



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2022 – 01:16 PM EDT

PDB ID : 7SAJ  
Title : Crystal Structure of LaM2 Nanobody bound to mCherry  
Authors : Cong, A.T.Q.; Schellenberg, M.J.  
Deposited on : 2021-09-22  
Resolution : 2.37 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

<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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

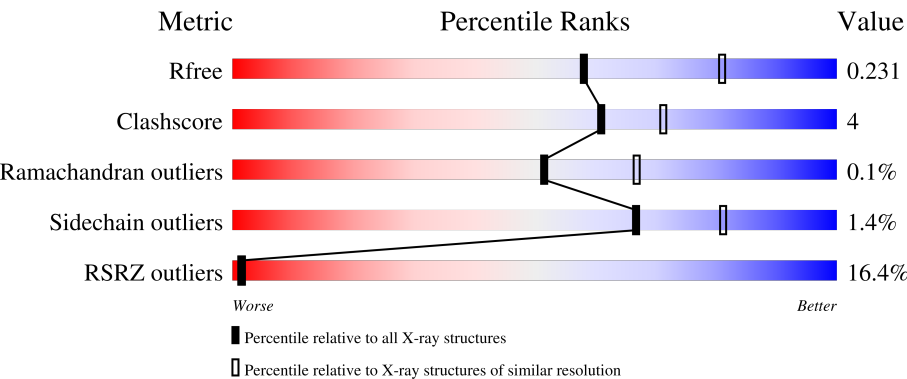
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 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	237	<div><div>9%</div><div><div></div><div>74%</div><div>17%</div><div>9%</div></div></div>
1	C	237	<div><div>13%</div><div><div></div><div>81%</div><div>9%</div><div>•</div><div>9%</div></div></div>
1	E	237	<div><div>7%</div><div><div></div><div>82%</div><div>8%</div><div>•</div><div>9%</div></div></div>
1	G	237	<div><div>14%</div><div><div></div><div>82%</div><div>9%</div><div>•</div><div>9%</div></div></div>
1	I	237	<div><div>58%</div><div><div></div><div>73%</div><div>16%</div><div>•</div><div>9%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	B	127	
2	D	127	
2	F	127	
2	H	127	
2	J	127	

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	I	66	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26588 atoms, of which 12935 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 mCherry.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	H	N	O	S	0	0	0
			3433	1111	1691	293	330	8			
1	C	216	Total	C	H	N	O	S	0	0	0
			3435	1111	1693	293	330	8			
1	E	216	Total	C	H	N	O	S	0	0	0
			3433	1111	1691	293	330	8			
1	G	216	Total	C	H	N	O	S	0	0	0
			3436	1111	1694	293	330	8			
1	I	216	Total	C	H	N	O	S	0	0	0
			3432	1111	1690	293	330	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP A0A366VY15
A	-6	ASN	-	expression tag	UNP A0A366VY15
A	-5	GLY	-	expression tag	UNP A0A366VY15
A	66	NRQ	MET	chromophore	UNP A0A366VY15
A	66	NRQ	TYR	chromophore	UNP A0A366VY15
A	66	NRQ	GLY	chromophore	UNP A0A366VY15
C	-7	SER	-	expression tag	UNP A0A366VY15
C	-6	ASN	-	expression tag	UNP A0A366VY15
C	-5	GLY	-	expression tag	UNP A0A366VY15
C	66	NRQ	MET	chromophore	UNP A0A366VY15
C	66	NRQ	TYR	chromophore	UNP A0A366VY15
C	66	NRQ	GLY	chromophore	UNP A0A366VY15
E	-7	SER	-	expression tag	UNP A0A366VY15
E	-6	ASN	-	expression tag	UNP A0A366VY15
E	-5	GLY	-	expression tag	UNP A0A366VY15
E	66	NRQ	MET	chromophore	UNP A0A366VY15
E	66	NRQ	TYR	chromophore	UNP A0A366VY15
E	66	NRQ	GLY	chromophore	UNP A0A366VY15
G	-7	SER	-	expression tag	UNP A0A366VY15

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ASN	-	expression tag	UNP A0A366VY15
G	-5	GLY	-	expression tag	UNP A0A366VY15
G	66	NRQ	MET	chromophore	UNP A0A366VY15
G	66	NRQ	TYR	chromophore	UNP A0A366VY15
G	66	NRQ	GLY	chromophore	UNP A0A366VY15
I	-7	SER	-	expression tag	UNP A0A366VY15
I	-6	ASN	-	expression tag	UNP A0A366VY15
I	-5	GLY	-	expression tag	UNP A0A366VY15
I	66	NRQ	MET	chromophore	UNP A0A366VY15
I	66	NRQ	TYR	chromophore	UNP A0A366VY15
I	66	NRQ	GLY	chromophore	UNP A0A366VY15

- Molecule 2 is a protein called nanobody LaM2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	124	Total	C	H	N	O	S	0	0	0
			1848	597	896	165	186	4			
2	D	124	Total	C	H	N	O	S	0	0	0
			1848	597	896	165	186	4			
2	F	124	Total	C	H	N	O	S	0	0	0
			1844	597	892	165	186	4			
2	H	124	Total	C	H	N	O	S	0	0	0
			1848	597	896	165	186	4			
2	J	124	Total	C	H	N	O	S	0	0	0
			1848	597	896	165	186	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	30	Total	O	0	0
			30	30		
3	C	38	Total	O	0	0
			38	38		
3	D	18	Total	O	0	0
			18	18		
3	E	14	Total	O	0	0
			14	14		
3	F	16	Total	O	0	0
			16	16		
3	G	10	Total	O	0	0
			10	10		

