



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 02:19 PM UTC

PDB ID : 7SAJ / pdb_00007saj
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

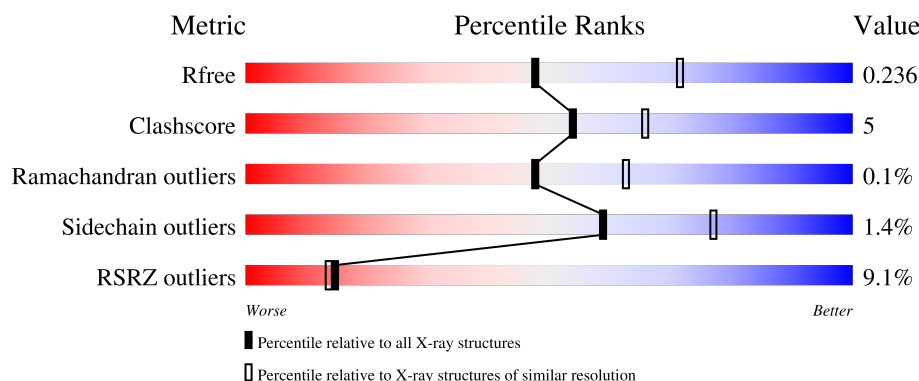
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (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 ≥ 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	3% 73% 16% • 9%
1	C	237	5% 80% 8% • 9%
1	E	237	3% 78% 12% • 9%
1	G	237	7% 78% 12% • 9%
1	I	237	35% 70% 18% •• 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	127	4% 92% 6%
2	D	127	6% 92% 6%
2	F	127	3% 92% 5%
2	H	127	3% 89% 7%
2	J	127	6% 87% 10%

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

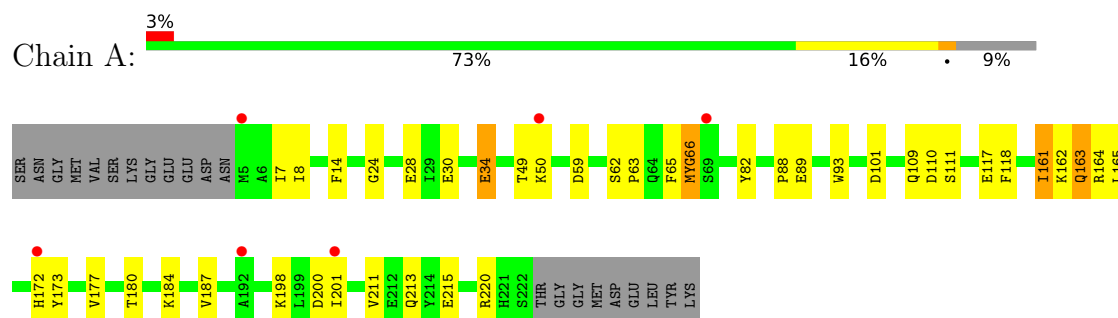
Continued from previous page...

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

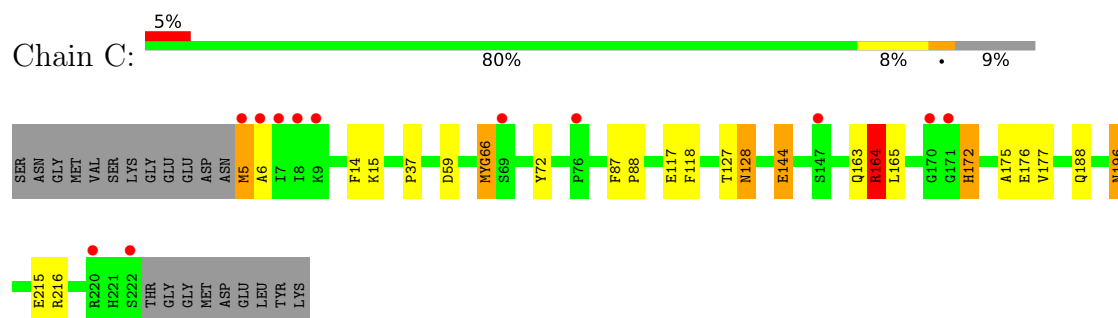
3 Residue-property plots [i](#)

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.

