



# Full wwPDB X-ray Structure Validation Report

May 6, 2014 – 09:02 AM EDT

PDB ID : 4OQW  
Title : Crystal structure of mCardinal far-red fluorescent protein  
Authors : Burg, J.S.; Chu, J.; Lam, A.J.; Lin, M.Z.; Garcia, K.C.  
Deposited on : 2014-02-10  
Resolution : 2.21 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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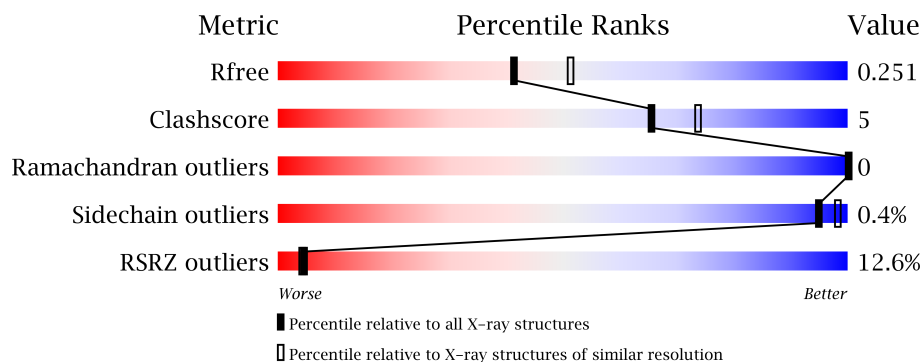
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.21 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))
$R_{free}$	66092	3340 (2.24-2.20)
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	228	
1	B	228	
1	C	228	
1	D	228	
1	E	228	
1	F	228	
1	G	228	
1	H	228	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27289 atoms, of which 12883 are hydrogens and 0 are deuterium.

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	226	Total	C	H	N	O	S	0	0	0
			3539	1148	1731	307	340	13			
1	B	224	Total	C	H	N	O	S	0	0	0
			3498	1136	1707	304	338	13			
1	C	223	Total	C	H	N	O	S	0	0	0
			3489	1133	1707	303	333	13			
1	D	226	Total	C	H	N	O	S	0	0	0
			3517	1143	1715	306	340	13			
1	E	214	Total	C	H	N	O	S	0	0	0
			3224	1064	1553	285	309	13			
1	F	215	Total	C	H	N	O	S	0	0	0
			3313	1085	1608	293	315	12			
1	G	212	Total	C	H	N	O	S	0	0	0
			3193	1060	1529	281	311	12			
1	H	196	Total	C	H	N	O	S	0	0	0
			2845	961	1333	250	288	13			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP D0VX33
A	0	LYS	-	EXPRESSION TAG	UNP D0VX33
A	1	GLY	-	EXPRESSION TAG	UNP D0VX33
A	2	GLU	-	EXPRESSION TAG	UNP D0VX33
A	6	LYS	THR	CONFLICT	UNP D0VX33
A	28	THR	SER	CONFLICT	UNP D0VX33
A	61	CYS	SER	CONFLICT	UNP D0VX33
A	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
A	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
A	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
A	67	LYS	HIS	CONFLICT	UNP D0VX33
A	80	PHE	TRP	CONFLICT	UNP D0VX33
A	104	VAL	ALA	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	LEU	ILE	CONFLICT	UNP D0VX33
A	143	THR	HIS	CONFLICT	UNP D0VX33
A	146	THR	MET	CONFLICT	UNP D0VX33
A	158	CYS	ALA	CONFLICT	UNP D0VX33
A	160	MET	LEU	CONFLICT	UNP D0VX33
A	171	HIS	ILE	CONFLICT	UNP D0VX33
A	174	LEU	PHE	CONFLICT	UNP D0VX33
A	194	PHE	TYR	CONFLICT	UNP D0VX33
A	197	ARG	TYR	CONFLICT	UNP D0VX33
A	207	ASN	LYS	CONFLICT	UNP D0VX33
B	-1	SER	-	EXPRESSION TAG	UNP D0VX33
B	0	LYS	-	EXPRESSION TAG	UNP D0VX33
B	1	GLY	-	EXPRESSION TAG	UNP D0VX33
B	2	GLU	-	EXPRESSION TAG	UNP D0VX33
B	6	LYS	THR	CONFLICT	UNP D0VX33
B	28	THR	SER	CONFLICT	UNP D0VX33
B	61	CYS	SER	CONFLICT	UNP D0VX33
B	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
B	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
B	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
B	67	LYS	HIS	CONFLICT	UNP D0VX33
B	80	PHE	TRP	CONFLICT	UNP D0VX33
B	104	VAL	ALA	CONFLICT	UNP D0VX33
B	121	LEU	ILE	CONFLICT	UNP D0VX33
B	143	THR	HIS	CONFLICT	UNP D0VX33
B	146	THR	MET	CONFLICT	UNP D0VX33
B	158	CYS	ALA	CONFLICT	UNP D0VX33
B	160	MET	LEU	CONFLICT	UNP D0VX33
B	171	HIS	ILE	CONFLICT	UNP D0VX33
B	174	LEU	PHE	CONFLICT	UNP D0VX33
B	194	PHE	TYR	CONFLICT	UNP D0VX33
B	197	ARG	TYR	CONFLICT	UNP D0VX33
B	207	ASN	LYS	CONFLICT	UNP D0VX33
C	-1	SER	-	EXPRESSION TAG	UNP D0VX33
C	0	LYS	-	EXPRESSION TAG	UNP D0VX33
C	1	GLY	-	EXPRESSION TAG	UNP D0VX33
C	2	GLU	-	EXPRESSION TAG	UNP D0VX33
C	6	LYS	THR	CONFLICT	UNP D0VX33
C	28	THR	SER	CONFLICT	UNP D0VX33
C	61	CYS	SER	CONFLICT	UNP D0VX33
C	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
C	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
C	67	LYS	HIS	CONFLICT	UNP D0VX33
C	80	PHE	TRP	CONFLICT	UNP D0VX33
C	104	VAL	ALA	CONFLICT	UNP D0VX33
C	121	LEU	ILE	CONFLICT	UNP D0VX33
C	143	THR	HIS	CONFLICT	UNP D0VX33
C	146	THR	MET	CONFLICT	UNP D0VX33
C	158	CYS	ALA	CONFLICT	UNP D0VX33
C	160	MET	LEU	CONFLICT	UNP D0VX33
C	171	HIS	ILE	CONFLICT	UNP D0VX33
C	174	LEU	PHE	CONFLICT	UNP D0VX33
C	194	PHE	TYR	CONFLICT	UNP D0VX33
C	197	ARG	TYR	CONFLICT	UNP D0VX33
C	207	ASN	LYS	CONFLICT	UNP D0VX33
D	-1	SER	-	EXPRESSION TAG	UNP D0VX33
D	0	LYS	-	EXPRESSION TAG	UNP D0VX33
D	1	GLY	-	EXPRESSION TAG	UNP D0VX33
D	2	GLU	-	EXPRESSION TAG	UNP D0VX33
D	6	LYS	THR	CONFLICT	UNP D0VX33
D	28	THR	SER	CONFLICT	UNP D0VX33
D	61	CYS	SER	CONFLICT	UNP D0VX33
D	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
D	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
D	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
D	67	LYS	HIS	CONFLICT	UNP D0VX33
D	80	PHE	TRP	CONFLICT	UNP D0VX33
D	104	VAL	ALA	CONFLICT	UNP D0VX33
D	121	LEU	ILE	CONFLICT	UNP D0VX33
D	143	THR	HIS	CONFLICT	UNP D0VX33
D	146	THR	MET	CONFLICT	UNP D0VX33
D	158	CYS	ALA	CONFLICT	UNP D0VX33
D	160	MET	LEU	CONFLICT	UNP D0VX33
D	171	HIS	ILE	CONFLICT	UNP D0VX33
D	174	LEU	PHE	CONFLICT	UNP D0VX33
D	194	PHE	TYR	CONFLICT	UNP D0VX33
D	197	ARG	TYR	CONFLICT	UNP D0VX33
D	207	ASN	LYS	CONFLICT	UNP D0VX33
E	-1	SER	-	EXPRESSION TAG	UNP D0VX33
E	0	LYS	-	EXPRESSION TAG	UNP D0VX33
E	1	GLY	-	EXPRESSION TAG	UNP D0VX33
E	2	GLU	-	EXPRESSION TAG	UNP D0VX33
E	6	LYS	THR	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
E	28	THR	SER	CONFLICT	UNP D0VX33
E	61	CYS	SER	CONFLICT	UNP D0VX33
E	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
E	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
E	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
E	67	LYS	HIS	CONFLICT	UNP D0VX33
E	80	PHE	TRP	CONFLICT	UNP D0VX33
E	104	VAL	ALA	CONFLICT	UNP D0VX33
E	121	LEU	ILE	CONFLICT	UNP D0VX33
E	143	THR	HIS	CONFLICT	UNP D0VX33
E	146	THR	MET	CONFLICT	UNP D0VX33
E	158	CYS	ALA	CONFLICT	UNP D0VX33
E	160	MET	LEU	CONFLICT	UNP D0VX33
E	171	HIS	ILE	CONFLICT	UNP D0VX33
E	174	LEU	PHE	CONFLICT	UNP D0VX33
E	194	PHE	TYR	CONFLICT	UNP D0VX33
E	197	ARG	TYR	CONFLICT	UNP D0VX33
E	207	ASN	LYS	CONFLICT	UNP D0VX33
F	-1	SER	-	EXPRESSION TAG	UNP D0VX33
F	0	LYS	-	EXPRESSION TAG	UNP D0VX33
F	1	GLY	-	EXPRESSION TAG	UNP D0VX33
F	2	GLU	-	EXPRESSION TAG	UNP D0VX33
F	6	LYS	THR	CONFLICT	UNP D0VX33
F	28	THR	SER	CONFLICT	UNP D0VX33
F	61	CYS	SER	CONFLICT	UNP D0VX33
F	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
F	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
F	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
F	67	LYS	HIS	CONFLICT	UNP D0VX33
F	80	PHE	TRP	CONFLICT	UNP D0VX33
F	104	VAL	ALA	CONFLICT	UNP D0VX33
F	121	LEU	ILE	CONFLICT	UNP D0VX33
F	143	THR	HIS	CONFLICT	UNP D0VX33
F	146	THR	MET	CONFLICT	UNP D0VX33
F	158	CYS	ALA	CONFLICT	UNP D0VX33
F	160	MET	LEU	CONFLICT	UNP D0VX33
F	171	HIS	ILE	CONFLICT	UNP D0VX33
F	174	LEU	PHE	CONFLICT	UNP D0VX33
F	194	PHE	TYR	CONFLICT	UNP D0VX33
F	197	ARG	TYR	CONFLICT	UNP D0VX33
F	207	ASN	LYS	CONFLICT	UNP D0VX33
G	-1	SER	-	EXPRESSION TAG	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	LYS	-	EXPRESSION TAG	UNP D0VX33
G	1	GLY	-	EXPRESSION TAG	UNP D0VX33
G	2	GLU	-	EXPRESSION TAG	UNP D0VX33
G	6	LYS	THR	CONFLICT	UNP D0VX33
G	28	THR	SER	CONFLICT	UNP D0VX33
G	61	CYS	SER	CONFLICT	UNP D0VX33
G	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
G	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
G	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
G	67	LYS	HIS	CONFLICT	UNP D0VX33
G	80	PHE	TRP	CONFLICT	UNP D0VX33
G	104	VAL	ALA	CONFLICT	UNP D0VX33
G	121	LEU	ILE	CONFLICT	UNP D0VX33
G	143	THR	HIS	CONFLICT	UNP D0VX33
G	146	THR	MET	CONFLICT	UNP D0VX33
G	158	CYS	ALA	CONFLICT	UNP D0VX33
G	160	MET	LEU	CONFLICT	UNP D0VX33
G	171	HIS	ILE	CONFLICT	UNP D0VX33
G	174	LEU	PHE	CONFLICT	UNP D0VX33
G	194	PHE	TYR	CONFLICT	UNP D0VX33
G	197	ARG	TYR	CONFLICT	UNP D0VX33
G	207	ASN	LYS	CONFLICT	UNP D0VX33
H	-1	SER	-	EXPRESSION TAG	UNP D0VX33
H	0	LYS	-	EXPRESSION TAG	UNP D0VX33
H	1	GLY	-	EXPRESSION TAG	UNP D0VX33
H	2	GLU	-	EXPRESSION TAG	UNP D0VX33
H	6	LYS	THR	CONFLICT	UNP D0VX33
H	28	THR	SER	CONFLICT	UNP D0VX33
H	61	CYS	SER	CONFLICT	UNP D0VX33
H	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
H	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
H	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
H	67	LYS	HIS	CONFLICT	UNP D0VX33
H	80	PHE	TRP	CONFLICT	UNP D0VX33
H	104	VAL	ALA	CONFLICT	UNP D0VX33
H	121	LEU	ILE	CONFLICT	UNP D0VX33
H	143	THR	HIS	CONFLICT	UNP D0VX33
H	146	THR	MET	CONFLICT	UNP D0VX33
H	158	CYS	ALA	CONFLICT	UNP D0VX33
H	160	MET	LEU	CONFLICT	UNP D0VX33
H	171	HIS	ILE	CONFLICT	UNP D0VX33
H	174	LEU	PHE	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
H	194	PHE	TYR	CONFLICT	UNP D0VX33
H	197	ARG	TYR	CONFLICT	UNP D0VX33
H	207	ASN	LYS	CONFLICT	UNP D0VX33

