



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:36 PM UTC

PDB ID : 7ZCT / pdb_00007zct
Title : Structure of the red fluorescent protein mScarlet3 at pH 7.5
Authors : Aumonier, S.; Dupuy, J.; Royant, A.
Deposited on : 2022-03-28
Resolution : 1.33 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

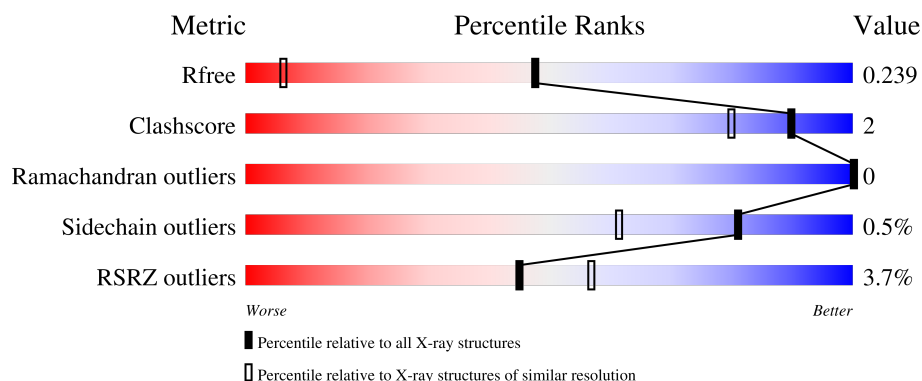
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.33 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2194 (1.36-1.32)
Clashscore	190562	2222 (1.36-1.32)
Ramachandran outliers	187476	2197 (1.36-1.32)
Sidechain outliers	187428	2197 (1.36-1.32)
RSRZ outliers	180081	2193 (1.36-1.32)