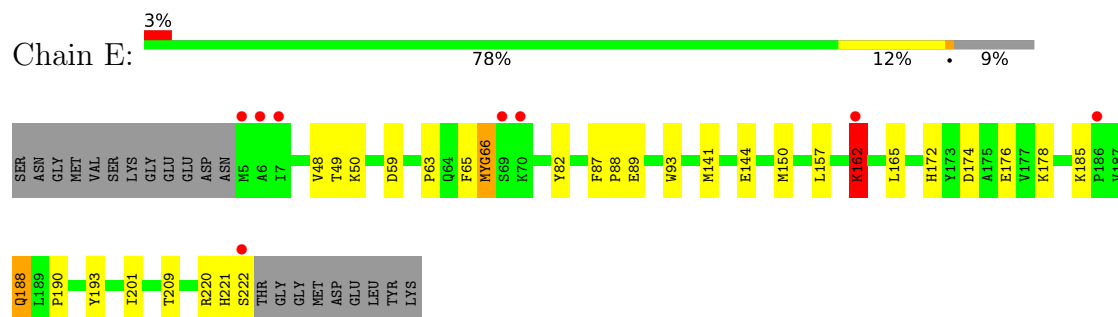
• Molecule 1: mCherry



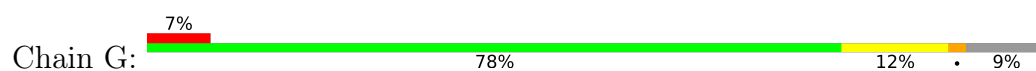
• Molecule 1: mCherry

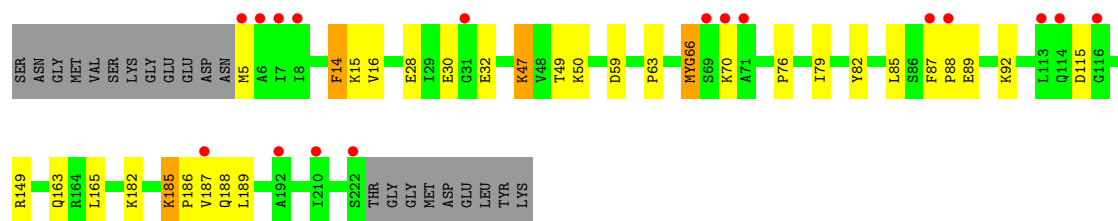


• Molecule 1: mCherry

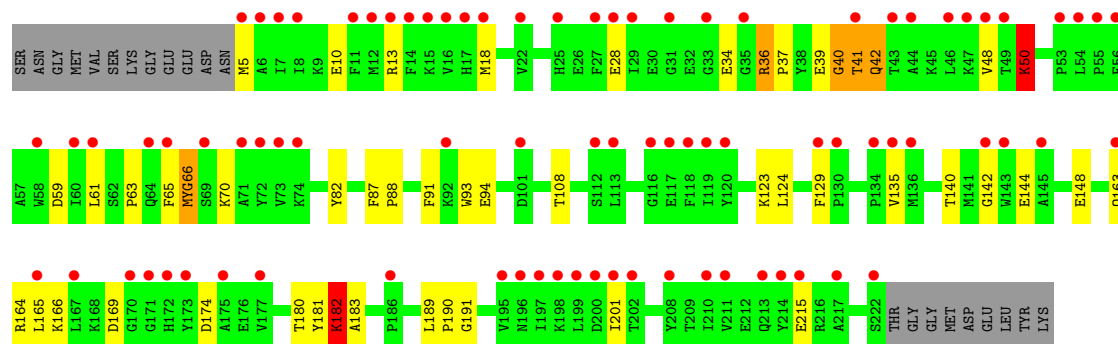


• Molecule 1: mCherry

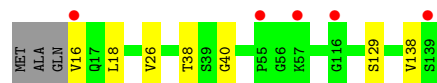
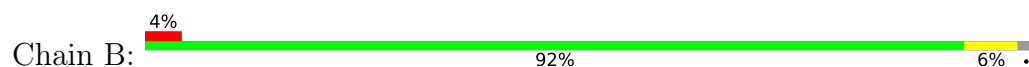