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total 132	O 132	0	0
2	B	103	Total 103	O 103	0	0
2	C	106	Total 106	O 106	0	0
2	D	91	Total 91	O 91	0	0
2	E	61	Total 61	O 61	0	0
2	F	57	Total 57	O 57	0	0
2	G	53	Total 53	O 53	0	0
2	H	68	Total 68	O 68	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.

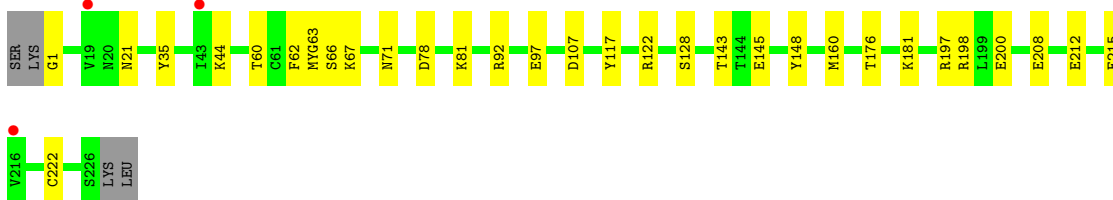
- Molecule 1: Fluorescent protein FP480

Chain A: 



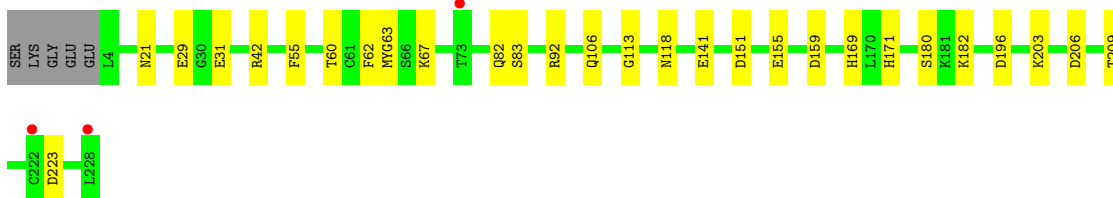
- Molecule 1: Fluorescent protein FP480

Chain B: 



- Molecule 1: Fluorescent protein FP480

Chain C: 



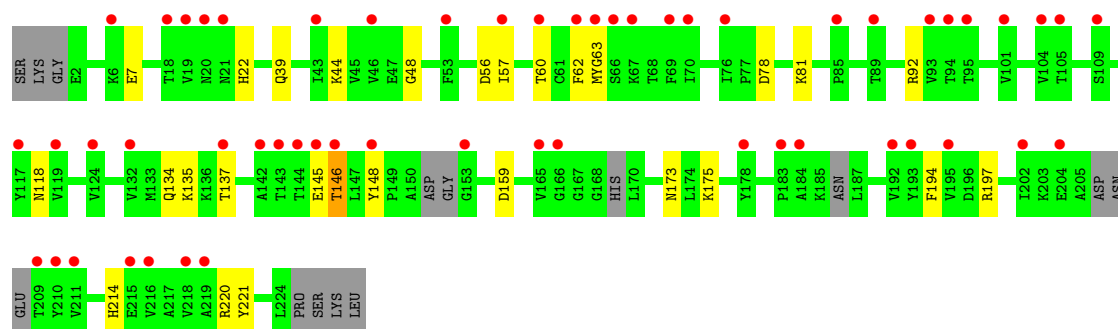
- Molecule 1: Fluorescent protein FP480

Chain D: 



