



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 02:16 PM EDT

PDB ID : 3RWA  
Title : Crystal structure of circular-permuted mKate  
Authors : Wang, Q.; Byrnes, L.; Sondermann, H.  
Deposited on : unknown  
Resolution : 1.67 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030345

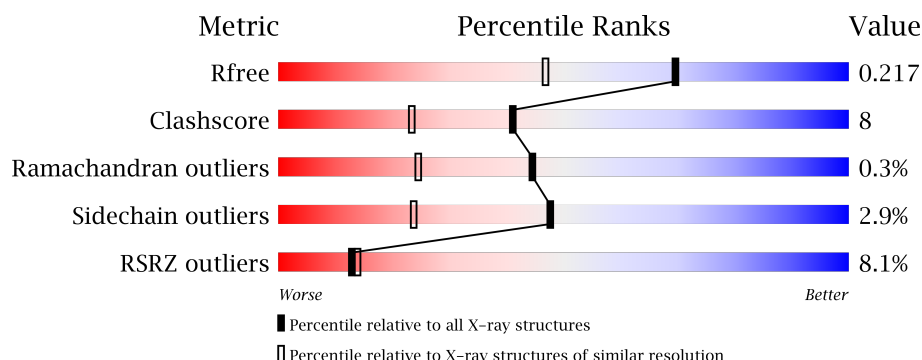
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.67 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.



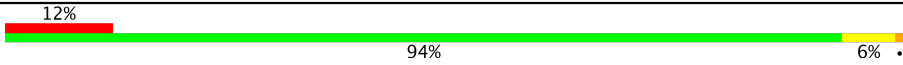
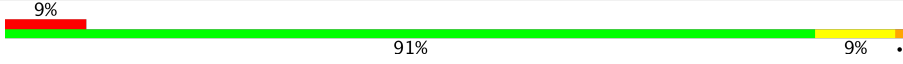
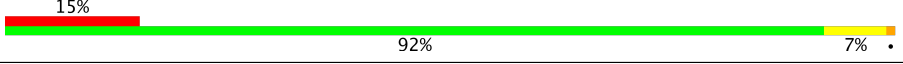
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5252 (1.70-1.66)
Clashscore	112137	5803 (1.70-1.66)
Ramachandran outliers	110173	5704 (1.70-1.66)
Sidechain outliers	110143	5703 (1.70-1.66)
RSRZ outliers	101464	5298 (1.70-1.66)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	233	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	B	233	<div> <div>2%</div> <div>90%</div> <div>9%</div> </div>
1	C	233	<div> <div>12%</div> <div>76%</div> <div>21%</div> </div>
1	D	233	<div> <div>6%</div> <div>93%</div> <div>6%</div> </div>
1	E	233	<div> <div>6%</div> <div>90%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
1	H	233	

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	NRQ	A	133	-	-	X	-
1	NRQ	C	133	-	-	X	-
1	NRQ	D	133	-	-	X	-
1	NRQ	F	133	-	-	X	-
1	NRQ	G	133	-	-	X	-
1	NRQ	H	133	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16152 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 Fluorescent protein FP480.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	B	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	C	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	D	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	E	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	F	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	G	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			
1	H	233	Total	C	N	O	S	0	0	0
			1839	1164	312	349	14			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LEU	PHE	See Remark 999	UNP D0VX33
A	30	ARG	TYR	See Remark 999	UNP D0VX33
A	64	ALA	-	linker	UNP D0VX33
A	65	GLY	-	linker	UNP D0VX33
A	66	GLY	-	linker	UNP D0VX33
A	67	THR	-	linker	UNP D0VX33
A	68	GLY	-	linker	UNP D0VX33
A	69	GLY	-	linker	UNP D0VX33
A	70	SER	-	linker	UNP D0VX33
A	111	MET	GLN	See Remark 999	UNP D0VX33
A	?	-	MET	chromophore	UNP D0VX33
A	?	-	TYR	chromophore	UNP D0VX33
A	133	NRQ	GLY	chromophore	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	137	LYS	HIS	See Remark 999	UNP D0VX33
A	150	PHE	TRP	See Remark 999	UNP D0VX33
A	213	SER	HIS	See Remark 999	UNP D0VX33
A	228	SER	ALA	See Remark 999	UNP D0VX33
A	230	MET	LEU	See Remark 999	UNP D0VX33
B	7	LEU	PHE	See Remark 999	UNP D0VX33
B	30	ARG	TYR	See Remark 999	UNP D0VX33
B	64	ALA	-	linker	UNP D0VX33
B	65	GLY	-	linker	UNP D0VX33
B	66	GLY	-	linker	UNP D0VX33
B	67	THR	-	linker	UNP D0VX33
B	68	GLY	-	linker	UNP D0VX33
B	69	GLY	-	linker	UNP D0VX33
B	70	SER	-	linker	UNP D0VX33
B	111	MET	GLN	See Remark 999	UNP D0VX33
B	?	-	MET	chromophore	UNP D0VX33
B	?	-	TYR	chromophore	UNP D0VX33
B	133	NRQ	GLY	chromophore	UNP D0VX33
B	137	LYS	HIS	See Remark 999	UNP D0VX33
B	150	PHE	TRP	See Remark 999	UNP D0VX33
B	213	SER	HIS	See Remark 999	UNP D0VX33
B	228	SER	ALA	See Remark 999	UNP D0VX33
B	230	MET	LEU	See Remark 999	UNP D0VX33
C	7	LEU	PHE	See Remark 999	UNP D0VX33
C	30	ARG	TYR	See Remark 999	UNP D0VX33
C	64	ALA	-	linker	UNP D0VX33
C	65	GLY	-	linker	UNP D0VX33
C	66	GLY	-	linker	UNP D0VX33
C	67	THR	-	linker	UNP D0VX33
C	68	GLY	-	linker	UNP D0VX33
C	69	GLY	-	linker	UNP D0VX33
C	70	SER	-	linker	UNP D0VX33
C	111	MET	GLN	See Remark 999	UNP D0VX33
C	?	-	MET	chromophore	UNP D0VX33
C	?	-	TYR	chromophore	UNP D0VX33
C	133	NRQ	GLY	chromophore	UNP D0VX33
C	137	LYS	HIS	See Remark 999	UNP D0VX33
C	150	PHE	TRP	See Remark 999	UNP D0VX33
C	213	SER	HIS	See Remark 999	UNP D0VX33
C	228	SER	ALA	See Remark 999	UNP D0VX33
C	230	MET	LEU	See Remark 999	UNP D0VX33
D	7	LEU	PHE	See Remark 999	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	ARG	TYR	See Remark 999	UNP D0VX33
D	64	ALA	-	linker	UNP D0VX33
D	65	GLY	-	linker	UNP D0VX33
D	66	GLY	-	linker	UNP D0VX33
D	67	THR	-	linker	UNP D0VX33
D	68	GLY	-	linker	UNP D0VX33
D	69	GLY	-	linker	UNP D0VX33
D	70	SER	-	linker	UNP D0VX33
D	111	MET	GLN	See Remark 999	UNP D0VX33
D	?	-	MET	chromophore	UNP D0VX33
D	?	-	TYR	chromophore	UNP D0VX33
D	133	NRQ	GLY	chromophore	UNP D0VX33
D	137	LYS	HIS	See Remark 999	UNP D0VX33
D	150	PHE	TRP	See Remark 999	UNP D0VX33
D	213	SER	HIS	See Remark 999	UNP D0VX33
D	228	SER	ALA	See Remark 999	UNP D0VX33
D	230	MET	LEU	See Remark 999	UNP D0VX33
E	7	LEU	PHE	See Remark 999	UNP D0VX33
E	30	ARG	TYR	See Remark 999	UNP D0VX33
E	64	ALA	-	linker	UNP D0VX33
E	65	GLY	-	linker	UNP D0VX33
E	66	GLY	-	linker	UNP D0VX33
E	67	THR	-	linker	UNP D0VX33
E	68	GLY	-	linker	UNP D0VX33
E	69	GLY	-	linker	UNP D0VX33
E	70	SER	-	linker	UNP D0VX33
E	111	MET	GLN	See Remark 999	UNP D0VX33
E	?	-	MET	chromophore	UNP D0VX33
E	?	-	TYR	chromophore	UNP D0VX33
E	133	NRQ	GLY	chromophore	UNP D0VX33
E	137	LYS	HIS	See Remark 999	UNP D0VX33
E	150	PHE	TRP	See Remark 999	UNP D0VX33
E	213	SER	HIS	See Remark 999	UNP D0VX33
E	228	SER	ALA	See Remark 999	UNP D0VX33
E	230	MET	LEU	See Remark 999	UNP D0VX33
F	7	LEU	PHE	See Remark 999	UNP D0VX33
F	30	ARG	TYR	See Remark 999	UNP D0VX33
F	64	ALA	-	linker	UNP D0VX33
F	65	GLY	-	linker	UNP D0VX33
F	66	GLY	-	linker	UNP D0VX33
F	67	THR	-	linker	UNP D0VX33
F	68	GLY	-	linker	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
F	69	GLY	-	linker	UNP D0VX33
F	70	SER	-	linker	UNP D0VX33
F	111	MET	GLN	See Remark 999	UNP D0VX33
F	?	-	MET	chromophore	UNP D0VX33
F	?	-	TYR	chromophore	UNP D0VX33
F	133	NRQ	GLY	chromophore	UNP D0VX33
F	137	LYS	HIS	See Remark 999	UNP D0VX33
F	150	PHE	TRP	See Remark 999	UNP D0VX33
F	213	SER	HIS	See Remark 999	UNP D0VX33
F	228	SER	ALA	See Remark 999	UNP D0VX33
F	230	MET	LEU	See Remark 999	UNP D0VX33
G	7	LEU	PHE	See Remark 999	UNP D0VX33
G	30	ARG	TYR	See Remark 999	UNP D0VX33
G	64	ALA	-	linker	UNP D0VX33
G	65	GLY	-	linker	UNP D0VX33
G	66	GLY	-	linker	UNP D0VX33
G	67	THR	-	linker	UNP D0VX33
G	68	GLY	-	linker	UNP D0VX33
G	69	GLY	-	linker	UNP D0VX33
G	70	SER	-	linker	UNP D0VX33
G	111	MET	GLN	See Remark 999	UNP D0VX33
G	?	-	MET	chromophore	UNP D0VX33
G	?	-	TYR	chromophore	UNP D0VX33
G	133	NRQ	GLY	chromophore	UNP D0VX33
G	137	LYS	HIS	See Remark 999	UNP D0VX33
G	150	PHE	TRP	See Remark 999	UNP D0VX33
G	213	SER	HIS	See Remark 999	UNP D0VX33
G	228	SER	ALA	See Remark 999	UNP D0VX33
G	230	MET	LEU	See Remark 999	UNP D0VX33
H	7	LEU	PHE	See Remark 999	UNP D0VX33
H	30	ARG	TYR	See Remark 999	UNP D0VX33
H	64	ALA	-	linker	UNP D0VX33
H	65	GLY	-	linker	UNP D0VX33
H	66	GLY	-	linker	UNP D0VX33
H	67	THR	-	linker	UNP D0VX33
H	68	GLY	-	linker	UNP D0VX33
H	69	GLY	-	linker	UNP D0VX33
H	70	SER	-	linker	UNP D0VX33
H	111	MET	GLN	See Remark 999	UNP D0VX33
H	?	-	MET	chromophore	UNP D0VX33
H	?	-	TYR	chromophore	UNP D0VX33
H	133	NRQ	GLY	chromophore	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
H	137	LYS	HIS	See Remark 999	UNP D0VX33
H	150	PHE	TRP	See Remark 999	UNP D0VX33
H	213	SER	HIS	See Remark 999	UNP D0VX33
H	228	SER	ALA	See Remark 999	UNP D0VX33
H	230	MET	LEU	See Remark 999	UNP D0VX33