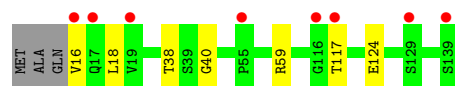
• Molecule 1: mCherry



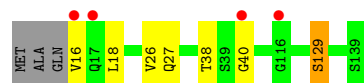
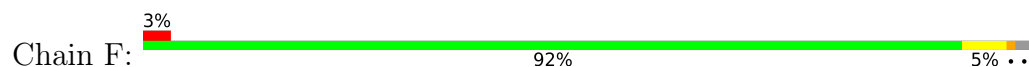
• Molecule 2: nanobody LaM2



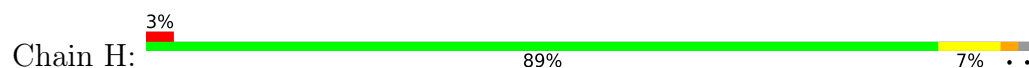
• Molecule 2: nanobody LaM2

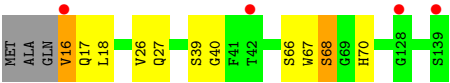


• Molecule 2: nanobody LaM2

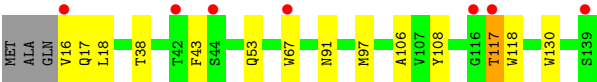
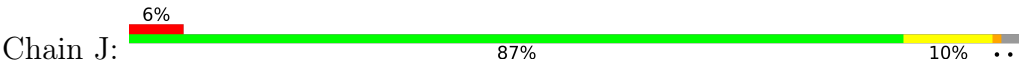