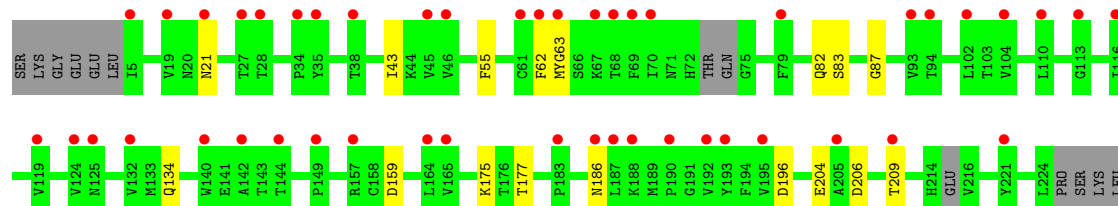
- Molecule 1: Fluorescent protein FP480

Chain E: 



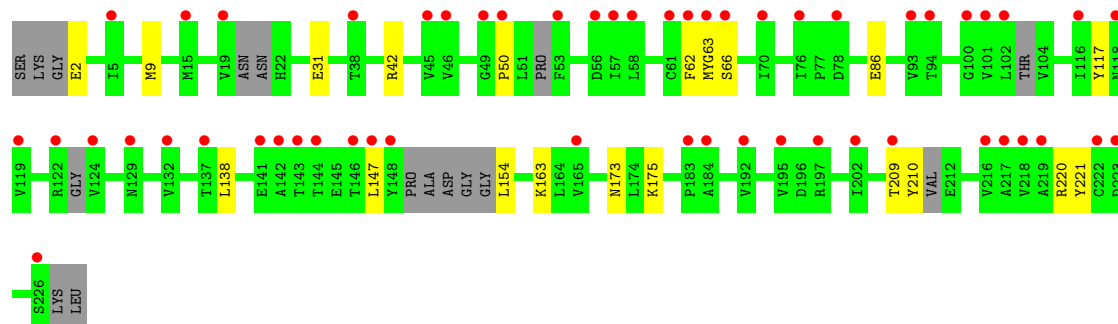
- Molecule 1: Fluorescent protein FP480

Chain F:



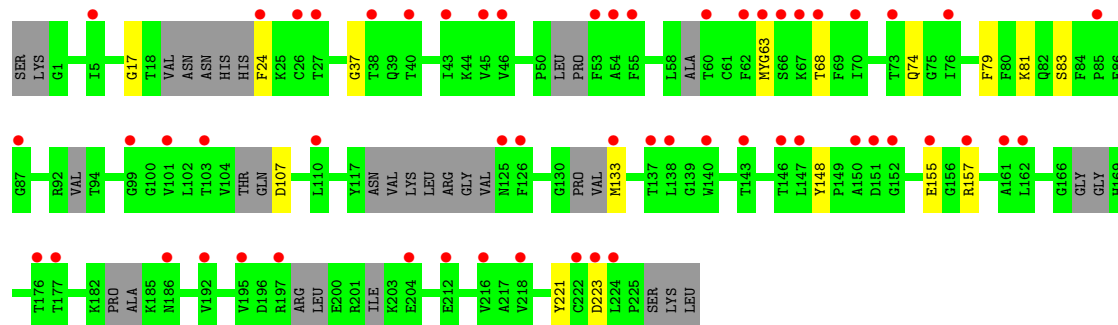
- Molecule 1: Fluorescent protein FP480

Chain G:



- Molecule 1: Fluorescent protein FP480

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	53.20Å 136.70Å 167.60Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	47.56 – 2.21 47.56 – 2.21	Depositor EDS
% Data completeness (in resolution range)	94.8 (47.56-2.21) 94.4 (47.56-2.21)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.223 , 0.251 0.223 , 0.251	Depositor DCC
$R_{free}$ test set	1996 reflections (1.76%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.1	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 26.1	EDS
Estimated twinning fraction	0.500 for h,-k,-l 0.387 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 113418 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/1803	0.47	0/2436
1	B	0.26	0/1786	0.46	0/2414
1	C	0.28	0/1777	0.49	0/2403
1	D	0.26	0/1797	0.45	0/2428
1	E	0.22	0/1659	0.41	0/2241
1	F	0.24	0/1697	0.44	0/2291
1	G	0.24	0/1649	0.44	0/2219
1	H	0.27	0/1490	0.43	0/2000
All	All	0.26	0/13658	0.45	0/18432