- Molecule 2 is water.

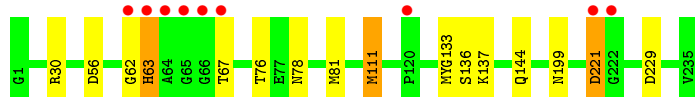
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	213	Total O 213 213	0	0
2	B	216	Total O 216 216	0	0
2	C	186	Total O 186 186	0	0
2	D	178	Total O 178 178	0	0
2	E	194	Total O 194 194	0	0
2	F	169	Total O 169 169	0	0
2	G	154	Total O 154 154	0	0
2	H	130	Total O 130 130	0	0



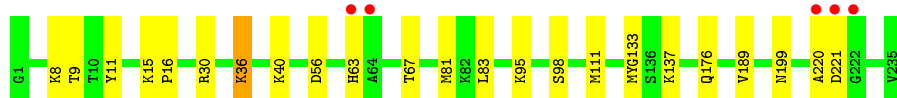
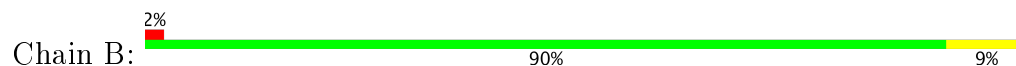
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

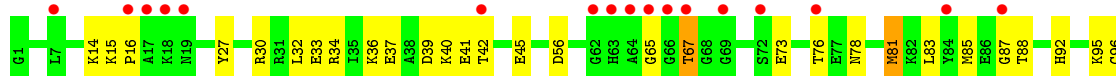
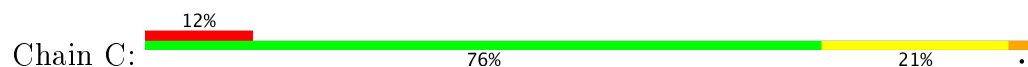
- Molecule 1: Fluorescent protein FP480



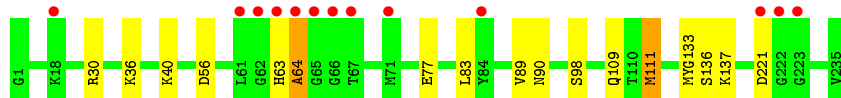
- Molecule 1: Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480

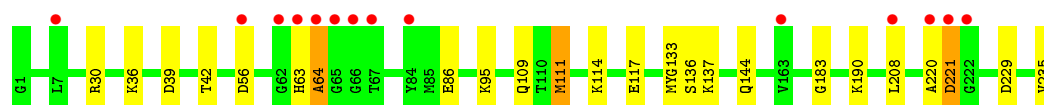


- Molecule 1: Fluorescent protein FP480

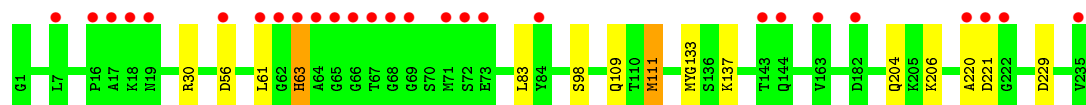
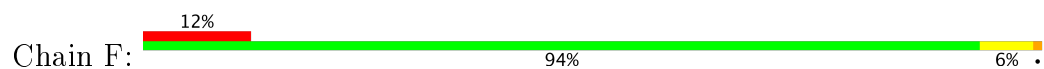