• Molecule 2: nanobody LaM2





● Molecule 2: nanobody LaM2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 99.1 (71.00-2.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.208 , 0.234 0.211 , 0.236	Depositor DCC
R_{free} test set	1590 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.55	5/1761 (0.3%)	0.51	2/2369 (0.1%)
1	C	0.82	13/1761 (0.7%)	0.54	0/2369
1	E	0.60	8/1761 (0.5%)	0.46	0/2369
1	G	0.69	11/1761 (0.6%)	0.52	0/2369
1	I	0.84	5/1761 (0.3%)	0.96	11/2369 (0.5%)
2	B	0.24	0/975	0.41	0/1321
2	D	0.23	0/975	0.42	0/1321
2	F	0.40	1/975 (0.1%)	0.43	0/1321
2	H	0.81	6/975 (0.6%)	0.62	3/1321 (0.2%)
2	J	0.21	0/975	0.40	0/1321
All	All	0.63	49/13680 (0.4%)	0.57	16/18450 (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 (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	42	GLN	N-CA	-17.67	1.24	1.46
1	I	40	GLY	C-N	17.57	1.55	1.33
1	I	182	LYS	C-N	17.18	1.57	1.33
1	C	177	VAL	C-O	-11.08	1.12	1.24
1	E	162	LYS	C-O	-9.39	1.13	1.24
2	H	17	GLN	C-O	-8.37	1.14	1.23
2	H	68	SER	N-CA	-8.37	1.35	1.46
2	H	18	LEU	C-O	-8.24	1.14	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176	GLU	C-O	-8.04	1.14	1.24
1	E	178	LYS	C-O	-8.02	1.14	1.24
1	G	149	ARG	C-O	-7.98	1.14	1.24
2	F	129	SER	C-O	-7.86	1.14	1.24
1	G	182	LYS	C-O	-7.55	1.15	1.23
1	A	162	LYS	C-O	-7.51	1.15	1.24
1	A	161	ILE	C-O	-7.38	1.15	1.23
1	C	164	ARG	C-O	-7.33	1.15	1.23
1	G	185	LYS	C-N	-7.21	1.25	1.33
1	G	163	GLN	C-O	-7.19	1.15	1.23
1	G	16	VAL	C-O	-7.08	1.16	1.23
1	C	163	GLN	C-O	-6.99	1.15	1.23
2	H	66	SER	C-O	-6.98	1.14	1.23
2	H	68	SER	C-O	-6.97	1.15	1.24
1	A	34	GLU	C-O	-6.94	1.15	1.23
1	E	176	GLU	C-O	-6.85	1.15	1.24
1	C	172	HIS	C-O	-6.70	1.15	1.23
1	C	175	ALA	C-O	-6.55	1.15	1.23
2	H	67	TRP	C-O	-6.41	1.16	1.24
1	A	117	GLU	C-O	-6.38	1.15	1.23
1	G	92	LYS	C-O	-6.21	1.16	1.23
1	C	196	ASN	C-O	-6.14	1.16	1.24
1	E	188	GLN	C-O	-6.11	1.16	1.23
1	A	163	GLN	C-O	-5.91	1.16	1.23
1	C	128	ASN	CA-CB	-5.84	1.44	1.53
1	G	15	LYS	C-O	-5.74	1.16	1.23
1	E	176	GLU	CA-C	-5.64	1.45	1.52
1	C	177	VAL	N-CA	-5.54	1.39	1.46
1	G	182	LYS	CA-C	-5.51	1.46	1.52
1	C	164	ARG	N-CA	-5.47	1.39	1.46
1	G	47	LYS	C-O	-5.37	1.17	1.23
1	I	50	LYS	C-O	-5.37	1.17	1.23
1	I	36	ARG	C-O	-5.35	1.20	1.25
1	E	176	GLU	CA-CB	-5.34	1.45	1.53
1	E	50	LYS	C-O	-5.34	1.17	1.23
1	E	49	THR	C-O	-5.32	1.17	1.24
1	C	144	GLU	C-O	-5.31	1.16	1.23
1	C	128	ASN	CA-C	-5.31	1.45	1.52
1	G	14	PHE	C-O	-5.21	1.17	1.23
1	G	186	PRO	C-O	-5.20	1.18	1.23
1	C	196	ASN	CA-CB	-5.15	1.46	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	181	TYR	O-C-N	18.52	145.14	123.29
1	I	181	TYR	CA-C-N	-16.93	94.36	122.29
1	I	181	TYR	C-N-CA	-16.93	94.36	122.29
1	I	41	THR	CA-C-N	-11.33	100.88	121.62
1	I	41	THR	C-N-CA	-11.33	100.88	121.62
1	I	182	LYS	O-C-N	-9.87	111.82	123.27
1	I	40	GLY	O-C-N	-9.46	110.40	122.70
1	I	41	THR	O-C-N	8.16	132.73	123.42
2	H	17	GLN	N-CA-C	8.09	123.00	108.69
1	I	40	GLY	CA-C-N	7.83	134.94	121.64
1	I	40	GLY	C-N-CA	7.83	134.94	121.64
2	H	67	TRP	CA-C-O	-6.88	113.19	120.63
2	H	67	TRP	N-CA-C	6.28	118.93	111.33
1	A	161	ILE	CB-CA-C	-5.91	100.55	111.18
1	I	48	VAL	CB-CA-C	-5.63	105.83	111.80
1	A	162	LYS	N-CA-C	-5.05	99.05	107.99

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	16	1
1	E	1742	1691	1694	20	1
1	G	1742	1694	1694	15	1
1	I	1742	1690	1694	29	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	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	129	2