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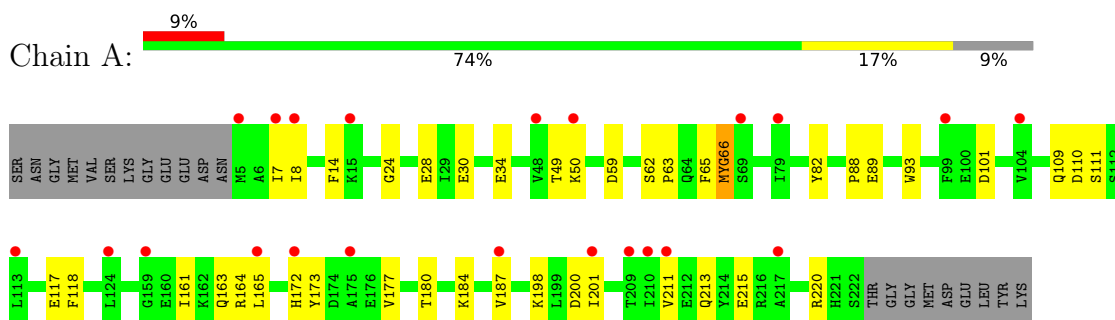
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	27	Total 27	O 27	0	0
3	I	2	Total 2	O 2	0	0
3	J	3	Total 3	O 3	0	0

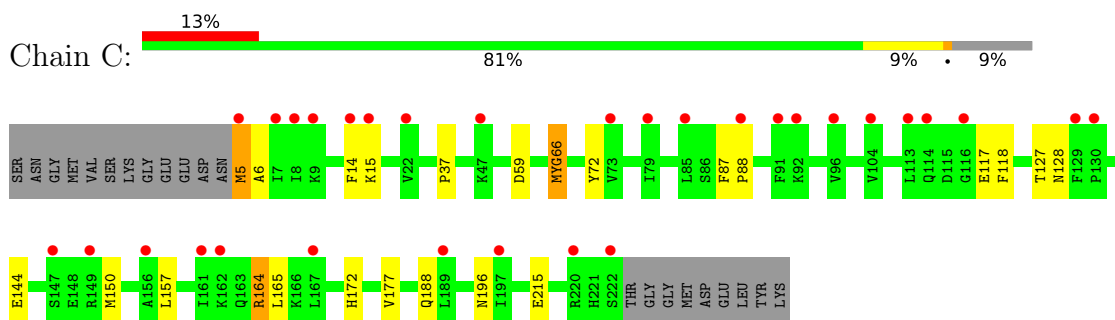
### 3 Residue-property plots [i](#)

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.

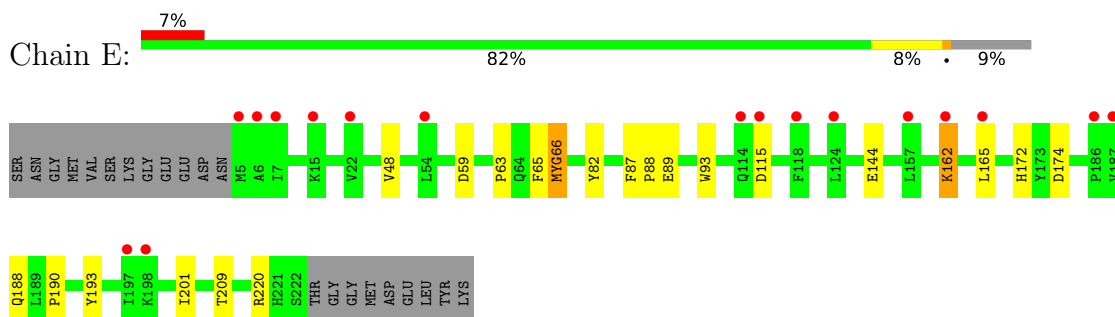
#### • Molecule 1: mCherry



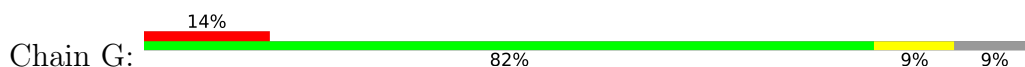
#### • Molecule 1: mCherry

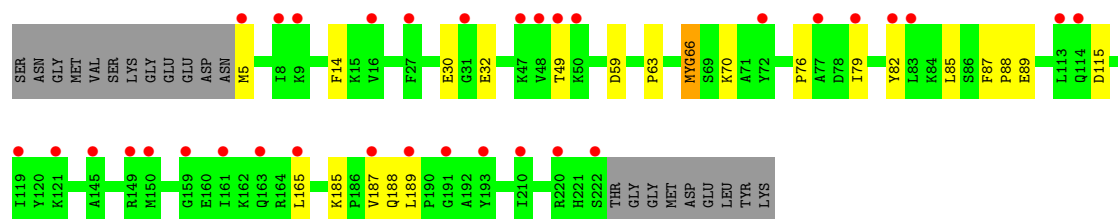


#### • Molecule 1: mCherry

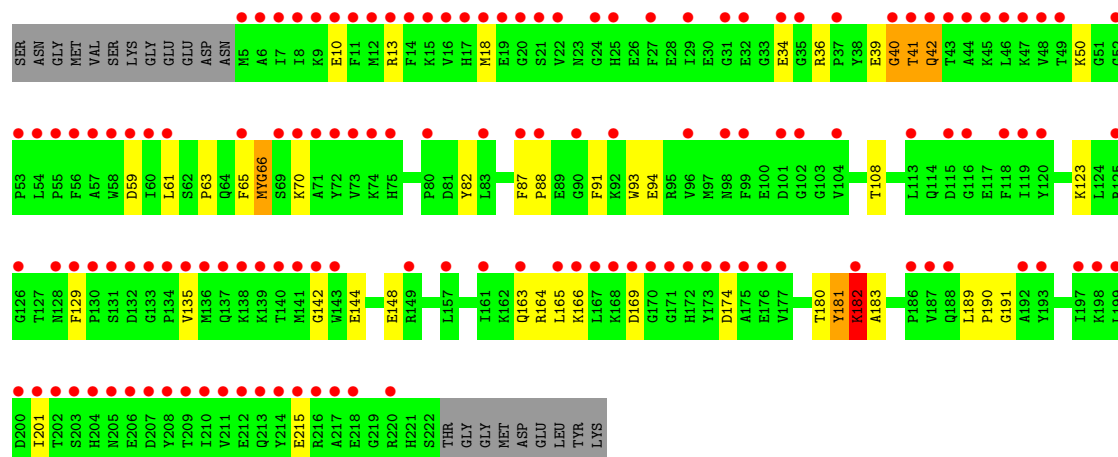
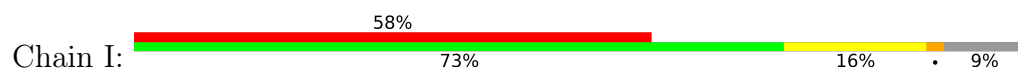