- Molecule 1: Fluorescent protein FP480

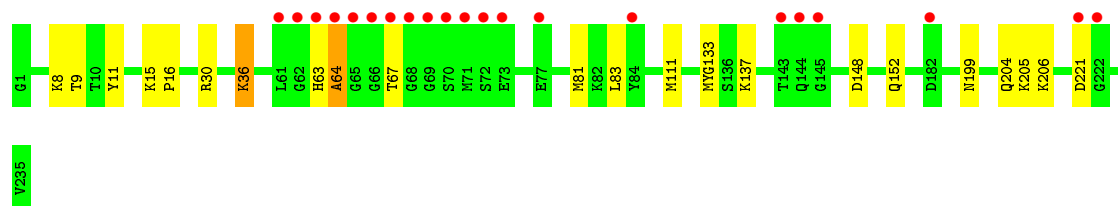




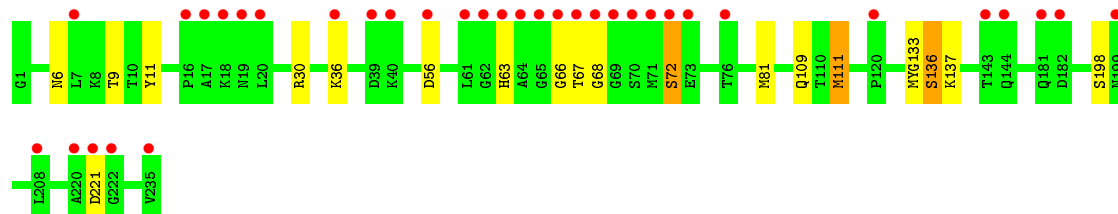
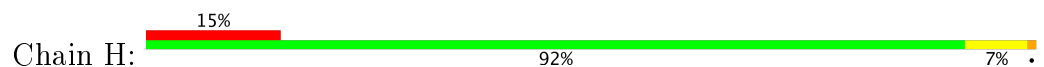
- Molecule 1: Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480



- Molecule 1: Fluorescent protein FP480



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.36Å 93.28Å 194.37Å 90.00° 96.52° 90.00°	Depositor
Resolution (Å)	38.31 – 1.67 38.31 – 1.67	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.31-1.67) 97.5 (38.31-1.67)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.73 (at 1.67Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.7.1_743	Depositor
R, $R_{free}$	0.182 , 0.215 0.193 , 0.217	Depositor DCC
$R_{free}$ test set	2000 reflections (0.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/1856	0.60	0/2502
1	B	0.38	0/1856	0.59	0/2502
1	C	0.31	0/1856	0.52	0/2502
1	D	0.36	0/1856	0.56	0/2502
1	E	0.34	0/1856	0.55	0/2502
1	F	0.35	0/1856	0.55	0/2502
1	G	0.34	0/1856	0.55	0/2502
1	H	0.31	0/1856	0.51	0/2502
All	All	0.35	0/14848	0.55	0/20016

There are no bond length outliers.

There are no bond angle outliers.

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	1839	0	1802	23	0
1	B	1839	0	1802	25	0
1	C	1839	0	1802	55	0
1	D	1839	0	1802	24	0
1	E	1839	0	1802	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1839	0	1802	23	0
1	G	1839	0	1802	32	0
1	H	1839	0	1802	22	0
2	A	213	0	0	5	0
2	B	216	0	0	3	0
2	C	186	0	0	3	0
2	D	178	0	0	0	0
2	E	194	0	0	6	0
2	F	169	0	0	3	0
2	G	154	0	0	3	0
2	H	130	0	0	2	0
All	All	16152	0	14416	236	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 8.