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1808	1731	2	17	1
1	B	1791	1707	0	23	0
1	C	1782	1707	0	23	0
1	D	1802	1715	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1671	1553	0	20	0
1	F	1705	1608	0	14	1
1	G	1664	1529	0	13	1
1	H	1512	1333	0	11	0
2	A	132	0	0	9	0
2	B	103	0	0	7	1
2	C	106	0	0	12	0
2	D	91	0	0	10	0
2	E	61	0	0	7	0
2	F	57	0	0	8	0
2	G	53	0	0	3	0
2	H	68	0	0	4	0
All	All	14406	12883	2	139	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (139) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:201:ARG:NH1	1:D:204:GLU:OE1	2.05	0.88
1:C:29:GLU:OE2	2:C:341:HOH:O	1.96	0.84
1:A:56:ASP:OD2	1:A:137:THR:OG1	1.98	0.81
1:H:107:ASP:OD2	2:H:313:HOH:O	2.03	0.77
1:C:42:ARG:NH1	2:C:402:HOH:O	2.18	0.77
1:B:145:GLU:OE1	2:B:374:HOH:O	2.05	0.73
1:E:44:LYS:NZ	2:E:319:HOH:O	2.21	0.72
1:E:159:ASP:OD1	1:E:173:ASN:ND2	2.22	0.72
1:D:204:GLU:OE2	2:D:369:HOH:O	2.07	0.72
1:D:6:LYS:NZ	2:D:311:HOH:O	2.22	0.71
1:G:31:GLU:OE2	2:G:350:HOH:O	2.08	0.71
1:H:68:THR:O	1:H:81:LYS:NZ	2.23	0.71
1:C:203:LYS:NZ	2:C:343:HOH:O	2.24	0.69
1:B:1:GLY:N	2:B:316:HOH:O	2.26	0.69
1:H:37:GLY:O	2:H:307:HOH:O	2.11	0.68
1:A:145:GLU:OE2	2:A:395:HOH:O	2.12	0.68
1:G:173:ASN:OD1	1:G:175:LYS:NZ	2.27	0.67
1:C:31:GLU:OE2	2:C:402:HOH:O	2.13	0.67
1:A:60:THR:OG1	2:A:368:HOH:O	2.13	0.66
1:B:97:GLU:OE2	1:D:157:ARG:NH2	2.28	0.66
1:B:208:GLU:OE2	2:B:356:HOH:O	2.14	0.66
1:F:196:ASP:OD2	2:F:320:HOH:O	2.15	0.65
1:A:141:GLU:OE2	1:A:169:HIS:NE2	2.30	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:72:HIS:NE2	2:D:377:HOH:O	2.30	0.64
1:C:155:GLU:OE1	2:C:338:HOH:O	2.15	0.63
1:A:203:LYS:NZ	2:A:327:HOH:O	2.31	0.62
1:C:63:NRQ:O2	1:C:67:LYS:NZ	2.31	0.62
1:H:133:MET:N	2:H:366:HOH:O	2.31	0.62
1:B:222:CYS:SG	1:D:198:ARG:NH2	2.73	0.62
1:G:2:GLU:OE1	1:G:2:GLU:N	2.34	0.61
1:E:145:GLU:OE1	1:E:197:ARG:NH2	2.35	0.60
1:D:197:ARG:NE	1:D:215:GLU:OE2	2.36	0.59
1:F:21:ASN:ND2	2:F:352:HOH:O	2.35	0.59
1:D:28:THR:OG1	2:D:372:HOH:O	2.17	0.58
1:B:66:SER:OG	1:B:117:TYR:OH	2.21	0.58
1:G:42:ARG:NH2	2:G:311:HOH:O	2.36	0.58
1:D:36:GLU:OE1	2:D:374:HOH:O	2.18	0.57
1:A:47:GLU:OE1	2:A:357:HOH:O	2.18	0.57
1:D:86:GLU:OE1	1:D:86:GLU:N	2.38	0.57
1:D:135:LYS:O	2:D:353:HOH:O	2.17	0.56
1:H:155:GLU:OE2	1:H:157:ARG:NH1	2.35	0.56
1:A:42:ARG:NH2	2:A:348:HOH:O	2.37	0.56
1:C:159:ASP:OD1	2:C:337:HOH:O	2.18	0.56
1:F:186:ASN:N	2:F:343:HOH:O	2.31	0.56
1:B:200:GLU:OE2	1:D:226:SER:OG	2.24	0.56
1:E:22:HIS:NE2	1:E:48:GLY:O	2.40	0.55
1:G:220:ARG:NH1	1:G:221:TYR:O	2.39	0.55
1:H:74:GLN:NE2	1:H:223:ASP:OD1	2.39	0.55
1:D:223:ASP:N	2:D:334:HOH:O	2.39	0.54
1:B:21:ASN:ND2	2:B:353:HOH:O	2.40	0.54
1:C:206:ASP:O	1:C:209:THR:OG1	2.25	0.54
1:A:122:ARG:NH2	2:A:314:HOH:O	2.39	0.53
1:B:63:NRQ:CA3	1:B:63:NRQ:N1	2.72	0.53
1:F:82:GLN:NE2	2:F:315:HOH:O	2.41	0.53
1:H:223:ASP:OD2	2:H:328:HOH:O	2.19	0.53
1:D:77:PRO:O	2:D:322:HOH:O	2.19	0.51
1:C:82:GLN:O	1:C:182:LYS:NZ	2.44	0.51
1:A:220:ARG:NH2	1:C:196:ASP:OD2	2.44	0.51
1:B:60:THR:O	1:B:92:ARG:NH1	2.42	0.50
1:D:226:SER:OG	1:D:226:SER:O	2.29	0.50
1:C:21:ASN:N	1:D:91:GLU:OE2	2.43	0.50
1:F:62:PHE:N	1:F:63:NRQ:CA1	2.74	0.50
1:B:44:LYS:NZ	2:B:335:HOH:O	2.43	0.50
1:E:134:GLN:NE2	2:E:310:HOH:O	2.43	0.50
1:C:62:PHE:N	1:C:63:NRQ:CA1	2.75	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:106:GLN:OE1	2:C:322:HOH:O	2.17	0.50
1:D:72:HIS:O	1:D:73:THR:OG1	2.31	0.49
1:E:56:ASP:N	2:E:320:HOH:O	2.46	0.48
1:F:134:GLN:NE2	2:F:351:HOH:O	2.46	0.48
1:C:223:ASP:N	2:C:302:HOH:O	2.38	0.48
1:D:54:ALA:HB1	1:D:137:THR:HG1	1.79	0.48
1:C:151:ASP:O	2:C:329:HOH:O	2.20	0.48
1:G:86:GLU:OE1	1:G:86:GLU:N	2.44	0.48
1:D:66:SER:OG	1:D:117:TYR:OH	2.32	0.48
1:E:135:LYS:N	2:E:343:HOH:O	2.42	0.48
1:A:63:NRQ:N1	1:A:63:NRQ:CA3	2.77	0.47
1:C:21:ASN:CA	1:D:91:GLU:OE2	2.62	0.47
1:E:78:ASP:OD2	1:E:81:LYS:NZ	2.48	0.47
1:D:62:PHE:N	1:D:63:NRQ:CA1	2.78	0.47
1:E:60:THR:O	1:E:92:ARG:NH1	2.45	0.47
1:F:204:GLU:OE1	1:F:204:GLU:N	2.42	0.47
1:B:35:TYR:O	1:B:71:ASN:ND2	2.42	0.46
1:F:177:THR:OG1	2:F:302:HOH:O	2.21	0.46
1:F:43:ILE:HG21	1:F:55:PHE:HZ	1.80	0.46
1:C:141:GLU:OE2	1:C:169:HIS:NE2	2.48	0.46
1:B:212:GLU:OE1	2:B:386:HOH:O	2.21	0.46
1:B:92:ARG:HE	1:B:176:THR:HG1	1.64	0.46
1:C:118:ASN:ND2	2:C:304:HOH:O	2.35	0.46
1:E:39:GLN:O	1:E:214:HIS:ND1	2.49	0.46
1:G:147:LEU:HB3	1:G:154:LEU:HD22	1.98	0.46
1:C:83:SER:OG	1:C:180:SER:OG	2.34	0.45
1:A:152:GLY:O	2:A:324:HOH:O	2.21	0.45
1:E:118:ASN:ND2	2:E:305:HOH:O	2.45	0.45
1:C:63:NRQ:N1	1:C:63:NRQ:CA3	2.79	0.45
1:B:143:THR:HG21	1:B:160:MET:HG2	1.98	0.44
1:G:9:MET:SD	2:G:316:HOH:O	2.61	0.44
1:A:11:MET:HE1	1:A:39:GLN:HB2	1.99	0.44
1:B:78:ASP:OD2	1:B:81:LYS:NZ	2.50	0.44
1:A:23:HIS:O	2:A:364:HOH:O	2.21	0.44
1:D:175:LYS:NZ	2:D:375:HOH:O	2.50	0.44
1:D:91:GLU:OE2	2:D:363:HOH:O	2.21	0.44
1:G:62:PHE:N	1:G:63:NRQ:CA1	2.80	0.44
1:C:113:GLY:O	2:C:357:HOH:O	2.21	0.44
1:B:62:PHE:N	1:B:63:NRQ:CA1	2.80	0.43
1:E:63:NRQ:N1	1:E:63:NRQ:CA3	2.81	0.43
1:B:198:ARG:NH2	1:D:222:CYS:SG	2.91	0.43
1:H:17:GLY:O	1:H:24:PHE:N	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:60:THR:O	1:C:92:ARG:NH1	2.52	0.43
1:E:146:THR:HG23	1:E:194:PHE:CE2	2.53	0.43
1:E:7:GLU:OE2	2:E:341:HOH:O	2.21	0.43
1:E:62:PHE:N	1:E:63:NRQ:CA1	2.82	0.43
1:F:206:ASP:O	1:F:209:THR:OG1	2.37	0.43
1:A:184:ALA:O	2:A:402:HOH:O	2.21	0.43
1:H:74:GLN:OE1	1:H:221:TYR:N	2.44	0.43
1:A:62:PHE:N	1:A:63:NRQ:CA1	2.82	0.43
1:G:63:NRQ:N1	1:G:63:NRQ:CA3	2.82	0.42
1:E:57:ILE:N	2:E:320:HOH:O	2.38	0.42
1:E:173:ASN:OD1	1:E:175:LYS:NZ	2.47	0.42
1:F:186:ASN:ND2	2:F:343:HOH:O	2.41	0.42
1:G:66:SER:OG	1:G:117:TYR:OH	2.35	0.42
1:D:63:NRQ:CA3	1:D:63:NRQ:N1	2.83	0.42
1:F:175:LYS:NZ	2:F:322:HOH:O	2.43	0.42
1:E:146:THR:HG22	1:E:148:TYR:HE2	1.85	0.42
1:F:63:NRQ:N1	1:F:63:NRQ:CA3	2.82	0.42
1:B:128:SER:O	2:B:375:HOH:O	2.21	0.42
1:B:107:ASP:OD1	1:B:181:MLY:HH11	2.20	0.41
1:G:138:LEU:N	1:G:163:MLY:O	2.46	0.41
1:H:79:PHE:O	1:H:83:SER:OG	2.33	0.41
1:A:105:THR:HG21	1:B:122:ARG:NH1	2.35	0.41
1:C:171:HIS:ND1	2:C:326:HOH:O	2.37	0.41
1:A:22:HIS:NE2	1:A:48:GLY:O	2.53	0.41
1:F:83:SER:O	1:F:87:GLY:N	2.47	0.41
1:E:56:ASP:OD2	1:E:137:THR:HB	2.20	0.41
1:B:197:ARG:HD3	1:B:215:GLU:OE2	2.21	0.41
1:G:50:PRO:HA	1:G:209:THR:HG22	2.03	0.41
1:H:63:NRQ:CA3	1:H:63:NRQ:N1	2.84	0.41
1:D:35:TYR:O	1:D:71:ASN:ND2	2.54	0.41
1:E:220:ARG:NH1	1:E:221:TYR:O	2.53	0.41
1:B:67:LYS:NZ	1:B:197:ARG:NH2	2.70	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	Distance(Å)	Clash(Å)
1:A:71:ASN:OD1	2:B:320:HOH:O[2_647]	2.11	0.09
1:F:159:ASP:OD2	1:G:173:ASN:ND2[2_656]	2.14	0.06