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 $\leq 5\%$. 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	227	2% 88% 7% 5%
1	B	227	5% 90% 5% 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3883 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 Red fluorescent protein drFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	11	0
			1816	1162	306	339	9			
1	B	215	Total	C	N	O	S	0	13	0
			1820	1164	307	339	10			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q9U6Y8
A	3	ASP	-	expression tag	UNP Q9U6Y8
A	4	SER	-	expression tag	UNP Q9U6Y8
A	5	THR	-	expression tag	UNP Q9U6Y8
A	6	GLU	-	expression tag	UNP Q9U6Y8
A	7	ALA	-	expression tag	UNP Q9U6Y8
A	18	HIS	ARG	engineered mutation	UNP Q9U6Y8
A	22	SER	THR	engineered mutation	UNP Q9U6Y8
A	23	MET	VAL	engineered mutation	UNP Q9U6Y8
A	42	THR	HIS	engineered mutation	UNP Q9U6Y8
A	43	GLN	ASN	engineered mutation	UNP Q9U6Y8
A	45	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	48	ARG	LYS	engineered mutation	UNP Q9U6Y8
A	58	SER	ALA	engineered mutation	UNP Q9U6Y8
A	67	NRQ	GLN	chromophore	UNP Q9U6Y8
A	?	-	TYR	chromophore	UNP Q9U6Y8
A	?	-	GLY	chromophore	UNP Q9U6Y8
A	71	ARG	LYS	engineered mutation	UNP Q9U6Y8
A	72	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	73	PHE	TYR	engineered mutation	UNP Q9U6Y8
A	74	THR	VAL	engineered mutation	UNP Q9U6Y8
A	84	TRP	LYS	engineered mutation	UNP Q9U6Y8
A	86	GLN	LEU	engineered mutation	UNP Q9U6Y8
A	105	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	107	SER	THR	engineered mutation	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	109	ALA	THR	engineered mutation	UNP Q9U6Y8
A	112	THR	SER	engineered mutation	UNP Q9U6Y8
A	115	GLU	GLN	engineered mutation	UNP Q9U6Y8
A	118	THR	CYS	engineered mutation	UNP Q9U6Y8
A	119	LEU	PHE	engineered mutation	UNP Q9U6Y8
A	125	LEU	PHE	engineered mutation	UNP Q9U6Y8
A	126	ARG	ILE	engineered mutation	UNP Q9U6Y8
A	128	THR	VAL	engineered mutation	UNP Q9U6Y8
A	132	PRO	SER	engineered mutation	UNP Q9U6Y8
A	154	GLU	ARG	engineered mutation	UNP Q9U6Y8
A	156	VAL	GLY	engineered mutation	UNP Q9U6Y8
A	161	ASP	GLU	engineered mutation	UNP Q9U6Y8
A	163	LYS	HIS	engineered mutation	UNP Q9U6Y8
A	164	MET	LYS	engineered mutation	UNP Q9U6Y8
A	167	ARG	LYS	engineered mutation	UNP Q9U6Y8
A	173	ARG	HIS	engineered mutation	UNP Q9U6Y8
A	176	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	177	ASP	GLU	engineered mutation	UNP Q9U6Y8
A	180	THR	SER	engineered mutation	UNP Q9U6Y8
A	181	THR	ILE	engineered mutation	UNP Q9U6Y8
A	183	ARG	MET	engineered mutation	UNP Q9U6Y8
A	190	MET	LEU	engineered mutation	UNP Q9U6Y8
A	193	ALA	TYR	engineered mutation	UNP Q9U6Y8
A	194	PHE	TYR	engineered mutation	UNP Q9U6Y8
A	195	ASN	TYR	engineered mutation	UNP Q9U6Y8
A	196	ILE	VAL	engineered mutation	UNP Q9U6Y8
A	198	ARG	SER	engineered mutation	UNP Q9U6Y8
A	211	VAL	ILE	engineered mutation	UNP Q9U6Y8
A	218	SER	THR	engineered mutation	UNP Q9U6Y8
A	219	VAL	GLU	engineered mutation	UNP Q9U6Y8
A	220	ALA	GLY	engineered mutation	UNP Q9U6Y8
A	223	SER	-	expression tag	UNP Q9U6Y8
A	224	THR	-	expression tag	UNP Q9U6Y8
A	225	GLY	-	expression tag	UNP Q9U6Y8
A	226	GLY	-	expression tag	UNP Q9U6Y8
A	227	SER	-	expression tag	UNP Q9U6Y8
A	228	GLY	-	expression tag	UNP Q9U6Y8
A	229	GLY	-	expression tag	UNP Q9U6Y8
A	230	SER	-	expression tag	UNP Q9U6Y8
B	2	MET	-	initiating methionine	UNP Q9U6Y8
B	3	ASP	-	expression tag	UNP Q9U6Y8
B	4	SER	-	expression tag	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	5	THR	-	expression tag	UNP Q9U6Y8
B	6	GLU	-	expression tag	UNP Q9U6Y8
B	7	ALA	-	expression tag	UNP Q9U6Y8
B	18	HIS	ARG	engineered mutation	UNP Q9U6Y8
B	22	SER	THR	engineered mutation	UNP Q9U6Y8
B	23	MET	VAL	engineered mutation	UNP Q9U6Y8
B	42	THR	HIS	engineered mutation	UNP Q9U6Y8
B	43	GLN	ASN	engineered mutation	UNP Q9U6Y8
B	45	ALA	VAL	engineered mutation	UNP Q9U6Y8
B	48	ARG	LYS	engineered mutation	UNP Q9U6Y8
B	58	SER	ALA	engineered mutation	UNP Q9U6Y8
B	?	-	GLN	deletion	UNP Q9U6Y8
B	?	-	TYR	deletion	UNP Q9U6Y8
B	67	NRQ	GLY	engineered mutation	UNP Q9U6Y8
B	71	ARG	LYS	engineered mutation	UNP Q9U6Y8
B	72	ALA	VAL	engineered mutation	UNP Q9U6Y8
B	73	PHE	TYR	engineered mutation	UNP Q9U6Y8
B	74	THR	VAL	engineered mutation	UNP Q9U6Y8
B	84	TRP	LYS	engineered mutation	UNP Q9U6Y8
B	86	GLN	LEU	engineered mutation	UNP Q9U6Y8
B	105	ALA	VAL	engineered mutation	UNP Q9U6Y8
B	107	SER	THR	engineered mutation	UNP Q9U6Y8
B	109	ALA	THR	engineered mutation	UNP Q9U6Y8
B	112	THR	SER	engineered mutation	UNP Q9U6Y8
B	115	GLU	GLN	engineered mutation	UNP Q9U6Y8
B	118	THR	CYS	engineered mutation	UNP Q9U6Y8
B	119	LEU	PHE	engineered mutation	UNP Q9U6Y8
B	125	LEU	PHE	engineered mutation	UNP Q9U6Y8
B	126	ARG	ILE	engineered mutation	UNP Q9U6Y8
B	128	THR	VAL	engineered mutation	UNP Q9U6Y8
B	132	PRO	SER	engineered mutation	UNP Q9U6Y8
B	154	GLU	ARG	engineered mutation	UNP Q9U6Y8
B	156	VAL	GLY	engineered mutation	UNP Q9U6Y8
B	161	ASP	GLU	engineered mutation	UNP Q9U6Y8
B	163	LYS	HIS	engineered mutation	UNP Q9U6Y8
B	164	MET	LYS	engineered mutation	UNP Q9U6Y8
B	167	ARG	LYS	engineered mutation	UNP Q9U6Y8
B	173	ARG	HIS	engineered mutation	UNP Q9U6Y8
B	176	ALA	VAL	engineered mutation	UNP Q9U6Y8
B	177	ASP	GLU	engineered mutation	UNP Q9U6Y8
B	180	THR	SER	engineered mutation	UNP Q9U6Y8
B	181	THR	ILE	engineered mutation	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	183	ARG	MET	engineered mutation	UNP Q9U6Y8
B	190	MET	LEU	engineered mutation	UNP Q9U6Y8
B	193	ALA	TYR	engineered mutation	UNP Q9U6Y8
B	194	PHE	TYR	engineered mutation	UNP Q9U6Y8
B	195	ASN	TYR	engineered mutation	UNP Q9U6Y8
B	196	ILE	VAL	engineered mutation	UNP Q9U6Y8
B	198	ARG	SER	engineered mutation	UNP Q9U6Y8
B	211	VAL	ILE	engineered mutation	UNP Q9U6Y8
B	218	SER	THR	engineered mutation	UNP Q9U6Y8
B	219	VAL	GLU	engineered mutation	UNP Q9U6Y8
B	220	ALA	GLY	engineered mutation	UNP Q9U6Y8
B	223	SER	-	expression tag	UNP Q9U6Y8
B	224	THR	-	expression tag	UNP Q9U6Y8
B	225	GLY	-	expression tag	UNP Q9U6Y8
B	226	GLY	-	expression tag	UNP Q9U6Y8
B	227	SER	-	expression tag	UNP Q9U6Y8
B	228	GLY	-	expression tag	UNP Q9U6Y8
B	229	GLY	-	expression tag	UNP Q9U6Y8
B	230	SER	-	expression tag	UNP Q9U6Y8