All (236) 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:63:HIS:CB	1:D:64:ALA:HB3	1.49	1.40
1:F:61:LEU:HD12	2:F:461:HOH:O	1.26	1.34
1:G:63:HIS:HB2	1:G:64:ALA:CB	1.58	1.32
1:G:63:HIS:CB	1:G:64:ALA:HB2	1.65	1.26
1:D:63:HIS:HB3	1:D:64:ALA:CB	1.72	1.18
1:E:63:HIS:CA	1:E:64:ALA:HB3	1.73	1.18
1:E:63:HIS:HA	1:E:64:ALA:CB	1.75	1.16
1:G:63:HIS:CA	1:G:64:ALA:HB2	1.81	1.11
1:G:63:HIS:HB2	1:G:64:ALA:HB2	1.10	1.05
1:G:63:HIS:CB	1:G:64:ALA:CB	2.30	1.01
1:E:63:HIS:HA	1:E:64:ALA:HB3	1.00	0.99
1:D:63:HIS:HA	1:D:64:ALA:HB2	1.41	0.99
1:D:63:HIS:CB	1:D:64:ALA:CB	2.32	0.99
1:C:130:THR:O	1:C:133:NRQ:C1	2.12	0.97
1:D:63:HIS:CA	1:D:64:ALA:CB	2.42	0.96
1:B:111:MET:HG3	1:B:133:NRQ:HE3	1.48	0.95
1:C:67:THR:HG23	2:C:362:HOH:O	1.64	0.95
1:H:111:MET:HG3	1:H:133:NRQ:CE	1.97	0.94
1:G:63:HIS:HA	1:G:64:ALA:HB2	1.50	0.92
1:C:39:ASP:HB2	1:C:42:THR:OG1	1.68	0.92
1:E:63:HIS:HB3	1:E:64:ALA:C	1.91	0.91
1:C:30:ARG:HH22	1:C:137:LYS:NZ	1.68	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:HIS:HB2	1:G:64:ALA:HB3	1.51	0.89
1:D:111:MET:HG3	1:D:133:NRQ:CE	2.04	0.88
1:D:111:MET:HG3	1:D:133:NRQ:HE3	1.56	0.86
1:B:111:MET:HG3	1:B:133:NRQ:CE	2.06	0.86
1:H:111:MET:HG3	1:H:133:NRQ:HE3	1.58	0.85
1:A:62:GLY:O	1:A:63:HIS:CG	2.30	0.84
1:E:183:GLY:O	2:E:470:HOH:O	1.96	0.83
1:F:63:HIS:O	1:F:63:HIS:CD2	2.30	0.83
1:D:63:HIS:HA	1:D:64:ALA:CB	2.05	0.83
1:A:111:MET:HG3	1:A:133:NRQ:CE	2.10	0.82
1:C:40:LYS:HE2	1:C:120:PRO:HG3	1.59	0.82
1:H:133:NRQ:N2	1:H:133:NRQ:HD2	1.94	0.81
1:F:63:HIS:O	1:F:63:HIS:CG	2.33	0.80
1:C:30:ARG:HH22	1:C:137:LYS:HZ1	1.29	0.79
1:E:133:NRQ:N2	1:E:133:NRQ:HD2	1.97	0.79
1:C:111:MET:HG3	1:C:133:NRQ:CE	2.13	0.79
1:G:111:MET:HG3	1:G:133:NRQ:CE	2.13	0.79
1:E:111:MET:HG3	1:E:133:NRQ:CE	2.14	0.78
1:H:111:MET:HG3	1:H:133:NRQ:HE1A	1.66	0.77
1:C:109:GLN:HE22	1:C:136:SER:HB3	1.49	0.77
1:D:133:NRQ:N2	1:D:133:NRQ:HD2	2.00	0.77
1:F:133:NRQ:HD2	1:F:133:NRQ:N2	1.99	0.77
1:B:133:NRQ:HD2	1:B:133:NRQ:N2	2.00	0.77
1:G:199:ASN:OD1	2:G:362:HOH:O	2.02	0.77
1:A:133:NRQ:N2	1:A:133:NRQ:HD2	2.00	0.76
1:H:109:GLN:HE22	1:H:136:SER:HB3	1.50	0.76
1:G:8:LYS:NZ	2:G:369:HOH:O	2.18	0.76
1:E:111:MET:HG3	1:E:133:NRQ:HE3	1.67	0.76
1:H:30:ARG:HH22	1:H:137:LYS:NZ	1.84	0.76
1:C:133:NRQ:HD2	1:C:133:NRQ:N2	2.00	0.76
1:G:133:NRQ:N2	1:G:133:NRQ:HD2	2.01	0.76
1:E:63:HIS:HB3	1:E:64:ALA:O	1.87	0.75
1:B:199:ASN:OD1	2:B:504:HOH:O	2.06	0.73
1:E:63:HIS:CB	1:E:64:ALA:HB3	2.18	0.72
1:D:63:HIS:HB3	1:D:64:ALA:HB3	0.75	0.72
1:A:111:MET:HG3	1:A:133:NRQ:HE3	1.70	0.71
1:F:30:ARG:HH22	1:F:137:LYS:NZ	1.88	0.71
1:G:111:MET:HG3	1:G:133:NRQ:HE3	1.72	0.71
1:A:199:ASN:OD1	2:A:412:HOH:O	2.07	0.71
1:F:133:NRQ:HA31	1:F:133:NRQ:N1	2.05	0.71
1:D:30:ARG:HH22	1:D:137:LYS:NZ	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ARG:HH22	1:E:137:LYS:NZ	1.88	0.71
1:B:220:ALA:O	1:B:221:ASP:CG	2.30	0.70
1:E:220:ALA:C	1:E:221:ASP:OD2	2.30	0.70
1:E:229:ASP:HB2	2:E:349:HOH:O	1.90	0.70
1:G:221:ASP:OD1	1:H:198:SER:OG	2.09	0.70
1:F:111:MET:HG3	1:F:133:NRQ:CE	2.21	0.70
1:F:220:ALA:O	1:F:221:ASP:CG	2.30	0.70
1:C:220:ALA:C	1:C:221:ASP:OD2	2.30	0.69
1:E:220:ALA:O	1:E:221:ASP:CG	2.30	0.69
1:A:63:HIS:C	1:A:63:HIS:HD1	1.96	0.69
1:A:30:ARG:HH22	1:A:137:LYS:NZ	1.91	0.68
1:B:111:MET:CG	1:B:133:NRQ:HE3	2.24	0.68
1:G:133:NRQ:N1	1:G:133:NRQ:HA31	2.09	0.68
1:H:133:NRQ:HA31	1:H:133:NRQ:N1	2.09	0.68
1:B:63:HIS:CE1	1:E:39:ASP:OD2	2.47	0.67
1:C:111:MET:HG3	1:C:133:NRQ:HE1A	1.76	0.67
1:E:39:ASP:HB3	1:E:42:THR:OG1	1.94	0.67
1:E:208:LEU:HD12	1:E:235:VAL:HG22	1.78	0.66
1:C:95:LYS:HB2	1:C:117:GLU:HB2	1.77	0.66
1:E:133:NRQ:HA31	1:E:133:NRQ:N1	2.11	0.65
1:B:30:ARG:HH22	1:B:137:LYS:NZ	1.93	0.65
1:C:130:THR:O	1:C:133:NRQ:N3	2.29	0.65
1:E:229:ASP:OD2	2:E:349:HOH:O	2.15	0.65
1:C:15:LYS:HG3	1:C:16:PRO:HD2	1.79	0.65
1:C:133:NRQ:HA31	1:C:133:NRQ:N1	2.11	0.65
1:D:133:NRQ:N1	1:D:133:NRQ:HA31	2.12	0.64
1:A:62:GLY:O	1:A:63:HIS:ND1	2.30	0.64
1:F:61:LEU:CD1	2:F:461:HOH:O	2.07	0.63
1:E:30:ARG:HH22	1:E:137:LYS:HZ3	1.46	0.63
1:B:8:LYS:NZ	2:B:402:HOH:O	2.30	0.63
1:H:6:ASN:ND2	2:H:360:HOH:O	2.06	0.63
1:C:30:ARG:NH2	1:C:137:LYS:NZ	2.43	0.63
1:D:111:MET:CG	1:D:133:NRQ:HE3	2.29	0.63
1:E:190:LYS:NZ	2:E:418:HOH:O	2.33	0.62
1:A:144:GLN:HG3	2:A:343:HOH:O	1.97	0.62
1:C:39:ASP:CB	1:C:42:THR:OG1	2.44	0.62
1:F:111:MET:HG3	1:F:133:NRQ:HE3	1.81	0.61
1:C:208:LEU:CD1	1:C:235:VAL:HG22	2.31	0.61
1:G:204:GLN:HB3	1:G:206:LYS:HE3	1.82	0.61
1:C:111:MET:HG3	1:C:133:NRQ:HE3	1.81	0.61
1:A:111:MET:HG3	1:A:133:NRQ:HE1A	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:MET:HG3	1:G:133:NRQ:HE1A	1.81	0.60
1:C:221:ASP:N	1:C:221:ASP:OD2	2.34	0.60
1:G:30:ARG:HH22	1:G:137:LYS:NZ	2.00	0.59
1:D:111:MET:HG3	1:D:133:NRQ:HE1A	1.83	0.59
1:D:30:ARG:HH22	1:D:137:LYS:HZ2	1.50	0.59
1:E:220:ALA:C	1:E:221:ASP:CG	2.63	0.57
1:C:85:MET:HB3	1:C:96:CYS:HB2	1.86	0.57
1:C:109:GLN:NE2	1:C:136:SER:HB3	2.19	0.57
1:A:133:NRQ:HA31	1:A:133:NRQ:N1	2.19	0.57
1:A:63:HIS:C	1:A:63:HIS:ND1	2.57	0.56
1:C:45:GLU:OE1	2:C:361:HOH:O	2.18	0.56
1:B:30:ARG:HH22	1:B:137:LYS:HZ1	1.54	0.56
1:C:83:LEU:HB3	1:C:98:SER:OG	2.04	0.56
1:F:30:ARG:HH22	1:F:137:LYS:HZ1	1.53	0.56
1:H:109:GLN:NE2	1:H:136:SER:HB3	2.19	0.56
1:B:133:NRQ:HA31	1:B:133:NRQ:N1	2.19	0.56
1:C:30:ARG:HH22	1:C:137:LYS:HZ2	1.46	0.56
1:E:133:NRQ:N2	1:E:133:NRQ:CD2	2.69	0.56
1:C:103:LYS:HB2	1:C:106:GLU:HB2	1.88	0.56
1:H:111:MET:CG	1:H:133:NRQ:CE	2.80	0.56