## 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	219/228 (96%)	217 (99%)	2 (1%)	0	100	100
1	B	217/228 (95%)	214 (99%)	3 (1%)	0	100	100
1	C	216/228 (95%)	213 (99%)	3 (1%)	0	100	100
1	D	219/228 (96%)	213 (97%)	6 (3%)	0	100	100
1	E	199/228 (87%)	197 (99%)	2 (1%)	0	100	100
1	F	204/228 (90%)	198 (97%)	6 (3%)	0	100	100
1	G	193/228 (85%)	189 (98%)	4 (2%)	0	100	100
1	H	167/228 (73%)	163 (98%)	4 (2%)	0	100	100
All	All	1634/1824 (90%)	1604 (98%)	30 (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	192/194 (99%)	192 (100%)	0	100	100
1	B	190/194 (98%)	189 (100%)	1 (0%)	94	97
1	C	189/194 (97%)	188 (100%)	1 (0%)	94	97
1	D	191/194 (98%)	191 (100%)	0	100	100
1	E	168/194 (87%)	167 (99%)	1 (1%)	92	96
1	F	175/194 (90%)	175 (100%)	0	100	100
1	G	165/194 (85%)	164 (99%)	1 (1%)	92	96
1	H	145/194 (75%)	144 (99%)	1 (1%)	91	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1415/1552 (91%)	1410 (100%)	5 (0%)	95 98

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	148	TYR
1	C	55	PHE
1	E	146	THR
1	G	210	TYR
1	H	148	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	71	ASN
1	A	129	ASN
1	A	134	GLN
1	A	213	GLN
1	B	41	GLN
1	B	71	ASN
1	B	74	GLN
1	B	118	ASN
1	B	125	ASN
1	B	134	GLN
1	B	173	ASN
1	C	41	GLN
1	C	74	GLN
1	C	118	ASN
1	C	125	ASN
1	C	173	ASN
1	C	186	ASN
1	D	71	ASN
1	D	82	GLN
1	D	111	GLN
1	D	118	ASN
1	D	173	ASN
1	D	186	ASN
1	E	118	ASN
1	E	125	ASN
1	E	134	GLN

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Mol	Chain	Res	Type
1	F	21	ASN
1	F	41	GLN
1	F	118	ASN
1	F	125	ASN
1	G	8	ASN
1	G	71	ASN
1	G	118	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

24 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	MLY	A	163	1	10,10,11	5.70	1 (10%)	9,11,13	1.32	1 (11%)
1	MLY	A	181	1	10,10,11	5.63	1 (10%)	9,11,13	1.47	1 (11%)
1	NRQ	A	63	1	24,24,25	6.43	13 (54%)	30,32,34	4.22	14 (46%)
1	MLY	B	163	1	10,10,11	5.49	1 (10%)	9,11,13	0.97	0
1	MLY	B	181	1	10,10,11	5.60	1 (10%)	9,11,13	1.49	1 (11%)
1	NRQ	B	63	1	24,24,25	6.36	14 (58%)	30,32,34	4.28	11 (36%)
1	MLY	C	163	1	10,10,11	5.50	1 (10%)	9,11,13	1.30	1 (11%)
1	MLY	C	181	1	10,10,11	5.57	1 (10%)	9,11,13	0.98	1 (11%)
1	NRQ	C	63	1	24,24,25	6.36	13 (54%)	30,32,34	4.10	12 (40%)
1	MLY	D	163	1	10,10,11	5.68	1 (10%)	9,11,13	0.96	1 (11%)
1	MLY	D	181	1	10,10,11	5.61	2 (20%)	9,11,13	1.47	1 (11%)
1	NRQ	D	63	1	24,24,25	6.47	14 (58%)	30,32,34	3.97	11 (36%)
1	MLY	E	163	1	10,10,11	5.64	1 (10%)	9,11,13	1.33	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	E	181	1	10,10,11	5.67	1 (10%)	9,11,13	0.91	0
1	NRQ	E	63	1	24,24,25	6.49	13 (54%)	30,32,34	4.18	11 (36%)
1	MLY	F	163	1	10,10,11	5.65	1 (10%)	9,11,13	1.05	1 (11%)
1	MLY	F	181	1	10,10,11	5.63	1 (10%)	9,11,13	1.30	1 (11%)
1	NRQ	F	63	1	24,24,25	6.44	13 (54%)	30,32,34	4.18	12 (40%)
1	MLY	G	163	1	10,10,11	5.51	1 (10%)	9,11,13	1.34	1 (11%)
1	MLY	G	181	1	10,10,11	5.60	1 (10%)	9,11,13	0.74	0
1	NRQ	G	63	1	24,24,25	6.48	14 (58%)	30,32,34	4.18	12 (40%)
1	MLY	H	163	1	10,10,11	5.68	1 (10%)	9,11,13	1.16	1 (11%)
1	MLY	H	181	1	10,10,11	5.62	1 (10%)	9,11,13	0.82	0
1	NRQ	H	63	1	24,24,25	6.48	14 (58%)	30,32,34	4.16	11 (36%)

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	MLY	A	163	1	-	0/7/9/11	0/0/0/0
1	MLY	A	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	A	63	1	-	0/9/31/32	0/2/2/2
1	MLY	B	163	1	-	0/7/9/11	0/0/0/0
1	MLY	B	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	B	63	1	-	0/9/31/32	0/2/2/2
1	MLY	C	163	1	-	0/7/9/11	0/0/0/0
1	MLY	C	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	C	63	1	-	0/9/31/32	0/2/2/2
1	MLY	D	163	1	-	0/7/9/11	0/0/0/0
1	MLY	D	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	D	63	1	-	0/9/31/32	0/2/2/2
1	MLY	E	163	1	-	0/7/9/11	0/0/0/0
1	MLY	E	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	E	63	1	-	0/9/31/32	0/2/2/2
1	MLY	F	163	1	-	0/7/9/11	0/0/0/0
1	MLY	F	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	F	63	1	-	0/9/31/32	0/2/2/2
1	MLY	G	163	1	-	0/7/9/11	0/0/0/0
1	MLY	G	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	G	63	1	-	0/9/31/32	0/2/2/2
1	MLY	H	163	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	H	181	1	-	0/7/9/11	0/0/0/0
1	NRQ	H	63	1	-	0/9/31/32	0/2/2/2

