



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 12:33 PM UTC

PDB ID : 5HZU / pdb_00005hzu
Title : Crystal structure of Dronpa-Ni²⁺
Authors : Hwang, K.Y.; Nam, K.H.
Deposited on : 2016-02-03
Resolution : 1.89 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

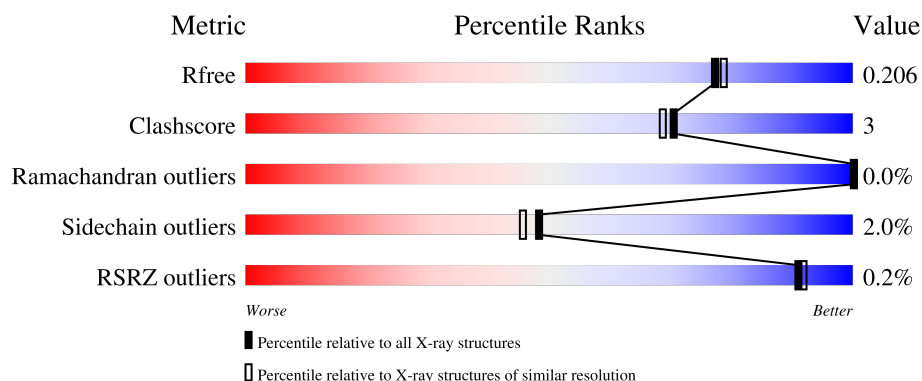
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	215	87% 12% .
1	B	215	87% 12% .
1	C	215	89% 9% ..
1	D	215	90% 8% ..
1	E	215	87% 12% .

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Mol	Chain	Length	Quality of chain
1	F	215	 93% 5% •
1	G	215	 85% 13% ••
1	H	215	 88% 11%
1	I	215	 92% 7% ••
1	J	215	 92% 7%
1	K	215	 89% 9% •
1	L	215	 91% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22735 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fluorescent protein Dronpa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	B	215	Total	C	N	O	S	0	0	0
			1736	1108	292	327	9			
1	C	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	D	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	E	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			
1	F	214	Total	C	N	O	S	0	0	0
			1727	1103	291	324	9			
1	G	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	H	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			
1	I	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	J	214	Total	C	N	O	S	0	0	0
			1727	1103	291	324	9			
1	K	213	Total	C	N	O	S	0	0	0
			1721	1100	290	322	9			
1	L	214	Total	C	N	O	S	0	0	0
			1730	1105	291	325	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	CYS	chromophore	UNP Q5TLG6
A	?	-	TYR	chromophore	UNP Q5TLG6
A	62	GYS	GLY	chromophore	UNP Q5TLG6
B	?	-	CYS	chromophore	UNP Q5TLG6
B	?	-	TYR	chromophore	UNP Q5TLG6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	62	GYS	GLY	chromophore	UNP Q5TLG6
C	?	-	CYS	chromophore	UNP Q5TLG6
C	?	-	TYR	chromophore	UNP Q5TLG6
C	62	GYS	GLY	chromophore	UNP Q5TLG6
D	?	-	CYS	chromophore	UNP Q5TLG6
D	?	-	TYR	chromophore	UNP Q5TLG6
D	62	GYS	GLY	chromophore	UNP Q5TLG6
E	?	-	CYS	chromophore	UNP Q5TLG6
E	?	-	TYR	chromophore	UNP Q5TLG6
E	62	GYS	GLY	chromophore	UNP Q5TLG6
F	?	-	CYS	chromophore	UNP Q5TLG6
F	?	-	TYR	chromophore	UNP Q5TLG6
F	62	GYS	GLY	chromophore	UNP Q5TLG6
G	?	-	CYS	chromophore	UNP Q5TLG6
G	?	-	TYR	chromophore	UNP Q5TLG6
G	62	GYS	GLY	chromophore	UNP Q5TLG6
H	?	-	CYS	chromophore	UNP Q5TLG6
H	?	-	TYR	chromophore	UNP Q5TLG6
H	62	GYS	GLY	chromophore	UNP Q5TLG6
I	?	-	CYS	chromophore	UNP Q5TLG6
I	?	-	TYR	chromophore	UNP Q5TLG6
I	62	GYS	GLY	chromophore	UNP Q5TLG6
J	?	-	CYS	chromophore	UNP Q5TLG6
J	?	-	TYR	chromophore	UNP Q5TLG6
J	62	GYS	GLY	chromophore	UNP Q5TLG6
K	?	-	CYS	chromophore	UNP Q5TLG6
K	?	-	TYR	chromophore	UNP Q5TLG6
K	62	GYS	GLY	chromophore	UNP Q5TLG6
L	?	-	CYS	chromophore	UNP Q5TLG6
L	?	-	TYR	chromophore	UNP Q5TLG6
L	62	GYS	GLY	chromophore	UNP Q5TLG6

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ni 2 2	0	0
2	B	2	Total Ni 2 2	0	0
2	C	2	Total Ni 2 2	0	0
2	D	2	Total Ni 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Ni 2	0	0
2	F	2	Total 2	Ni 2	0	0
2	G	2	Total 2	Ni 2	0	0
2	H	2	Total 2	Ni 2	0	0
2	I	2	Total 2	Ni 2	0	0
2	J	2	Total 2	Ni 2	0	0
2	K	3	Total 3	Ni 3	0	0
2	L	2	Total 2	Ni 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total 168	O 168	0	0
3	B	155	Total 155	O 155	0	0
3	C	166	Total 166	O 166	0	0
3	D	161	Total 161	O 161	0	0
3	E	173	Total 173	O 173	0	0
3	F	170	Total 170	O 170	0	0
3	G	156	Total 156	O 156	0	0
3	H	164	Total 164	O 164	0	0
3	I	154	Total 154	O 154	0	0
3	J	160	Total 160	O 160	0	0
3	K	193	Total 193	O 193	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	184	Total 184	O 184	0	0

3 Residue-property plots

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.