1:H:30:ARG:HH22	1:H:137:LYS:HZ2	1.51	0.56
1:G:63:HIS:CB	1:G:64:ALA:HB3	2.21	0.55
1:C:40:LYS:O	1:C:41:GLU:HB2	2.06	0.55
1:E:111:MET:HG3	1:E:133:NRQ:HE1A	1.88	0.55
1:C:33:GLU:OE2	1:F:61:LEU:HG	2.07	0.55
1:E:144:GLN:HG3	2:E:314:HOH:O	2.05	0.54
1:F:229:ASP:OD2	2:F:334:HOH:O	2.18	0.54
1:A:30:ARG:HH22	1:A:137:LYS:HZ3	1.55	0.54
1:H:133:NRQ:N2	1:H:133:NRQ:CD2	2.66	0.54
1:B:63:HIS:HE1	1:E:39:ASP:OD2	1.88	0.53
1:H:30:ARG:HH22	1:H:137:LYS:HZ3	1.53	0.53
1:H:111:MET:CG	1:H:133:NRQ:HE3	2.35	0.53
1:B:133:NRQ:N2	1:B:133:NRQ:CD2	2.71	0.53
1:C:95:LYS:HB2	1:C:117:GLU:CB	2.38	0.53
1:C:40:LYS:HE2	1:C:120:PRO:CG	2.34	0.53
1:C:220:ALA:O	1:C:222:GLY:N	2.42	0.53
1:A:133:NRQ:CD2	1:A:133:NRQ:N2	2.72	0.52
1:E:39:ASP:HB3	1:E:42:THR:HG1	1.72	0.52
1:C:39:ASP:HB2	1:C:42:THR:HG1	1.71	0.52
1:D:109:GLN:HE22	1:D:136:SER:HB3	1.73	0.52
1:C:229:ASP:HB2	2:C:332:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:NRQ:N2	1:G:133:NRQ:CD2	2.71	0.51
1:E:208:LEU:CD1	1:E:235:VAL:HG22	2.40	0.51
1:C:39:ASP:CB	1:C:42:THR:HG1	2.23	0.51
1:D:133:NRQ:CD2	1:D:133:NRQ:N2	2.71	0.51
1:C:30:ARG:NH2	1:C:137:LYS:HZ2	2.07	0.51
1:C:81:MET:HE3	1:C:100:GLY:HA3	1.91	0.51
1:C:76:THR:OG1	1:C:78:ASN:O	2.28	0.51
1:D:89:VAL:O	1:D:90:ASN:HB2	2.11	0.50
1:D:111:MET:CG	1:D:133:NRQ:CE	2.85	0.50
1:C:27:TYR:N	1:C:27:TYR:CD1	2.80	0.50
1:C:133:NRQ:CD2	1:C:133:NRQ:N2	2.72	0.50
1:F:220:ALA:O	1:F:221:ASP:OD2	2.30	0.49
1:D:63:HIS:CG	1:D:64:ALA:HB3	2.38	0.48
1:A:229:ASP:OD2	2:A:386:HOH:O	2.20	0.48
1:A:30:ARG:HH22	1:A:137:LYS:HZ2	1.61	0.48
1:C:208:LEU:HD11	1:C:235:VAL:HG22	1.94	0.48
1:F:111:MET:HG3	1:F:133:NRQ:HE1A	1.94	0.48
1:A:111:MET:CG	1:A:133:NRQ:HE3	2.42	0.48
2:A:512:HOH:O	1:C:198:SER:HB3	2.13	0.48
1:B:111:MET:HG3	1:B:133:NRQ:HE1A	1.94	0.48
1:C:95:LYS:NZ	1:C:117:GLU:OE2	2.46	0.48
1:F:30:ARG:HH22	1:F:137:LYS:HZ2	1.60	0.47
1:G:133:NRQ:N1	1:G:133:NRQ:CA3	2.77	0.47
1:B:95:LYS:NZ	2:B:511:HOH:O	2.48	0.47
1:A:76:THR:OG1	1:A:78:ASN:O	2.33	0.47
1:B:36:LYS:HE3	1:B:36:LYS:HB2	1.66	0.47
1:B:67:THR:CG2	1:E:114:LYS:HE2	2.45	0.47
1:F:83:LEU:HB3	1:F:98:SER:OG	2.15	0.46
1:H:133:NRQ:CA3	1:H:133:NRQ:N1	2.78	0.46
1:E:109:GLN:HE22	1:E:136:SER:HB3	1.80	0.46
1:C:30:ARG:NH2	1:C:137:LYS:HZ1	2.07	0.46
1:A:136:SER:N	2:A:325:HOH:O	2.49	0.45
1:E:63:HIS:HB3	1:E:64:ALA:CA	2.46	0.45
1:H:111:MET:CG	1:H:133:NRQ:HE1A	2.41	0.45
1:D:30:ARG:HH22	1:D:137:LYS:HZ3	1.62	0.45
1:C:133:NRQ:N1	1:C:133:NRQ:CA3	2.80	0.45
1:F:133:NRQ:CD2	1:F:133:NRQ:N2	2.71	0.45
1:G:148:ASP:O	1:G:152:GLN:HG3	2.16	0.45
1:C:15:LYS:HE3	1:C:156:GLU:OE2	2.17	0.45
1:C:83:LEU:C	1:C:83:LEU:HD23	2.36	0.45
1:B:220:ALA:O	1:B:221:ASP:OD2	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:GLU:CD	1:C:112:ARG:HE	2.20	0.45
1:E:220:ALA:O	1:E:221:ASP:OD2	2.34	0.45
1:D:133:NRQ:N1	1:D:133:NRQ:CA3	2.79	0.44
1:C:87:GLY:HA3	1:C:191:ILE:HB	2.00	0.44
1:G:63:HIS:ND1	1:G:64:ALA:HB3	2.33	0.44
1:C:34:ARG:HD3	1:C:37:GLU:HB3	1.99	0.44
1:G:15:LYS:HG3	1:G:16:PRO:HD2	1.99	0.44
1:A:111:MET:CG	1:A:133:NRQ:CE	2.91	0.44
1:A:133:NRQ:N1	1:A:133:NRQ:CA3	2.82	0.43
1:B:83:LEU:HB3	1:B:98:SER:OG	2.19	0.43
1:E:229:ASP:CB	2:E:349:HOH:O	2.58	0.43
1:G:30:ARG:HH22	1:G:137:LYS:HZ2	1.67	0.43
1:G:63:HIS:HA	1:G:64:ALA:CB	2.26	0.43
1:F:133:NRQ:N1	1:F:133:NRQ:CA3	2.78	0.42
1:B:67:THR:HG23	1:E:114:LYS:HE2	2.02	0.42
1:B:133:NRQ:N1	1:B:133:NRQ:CA3	2.82	0.42
1:E:95:LYS:HB2	1:E:117:GLU:HB2	2.01	0.42
1:E:111:MET:CG	1:E:133:NRQ:HE3	2.45	0.42
1:F:220:ALA:C	1:F:221:ASP:CG	2.78	0.42
1:G:9:THR:HG21	1:G:11:TYR:CZ	2.54	0.42
1:A:63:HIS:O	1:A:63:HIS:ND1	2.30	0.42
1:B:15:LYS:HG3	1:B:16:PRO:HD2	2.01	0.42
1:C:14:LYS:HB2	1:C:156:GLU:HB3	2.01	0.42
1:G:205:LYS:NZ	2:G:451:HOH:O	2.32	0.42
1:C:123:PHE:CD1	1:C:127:ILE:HD11	2.54	0.41
1:F:204:GLN:HB3	1:F:206:LYS:HE3	2.03	0.41
1:E:133:NRQ:CA3	1:E:133:NRQ:N1	2.81	0.41
1:F:111:MET:CG	1:F:133:NRQ:HE3	2.49	0.41
1:G:111:MET:CG	1:G:133:NRQ:HE3	2.47	0.41
1:B:9:THR:HG21	1:B:11:TYR:CZ	2.56	0.41
1:C:40:LYS:HE3	1:C:40:LYS:HB3	1.91	0.41
1:H:72:SER:HB3	2:H:382:HOH:O	2.19	0.41
1:D:63:HIS:CA	1:D:64:ALA:HB2	2.12	0.41
1:A:221:ASP:O	1:A:221:ASP:CG	2.59	0.41
1:H:109:GLN:OE1	1:H:136:SER:CB	2.69	0.41
1:B:176:GLN:HG2	1:B:189:VAL:HG22	2.02	0.41
1:B:30:ARG:HH22	1:B:137:LYS:HZ2	1.67	0.41
1:G:30:ARG:HH22	1:G:137:LYS:HZ3	1.67	0.41
1:H:66:GLY:C	1:H:68:GLY:H	2.24	0.41
1:H:111:MET:HB3	1:H:111:MET:HE2	1.97	0.41
1:E:86:GLU:HG3	1:E:95:LYS:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:LEU:C	1:G:83:LEU:HD23	2.41	0.41
1:C:88:THR:HA	1:C:92:HIS:O	2.21	0.40
1:D:83:LEU:HB3	1:D:98:SER:OG	2.21	0.40
1:F:109:GLN:HG3	1:F:133:NRQ:HE2A	2.03	0.40
1:H:9:THR:HG21	1:H:11:TYR:CZ	2.57	0.40
1:C:104:PRO:HA	1:C:139:PHE:HA	2.02	0.40
1:C:32:LEU:C	1:C:32:LEU:HD23	2.41	0.40
1:G:111:MET:CG	1:G:133:NRQ:CE	2.95	0.40
1:G:36:LYS:HB2	1:G:36:LYS:HE2	1.48	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	228/233 (98%)	219 (96%)	9 (4%)	0	100	100
1	B	228/233 (98%)	224 (98%)	4 (2%)	0	100	100
1	C	228/233 (98%)	220 (96%)	6 (3%)	2 (1%)	20	5
1	D	228/233 (98%)	221 (97%)	6 (3%)	1 (0%)	38	18
1	E	228/233 (98%)	218 (96%)	9 (4%)	1 (0%)	38	18
1	F	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
1	G	228/233 (98%)	222 (97%)	5 (2%)	1 (0%)	38	18
1	H	228/233 (98%)	223 (98%)	5 (2%)	0	100	100
All	All	1824/1864 (98%)	1770 (97%)	49 (3%)	5 (0%)	44	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	ALA