#### • Molecule 1: mCherry





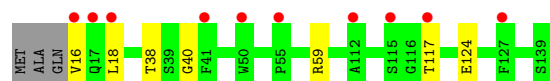
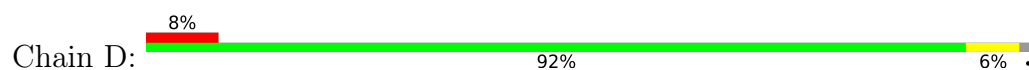
• Molecule 1: mCherry



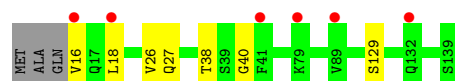
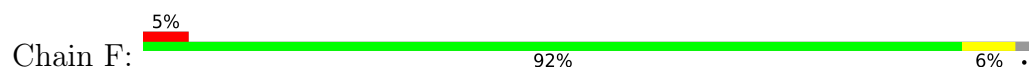
• Molecule 2: nanobody LaM2



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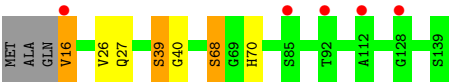
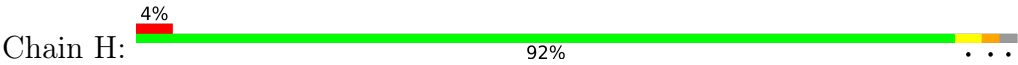


• Molecule 2: nanobody LaM2

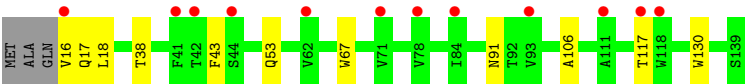
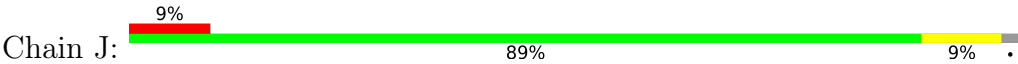


• Molecule 2: nanobody LaM2





● Molecule 2: nanobody LaM2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	171.44Å 160.56Å 88.79Å 90.00° 109.02° 90.00°	Depositor
Resolution (Å)	71.00 – 2.37 71.00 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.0 (71.00-2.37) 99.0 (71.00-2.37)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.208 , 0.234 0.207 , 0.231	Depositor DCC
$R_{free}$ test set	1589 reflections (1.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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

