)	869 (98%)	17 (2%)	2 (0%)	52 63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	6	GLU
1	D	5	GLY

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	200/229 (87%)	196 (98%)	4 (2%)	63 77
1	B	197/229 (86%)	193 (98%)	4 (2%)	63 77
1	C	200/229 (87%)	192 (96%)	8 (4%)	38 49
1	D	200/229 (87%)	192 (96%)	8 (4%)	38 49
All	All	797/916 (87%)	773 (97%)	24 (3%)	48 62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	196	LEU
1	A	215	LYS
1	A	232	HIS
1	B	91	GLU
1	B	157	LYS
1	B	158	GLN
1	B	185	GLN
1	C	4	LYS

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Mol	Chain	Res	Type
1	C	7	GLU
1	C	91	GLU
1	C	127	LYS
1	C	138	LEU
1	C	158	GLN
1	C	165	ASN
1	C	181	ASP
1	D	3	SER
1	D	10	THR
1	D	91	GLU
1	D	127	LYS
1	D	158	GLN
1	D	165	ASN
1	D	194	VAL
1	D	230	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	HIS
1	B	185	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PIA	A	68	1	21,21,22	4.22	7 (33%)	26,29,31	4.48	14 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	PIA	B	68	1	21,21,22	4.10	8 (38%)	26,29,31	4.21	9 (34%)
1	PIA	C	68	1	21,21,22	3.81	8 (38%)	26,29,31	3.57	8 (30%)
1	PIA	D	68	1	21,21,22	4.14	8 (38%)	26,29,31	3.60	4 (15%)

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

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PIA	CA2-C2	-16.35	1.31	1.48
1	D	68	PIA	CA2-C2	-15.65	1.31	1.48
1	B	68	PIA	CA2-C2	-15.21	1.32	1.48
1	C	68	PIA	CA2-C2	-14.62	1.33	1.48
1	A	68	PIA	CA2-N2	-5.32	1.26	1.38
1	B	68	PIA	CA2-N2	-5.23	1.27	1.38
1	D	68	PIA	CA2-N2	-4.92	1.27	1.38
1	B	68	PIA	C2-N3	-4.74	1.28	1.39
1	D	68	PIA	C2-N3	-4.72	1.28	1.39
1	D	68	PIA	CG2-CB2	-4.72	1.37	1.46
1	C	68	PIA	CA2-N2	-4.68	1.28	1.38
1	B	68	PIA	C1-N3	-4.47	1.29	1.37
1	B	68	PIA	CG2-CB2	-4.46	1.38	1.46
1	A	68	PIA	C2-N3	-4.39	1.28	1.39
1	D	68	PIA	C1-N3	-4.20	1.29	1.37
1	C	68	PIA	CG2-CB2	-4.05	1.39	1.46
1	A	68	PIA	CG2-CB2	-4.03	1.39	1.46
1	A	68	PIA	C1-N3	-3.89	1.30	1.37
1	C	68	PIA	C2-N3	-3.82	1.30	1.39
1	C	68	PIA	C1-N3	-3.60	1.30	1.37
1	B	68	PIA	C1-N2	-3.00	1.27	1.32
1	D	68	PIA	C1-N2	-2.53	1.28	1.32
1	A	68	PIA	C1-N2	-2.49	1.28	1.32
1	D	68	PIA	CA3-N3	-2.47	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	68	PIA	OH-CZ	-2.22	1.31	1.37
1	B	68	PIA	CA1-N1	-2.10	1.41	1.48
1	C	68	PIA	C1-N2	-2.10	1.28	1.32
1	D	68	PIA	CB2-CA2	-2.09	1.33	1.35
1	A	68	PIA	CD2-CG2	-2.08	1.35	1.39
1	C	68	PIA	CB2-CA2	-2.08	1.33	1.35
1	B	68	PIA	OH-CZ	-2.06	1.32	1.37