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Mol	Chain	Res	Type
1	G	64	ALA
1	C	221	ASP
1	C	65	GLY
1	E	64	ALA

### 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	197/197 (100%)	191 (97%)	6 (3%)	46	22
1	B	197/197 (100%)	193 (98%)	4 (2%)	60	40
1	C	197/197 (100%)	187 (95%)	10 (5%)	28	8
1	D	197/197 (100%)	191 (97%)	6 (3%)	46	22
1	E	197/197 (100%)	193 (98%)	4 (2%)	60	40
1	F	197/197 (100%)	194 (98%)	3 (2%)	70	52
1	G	197/197 (100%)	194 (98%)	3 (2%)	70	52
1	H	197/197 (100%)	188 (95%)	9 (5%)	31	10
All	All	1576/1576 (100%)	1531 (97%)	45 (3%)	48	24

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	63	HIS
1	A	67	THR
1	A	81	MET
1	A	111	MET
1	A	221	ASP
1	B	36	LYS
1	B	40	LYS
1	B	56	ASP
1	B	81	MET
1	C	36	LYS

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Mol	Chain	Res	Type
1	C	56	ASP
1	C	67	THR
1	C	73	GLU
1	C	81	MET
1	C	99	GLU
1	C	106	GLU
1	C	111	MET
1	C	136	SER
1	C	221	ASP
1	D	36	LYS
1	D	40	LYS
1	D	56	ASP
1	D	77	GLU
1	D	111	MET
1	D	221	ASP
1	E	36	LYS
1	E	56	ASP
1	E	111	MET
1	E	221	ASP
1	F	56	ASP
1	F	63	HIS
1	F	111	MET
1	G	36	LYS
1	G	67	THR
1	G	81	MET
1	H	36	LYS
1	H	56	ASP
1	H	63	HIS
1	H	67	THR
1	H	72	SER
1	H	81	MET
1	H	111	MET
1	H	136	SER
1	H	221	ASP

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

Mol	Chain	Res	Type
1	B	63	HIS
1	F	63	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	133	1	23,24,25	5.73	7 (30%)	25,32,34	4.34	8 (32%)
1	NRQ	B	133	1	23,24,25	5.73	7 (30%)	25,32,34	4.38	8 (32%)
1	NRQ	C	133	1	23,24,25	5.71	7 (30%)	25,32,34	4.37	7 (28%)
1	NRQ	D	133	1	23,24,25	5.71	7 (30%)	25,32,34	4.42	8 (32%)
1	NRQ	E	133	1	23,24,25	5.72	7 (30%)	25,32,34	4.41	7 (28%)
1	NRQ	F	133	1	23,24,25	5.74	7 (30%)	25,32,34	4.33	7 (28%)
1	NRQ	G	133	1	23,24,25	5.72	7 (30%)	25,32,34	4.34	8 (32%)
1	NRQ	H	133	1	23,24,25	5.74	7 (30%)	25,32,34	4.43	7 (28%)