### 5.1 Standard geometry

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	0.49	1/1761 (0.1%)	0.57	1/2369 (0.0%)
1	C	0.64	1/1761 (0.1%)	0.58	0/2369
1	E	0.49	1/1761 (0.1%)	0.55	0/2369
1	G	0.54	0/1761	0.56	0/2369
1	I	0.58	3/1761 (0.2%)	0.79	9/2369 (0.4%)
2	B	0.34	0/975	0.52	0/1321
2	D	0.35	0/975	0.52	0/1321
2	F	0.42	0/975	0.53	0/1321
2	H	0.71	1/975 (0.1%)	0.63	0/1321
2	J	0.31	0/975	0.50	0/1321
All	All	0.51	7/13680 (0.1%)	0.59	10/18450 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	42	GLN	N-CA	-11.04	1.24	1.46
1	I	182	LYS	C-N	10.38	1.57	1.34
1	I	40	GLY	C-N	9.36	1.55	1.34
2	H	68	SER	N-CA	-5.64	1.35	1.46
1	C	177	VAL	C-O	-5.58	1.12	1.23
1	E	162	LYS	C-O	-5.32	1.13	1.23
1	A	117	GLU	CD-OE1	-5.01	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	181	TYR	O-C-N	14.03	145.14	122.70
1	I	181	TYR	C-N-CA	-10.94	94.36	121.70
1	I	181	TYR	CA-C-N	-10.69	93.67	117.20
1	I	41	THR	C-N-CA	-8.33	100.88	121.70
1	I	40	GLY	O-C-N	-7.69	110.40	122.70
1	I	182	LYS	O-C-N	-6.80	111.82	122.70
1	I	41	THR	O-C-N	6.27	132.73	122.70
1	I	41	THR	CA-C-N	-5.70	104.66	117.20
1	A	161	ILE	CB-CA-C	-5.52	100.55	111.60
1	I	40	GLY	C-N-CA	5.30	134.94	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	182	LYS	Mainchain
1	I	40	GLY	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1742	1691	1694	30	0
1	C	1742	1693	1694	15	1
1	E	1742	1691	1694	15	1
1	G	1742	1694	1694	14	1
1	I	1742	1690	1694	25	1
2	B	952	896	896	3	0
2	D	952	896	896	4	0
2	F	952	892	896	3	0
2	H	952	896	896	5	0
2	J	952	896	896	6	0
3	A	25	0	0	1	0
3	B	30	0	0	0	0
3	C	38	0	0	0	0
3	D	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	14	0	0	1	0
3	F	16	0	0	0	0
3	G	10	0	0	0	0
3	H	27	0	0	0	0
3	I	2	0	0	0	0
3	J	3	0	0	0	0
All	All	13653	12935	12950	118	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (118) 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)
2:H:16:VAL:CG2	2:H:40:GLY:HA3	2.01	0.90
2:H:16:VAL:HG23	2:H:40:GLY:HA3	1.53	0.89
1:I:10:GLU:O	1:I:36:ARG:HG2	1.75	0.85
1:A:201:ILE:HD12	1:A:211:VAL:CG1	2.16	0.76
1:A:201:ILE:HD13	1:A:213:GLN:HG2	1.70	0.72
1:G:66:NRQ:O2	1:G:70:LYS:NZ	2.24	0.70
1:C:144:GLU:OE2	1:C:172:HIS:NE2	2.25	0.69
1:I:65:PHE:O	1:I:66:NRQ:HB11	1.92	0.69
1:I:10:GLU:O	1:I:36:ARG:CG	2.43	0.66
2:F:18:LEU:HD22	2:F:38:THR:HG22	1.79	0.65
2:D:18:LEU:HD22	2:D:38:THR:HG22	1.81	0.63
2:D:117:THR:HG23	3:D:209:HOH:O	1.99	0.62
1:C:164:ARG:NH1	1:C:172:HIS:CG	2.68	0.62
1:I:70:LYS:NZ	1:I:148:GLU:OE1	2.30	0.61
2:B:16:VAL:HG12	2:B:40:GLY:HA3	1.83	0.60
1:A:82:TYR:CE1	1:A:187:VAL:HG23	2.37	0.58
1:A:8:ILE:HD12	1:A:118:PHE:HZ	1.69	0.58
1:G:85:LEU:HB2	1:G:187:VAL:HG11	1.85	0.58
1:C:15:LYS:NZ	1:C:117:GLU:OE1	2.36	0.57
1:E:144:GLU:OE2	1:E:172:HIS:NE2	2.33	0.57
1:A:8:ILE:HD12	1:A:118:PHE:CZ	2.39	0.57
2:F:16:VAL:HG12	2:F:40:GLY:HA3	1.87	0.56
1:I:129:PHE:CE2	1:I:135:VAL:HG21	2.41	0.55
1:E:48:VAL:HG21	1:E:209:THR:HG22	1.89	0.55
1:C:59:ASP:HB3	1:C:165:LEU:HD21	1.89	0.55
1:G:30:GLU:HG3	1:G:49:THR:HG21	1.88	0.55
1:E:48:VAL:O	1:E:48:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HH22	1:A:172:HIS:HB2	1.72	0.54
1:E:201:ILE:HD11	3:E:301:HOH:O	2.08	0.53
1:I:164:ARG:NH2	1:I:174:ASP:OD2	2.41	0.53
1:A:59:ASP:HB3	1:A:165:LEU:HD21	1.92	0.52
1:A:201:ILE:HD12	1:A:211:VAL:HG11	1.90	0.52
1:C:164:ARG:HH12	1:C:172:HIS:CG	2.27	0.51
1:I:66:NRQ:N2	1:I:66:NRQ:HD1	2.26	0.51
1:A:164:ARG:NH2	1:A:172:HIS:CB	2.75	0.50
1:I:13:ARG:NH2	1:I:34:GLU:OE1	2.44	0.50
1:G:187:VAL:HG12	1:G:188:GLN:N	2.26	0.50
1:C:66:NRQ:HD1	1:C:66:NRQ:N2	2.26	0.50
1:G:14:PHE:C	1:G:14:PHE:CD1	2.85	0.50
1:C:5:MET:O	1:C:6:ALA:HB3	2.12	0.49
1:C:127:THR:O	1:C:128:ASN:HB2	2.12	0.49
1:A:89:GLU:OE1	1:A:89:GLU:N	2.43	0.49
2:H:16:VAL:HG23	2:H:39:SER:O	2.13	0.49
1:A:201:ILE:CD1	1:A:213:GLN:HG2	2.41	0.48
1:I:142:GLY:O	1:I:165:LEU:HD23	2.13	0.48
1:E:59:ASP:HB3	1:E:165:LEU:HD21	1.96	0.48
1:I:94:GLU:HG3	2:J:67:TRP:CZ2	2.48	0.48
1:E:66:NRQ:HA31	1:E:66:NRQ:N1	2.29	0.47
1:A:163:GLN:OE1	1:A:177:VAL:HG21	2.15	0.47
1:E:87:PHE:HB3	1:E:88:PRO:HA	1.96	0.47
2:J:18:LEU:HD22	2:J:38:THR:HG22	1.96	0.47
2:B:18:LEU:HD22	2:B:38:THR:HG22	1.97	0.46
1:G:82:TYR:CD1	1:G:189:LEU:HD23	2.51	0.46
1:G:87:PHE:HB3	1:G:88:PRO:HA	1.98	0.46
1:I:82:TYR:HB2	1:I:190:PRO:HD3	1.98	0.46
1:G:59:ASP:HB3	1:G:165:LEU:HD21	1.97	0.46
1:G:59:ASP:O	1:G:63:PRO:HD3	2.16	0.46
1:I:66:NRQ:HD1	1:I:215:GLU:OE1	2.16	0.46
1:A:65:PHE:O	1:A:66:NRQ:C3	2.64	0.45
1:A:59:ASP:O	1:A:63:PRO:HD3	2.16	0.45
1:I:59:ASP:O	1:I:63:PRO:HD3	2.16	0.45
1:A:66:NRQ:HD1	1:A:215:GLU:OE1	2.16	0.45
1:G:30:GLU:CG	1:G:49:THR:HG21	2.47	0.45
2:H:68:SER:HB2	2:H:70:HIS:CD2	2.52	0.45
1:A:24:GLY:O	3:A:301:HOH:O	2.21	0.45
1:I:91:PHE:HB2	1:I:182:LYS:O	2.17	0.45
2:J:53:GLN:O	2:J:106:ALA:HB1	2.17	0.45
1:A:28:GLU:CD	1:A:50:LYS:HD2	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:GLU:OE1	1:G:185:LYS:HD3	2.17	0.45
1:C:66:NRQ:HD1	1:C:215:GLU:OE1	2.17	0.45
1:C:87:PHE:HB3	1:C:88:PRO:HA	1.99	0.44
1:I:41:THR:O	1:I:42:GLN:HB3	2.16	0.44
1:I:108:THR:HG22	1:I:123:LYS:HB2	1.99	0.44
2:J:43:PHE:CD2	2:J:91:ASN:HA	2.52	0.44
1:A:7:ILE:HD13	1:A:88:PRO:HD3	1.99	0.44
1:A:30:GLU:HG3	1:A:49:THR:HG21	1.98	0.44
1:A:198:LYS:HE3	1:A:200:ASP:OD2	2.17	0.44
1:E:82:TYR:HB2	1:E:190:PRO:HD3	2.00	0.44
1:A:66:NRQ:OH	1:A:163:GLN:NE2	2.50	0.44
1:A:82:TYR:CD1	1:A:187:VAL:HG23	2.52	0.44
2:D:59:ARG:NH2	2:D:124:GLU:OE2	2.48	0.43
2:J:38:THR:HG21	2:J:43:PHE:CD1	2.54	0.43
1:I:182:LYS:HG2	1:I:183:ALA:N	2.34	0.43
1:E:48:VAL:CG2	1:E:209:THR:HG22	2.49	0.43
1:C:150:MET:HE2	1:C:157:LEU:HD21	2.01	0.42
1:A:65:PHE:O	1:A:66:NRQ:CA3	2.67	0.42
1:I:201:ILE:HD12	1:I:201:ILE:H	1.84	0.42
1:A:14:PHE:CB	1:A:118:PHE:HB2	2.51	0.41
1:A:66:NRQ:HD1	1:A:66:NRQ:N2	2.35	0.41
1:C:164:ARG:HH11	1:C:164:ARG:HG2	1.85	0.41
1:E:65:PHE:O	1:E:66:NRQ:CB1	2.68	0.41
1:A:93:TRP:HA	1:A:180:THR:O	2.20	0.41
1:A:101:ASP:OD1	1:A:173:TYR:OH	2.34	0.41
2:D:16:VAL:HG12	2:D:40:GLY:HA3	2.02	0.41
1:G:76:PRO:HG2	1:G:79:ILE:HD12	2.03	0.41
1:C:5:MET:HB2	1:C:6:ALA:H	1.40	0.41
1:C:37:PRO:HA	1:C:72:TYR:HA	2.02	0.41
1:E:193:TYR:HB2	1:E:220:ARG:O	2.20	0.41
1:I:93:TRP:HA	1:I:180:THR:O	2.21	0.41
1:I:144:GLU:HG2	1:I:166:LYS:HE3	2.03	0.41
1:A:62:SER:N	1:A:63:PRO:CD	2.84	0.41
1:C:14:PHE:CB	1:C:118:PHE:HB2	2.51	0.41
1:E:66:NRQ:HA32	1:E:93:TRP:CZ2	2.55	0.41
1:I:87:PHE:HB3	1:I:88:PRO:HA	2.03	0.41
1:E:162:LYS:HE2	1:E:174:ASP:HB3	2.03	0.41
1:I:42:GLN:HG3	1:I:66:NRQ:SD	2.61	0.41
1:A:110:ASP:OD1	1:A:184:LYS:NZ	2.50	0.40
1:I:18:MET:SD	1:I:65:PHE:CZ	3.14	0.40
2:B:26:VAL:O	2:B:138:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:VAL:HG22	2:F:27:GLN:N	2.36	0.40
1:G:85:LEU:CB	1:G:187:VAL:HG11	2.51	0.40
2:H:26:VAL:HG22	2:H:27:GLN:N	2.36	0.40
1:A:109:GLN:NE2	1:A:111:SER:OG	2.52	0.40
1:E:188:GLN:NE2	2:J:130:TRP:O	2.54	0.40
1:G:66:NRQ:C2	1:G:70:LYS:NZ	2.85	0.40
1:I:82:TYR:CD1	1:I:189:LEU:HD23	2.56	0.40
1:E:59:ASP:O	1:E:63:PRO:HD3	2.21	0.40
1:I:18:MET:HE1	1:I:61:LEU:HD22	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:GLU:OE2	1:G:115:ASP:H[4_445]	1.45	0.15
1:C:188:GLN:OE1	1:I:191:GLY:H[1_556]	1.59	0.01