- Molecule 2 is water.

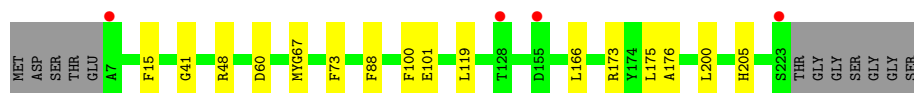
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	118	Total O 120 120	0	2
2	B	126	Total O 127 127	0	3

3 Residue-property plots [i](#)

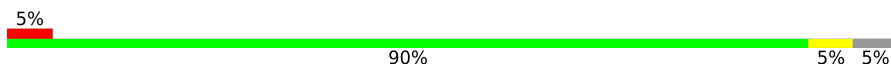
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

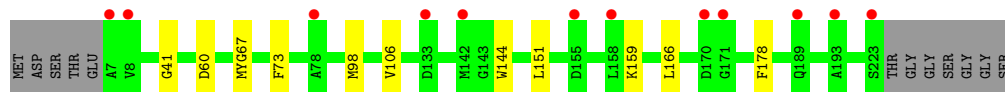
- Molecule 1: Red fluorescent protein drFP583

Chain A: 



- Molecule 1: Red fluorescent protein drFP583

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.23Å 61.86Å 110.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.78 – 1.33 42.78 – 1.33	Depositor EDS
% Data completeness (in resolution range)	97.3 (42.78-1.33) 97.5 (42.78-1.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.33Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.228 0.209 , 0.239	Depositor DCC
R_{free} test set	1157 reflections (1.26%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3883	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NRQ

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	0.95	1/1854 (0.1%)	1.11	1/2499 (0.0%)
1	B	0.91	0/1866	1.06	0/2515
All	All	0.93	1/3720 (0.0%)	1.09	1/5014 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	HIS	CE1-NE2	5.13	1.37	1.32

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	PHE	CB-CA-C	5.54	117.42	109.11

There are no chirality outliers.

There are no planarity outliers.

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	1816	0	1772	7	0
1	B	1820	0	1777	6	0
2	A	120	0	0	0	0
2	B	127	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3883	0	3549	13	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 2.