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	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	B	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	C	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	D	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	E	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	F	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	G	133	1	-	0/9/31/32	0/2/2/2
1	NRQ	H	133	1	-	0/9/31/32	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	133	NRQ	CA2-C2	-12.93	1.35	1.48
1	H	133	NRQ	CA2-C2	-12.91	1.35	1.48
1	B	133	NRQ	CA2-C2	-12.90	1.35	1.48
1	D	133	NRQ	CA2-C2	-12.89	1.35	1.48
1	F	133	NRQ	CA2-C2	-12.86	1.35	1.48
1	G	133	NRQ	CA2-C2	-12.85	1.35	1.48
1	E	133	NRQ	CA2-C2	-12.84	1.35	1.48
1	C	133	NRQ	CA2-C2	-12.80	1.35	1.48
1	D	133	NRQ	CE1-CZ	2.52	1.43	1.38
1	G	133	NRQ	CE1-CZ	2.53	1.43	1.38
1	A	133	NRQ	CE1-CZ	2.55	1.43	1.38
1	C	133	NRQ	CE1-CZ	2.56	1.43	1.38
1	B	133	NRQ	CE1-CZ	2.57	1.43	1.38
1	E	133	NRQ	CE1-CZ	2.58	1.44	1.38
1	H	133	NRQ	CE1-CZ	2.59	1.44	1.38
1	F	133	NRQ	CE1-CZ	2.61	1.44	1.38
1	B	133	NRQ	CG2-CB2	3.07	1.53	1.46
1	A	133	NRQ	CG2-CB2	3.08	1.53	1.46
1	H	133	NRQ	CG2-CB2	3.09	1.53	1.46
1	E	133	NRQ	CG2-CB2	3.11	1.53	1.46
1	F	133	NRQ	CG2-CB2	3.11	1.53	1.46
1	G	133	NRQ	CG2-CB2	3.12	1.53	1.46
1	D	133	NRQ	CG2-CB2	3.12	1.53	1.46
1	C	133	NRQ	CG2-CB2	3.13	1.53	1.46
1	B	133	NRQ	CD2-CG2	4.83	1.48	1.39
1	E	133	NRQ	CD2-CG2	4.83	1.48	1.39
1	C	133	NRQ	CD2-CG2	4.83	1.48	1.39
1	G	133	NRQ	CD2-CG2	4.84	1.48	1.39
1	A	133	NRQ	CD2-CG2	4.84	1.48	1.39
1	D	133	NRQ	CD2-CG2	4.84	1.48	1.39
1	F	133	NRQ	CD2-CG2	4.89	1.48	1.39
1	H	133	NRQ	CD2-CG2	4.90	1.48	1.39
1	G	133	NRQ	CA1-N1	7.22	1.45	1.27
1	B	133	NRQ	CA1-N1	7.22	1.45	1.27
1	E	133	NRQ	CA1-N1	7.23	1.45	1.27
1	A	133	NRQ	CA1-N1	7.23	1.45	1.27
1	C	133	NRQ	CA1-N1	7.23	1.45	1.27
1	H	133	NRQ	CA1-N1	7.24	1.45	1.27
1	F	133	NRQ	CA1-N1	7.24	1.45	1.27
1	D	133	NRQ	CA1-N1	7.26	1.45	1.27
1	D	133	NRQ	O2-C2	7.85	1.40	1.23
1	A	133	NRQ	O2-C2	7.86	1.40	1.23
1	C	133	NRQ	O2-C2	7.88	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	133	NRQ	O2-C2	7.89	1.40	1.23
1	B	133	NRQ	O2-C2	7.89	1.40	1.23
1	F	133	NRQ	O2-C2	7.89	1.40	1.23
1	H	133	NRQ	O2-C2	7.91	1.40	1.23
1	E	133	NRQ	O2-C2	7.93	1.40	1.23
1	D	133	NRQ	CB2-CA2	20.37	1.53	1.35
1	C	133	NRQ	CB2-CA2	20.40	1.53	1.35
1	E	133	NRQ	CB2-CA2	20.42	1.53	1.35
1	A	133	NRQ	CB2-CA2	20.43	1.53	1.35
1	G	133	NRQ	CB2-CA2	20.46	1.53	1.35
1	H	133	NRQ	CB2-CA2	20.49	1.53	1.35
1	B	133	NRQ	CB2-CA2	20.51	1.53	1.35
1	F	133	NRQ	CB2-CA2	20.54	1.53	1.35

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	133	NRQ	CG2-CB2-CA2	-14.50	113.35	130.19
1	D	133	NRQ	CG2-CB2-CA2	-14.17	113.73	130.19
1	E	133	NRQ	CG2-CB2-CA2	-14.15	113.75	130.19
1	G	133	NRQ	CG2-CB2-CA2	-14.00	113.92	130.19
1	B	133	NRQ	CG2-CB2-CA2	-13.85	114.10	130.19
1	C	133	NRQ	CG2-CB2-CA2	-13.84	114.12	130.19
1	A	133	NRQ	CG2-CB2-CA2	-13.79	114.18	130.19
1	F	133	NRQ	CG2-CB2-CA2	-13.74	114.22	130.19
1	B	133	NRQ	O2-C2-CA2	-9.93	125.62	130.97
1	D	133	NRQ	O2-C2-CA2	-9.88	125.64	130.97
1	C	133	NRQ	O2-C2-CA2	-9.84	125.67	130.97
1	E	133	NRQ	O2-C2-CA2	-9.81	125.68	130.97
1	F	133	NRQ	O2-C2-CA2	-9.67	125.76	130.97
1	G	133	NRQ	O2-C2-CA2	-9.59	125.80	130.97
1	H	133	NRQ	O2-C2-CA2	-9.58	125.80	130.97
1	A	133	NRQ	O2-C2-CA2	-9.56	125.82	130.97
1	E	133	NRQ	N3-C1-N2	-3.89	108.32	113.31
1	H	133	NRQ	N3-C1-N2	-3.87	108.35	113.31
1	A	133	NRQ	N3-C1-N2	-3.85	108.37	113.31
1	D	133	NRQ	N3-C1-N2	-3.85	108.37	113.31
1	G	133	NRQ	N3-C1-N2	-3.84	108.38	113.31
1	F	133	NRQ	N3-C1-N2	-3.83	108.39	113.31
1	B	133	NRQ	N3-C1-N2	-3.82	108.40	113.31
1	C	133	NRQ	N3-C1-N2	-3.80	108.43	113.31
1	H	133	NRQ	CB1-CA1-N1	-3.38	113.66	125.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	133	NRQ	CB1-CA1-N1	-3.33	113.86	125.34
1	A	133	NRQ	CB1-CA1-N1	-3.30	113.95	125.34
1	G	133	NRQ	CB1-CA1-N1	-3.29	113.99	125.34
1	F	133	NRQ	CB1-CA1-N1	-3.28	114.03	125.34
1	D	133	NRQ	CB1-CA1-N1	-3.27	114.06	125.34
1	B	133	NRQ	CB1-CA1-N1	-3.26	114.08	125.34
1	C	133	NRQ	CB1-CA1-N1	-3.25	114.13	125.34
1	B	133	NRQ	O3-C3-CA3	-2.05	119.59	126.38
1	G	133	NRQ	O3-C3-CA3	-2.03	119.68	126.38
1	A	133	NRQ	O3-C3-CA3	-2.01	119.73	126.38
1	D	133	NRQ	O3-C3-CA3	-2.00	119.77	126.38
1	G	133	NRQ	CE-SD-CG1	2.48	109.27	100.35
1	B	133	NRQ	CE-SD-CG1	2.52	109.41	100.35
1	A	133	NRQ	CE-SD-CG1	2.52	109.41	100.35
1	E	133	NRQ	CE-SD-CG1	2.54	109.46	100.35
1	D	133	NRQ	CE-SD-CG1	2.56	109.52	100.35
1	H	133	NRQ	CE-SD-CG1	2.56	109.54	100.35
1	C	133	NRQ	CE-SD-CG1	2.56	109.54	100.35
1	F	133	NRQ	CE-SD-CG1	2.57	109.59	100.35
1	H	133	NRQ	CG1-CB1-CA1	2.67	117.36	112.67
1	E	133	NRQ	CG1-CB1-CA1	2.70	117.42	112.67
1	F	133	NRQ	CG1-CB1-CA1	2.72	117.46	112.67
1	A	133	NRQ	CG1-CB1-CA1	2.75	117.51	112.67
1	G	133	NRQ	CG1-CB1-CA1	2.76	117.52	112.67
1	B	133	NRQ	CG1-CB1-CA1	2.77	117.54	112.67
1	D	133	NRQ	CG1-CB1-CA1	2.79	117.57	112.67
1	C	133	NRQ	CG1-CB1-CA1	2.95	117.86	112.67
1	G	133	NRQ	CA2-C2-N3	11.15	108.27	103.30
1	F	133	NRQ	CA2-C2-N3	11.29	108.33	103.30
1	H	133	NRQ	CA2-C2-N3	11.35	108.36	103.30
1	E	133	NRQ	CA2-C2-N3	11.38	108.37	103.30
1	C	133	NRQ	CA2-C2-N3	11.38	108.38	103.30
1	D	133	NRQ	CA2-C2-N3	11.43	108.40	103.30
1	A	133	NRQ	CA2-C2-N3	11.43	108.40	103.30
1	B	133	NRQ	CA2-C2-N3	11.48	108.42	103.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	133	NRQ	9	0
1	B	133	NRQ	8	0
1	C	133	NRQ	9	0
1	D	133	NRQ	9	0
1	E	133	NRQ	8	0
1	F	133	NRQ	9	0
1	G	133	NRQ	9	0
1	H	133	NRQ	10	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	132:PHE	C	133:NRQ	N1	1.65
1	D	132:PHE	C	133:NRQ	N1	1.62
1	E	133:NRQ	C3	136:SER	N	1.60