## 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	211/237 (89%)	208 (99%)	3 (1%)	0	100	100
1	C	211/237 (89%)	207 (98%)	4 (2%)	0	100	100
1	E	211/237 (89%)	208 (99%)	3 (1%)	0	100	100
1	G	211/237 (89%)	207 (98%)	4 (2%)	0	100	100
1	I	211/237 (89%)	205 (97%)	6 (3%)	0	100	100
2	B	122/127 (96%)	117 (96%)	4 (3%)	1 (1%)	19	27
2	D	122/127 (96%)	116 (95%)	6 (5%)	0	100	100
2	F	122/127 (96%)	117 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
2	J	122/127 (96%)	114 (93%)	8 (7%)	0	100	100
All	All	1665/1820 (92%)	1616 (97%)	48 (3%)	1 (0%)	51	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	129	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/200 (92%)	181 (99%)	2 (1%)	73	86
1	C	183/200 (92%)	180 (98%)	3 (2%)	62	78
1	E	183/200 (92%)	182 (100%)	1 (0%)	88	95
1	G	183/200 (92%)	181 (99%)	2 (1%)	73	86
1	I	183/200 (92%)	178 (97%)	5 (3%)	44	62
2	B	99/101 (98%)	98 (99%)	1 (1%)	76	87
2	D	99/101 (98%)	99 (100%)	0	100	100
2	F	99/101 (98%)	98 (99%)	1 (1%)	76	87
2	H	99/101 (98%)	97 (98%)	2 (2%)	55	72
2	J	99/101 (98%)	96 (97%)	3 (3%)	41	59
All	All	1410/1505 (94%)	1390 (99%)	20 (1%)	67	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	220	ARG
2	B	39	SER

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Mol	Chain	Res	Type
1	C	5	MET
1	C	164	ARG
1	C	196	ASN
1	E	115	ASP
2	F	129	SER
1	G	5	MET
1	G	32	GLU
2	H	16	VAL
2	H	39	SER
1	I	39	GLU
1	I	50	LYS
1	I	163	GLN
1	I	169	ASP
1	I	181	TYR
2	J	16	VAL
2	J	17	GLN
2	J	117	THR

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

Mol	Chain	Res	Type
1	A	163	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	E	66	1	23,24,25	2.48	8 (34%)	23,32,34	2.93	7 (30%)
1	NRQ	C	66	1	23,24,25	2.43	7 (30%)	23,32,34	3.38	8 (34%)
1	NRQ	I	66	1	23,24,25	2.42	8 (34%)	23,32,34	3.31	8 (34%)
1	NRQ	G	66	1	23,24,25	2.44	8 (34%)	23,32,34	3.34	7 (30%)
1	NRQ	A	66	1	23,24,25	2.52	7 (30%)	23,32,34	3.72	9 (39%)