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

All (129) 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:I:18:MET:HE1	1:I:61:LEU:HD22	1.72	0.71
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
1:C:216:ARG:NH1	1:E:141:MET:HE2	2.12	0.64
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:16:VAL:HG12	2:F:40:GLY:HA3	1.87	0.56
1:C:216:ARG:HH11	1:E:141:MET:HE2	1.69	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:G:14:PHE:C	1:G:14:PHE:CD1	2.85	0.55
1:E:48:VAL:O	1:E:48:VAL:HG23	2.07	0.55
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:E:150:MET:HE3	1:E:157:LEU:HG	1.91	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:A:28:GLU:CD	1:A:50:LYS:HD2	2.38	0.49
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:I:5:MET:HE2	1:I:5:MET:HA	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:28:GLU:CD	1:G:50:LYS:HD2	2.42	0.45
1:C:87:PHE:HB3	1:C:88:PRO:HA	1.99	0.44
1:E:221:HIS:O	1:E:222:SER:C	2.60	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
2:J:97:MET:HE1	2:J:108:TYR:CZ	2.51	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
2:J:117:THR:O	2:J:118:TRP:C	2.61	0.43
1:E:48:VAL:CG2	1:E:209:THR:HG22	2.49	0.43
1:I:59:ASP:OD2	1:I:140:THR:OG1	2.31	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:MET:HE3	1:I:124:LEU:HB3	2.02	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
1:E:89:GLU:CD	1:E:185:LYS:HD3	2.46	0.40
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:I:28:GLU:CD	1:I:50:LYS:HE2	2.47	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

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%)	16	23
2	D	122/127 (96%)	116 (95%)	6 (5%)	0	100	100
2	F	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
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%)	48	62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	129	SER

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	183/200 (92%)	180 (98%)	3 (2%)	55	74
1	C	183/200 (92%)	180 (98%)	3 (2%)	55	74
1	E	183/200 (92%)	182 (100%)	1 (0%)	81	90
1	G	183/200 (92%)	180 (98%)	3 (2%)	55	74
1	I	183/200 (92%)	178 (97%)	5 (3%)	39	59
2	B	99/101 (98%)	99 (100%)	0	100	100
2	D	99/101 (98%)	99 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	99/101 (98%)	98 (99%)	1 (1%)	68	82
2	H	99/101 (98%)	98 (99%)	1 (1%)	68	82
2	J	99/101 (98%)	96 (97%)	3 (3%)	36	56
All	All	1410/1505 (94%)	1390 (99%)	20 (1%)	59	77

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

Mol	Chain	Res	Type
1	A	34	GLU
1	A	161	ILE
1	A	220	ARG
1	C	5	MET
1	C	164	ARG
1	C	196	ASN
1	E	162	LYS
2	F	129	SER
1	G	5	MET
1	G	32	GLU
1	G	47	LYS
2	H	16	VAL
1	I	37	PRO
1	I	39	GLU
1	I	50	LYS
1	I	163	GLN
1	I	169	ASP
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	163	GLN
1	A	188	GLN
2	D	135	GLN
2	F	96	GLN
2	F	98	ASN
1	G	98	ASN
1	G	188	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	42	GLN
1	I	172	HIS
1	I	205	ASN

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	I	66	1	24,24,25	2.45	8 (33%)	24,32,34	2.71	6 (25%)
1	NRQ	C	66	1	24,24,25	2.49	8 (33%)	24,32,34	2.74	6 (25%)
1	NRQ	G	66	1	24,24,25	2.46	9 (37%)	24,32,34	2.54	5 (20%)
1	NRQ	A	66	1	24,24,25	2.69	8 (33%)	24,32,34	3.01	8 (33%)
1	NRQ	E	66	1	24,24,25	2.53	9 (37%)	24,32,34	2.28	6 (25%)