## 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<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	232/233 (99%)	0.31	9 (3%) 40 44	9, 15, 29, 65	0
1	B	232/233 (99%)	0.06	5 (2%) 62 67	9, 15, 28, 37	0
1	C	232/233 (99%)	0.75	27 (11%) 5 6	11, 17, 34, 67	0
1	D	232/233 (99%)	0.29	13 (5%) 25 26	11, 17, 34, 65	0
1	E	232/233 (99%)	0.35	14 (6%) 23 23	11, 17, 32, 69	0
1	F	232/233 (99%)	0.61	27 (11%) 5 6	11, 18, 40, 66	0
1	G	232/233 (99%)	0.56	21 (9%) 10 10	12, 19, 41, 71	0
1	H	232/233 (99%)	0.96	35 (15%) 3 2	13, 25, 43, 69	0
All	All	1856/1864 (99%)	0.49	151 (8%) 13 14	9, 18, 37, 71	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	64	ALA	23.4
1	G	65	GLY	20.1
1	H	64	ALA	19.2
1	A	64	ALA	19.0
1	H	63	HIS	16.0
1	F	65	GLY	15.8
1	H	66	GLY	14.9
1	H	65	GLY	13.4
1	E	65	GLY	13.3
1	F	64	ALA	13.2
1	G	64	ALA	13.1
1	G	66	GLY	12.9
1	E	64	ALA	12.6
1	C	63	HIS	12.2
1	D	62	GLY	12.0
1	A	63	HIS	11.5

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Mol	Chain	Res	Type	RSRZ
1	F	63	HIS	11.3
1	G	63	HIS	11.2
1	F	62	GLY	11.2
1	E	63	HIS	11.1
1	G	67	THR	10.9
1	D	63	HIS	10.0
1	D	64	ALA	10.0
1	F	67	THR	9.6
1	E	221	ASP	9.5
1	D	65	GLY	9.5
1	E	66	GLY	9.2
1	C	66	GLY	8.8
1	A	65	GLY	8.7
1	G	62	GLY	8.5
1	D	222	GLY	8.5
1	G	68	GLY	8.4
1	A	222	GLY	8.2
1	C	221	ASP	8.0
1	H	67	THR	8.0
1	F	61	LEU	8.0
1	C	65	GLY	7.8
1	H	221	ASP	7.8
1	G	222	GLY	7.5
1	H	62	GLY	7.3
1	H	61	LEU	7.3
1	A	66	GLY	7.3
1	F	66	GLY	7.0
1	H	71	MET	6.9
1	A	221	ASP	6.7
1	D	221	ASP	6.2
1	C	222	GLY	6.0
1	C	67	THR	5.9
1	E	67	THR	5.7
1	B	221	ASP	5.7
1	D	66	GLY	5.7
1	C	62	GLY	5.0
1	F	221	ASP	5.0
1	H	222	GLY	4.9
1	G	221	ASP	4.9
1	F	71	MET	4.9
1	G	71	MET	4.8
1	B	222	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	222	GLY	4.8
1	H	143	THR	4.7
1	A	62	GLY	4.7
1	D	223	GLY	4.6
1	H	18	LYS	4.6
1	F	17	ALA	4.4
1	C	19	ASN	4.3
1	H	73	GLU	4.1
1	G	143	THR	4.0
1	H	17	ALA	4.0
1	E	62	GLY	4.0
1	F	222	GLY	4.0
1	H	69	GLY	3.9
1	H	70	SER	3.8
1	H	182	ASP	3.8
1	H	235	VAL	3.7
1	G	70	SER	3.7
1	H	68	GLY	3.6
1	C	18	LYS	3.6
1	F	235	VAL	3.5
1	H	76	THR	3.5
1	D	67	THR	3.4
1	F	56	ASP	3.4
1	B	63	HIS	3.3
1	E	220	ALA	3.3
1	F	18	LYS	3.3
1	C	69	GLY	3.3
1	H	16	PRO	3.3
1	F	84	TYR	3.3
1	H	144	GLN	3.2
1	H	56	ASP	3.2
1	C	116	VAL	3.2
1	G	84	TYR	3.1
1	G	69	GLY	3.0
1	H	220	ALA	2.9
1	C	16	PRO	2.9
1	C	87	GLY	2.8
1	B	220	ALA	2.8
1	F	68	GLY	2.8
1	D	61	LEU	2.8
1	E	56	ASP	2.7
1	G	144	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	19	ASN	2.7
1	G	72	SER	2.7
1	H	7	LEU	2.7
1	H	208	LEU	2.7
1	H	72	SER	2.6
1	C	42	THR	2.6
1	F	163	VAL	2.6
1	E	208	LEU	2.6
1	C	17	ALA	2.5
1	H	20	LEU	2.5
1	H	199	ASN	2.5
1	G	182	ASP	2.5
1	F	73	GLU	2.5
1	C	131	SER	2.5
1	A	67	THR	2.4
1	F	7	LEU	2.4
1	D	18	LYS	2.4
1	H	39	ASP	2.4
1	F	144	GLN	2.4
1	C	72	SER	2.4
1	C	127	ILE	2.4
1	F	69	GLY	2.3
1	D	71	MET	2.3
1	G	77	GLU	2.3
1	C	84	TYR	2.3
1	C	100	GLY	2.3
1	C	208	LEU	2.3
1	E	84	TYR	2.3
1	F	182	ASP	2.2
1	F	19	ASN	2.2
1	C	76	THR	2.2
1	C	235	VAL	2.2
1	A	120	PRO	2.2
1	C	7	LEU	2.2
1	E	7	LEU	2.2
1	G	61	LEU	2.2
1	F	220	ALA	2.2
1	D	84	TYR	2.1
1	H	181	GLN	2.1
1	F	72	SER	2.1
1	G	73	GLU	2.1
1	H	36	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	163	VAL	2.1
1	E	163	VAL	2.1
1	C	130	THR	2.0
1	H	40	LYS	2.0
1	F	143	THR	2.0
1	F	16	PRO	2.0
1	H	120	PRO	2.0
1	B	64	ALA	2.0
1	G	145	GLY	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<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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	NRQ	D	133	23/24	0.90	0.14	-	14,18,24,25	0
1	NRQ	B	133	23/24	0.91	0.13	-	11,15,22,23	0
1	NRQ	A	133	23/24	0.91	0.14	-	12,15,22,25	0
1	NRQ	C	133	23/24	0.88	0.15	-	15,17,25,27	0
1	NRQ	F	133	23/24	0.91	0.13	-	14,18,26,28	0
1	NRQ	E	133	23/24	0.89	0.15	-	15,17,25,28	0
1	NRQ	G	133	23/24	0.89	0.13	-	16,19,25,27	0
1	NRQ	H	133	23/24	0.88	0.14	-	19,23,31,34	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.