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	E	66	1	-	4/9/31/32	0/2/2/2
1	NRQ	C	66	1	-	4/9/31/32	0/2/2/2
1	NRQ	I	66	1	-	4/9/31/32	0/2/2/2
1	NRQ	G	66	1	-	4/9/31/32	0/2/2/2
1	NRQ	A	66	1	-	4/9/31/32	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	NRQ	C1-N3	6.62	1.49	1.38
1	E	66	NRQ	CA2-C2	6.25	1.54	1.48
1	I	66	NRQ	CA2-C2	6.25	1.54	1.48
1	G	66	NRQ	CA2-C2	6.23	1.54	1.48
1	C	66	NRQ	CA2-C2	5.43	1.54	1.48
1	C	66	NRQ	C1-N3	5.40	1.47	1.38
1	E	66	NRQ	C1-N3	5.33	1.47	1.38
1	A	66	NRQ	CA2-C2	4.96	1.53	1.48
1	I	66	NRQ	C1-N3	4.88	1.46	1.38
1	A	66	NRQ	C1-N2	4.86	1.43	1.33
1	G	66	NRQ	C1-N2	4.76	1.43	1.33
1	G	66	NRQ	C1-N3	4.72	1.46	1.38
1	E	66	NRQ	C1-N2	4.54	1.43	1.33
1	C	66	NRQ	C1-N2	4.19	1.42	1.33
1	I	66	NRQ	C1-N2	4.09	1.42	1.33
1	I	66	NRQ	C2-N3	4.08	1.49	1.39
1	C	66	NRQ	C2-N3	4.06	1.49	1.39
1	I	66	NRQ	CG2-CB2	3.99	1.54	1.46
1	A	66	NRQ	C2-N3	3.88	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	NRQ	CG2-CB2	3.73	1.54	1.46
1	G	66	NRQ	CG2-CB2	3.68	1.53	1.46
1	E	66	NRQ	CG2-CB2	3.63	1.53	1.46
1	G	66	NRQ	C2-N3	3.61	1.48	1.39
1	E	66	NRQ	C2-N3	3.60	1.48	1.39
1	A	66	NRQ	CG2-CB2	3.59	1.53	1.46
1	C	66	NRQ	CB2-CA2	-3.47	1.32	1.35
1	A	66	NRQ	CB2-CA2	-3.16	1.32	1.35
1	E	66	NRQ	CB2-CA2	-3.05	1.32	1.35
1	G	66	NRQ	CB2-CA2	-2.75	1.32	1.35
1	I	66	NRQ	CB2-CA2	-2.60	1.32	1.35
1	G	66	NRQ	O2-C2	-2.27	1.18	1.23
1	E	66	NRQ	O2-C2	-2.22	1.18	1.23
1	E	66	NRQ	CA2-N2	2.21	1.43	1.38
1	C	66	NRQ	O2-C2	-2.18	1.18	1.23
1	G	66	NRQ	CA2-N2	2.15	1.43	1.38
1	I	66	NRQ	O2-C2	-2.05	1.18	1.23
1	A	66	NRQ	O2-C2	-2.03	1.18	1.23
1	I	66	NRQ	CA2-N2	2.02	1.42	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	NRQ	CA2-C2-N3	10.45	108.31	103.37
1	A	66	NRQ	CA2-C2-N3	10.24	108.21	103.37
1	A	66	NRQ	O2-C2-CA2	-10.15	125.26	130.96
1	G	66	NRQ	O2-C2-CA2	-9.68	125.53	130.96
1	C	66	NRQ	O2-C2-CA2	-9.26	125.76	130.96
1	C	66	NRQ	CA2-C2-N3	9.06	107.66	103.37
1	E	66	NRQ	CA2-C2-N3	8.83	107.55	103.37
1	I	66	NRQ	CA2-C2-N3	8.65	107.46	103.37
1	I	66	NRQ	O2-C2-CA2	-8.47	126.20	130.96
1	E	66	NRQ	O2-C2-CA2	-7.40	126.81	130.96
1	I	66	NRQ	CG2-CB2-CA2	-5.67	123.00	129.94
1	A	66	NRQ	CG2-CB2-CA2	-5.04	123.76	129.94
1	C	66	NRQ	CG2-CB2-CA2	-4.96	123.86	129.94
1	A	66	NRQ	C2-CA2-N2	-4.74	105.61	108.93
1	I	66	NRQ	C2-CA2-N2	-4.45	105.82	108.93
1	C	66	NRQ	C2-CA2-N2	-4.44	105.83	108.93
1	G	66	NRQ	C2-CA2-N2	-4.43	105.83	108.93
1	I	66	NRQ	CB2-CA2-C2	4.06	127.12	122.28
1	A	66	NRQ	CA2-N2-C1	4.00	111.66	104.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	NRQ	CG2-CB2-CA2	-3.93	125.13	129.94
1	C	66	NRQ	CA2-N2-C1	3.55	110.83	104.33
1	E	66	NRQ	C2-CA2-N2	-3.55	106.44	108.93
1	A	66	NRQ	N3-C1-N2	-3.32	108.90	113.28
1	C	66	NRQ	CB2-CA2-C2	3.29	126.20	122.28
1	I	66	NRQ	CA2-N2-C1	3.20	110.18	104.33
1	E	66	NRQ	CE-SD-CG1	2.95	110.53	100.40
1	A	66	NRQ	CA3-N3-C1	2.77	133.65	128.22
1	I	66	NRQ	O3-C3-CA3	-2.71	118.22	126.39
1	E	66	NRQ	CA2-N2-C1	2.69	109.25	104.33
1	G	66	NRQ	CA2-N2-C1	2.64	109.15	104.33
1	A	66	NRQ	CE-SD-CG1	2.55	109.17	100.40
1	I	66	NRQ	CE-SD-CG1	2.29	108.28	100.40
1	G	66	NRQ	O3-C3-CA3	-2.28	119.50	126.39
1	C	66	NRQ	CE-SD-CG1	2.24	108.11	100.40
1	E	66	NRQ	CD1-CG2-CD2	2.12	120.77	117.64
1	A	66	NRQ	CD1-CG2-CD2	2.12	120.77	117.64
1	G	66	NRQ	CE-SD-CG1	2.06	107.47	100.40
1	G	66	NRQ	CD1-CG2-CD2	2.03	120.65	117.64
1	C	66	NRQ	N3-C1-N2	-2.02	110.61	113.28