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

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	NRQ	C1-N3	6.67	1.49	1.38
1	E	66	NRQ	CA2-C2	5.77	1.54	1.48
1	I	66	NRQ	CA2-C2	5.76	1.54	1.48
1	G	66	NRQ	CA2-C2	5.75	1.54	1.48
1	A	66	NRQ	C1-CA1	5.48	1.56	1.48
1	C	66	NRQ	C1-N3	5.48	1.47	1.38
1	E	66	NRQ	C1-N3	5.41	1.47	1.38
1	A	66	NRQ	C1-N2	5.03	1.43	1.33
1	C	66	NRQ	CA2-C2	5.01	1.54	1.48
1	I	66	NRQ	C1-N3	4.97	1.46	1.38
1	G	66	NRQ	C1-N2	4.93	1.43	1.33
1	G	66	NRQ	C1-N3	4.81	1.46	1.38
1	E	66	NRQ	C1-N2	4.70	1.43	1.33
1	A	66	NRQ	CA2-C2	4.59	1.53	1.48
1	C	66	NRQ	C1-N2	4.33	1.42	1.33
1	I	66	NRQ	C1-N2	4.23	1.42	1.33
1	I	66	NRQ	CG2-CB2	4.17	1.54	1.46
1	I	66	NRQ	C2-N3	4.12	1.49	1.40
1	C	66	NRQ	C1-CA1	4.11	1.54	1.48
1	C	66	NRQ	C2-N3	4.11	1.49	1.40
1	E	66	NRQ	C1-CA1	4.00	1.53	1.48
1	A	66	NRQ	C2-N3	3.92	1.49	1.40
1	C	66	NRQ	CG2-CB2	3.89	1.54	1.46
1	G	66	NRQ	CG2-CB2	3.84	1.53	1.46
1	E	66	NRQ	CG2-CB2	3.79	1.53	1.46
1	A	66	NRQ	CG2-CB2	3.75	1.53	1.46
1	G	66	NRQ	C2-N3	3.64	1.48	1.40
1	E	66	NRQ	C2-N3	3.64	1.48	1.40
1	G	66	NRQ	C1-CA1	3.44	1.53	1.48
1	I	66	NRQ	C1-CA1	3.43	1.53	1.48
1	C	66	NRQ	CB2-CA2	-3.08	1.32	1.35
1	A	66	NRQ	CB2-CA2	-2.81	1.32	1.35
1	E	66	NRQ	CB2-CA2	-2.71	1.32	1.35
1	G	66	NRQ	CB2-CA2	-2.45	1.32	1.35
1	G	66	NRQ	O2-C2	-2.33	1.18	1.23
1	I	66	NRQ	CB2-CA2	-2.32	1.32	1.35
1	E	66	NRQ	O2-C2	-2.27	1.18	1.23
1	C	66	NRQ	O2-C2	-2.23	1.18	1.23
1	E	66	NRQ	CA2-N2	2.17	1.43	1.38
1	G	66	NRQ	CA2-N2	2.12	1.43	1.38
1	I	66	NRQ	O2-C2	-2.09	1.18	1.23
1	A	66	NRQ	O2-C2	-2.07	1.18	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	NRQ	O2-C2-CA2	-9.02	125.26	131.02
1	G	66	NRQ	O2-C2-CA2	-8.61	125.53	131.02
1	C	66	NRQ	O2-C2-CA2	-8.24	125.76	131.02
1	I	66	NRQ	O2-C2-CA2	-7.55	126.20	131.02
1	E	66	NRQ	O2-C2-CA2	-6.61	126.81	131.02
1	I	66	NRQ	CG2-CB2-CA2	-5.78	123.00	129.87
1	G	66	NRQ	CA2-C2-N3	5.73	108.31	103.50
1	A	66	NRQ	CA2-C2-N3	5.61	108.21	103.50
1	A	66	NRQ	CG2-CB2-CA2	-5.13	123.76	129.87
1	C	66	NRQ	CG2-CB2-CA2	-5.05	123.86	129.87
1	C	66	NRQ	CA2-C2-N3	4.95	107.66	103.50
1	E	66	NRQ	CA2-C2-N3	4.82	107.55	103.50
1	I	66	NRQ	CA2-C2-N3	4.72	107.46	103.50
1	A	66	NRQ	C2-CA2-N2	-4.66	105.61	108.95
1	I	66	NRQ	C2-CA2-N2	-4.37	105.82	108.95
1	C	66	NRQ	C2-CA2-N2	-4.36	105.83	108.95
1	G	66	NRQ	C2-CA2-N2	-4.36	105.83	108.95
1	A	66	NRQ	CA2-N2-C1	4.11	111.66	104.09
1	E	66	NRQ	CG2-CB2-CA2	-3.99	125.13	129.87
1	I	66	NRQ	CB2-CA2-C2	3.93	127.12	122.36
1	C	66	NRQ	CA2-N2-C1	3.66	110.83	104.09
1	E	66	NRQ	C2-CA2-N2	-3.50	106.44	108.95
1	I	66	NRQ	CA2-N2-C1	3.31	110.18	104.09
1	C	66	NRQ	CB2-CA2-C2	3.17	126.20	122.36
1	A	66	NRQ	N3-C1-N2	-3.14	108.90	112.62
1	E	66	NRQ	CA2-N2-C1	2.80	109.25	104.09
1	G	66	NRQ	CA2-N2-C1	2.75	109.15	104.09
1	A	66	NRQ	CA3-N3-C1	2.67	133.65	128.39
1	E	66	NRQ	CD1-CG2-CD2	2.10	120.77	117.65
1	A	66	NRQ	CD1-CG2-CD2	2.10	120.77	117.65
1	G	66	NRQ	CD1-CG2-CD2	2.02	120.65	117.65