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63	NRQ	CB2-CA2	22.73	1.51	1.35
1	H	63	NRQ	CB2-CA2	22.55	1.51	1.35
1	G	63	NRQ	CB2-CA2	22.51	1.51	1.35
1	F	63	NRQ	CB2-CA2	22.39	1.51	1.35
1	A	63	NRQ	CB2-CA2	22.31	1.51	1.35
1	D	63	NRQ	CB2-CA2	22.05	1.50	1.35
1	B	63	NRQ	CB2-CA2	21.89	1.50	1.35
1	C	63	NRQ	CB2-CA2	21.88	1.50	1.35
1	A	163	MLY	O-C	17.91	1.23	1.11
1	D	163	MLY	O-C	17.85	1.23	1.11
1	H	163	MLY	O-C	17.82	1.23	1.11
1	E	181	MLY	O-C	17.79	1.23	1.11
1	F	163	MLY	O-C	17.74	1.23	1.11
1	E	163	MLY	O-C	17.69	1.23	1.11
1	A	181	MLY	O-C	17.66	1.23	1.11
1	H	181	MLY	O-C	17.63	1.23	1.11
1	F	181	MLY	O-C	17.60	1.23	1.11
1	B	181	MLY	O-C	17.59	1.23	1.11
1	D	181	MLY	O-C	17.59	1.23	1.11
1	G	181	MLY	O-C	17.52	1.23	1.11
1	C	181	MLY	O-C	17.49	1.23	1.11
1	G	163	MLY	O-C	17.31	1.23	1.11
1	C	163	MLY	O-C	17.26	1.23	1.11
1	B	163	MLY	O-C	17.23	1.23	1.11
1	D	63	NRQ	O3-C3	16.48	1.22	1.11
1	H	63	NRQ	O3-C3	16.05	1.22	1.11
1	A	63	NRQ	O3-C3	16.02	1.22	1.11
1	G	63	NRQ	O3-C3	16.01	1.22	1.11
1	F	63	NRQ	O3-C3	15.96	1.22	1.11
1	B	63	NRQ	O3-C3	15.90	1.22	1.11
1	E	63	NRQ	O3-C3	15.85	1.22	1.11
1	C	63	NRQ	O3-C3	15.80	1.22	1.11
1	B	63	NRQ	CA2-C2	-9.21	1.38	1.48
1	D	63	NRQ	CA2-C2	-9.20	1.38	1.48
1	C	63	NRQ	CA2-C2	-9.17	1.38	1.48
1	G	63	NRQ	CA2-C2	-9.14	1.38	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	CA2-C2	-9.12	1.38	1.48
1	F	63	NRQ	CA2-C2	-8.91	1.39	1.48
1	E	63	NRQ	CA2-C2	-8.90	1.39	1.48
1	H	63	NRQ	CA2-C2	-8.82	1.39	1.48
1	E	63	NRQ	O2-C2	7.29	1.38	1.23
1	H	63	NRQ	O2-C2	7.24	1.38	1.23
1	D	63	NRQ	O2-C2	7.21	1.38	1.23
1	F	63	NRQ	O2-C2	7.18	1.38	1.23
1	B	63	NRQ	O2-C2	7.13	1.38	1.23
1	A	63	NRQ	O2-C2	7.11	1.38	1.23
1	G	63	NRQ	O2-C2	7.08	1.38	1.23
1	C	63	NRQ	O2-C2	7.04	1.38	1.23
1	D	63	NRQ	CA1-N1	5.44	1.42	1.27
1	H	63	NRQ	CA1-N1	5.43	1.42	1.27
1	C	63	NRQ	CA1-N1	5.42	1.42	1.27
1	F	63	NRQ	CA1-N1	5.40	1.42	1.27
1	E	63	NRQ	CA1-N1	5.37	1.42	1.27
1	A	63	NRQ	CA1-N1	5.35	1.42	1.27
1	G	63	NRQ	CA1-N1	5.34	1.42	1.27
1	B	63	NRQ	CA1-N1	5.19	1.42	1.27
1	E	63	NRQ	CG2-CB2	4.22	1.55	1.46
1	F	63	NRQ	CG2-CB2	4.14	1.55	1.46
1	D	63	NRQ	CG2-CB2	4.14	1.55	1.46
1	H	63	NRQ	CG2-CB2	4.13	1.55	1.46
1	G	63	NRQ	CG2-CB2	4.09	1.55	1.46
1	A	63	NRQ	CG2-CB2	4.06	1.55	1.46
1	B	63	NRQ	CG2-CB2	4.04	1.55	1.46
1	C	63	NRQ	CG2-CB2	3.98	1.55	1.46
1	G	63	NRQ	CA2-N2	3.40	1.45	1.38
1	E	63	NRQ	CA2-N2	3.36	1.45	1.38
1	F	63	NRQ	CA2-N2	3.35	1.45	1.38
1	H	63	NRQ	CA2-N2	3.35	1.45	1.38
1	G	63	NRQ	CA3-N3	-3.29	1.44	1.46
1	D	63	NRQ	CA2-N2	3.29	1.45	1.38
1	C	63	NRQ	CA2-N2	3.22	1.45	1.38
1	B	63	NRQ	CA2-N2	3.21	1.45	1.38
1	A	63	NRQ	CA2-N2	3.14	1.45	1.38
1	E	63	NRQ	CA3-N3	-3.09	1.44	1.46
1	E	63	NRQ	CE1-CD1	3.07	1.44	1.38
1	C	63	NRQ	CE1-CD1	3.00	1.44	1.38
1	H	63	NRQ	CA3-N3	-2.99	1.44	1.46
1	F	63	NRQ	CE1-CD1	2.97	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	NRQ	CE1-CD1	2.97	1.44	1.38
1	H	63	NRQ	CE1-CD1	2.97	1.44	1.38
1	B	63	NRQ	OH-CZ	2.93	1.44	1.37
1	D	63	NRQ	CE1-CD1	2.92	1.44	1.38
1	C	63	NRQ	CA3-N3	-2.91	1.44	1.46
1	A	63	NRQ	CE1-CD1	2.89	1.44	1.38
1	D	63	NRQ	CA3-N3	-2.87	1.44	1.46
1	D	63	NRQ	OH-CZ	2.85	1.44	1.37
1	F	63	NRQ	CA3-N3	-2.82	1.44	1.46
1	B	63	NRQ	CE1-CD1	2.81	1.44	1.38
1	H	63	NRQ	OH-CZ	2.80	1.44	1.37
1	A	63	NRQ	OH-CZ	2.79	1.44	1.37
1	E	63	NRQ	C2-N3	2.79	1.45	1.39
1	G	63	NRQ	OH-CZ	2.76	1.44	1.37
1	F	63	NRQ	OH-CZ	2.75	1.44	1.37
1	C	63	NRQ	OH-CZ	2.75	1.44	1.37
1	E	63	NRQ	OH-CZ	2.75	1.44	1.37
1	F	63	NRQ	C2-N3	2.70	1.45	1.39
1	H	63	NRQ	C2-N3	2.68	1.45	1.39
1	A	63	NRQ	C2-N3	2.68	1.45	1.39
1	B	63	NRQ	C2-N3	2.60	1.45	1.39
1	D	63	NRQ	C2-N3	2.53	1.45	1.39
1	G	63	NRQ	C2-N3	2.52	1.45	1.39
1	B	63	NRQ	CA3-N3	-2.50	1.44	1.46
1	C	63	NRQ	C2-N3	2.45	1.45	1.39
1	A	63	NRQ	CA3-N3	-2.42	1.44	1.46
1	F	63	NRQ	CA3-C3	2.36	1.51	1.48
1	H	63	NRQ	CA3-C3	2.36	1.51	1.48
1	B	63	NRQ	CE2-CZ	2.24	1.43	1.38
1	E	63	NRQ	CA3-C3	2.21	1.51	1.48
1	H	63	NRQ	CE2-CZ	2.18	1.43	1.38
1	C	63	NRQ	CE2-CZ	2.17	1.43	1.38
1	C	63	NRQ	C1-N2	2.16	1.37	1.33
1	G	63	NRQ	CE2-CZ	2.14	1.43	1.38
1	A	63	NRQ	CE2-CZ	2.11	1.43	1.38
1	B	63	NRQ	CA3-C3	2.11	1.51	1.48
1	G	63	NRQ	C1-N2	2.11	1.37	1.33
1	D	63	NRQ	CE2-CZ	2.11	1.43	1.38
1	B	63	NRQ	C1-N2	2.10	1.37	1.33
1	E	63	NRQ	CE2-CZ	2.10	1.43	1.38
1	D	181	MLY	CA-C	2.09	1.53	1.49
1	H	63	NRQ	C1-N2	2.09	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	NRQ	CA3-C3	2.08	1.51	1.48
1	F	63	NRQ	CE2-CZ	2.06	1.43	1.38
1	D	63	NRQ	C1-N2	2.04	1.37	1.33
1	A	63	NRQ	C1-N2	2.03	1.37	1.33
1	D	63	NRQ	CA3-C3	2.00	1.51	1.48