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	NRQ	CA1-CB1-CG1-SD
1	A	66	NRQ	N2-CA2-CB2-CG2
1	A	66	NRQ	C2-CA2-CB2-CG2
1	C	66	NRQ	CA1-CB1-CG1-SD
1	C	66	NRQ	N2-CA2-CB2-CG2
1	C	66	NRQ	C2-CA2-CB2-CG2
1	E	66	NRQ	CA1-CB1-CG1-SD
1	E	66	NRQ	N2-CA2-CB2-CG2
1	E	66	NRQ	C2-CA2-CB2-CG2
1	G	66	NRQ	CA1-CB1-CG1-SD
1	G	66	NRQ	N2-CA2-CB2-CG2
1	G	66	NRQ	C2-CA2-CB2-CG2
1	I	66	NRQ	CA1-CB1-CG1-SD
1	I	66	NRQ	N2-CA2-CB2-CG2
1	I	66	NRQ	C2-CA2-CB2-CG2
1	E	66	NRQ	CB1-CG1-SD-CE
1	A	66	NRQ	CB1-CG1-SD-CE

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Mol	Chain	Res	Type	Atoms
1	C	66	NRQ	CB1-CG1-SD-CE
1	I	66	NRQ	CB1-CG1-SD-CE
1	G	66	NRQ	CB1-CG1-SD-CE

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	66	NRQ	3	0
1	C	66	NRQ	2	0
1	I	66	NRQ	4	0
1	G	66	NRQ	2	0
1	A	66	NRQ	5	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	215/237 (90%)	1.17	22 (10%) 6 7	41, 64, 91, 126	0
1	C	215/237 (90%)	1.31	31 (14%) 2 2	45, 63, 91, 143	0
1	E	215/237 (90%)	1.10	17 (7%) 12 13	48, 67, 92, 124	0
1	G	215/237 (90%)	1.28	33 (15%) 2 2	50, 74, 106, 122	0
1	I	215/237 (90%)	3.25	137 (63%) 0 0	70, 112, 148, 167	0
2	B	124/127 (97%)	1.11	5 (4%) 38 41	43, 54, 78, 109	0
2	D	124/127 (97%)	1.20	10 (8%) 12 13	46, 58, 90, 110	0
2	F	124/127 (97%)	1.03	6 (4%) 30 33	43, 54, 81, 104	0
2	H	124/127 (97%)	1.07	5 (4%) 38 41	45, 55, 71, 88	0
2	J	124/127 (97%)	1.17	12 (9%) 7 8	57, 69, 91, 112	0
All	All	1695/1820 (93%)	1.44	278 (16%) 1 1	41, 67, 119, 167	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	5	MET	11.8
1	I	167	LEU	11.6
1	I	6	ALA	11.2
1	I	16	VAL	9.0
1	I	11	PHE	8.9
1	I	208	TYR	8.5
1	I	206	GLU	8.1
1	I	65	PHE	8.1
1	I	199	LEU	8.1
1	I	60	ILE	8.0
1	I	8	ILE	8.0
1	I	46	LEU	7.8
1	I	136	MET	7.6