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

Continued on next page...

Continued from previous page...

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/237 (90%)	0.50	6 (2%) 55 54	45, 70, 100, 142	0
1	C	215/237 (90%)	0.53	12 (5%) 30 29	50, 69, 100, 160	0
1	E	215/237 (90%)	0.58	8 (3%) 45 45	52, 73, 100, 136	0
1	G	215/237 (90%)	0.92	17 (7%) 18 17	54, 81, 115, 135	0
1	I	215/237 (90%)	1.91	84 (39%) 1 0	76, 123, 164, 183	0
2	B	124/127 (97%)	0.33	5 (4%) 42 42	47, 59, 87, 118	0
2	D	124/127 (97%)	0.53	8 (6%) 25 23	51, 64, 97, 123	0
2	F	124/127 (97%)	0.33	4 (3%) 50 50	48, 59, 89, 115	0
2	H	124/127 (97%)	0.21	4 (3%) 50 50	50, 60, 80, 99	0
2	J	124/127 (97%)	0.74	7 (5%) 30 29	62, 76, 98, 123	0
All	All	1695/1820 (93%)	0.72	155 (9%) 15 14	45, 73, 132, 183	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	16	VAL	8.4
1	I	65	PHE	6.5
2	D	16	VAL	6.2
2	F	16	VAL	5.7
1	E	5	MET	5.7
1	I	7	ILE	5.7
1	I	199	LEU	5.5
1	I	48	VAL	5.4
2	B	16	VAL	5.4
2	H	16	VAL	5.3
1	I	16	VAL	5.1
1	G	6	ALA	4.9
1	I	8	ILE	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	6	ALA	4.7
1	C	5	MET	4.6
1	I	46	LEU	4.6
1	I	211	VAL	4.6
1	E	6	ALA	4.5
1	I	11	PHE	4.5
1	I	5	MET	4.2
1	I	201	ILE	4.0
2	D	116	GLY	4.0
2	D	117	THR	3.9
1	A	5	MET	3.9
2	J	116	GLY	3.9
1	G	5	MET	3.8
1	I	175	ALA	3.8
1	I	33	GLY	3.7
1	I	214	TYR	3.7
1	I	18	MET	3.7
1	I	44	ALA	3.6
1	I	69	SER	3.6
1	I	61	LEU	3.6
1	I	71	ALA	3.6
1	I	210	ILE	3.5
1	I	6	ALA	3.5
1	I	143	TRP	3.5
2	J	139	SER	3.4
1	I	49	THR	3.4
1	G	114	GLN	3.4
1	I	15	LYS	3.4
1	I	43	THR	3.4
2	D	139	SER	3.4
1	I	27	PHE	3.3
1	E	222	SER	3.3
1	I	101	ASP	3.3
1	I	197	ILE	3.3
1	C	7	ILE	3.3
2	D	55	PRO	3.3
1	I	217	ALA	3.2
1	I	31	GLY	3.2
1	I	119	ILE	3.2
1	I	170	GLY	3.2
1	E	7	ILE	3.2
1	I	135	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	213	GLN	3.1
1	I	72	TYR	3.1
1	I	173	TYR	3.1
1	C	8	ILE	3.1
1	G	7	ILE	3.1
1	I	58	TRP	3.1
1	I	120	TYR	3.0