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	NRQ	CG2-CB2-CA2	-13.25	115.39	130.12
1	F	63	NRQ	CG2-CB2-CA2	-12.98	115.69	130.12
1	H	63	NRQ	CG2-CB2-CA2	-12.83	115.86	130.12
1	G	63	NRQ	CG2-CB2-CA2	-12.33	116.42	130.12
1	D	63	NRQ	CG2-CB2-CA2	-12.04	116.73	130.12
1	B	63	NRQ	C1-CA1-N1	-11.96	107.67	121.83
1	B	63	NRQ	CG2-CB2-CA2	-11.87	116.92	130.12
1	C	63	NRQ	CG2-CB2-CA2	-11.68	117.14	130.12
1	A	63	NRQ	CG2-CB2-CA2	-10.87	118.04	130.12
1	A	63	NRQ	O2-C2-CA2	-10.65	124.97	130.93
1	A	63	NRQ	C1-CA1-N1	-9.98	110.00	121.83
1	C	63	NRQ	C1-CA1-N1	-9.93	110.07	121.83
1	C	63	NRQ	O2-C2-CA2	-9.56	125.58	130.93
1	F	63	NRQ	O2-C2-CA2	-9.51	125.61	130.93
1	G	63	NRQ	C1-CA1-N1	-9.39	110.71	121.83
1	A	63	NRQ	CA2-C2-N3	9.29	108.33	103.43
1	E	63	NRQ	C1-CA1-N1	-9.26	110.85	121.83
1	H	63	NRQ	O2-C2-CA2	-9.19	125.79	130.93
1	B	63	NRQ	O2-C2-CA2	-9.16	125.80	130.93
1	H	63	NRQ	C1-CA1-N1	-9.15	110.98	121.83
1	F	63	NRQ	C1-CA1-N1	-9.11	111.03	121.83
1	D	63	NRQ	O2-C2-CA2	-9.08	125.85	130.93
1	G	63	NRQ	CA2-C2-N3	9.04	108.20	103.43
1	C	63	NRQ	CA2-C2-N3	8.94	108.15	103.43
1	E	63	NRQ	O2-C2-CA2	-8.78	126.01	130.93
1	B	63	NRQ	CA2-C2-N3	8.67	108.00	103.43
1	G	63	NRQ	O2-C2-CA2	-8.59	126.12	130.93
1	D	63	NRQ	C1-CA1-N1	-8.54	111.71	121.83
1	F	63	NRQ	CA2-C2-N3	8.53	107.93	103.43
1	H	63	NRQ	CA2-C2-N3	8.45	107.89	103.43
1	D	63	NRQ	CA2-C2-N3	8.25	107.78	103.43
1	E	63	NRQ	CA2-C2-N3	8.18	107.75	103.43
1	E	63	NRQ	CB1-CA1-N1	-6.34	112.75	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	NRQ	CB1-CA1-N1	-6.22	112.97	125.10
1	H	63	NRQ	CB1-CA1-N1	-6.12	113.17	125.10
1	F	63	NRQ	CB1-CA1-N1	-5.78	113.84	125.10
1	D	63	NRQ	CB1-CA1-N1	-5.01	115.33	125.10
1	G	63	NRQ	C2-CA2-N2	-4.73	105.28	108.89
1	C	63	NRQ	CB1-CA1-N1	-4.67	116.00	125.10
1	A	63	NRQ	C2-CA2-N2	-4.60	105.38	108.89
1	E	63	NRQ	C2-CA2-N2	-4.48	105.47	108.89
1	F	63	NRQ	C2-CA2-N2	-4.43	105.51	108.89
1	H	63	NRQ	C2-CA2-N2	-4.38	105.55	108.89
1	B	63	NRQ	CB1-CA1-N1	-4.35	116.63	125.10
1	C	63	NRQ	C2-CA2-N2	-4.10	105.76	108.89
1	E	63	NRQ	N3-C1-N2	-4.10	108.55	113.38
1	D	63	NRQ	N3-C1-N2	-4.07	108.58	113.38
1	D	63	NRQ	C2-CA2-N2	-4.02	105.83	108.89
1	G	63	NRQ	N3-C1-N2	-4.00	108.67	113.38
1	B	63	NRQ	N3-C1-N2	-3.99	108.68	113.38
1	A	63	NRQ	N3-C1-N2	-3.98	108.69	113.38
1	A	181	MLY	C-CA-N	-3.98	109.86	113.83
1	H	63	NRQ	N3-C1-N2	-3.95	108.72	113.38
1	B	63	NRQ	C2-CA2-N2	-3.94	105.89	108.89
1	B	181	MLY	C-CA-N	-3.93	109.90	113.83
1	D	181	MLY	C-CA-N	-3.90	109.93	113.83
1	C	63	NRQ	N3-C1-N2	-3.84	108.86	113.38
1	A	63	NRQ	CB1-CA1-N1	-3.79	117.70	125.10
1	F	63	NRQ	N3-C1-N2	-3.77	108.93	113.38
1	F	181	MLY	C-CA-N	-3.68	110.16	113.83
1	G	163	MLY	C-CA-N	-3.59	110.24	113.83
1	A	63	NRQ	CE-SD-CG1	3.54	112.98	100.38
1	E	163	MLY	C-CA-N	-3.52	110.31	113.83
1	A	163	MLY	C-CA-N	-3.44	110.40	113.83
1	C	163	MLY	C-CA-N	-3.33	110.50	113.83
1	G	63	NRQ	CB1-CA1-C1	-3.12	110.34	118.19
1	B	63	NRQ	CA3-N3-C1	3.07	129.48	124.18
1	E	63	NRQ	CE-SD-CG1	3.07	111.32	100.38
1	H	63	NRQ	CE-SD-CG1	3.06	111.28	100.38
1	B	63	NRQ	CB1-CA1-C1	-3.00	110.63	118.19
1	B	63	NRQ	CE-SD-CG1	2.99	111.03	100.38
1	A	63	NRQ	CA2-N2-C1	2.98	109.75	104.10
1	D	63	NRQ	CE-SD-CG1	2.98	110.99	100.38
1	H	163	MLY	C-CA-N	-2.98	110.86	113.83
1	E	63	NRQ	CA2-N2-C1	2.98	109.74	104.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63	NRQ	CA3-N3-C1	2.93	129.23	124.18
1	G	63	NRQ	CA2-N2-C1	2.85	109.50	104.10
1	C	63	NRQ	CE-SD-CG1	2.85	110.52	100.38
1	H	63	NRQ	CA2-N2-C1	2.84	109.49	104.10
1	A	63	NRQ	CA3-N3-C1	2.83	129.06	124.18
1	F	63	NRQ	CE-SD-CG1	2.82	110.43	100.38
1	A	63	NRQ	CB1-CG1-SD	-2.80	105.93	112.89
1	F	63	NRQ	CA2-N2-C1	2.80	109.41	104.10
1	C	63	NRQ	CA3-N3-C1	2.79	128.99	124.18
1	B	63	NRQ	CA2-N2-C1	2.77	109.35	104.10
1	D	63	NRQ	CA2-N2-C1	2.77	109.35	104.10
1	G	63	NRQ	CE-SD-CG1	2.76	110.21	100.38
1	A	63	NRQ	CB1-CA1-C1	-2.76	111.23	118.19
1	C	63	NRQ	CA2-N2-C1	2.67	109.16	104.10
1	E	63	NRQ	CB1-CA1-C1	-2.65	111.52	118.19
1	D	63	NRQ	CA3-N3-C1	2.64	128.74	124.18
1	H	63	NRQ	CB1-CA1-C1	-2.60	111.64	118.19
1	F	163	MLY	C-CA-N	-2.57	111.26	113.83
1	D	63	NRQ	CB1-CG1-SD	-2.42	106.88	112.89
1	H	63	NRQ	CA3-N3-C1	2.42	128.35	124.18
1	E	63	NRQ	CA3-N3-C1	2.37	128.26	124.18
1	A	63	NRQ	CG1-CB1-CA1	2.32	116.71	112.37
1	F	63	NRQ	CA3-N3-C1	2.31	128.16	124.18
1	C	181	MLY	C-CA-N	-2.28	111.55	113.83
1	F	63	NRQ	CB1-CA1-C1	-2.25	112.53	118.19
1	C	63	NRQ	CB1-CG1-SD	-2.22	107.39	112.89
1	D	163	MLY	C-CA-N	-2.14	111.69	113.83
1	F	63	NRQ	CB1-CG1-SD	-2.10	107.67	112.89
1	A	63	NRQ	CA1-C1-N3	2.10	127.12	124.42
1	C	63	NRQ	CB1-CA1-C1	-2.10	112.90	118.19
1	G	63	NRQ	CB1-CG1-SD	-2.01	107.89	112.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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<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	226/228 (99%)	0.04	1 (0%) 90 92	7, 16, 38, 69	0
1	B	224/228 (98%)	0.04	3 (1%) 74 74	8, 19, 35, 51	0
1	C	223/228 (97%)	0.04	3 (1%) 74 74	9, 21, 43, 76	0
1	D	226/228 (99%)	0.04	0 100 100	11, 21, 51, 78	0
1	E	214/228 (93%)	1.33	55 (25%) 1 1	33, 64, 90, 157	0
1	F	215/228 (94%)	1.20	47 (21%) 1 1	31, 62, 89, 130	0
1	G	212/228 (92%)	1.31	54 (25%) 1 1	35, 63, 89, 127	0
1	H	196/228 (85%)	1.60	56 (28%) 1 1	39, 69, 97, 120	0
All	All	1736/1824 (95%)	0.67	219 (12%) 4 4	7, 41, 85, 157	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	63	NRQ	17.4
1	F	63	NRQ	13.2
1	H	151	ASP	8.9
1	H	216	VAL	7.5
1	H	63	NRQ	7.5
1	H	101	VAL	7.4
1	G	101	VAL	7.4
1	G	100	GLY	7.0
1	G	218	VAL	6.9
1	H	140	TRP	6.9
1	H	99	GLY	6.4
1	G	192	VAL	6.0
1	E	119	VAL	5.8
1	E	137	THR	5.8
1	H	62	PHE	5.8
1	G	93	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	217	ALA	5.5
1	G	102	LEU	5.4
1	H	218	VAL	5.3
1	F	68	THR	5.3
1	G	195	VAL	5.2
1	F	183	PRO	5.1
1	H	223	ASP	5.1
1	F	70	ILE	5.0
1	H	76	ILE	5.0
1	H	222	CYS	5.0
1	E	62	PHE	5.0
1	H	137	THR	4.9
1	F	195	VAL	4.8
1	H	195	VAL	4.7
1	G	70	ILE	4.6
1	E	57	ILE	4.5
1	E	70	ILE	4.5
1	H	146	THR	4.5
1	H	150	ALA	4.5
1	G	165	VAL	4.4
1	F	19	VAL	4.3
1	G	63	NRQ	4.2
1	H	224	LEU	4.2
1	F	192	VAL	4.1
1	C	228	LEU	4.1
1	E	210	TYR	4.1
1	E	146	THR	4.0
1	G	119	VAL	4.0
1	F	187	LEU	4.0
1	E	18	THR	4.0
1	H	43	ILE	3.9
1	G	49	GLY	3.9
1	F	94	THR	3.9
1	E	195	VAL	3.8
1	G	53	PHE	3.8
1	G	219	ALA	3.8
1	E	183	PRO	3.8
1	E	46	VAL	3.8
1	H	192	VAL	3.8
1	E	104	VAL	3.7
1	E	93	VAL	3.7
1	G	146	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	209	THR	3.7
1	G	94	THR	3.6
1	H	67	LYS	3.6
1	E	218	VAL	3.6
1	F	27	THR	3.6
1	G	222	CYS	3.5
1	H	53	PHE	3.5
1	G	45	VAL	3.5
1	G	148	TYR	3.5
1	H	161	ALA	3.4
1	E	216	VAL	3.4
1	F	61	CYS	3.4
1	E	89	THR	3.4
1	F	104	VAL	3.4
1	G	226	SER	3.4
1	F	62	PHE	3.4
1	H	26	CYS	3.3
1	H	177	THR	3.3
1	H	70	ILE	3.3
1	G	183	PRO	3.3
1	G	61	CYS	3.3
1	E	184	ALA	3.3
1	G	144	THR	3.3
1	E	43	ILE	3.3
1	E	76	ILE	3.3
1	F	186	ASN	3.3
1	G	5	ILE	3.2
1	F	119	VAL	3.2
1	E	193	TYR	3.2
1	E	219	ALA	3.2
1	F	5	ILE	3.2
1	H	133	MET	3.2
1	H	60	THR	3.2
1	G	124	VAL	3.2
1	E	143	THR	3.2
1	F	46	VAL	3.1
1	G	19	VAL	3.1
1	G	132	VAL	3.1
1	F	38	THR	3.1
1	H	126	PHE	3.1
1	F	132	VAL	3.1
1	H	157	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	132	VAL	3.1
1	G	184	ALA	3.1
1	F	35	TYR	3.0
1	H	204	GLU	3.0
1	E	192	VAL	3.0
1	F	45	VAL	3.0
1	H	45	VAL	3.0
1	H	46	VAL	3.0
1	F	113	GLY	3.0
1	E	148	TYR	3.0
1	E	60	THR	3.0
1	G	57	ILE	3.0
1	H	155	GLU	3.0
1	G	137	THR	2.9
1	G	118	ASN	2.9
1	F	79	PHE	2.9
1	E	144	THR	2.9
1	H	138	LEU	2.9
1	E	165	VAL	2.9
1	F	140	TRP	2.9
1	G	38	THR	2.9
1	G	216	VAL	2.9
1	G	143	THR	2.8
1	G	141	GLU	2.8
1	G	202	ILE	2.8
1	H	40	THR	2.8
1	G	15	MET	2.7
1	F	124	VAL	2.7
1	E	117	TYR	2.7
1	E	153	GLY	2.7
1	E	211	VAL	2.7
1	F	110	LEU	2.7
1	E	109	SER	2.7
1	G	66	SER	2.7
1	H	24	PHE	2.7
1	C	222	CYS	2.7
1	F	93	VAL	2.7
1	H	85	PRO	2.7
1	A	202	ILE	2.6
1	H	87	GLY	2.6
1	E	178	TYR	2.6
1	F	69	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	62	PHE	2.6
1	H	38	THR	2.6
1	E	202	ILE	2.6
1	F	165	VAL	2.6
1	G	76	ILE	2.6
1	H	54	ALA	2.6
1	E	53	PHE	2.6
1	H	55	PHE	2.5
1	H	212	GLU	2.5
1	H	27	THR	2.5
1	E	142	ALA	2.5
1	F	142	ALA	2.5
1	E	66	SER	2.5
1	C	73	THR	2.5
1	F	125	ASN	2.5
1	F	205	ALA	2.5
1	E	94	THR	2.5
1	E	20	ASN	2.5
1	E	95	THR	2.5
1	F	149	PRO	2.5
1	G	197	ARG	2.5
1	H	186	ASN	2.5
1	H	143	THR	2.4
1	H	176	THR	2.4
1	E	21	ASN	2.4
1	E	101	VAL	2.4
1	H	103	THR	2.4
1	G	147	LEU	2.4
1	F	67	LYS	2.4
1	G	116	ILE	2.4
1	B	216	VAL	2.4
1	E	209	THR	2.4
1	G	223	ASP	2.3
1	G	78	ASP	2.3
1	G	46	VAL	2.3
1	E	85	PRO	2.3
1	B	19	VAL	2.3
1	E	69	PHE	2.3
1	H	5	ILE	2.3
1	F	28	THR	2.3
1	F	193	TYR	2.2
1	H	197	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	190	PRO	2.2
1	F	144	THR	2.2
1	H	68	THR	2.2
1	G	122	ARG	2.2
1	H	110	LEU	2.2
1	E	204	GLU	2.2
1	E	166	GLY	2.2
1	E	6	LYS	2.2
1	E	215	GLU	2.2
1	E	105	THR	2.2
1	F	209	THR	2.2
1	H	152	GLY	2.1
1	H	162	LEU	2.1
1	E	19	VAL	2.1
1	G	142	ALA	2.1
1	G	56	ASP	2.1
1	G	129	ASN	2.1
1	F	102	LEU	2.1
1	F	34	PRO	2.1
1	F	221	TYR	2.1
1	H	125	ASN	2.1
1	H	66	SER	2.1
1	E	67	LYS	2.1
1	F	164	LEU	2.1
1	F	21	ASN	2.1
1	F	188	LYS	2.1
1	H	73	THR	2.1
1	G	58	LEU	2.0
1	E	124	VAL	2.0
1	G	50	PRO	2.0
1	B	43	ILE	2.0
1	F	116	ILE	2.0
1	E	145	GLU	2.0
1	H	147	LEU	2.0
1	F	157	ARG	2.0