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Mol	Chain	Res	Type	RSRZ
1	I	119	ILE	7.6
1	I	139	LYS	7.5
1	I	72	TYR	7.2
1	I	169	ASP	7.2
1	I	168	LYS	7.2
1	I	143	TRP	7.0
2	J	16	VAL	6.7
1	I	173	TYR	6.7
1	I	129	PHE	6.4
1	I	135	VAL	6.4
1	I	210	ILE	6.4
1	I	141	MET	6.3
1	I	137	GLN	6.2
1	I	201	ILE	6.0
1	I	113	LEU	6.0
1	I	203	SER	5.9
1	I	211	VAL	5.9
1	I	56	PHE	5.9
1	I	101	ASP	5.9
1	I	171	GLY	5.6
1	I	170	GLY	5.6
1	I	212	GLU	5.6
1	I	130	PRO	5.4
1	I	213	GLN	5.4
1	I	47	LYS	5.4
1	I	87	PHE	5.4
1	I	53	PRO	5.2
1	I	88	PRO	5.2
1	I	43	THR	5.0
1	C	8	ILE	4.9
1	I	133	GLY	4.8
1	I	99	PHE	4.8
1	I	92	LYS	4.8
1	I	134	PRO	4.7
1	I	138	LYS	4.7
1	I	15	LYS	4.7
1	I	14	PHE	4.7
1	I	197	ILE	4.4
1	I	74	LYS	4.4
1	I	98	ASN	4.4
1	I	204	HIS	4.3
1	I	45	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	18	MET	4.3
1	I	27	PHE	4.2
1	I	175	ALA	4.2
1	I	174	ASP	4.2
1	I	165	LEU	4.1
1	A	5	MET	4.1
1	I	29	ILE	4.0
1	I	22	VAL	4.0
1	I	13	ARG	4.0
1	I	9	LYS	4.0
1	I	54	LEU	4.0
1	I	217	ALA	3.9
1	G	210	ILE	3.9
1	I	69	SER	3.9
1	I	118	PHE	3.9
1	I	188	GLN	3.9
1	I	35	GLY	3.8
1	G	113	LEU	3.8
1	I	37	PRO	3.8
1	G	50	LYS	3.8
1	I	49	THR	3.8
1	C	220	ARG	3.7
1	I	198	LYS	3.7
1	I	209	THR	3.7
1	I	200	ASP	3.6
1	I	172	HIS	3.6
1	I	218	GLU	3.5
1	C	114	GLN	3.5
2	D	41	PHE	3.5
1	C	5	MET	3.5
1	I	48	VAL	3.5
1	I	131	SER	3.5
1	I	83	LEU	3.4
1	I	96	VAL	3.4
1	I	216	ARG	3.4
2	D	55	PRO	3.4
1	I	140	THR	3.4
1	C	9	LYS	3.4
2	D	117	THR	3.4
1	I	17	HIS	3.3
1	A	50	LYS	3.3
1	I	214	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	172	HIS	3.3
2	B	55	PRO	3.3
2	B	16	VAL	3.3
1	I	12	MET	3.2
1	C	149	ARG	3.2
1	I	115	ASP	3.2
1	I	41	THR	3.2
1	G	47	LYS	3.2
1	A	210	ILE	3.1
1	I	215	GLU	3.1
2	B	19	VAL	3.1
1	I	132	ASP	3.1
1	I	187	VAL	3.1
1	I	149	ARG	3.1
1	E	15	LYS	3.1
1	I	70	LYS	3.1
1	I	58	TRP	3.1
1	I	61	LEU	3.1
1	G	77	ALA	3.0
2	D	16	VAL	3.0
1	G	161	ILE	3.0
1	I	220	ARG	3.0
1	G	9	LYS	3.0
1	I	126	GLY	3.0
1	C	7	ILE	3.0
1	G	48	VAL	3.0
1	A	165	LEU	2.9
1	C	113	LEU	2.9
1	I	42	GLN	2.9
1	I	59	ASP	2.9
1	I	44	ALA	2.9
1	C	161	ILE	2.9
1	I	202	THR	2.9
1	I	116	GLY	2.8
1	E	157	LEU	2.8
1	G	114	GLN	2.8
1	I	73	VAL	2.8
1	I	40	GLY	2.8
1	I	10	GLU	2.8
2	J	41	PHE	2.8
2	F	16	VAL	2.8
2	F	79	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	113	LEU	2.7
2	D	17	GLN	2.7
1	I	161	ILE	2.7
1	I	120	TYR	2.7
1	I	71	ALA	2.7
1	G	187	VAL	2.7
1	I	176	GLU	2.7
1	G	5	MET	2.7
1	I	7	ILE	2.7
1	I	207	ASP	2.7
1	I	163	GLN	2.6
1	G	83	LEU	2.6
1	G	149	ARG	2.6
1	I	166	LYS	2.6
1	A	201	ILE	2.6
1	I	75	HIS	2.6
1	G	193	TYR	2.6
1	C	147	SER	2.6
1	G	8	ILE	2.6
1	I	19	GLU	2.6
1	C	222	SER	2.6
2	D	18	LEU	2.6
2	D	115	SER	2.6
1	I	192	ALA	2.6
1	E	197	ILE	2.6
1	E	115	ASP	2.6
1	C	85	LEU	2.6
1	E	6	ALA	2.6
1	I	128	ASN	2.6
2	D	127	PHE	2.5
1	A	15	LYS	2.5
1	I	20	GLY	2.5
2	J	44	SER	2.5
1	C	104	VAL	2.5
2	H	16	VAL	2.5
2	J	42	THR	2.5
1	I	32	GLU	2.5
2	J	84	ILE	2.5
1	C	96	VAL	2.5
1	C	15	LYS	2.5
1	C	189	LEU	2.5
1	I	125	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	175	ALA	2.4
1	I	90	GLY	2.4
1	I	142	GLY	2.4
1	G	165	LEU	2.4
2	J	93	VAL	2.4
2	J	117	THR	2.4
1	G	222	SER	2.4
1	I	177	VAL	2.4
1	G	72	TYR	2.4
1	G	189	LEU	2.4
1	E	5	MET	2.4
1	C	14	PHE	2.4
1	C	47	LYS	2.4
1	G	145	ALA	2.4
1	I	34	GLU	2.4
1	I	25	HIS	2.3
1	I	102	GLY	2.3
1	I	55	PRO	2.3
1	A	99	PHE	2.3
1	G	220	ARG	2.3
1	A	187	VAL	2.3
1	C	91	PHE	2.3
1	C	197	ILE	2.3
1	I	57	ALA	2.3
1	A	104	VAL	2.3
1	A	7	ILE	2.3
1	A	8	ILE	2.3
2	D	112	ALA	2.3
1	E	54	LEU	2.3
2	J	118	TRP	2.3
1	C	79	ILE	2.3
1	I	157	LEU	2.3
1	I	31	GLY	2.3
2	D	50	TRP	2.3
2	J	71	VAL	2.3
1	C	88	PRO	2.3
1	G	163	GLN	2.3
2	F	18	LEU	2.2
1	E	162	LYS	2.2
1	I	182	LYS	2.2
1	C	22	VAL	2.2
2	F	89	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	80	PRO	2.2
2	J	111	ALA	2.2
2	H	128	GLY	2.2
2	F	132	GLN	2.2
1	A	217	ALA	2.2
1	E	124	LEU	2.2
1	I	205	ASN	2.2
2	B	48	MET	2.2
2	J	62	VAL	2.2
1	E	198	LYS	2.2
1	I	186	PRO	2.2
1	A	159	GLY	2.2
1	C	116	GLY	2.2
1	C	129	PHE	2.2
1	I	104	VAL	2.2
1	G	82	TYR	2.1
2	J	78	VAL	2.1
2	H	92	THR	2.1
1	C	167	LEU	2.1
1	G	121	LYS	2.1
1	C	73	VAL	2.1
1	G	49	THR	2.1
1	G	119	ILE	2.1
1	G	31	GLY	2.1
1	A	209	THR	2.1
1	E	114	GLN	2.1
1	G	79	ILE	2.1
1	E	165	LEU	2.1
1	G	159	GLY	2.1
2	H	85	SER	2.1
1	E	118	PHE	2.1
2	B	56	GLY	2.1
1	A	79	ILE	2.1
1	C	92	LYS	2.1
1	C	162	LYS	2.1
1	A	211	VAL	2.1
1	I	21	SER	2.1
1	E	186	PRO	2.1
1	G	150	MET	2.1
1	C	130	PRO	2.1
1	E	7	ILE	2.0
1	G	191	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	48	VAL	2.0
1	E	22	VAL	2.0
1	E	187	VAL	2.0
1	G	16	VAL	2.0
1	I	193	TYR	2.0
2	F	41	PHE	2.0
1	A	124	LEU	2.0
1	I	52	GLY	2.0
1	G	27	PHE	2.0
1	I	24	GLY	2.0
1	A	69	SER	2.0
1	C	156	ALA	2.0
2	H	112	ALA	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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	NRQ	I	66	23/24	0.72	0.44	117,132,160,161	0
1	NRQ	A	66	23/24	0.81	0.28	76,98,120,120	0
1	NRQ	E	66	23/24	0.84	0.28	72,86,103,106	0
1	NRQ	C	66	23/24	0.86	0.33	75,87,105,105	0
1	NRQ	G	66	23/24	0.87	0.29	78,95,115,115	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.