1	I	118	PHE	3.0
1	I	14	PHE	3.0
2	B	55	PRO	3.0
1	I	215	GLU	3.0
1	I	222	SER	2.9
2	J	44	SER	2.9
1	I	64	GLN	2.9
2	F	17	GLN	2.9
1	I	165	LEU	2.8
1	I	113	LEU	2.8
1	I	200	ASP	2.8
1	I	145	ALA	2.8
1	I	136	MET	2.8
2	J	117	THR	2.7
1	I	134	PRO	2.7
1	I	54	LEU	2.7
1	G	187	VAL	2.7
1	I	167	LEU	2.7
1	E	162	LYS	2.7
1	I	208	TYR	2.7
1	G	116	GLY	2.7
1	I	22	VAL	2.6
1	G	88	PRO	2.6
1	A	192	ALA	2.6
1	A	201	ILE	2.6
1	E	186	PRO	2.6
1	I	186	PRO	2.6
1	A	50	LYS	2.6
1	E	69	SER	2.6
2	B	57	LYS	2.6
1	I	130	PRO	2.6
1	I	116	GLY	2.5
1	I	202	THR	2.5
1	I	29	ILE	2.5
1	I	41	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	113	LEU	2.5
1	C	9	LYS	2.5
1	I	129	PHE	2.5
1	I	60	ILE	2.5
1	I	198	LYS	2.5
1	I	73	VAL	2.4
1	G	222	SER	2.4
1	I	92	LYS	2.4
1	A	69	SER	2.4
1	I	112	SER	2.4
1	I	195	VAL	2.4
1	A	172	HIS	2.4
1	I	53	PRO	2.3
1	I	177	VAL	2.3
2	J	42	THR	2.3
1	G	31	GLY	2.3
2	B	139	SER	2.3
2	H	139	SER	2.3
1	I	142	GLY	2.3
1	C	222	SER	2.3
2	D	129	SER	2.3
1	I	35	GLY	2.2
1	G	192	ALA	2.2
1	C	220	ARG	2.2
1	I	12	MET	2.2
1	I	13	ARG	2.2
1	I	171	GLY	2.2
1	G	210	ILE	2.2
1	G	87	PHE	2.2
1	I	196	ASN	2.2
1	G	70	LYS	2.2
2	F	40	GLY	2.2
2	D	19	VAL	2.1
1	I	55	PRO	2.1
2	H	128	GLY	2.1
1	G	8	ILE	2.1
1	I	56	PHE	2.1
1	I	163	GLN	2.1
1	C	69	SER	2.1
1	G	69	SER	2.1
1	I	28	GLU	2.1
1	I	117	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	76	PRO	2.1
2	H	42	THR	2.1
2	D	17	GLN	2.1
2	B	116	GLY	2.1
2	J	67	TRP	2.1
1	I	74	LYS	2.0
1	G	71	ALA	2.0
1	I	17	HIS	2.0
1	I	25	HIS	2.0
1	C	170	GLY	2.0
1	C	171	GLY	2.0
2	F	116	GLY	2.0
1	I	47	LYS	2.0
1	C	147	SER	2.0
1	I	172	HIS	2.0
1	E	70	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	NRQ	I	66	23/24	0.81	0.25	117,132,160,161	0
1	NRQ	E	66	23/24	0.83	0.22	72,86,103,106	0
1	NRQ	G	66	23/24	0.84	0.22	78,95,115,115	0
1	NRQ	A	66	23/24	0.86	0.23	76,98,120,120	0
1	NRQ	C	66	23/24	0.89	0.20	75,87,105,105	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.