All (13) 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:41:GLY:HA2	1:A:73:PHE:O	2.04	0.58
1:B:98[B]:MET:HE3	1:B:106:VAL:HB	1.93	0.50
1:B:98[B]:MET:SD	1:B:178:PHE:CZ	3.06	0.49
1:B:41:GLY:HA2	1:B:73:PHE:O	2.15	0.46
1:A:60:ASP:HB3	1:A:166:LEU:HD21	1.99	0.44
1:B:151:LEU:HA	1:B:159:LYS:O	2.17	0.44
1:B:60:ASP:HB3	1:B:166:LEU:HD21	2.00	0.43
1:A:100:PHE:CD2	1:A:176:ALA:HB2	2.54	0.42
1:A:200[B]:LEU:C	1:A:200[B]:LEU:HD23	2.45	0.41
1:A:15:PHE:HA	1:A:119:LEU:O	2.20	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.95	0.41
1:B:144:TRP:CZ3	1:B:166:LEU:HG	2.56	0.41
1:A:101[B]:GLU:HG3	1:A:175:LEU:HB2	2.03	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	221/227 (97%)	218 (99%)	3 (1%)	0	100	100
1	B	223/227 (98%)	219 (98%)	4 (2%)	0	100	100
All	All	444/454 (98%)	437 (98%)	7 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/191 (102%)	192 (99%)	2 (1%)	68	37
1	B	194/191 (102%)	194 (100%)	0	100	100
All	All	388/382 (102%)	386 (100%)	2 (0%)	81	61

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	173	ARG

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	110	GLN
1	B	99	ASN
1	B	110	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	NRQ	A	67	1	24,24,25	2.08	5 (20%)	24,32,34	2.21	9 (37%)
1	NRQ	B	67	1	24,24,25	2.47	4 (16%)	24,32,34	2.42	8 (33%)

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	NRQ	A	67	1	-	0/9/31/32	0/2/2/2
1	NRQ	B	67	1	-	0/9/31/32	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	NRQ	CB2-CA2	10.05	1.44	1.35
1	A	67	NRQ	CB2-CA2	8.02	1.42	1.35
1	B	67	NRQ	CA2-C2	-3.69	1.44	1.48
1	A	67	NRQ	C1-N2	3.14	1.39	1.33
1	B	67	NRQ	C2-N3	-3.12	1.32	1.40
1	A	67	NRQ	C2-N3	-2.98	1.33	1.40
1	A	67	NRQ	O2-C2	2.39	1.27	1.23
1	A	67	NRQ	CE2-CD2	2.18	1.42	1.38
1	B	67	NRQ	C1-N2	2.17	1.37	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	NRQ	O2-C2-CA2	-7.98	125.93	131.02
1	A	67	NRQ	CA2-C2-N3	6.37	108.85	103.50
1	B	67	NRQ	CA2-C2-N3	4.21	107.04	103.50
1	A	67	NRQ	CD1-CG2-CD2	3.81	123.30	117.65
1	B	67	NRQ	CD1-CG2-CD2	3.48	122.82	117.65
1	B	67	NRQ	CE2-CD2-CG2	-3.36	116.88	121.22
1	A	67	NRQ	O2-C2-CA2	-3.18	128.99	131.02
1	A	67	NRQ	CE2-CD2-CG2	-3.11	117.21	121.22
1	B	67	NRQ	C3-CA3-N3	2.75	118.69	112.43
1	A	67	NRQ	O3-C3-CA3	-2.60	113.77	125.47
1	A	67	NRQ	CA3-N3-C1	2.57	133.46	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	NRQ	CD1-CG2-CB2	-2.53	112.52	121.22
1	B	67	NRQ	O3-C3-CA3	-2.52	114.14	125.47
1	A	67	NRQ	CD1-CG2-CB2	-2.51	112.60	121.22
1	A	67	NRQ	C3-CA3-N3	2.17	117.38	112.43
1	A	67	NRQ	CE1-CD1-CG2	-2.05	118.57	121.22
1	B	67	NRQ	CB2-CA2-C2	-2.02	119.91	122.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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, 95th 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	214/227 (94%)	0.46	4 (1%) 66 75	8, 18, 29, 37	11 (5%)
1	B	214/227 (94%)	0.45	12 (5%) 30 41	8, 18, 29, 52	13 (6%)
All	All	428/454 (94%)	0.46	16 (3%) 45 57	8, 18, 29, 52	24 (5%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	5.1
1	B	170	ASP	5.1
1	A	7	ALA	3.9
1	B	171	GLY	3.3
1	A	155	ASP	3.3
1	B	155	ASP	3.3
1	B	223	SER	3.0
1	A	223	SER	2.7
1	B	78	ALA	2.7
1	B	158	LEU	2.7
1	B	133	ASP	2.5
1	B	142	MET	2.2
1	B	8	VAL	2.1
1	A	128	THR	2.1
1	B	193	ALA	2.1
1	B	189	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NRQ	A	67	23/24	0.98	0.05	12,13,15,17	0
1	NRQ	B	67	23/24	0.98	0.05	12,14,16,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.