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

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	NRQ	F	63	23/24	0.35	2.90	85,112,126,143	0
1	NRQ	E	63	23/24	0.42	2.58	132,143,153,161	0
1	NRQ	C	63	23/24	0.16	1.62	14,18,22,28	0
1	NRQ	A	63	23/24	0.16	1.61	9,14,22,30	0
1	NRQ	B	63	23/24	0.16	1.55	15,19,31,43	0
1	MLY	F	163	11/12	0.30	1.09	77,93,111,113	0
1	MLY	E	181	11/12	0.27	0.85	49,62,72,73	0
1	MLY	D	163	11/12	0.16	0.71	14,23,57,57	0
1	MLY	B	181	11/12	0.13	0.67	16,21,41,45	0
1	NRQ	D	63	23/24	0.14	0.57	12,18,32,43	0
1	MLY	B	163	11/12	0.15	0.51	15,23,33,33	0
1	MLY	A	163	11/12	0.13	0.16	8,11,25,25	0
1	NRQ	H	63	23/24	0.26	0.13	52,87,96,104	0
1	MLY	C	163	11/12	0.13	0.06	9,15,35,35	0
1	MLY	C	181	11/12	0.15	0.04	19,32,59,59	0
1	NRQ	G	63	23/24	0.21	0.03	42,59,67,98	0
1	MLY	E	163	11/12	0.20	-0.07	52,65,73,73	0
1	MLY	D	181	11/12	0.13	-0.13	14,18,48,48	0
1	MLY	F	181	11/12	0.19	-0.19	37,45,50,54	0
1	MLY	G	163	11/12	0.18	-0.32	33,49,58,61	0
1	MLY	H	181	11/12	0.18	-0.33	51,65,77,81	0
1	MLY	A	181	11/12	0.12	-0.58	10,17,32,32	0
1	MLY	G	181	11/12	0.14	-0.64	40,52,76,79	0
1	MLY	H	163	11/12	0.19	-0.86	48,61,73,73	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.