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	68	PIA	CB2-CA2-N2	-8.59	113.48	128.71
1	C	68	PIA	CB2-CA2-N2	-7.88	114.74	128.71
1	A	68	PIA	CB2-CA2-N2	-7.67	115.12	128.71
1	B	68	PIA	CB2-CA2-N2	-7.63	115.19	128.71
1	A	68	PIA	O2-C2-CA2	-6.04	127.50	130.97
1	B	68	PIA	O2-C2-CA2	-4.42	128.43	130.97
1	B	68	PIA	C2-CA2-N2	-4.20	105.84	109.03
1	A	68	PIA	C2-CA2-N2	-3.59	106.30	109.03
1	C	68	PIA	O2-C2-CA2	-2.75	129.39	130.97
1	A	68	PIA	CD1-CE1-CZ	-2.44	117.06	119.86
1	D	68	PIA	O2-C2-CA2	-2.33	129.63	130.97
1	C	68	PIA	N3-C1-N2	-2.33	109.80	111.53
1	A	68	PIA	N3-C1-N2	-2.24	109.87	111.53
1	A	68	PIA	CE2-CD2-CG2	-2.20	118.57	121.29
1	A	68	PIA	CA1-C1-N2	-2.13	120.65	123.71
1	B	68	PIA	N3-C1-N2	-2.09	109.98	111.53
1	C	68	PIA	C2-CA2-N2	-2.01	107.50	109.03
1	C	68	PIA	CA1-C1-N3	2.04	127.45	124.98
1	A	68	PIA	CA3-N3-C1	2.16	129.76	127.38
1	A	68	PIA	CD2-CE2-CZ	2.32	122.53	119.86
1	A	68	PIA	CE1-CD1-CG2	2.33	124.16	121.29
1	B	68	PIA	CA3-N3-C1	2.97	130.65	127.38
1	C	68	PIA	CA2-N2-C1	3.25	108.27	105.54
1	B	68	PIA	CA1-C1-N3	3.38	129.06	124.98
1	A	68	PIA	CA1-C1-N3	3.72	129.47	124.98
1	A	68	PIA	CA2-N2-C1	3.91	108.83	105.54
1	B	68	PIA	CA2-N2-C1	4.11	108.99	105.54
1	C	68	PIA	CA2-C2-N3	9.98	108.31	103.37
1	D	68	PIA	CA2-C2-N3	10.24	108.44	103.37
1	C	68	PIA	CB2-CA2-C2	11.00	137.71	122.24
1	D	68	PIA	CB2-CA2-C2	11.34	138.19	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	PIA	CB2-CA2-C2	11.54	138.47	122.24
1	B	68	PIA	CB2-CA2-C2	11.82	138.87	122.24
1	B	68	PIA	CA2-C2-N3	12.87	109.74	103.37
1	A	68	PIA	CA2-C2-N3	14.20	110.40	103.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	68	PIA	1	0
1	B	68	PIA	1	0
1	C	68	PIA	2	0
1	D	68	PIA	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	227/264 (85%)	0.35	6 (2%)	59	71	28, 41, 65, 91	0
1	B	225/264 (85%)	0.25	3 (1%)	79	87	23, 33, 50, 90	0
1	C	227/264 (85%)	0.50	9 (3%)	42	56	30, 43, 69, 94	0
1	D	227/264 (85%)	0.44	9 (3%)	42	56	23, 37, 65, 92	0
All	All	906/1056 (85%)	0.38	27 (2%)	54	66	23, 39, 65, 94	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	GLY	4.6
1	B	3	SER	4.0
1	A	3	SER	3.7
1	B	232	HIS	3.5
1	D	134	ASP	3.2
1	D	191	ASP	3.2
1	A	158	GLN	3.1
1	D	3	SER	3.1
1	C	52	GLY	3.1
1	C	191	ASP	2.9
1	C	53	LYS	2.9
1	D	133	GLU	2.9
1	C	3	SER	2.7
1	C	6	GLU	2.5
1	D	158	GLN	2.5
1	C	134	ASP	2.5
1	C	7	GLU	2.4
1	A	4	LYS	2.4
1	A	190	GLY	2.3
1	D	213	ASN	2.3
1	A	191	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	113	VAL	2.2
1	D	193	PRO	2.2
1	B	4	LYS	2.2
1	D	183	TYR	2.1
1	A	137	ILE	2.1
1	C	215	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
1	PIA	B	68	20/21	0.94	0.15	-	24,29,32,37	0
1	PIA	A	68	20/21	0.94	0.14	-	29,33,38,39	0
1	PIA	D	68	20/21	0.93	0.15	-	26,31,36,36	0
1	PIA	C	68	20/21	0.90	0.16	-	30,35,39,41	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.