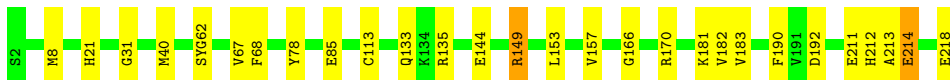
• Molecule 1: Fluorescent protein Dronpa

Chain A: 



• Molecule 1: Fluorescent protein Dronpa

Chain B: 



• Molecule 1: Fluorescent protein Dronpa

Chain C: 



• Molecule 1: Fluorescent protein Dronpa

Chain D: 



• Molecule 1: Fluorescent protein Dronpa

Chain E: 



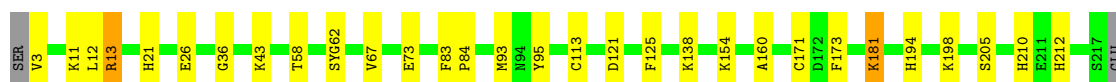
• Molecule 1: Fluorescent protein Dronpa

Chain F:  93% 5% .



- Molecule 1: Fluorescent protein Dronpa

Chain G:  85% 13% ..



- Molecule 1: Fluorescent protein Dronpa

Chain H:  88% 11%



- Molecule 1: Fluorescent protein Dronpa

Chain I:  92% 7% ..



- Molecule 1: Fluorescent protein Dronpa

Chain J:  92% 7%



- Molecule 1: Fluorescent protein Dronpa

Chain K:  89% 9% .



- Molecule 1: Fluorescent protein Dronpa

Chain L:  91% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.37Å 109.40Å 72.09Å 71.11° 85.97° 61.30°	Depositor
Resolution (Å)	29.03 – 1.89 29.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.03-1.89) 94.0 (29.03-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.151 , 0.199 0.161 , 0.206	Depositor DCC
R_{free} test set	9967 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22735	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.23	4/1745 (0.2%)	1.08	2/2355 (0.1%)
1	B	1.27	4/1760 (0.2%)	1.12	2/2375 (0.1%)
1	C	1.22	3/1745 (0.2%)	1.12	1/2355 (0.0%)
1	D	1.27	2/1745 (0.1%)	1.10	0/2355
1	E	1.36	7/1754 (0.4%)	1.10	3/2367 (0.1%)
1	F	1.34	3/1751 (0.2%)	1.12	1/2363 (0.0%)
1	G	1.27	3/1745 (0.2%)	1.09	3/2355 (0.1%)
1	H	1.22	0/1754	1.10	0/2367
1	I	1.22	1/1745 (0.1%)	1.13	1/2355 (0.0%)
1	J	1.25	1/1751 (0.1%)	1.13	2/2363 (0.1%)
1	K	1.36	5/1745 (0.3%)	1.12	0/2355
1	L	1.34	3/1754 (0.2%)	1.13	3/2367 (0.1%)
All	All	1.28	36/20994 (0.2%)	1.11	18/28332 (0.1%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	170	ARG	C-O	8.59	1.34	1.23
1	K	123	VAL	C-O	6.75	1.31	1.23
1	G	13	ARG	N-CA	-6.54	1.37	1.46
1	L	174	LYS	N-CA	-6.35	1.39	1.46
1	E	116	TYR	CA-C	-6.24	1.45	1.52
1	K	120	PHE	N-CA	6.23	1.53	1.46
1	L	162	SER	C-O	-6.00	1.16	1.23
1	K	188	TYR	N-CA	5.77	1.53	1.46
1	F	26	GLU	CA-C	-5.76	1.45	1.52
1	E	26	GLU	CA-C	-5.68	1.45	1.52
1	E	174	LYS	C-O	-5.66	1.17	1.24
1	A	174	LYS	N-CA	5.62	1.53	1.46
1	B	40	MET	N-CA	-5.58	1.39	1.46
1	L	67	VAL	C-O	-5.57	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	GLY	N-CA	5.57	1.51	1.45
1	D	176	THR	C-O	-5.52	1.17	1.24
1	G	160	ALA	C-O	5.51	1.30	1.23
1	C	159	MET	C-O	5.50	1.30	1.23
1	C	190	PHE	C-O	5.49	1.30	1.23
1	J	123	VAL	C-O	5.49	1.30	1.23
1	E	58	THR	C-O	5.48	1.30	1.24
1	A	75	ILE	C-O	-5.38	1.18	1.24
1	E	120	PHE	C-O	-5.36	1.18	1.23
1	K	7	ASP	C-O	-5.34	1.18	1.24
1	B	153	LEU	C-O	-5.31	1.17	1.24
1	D	69	ALA	C-O	-5.29	1.17	1.23
1	I	215	ALA	C-O	5.29	1.30	1.23
1	G	121	ASP	C-O	5.21	1.30	1.24
1	F	171	CYS	C-O	5.17	1.29	1.23
1	A	16	GLY	CA-C	-5.14	1.46	1.51
1	F	21	HIS	C-O	-5.14	1.18	1.24
1	E	27	GLY	C-O	-5.07	1.17	1.24
1	K	157	VAL	N-CA	-5.04	1.40	1.46
1	A	89	TRP	C-O	5.02	1.30	1.23
1	B	190	PHE	C-O	5.01	1.30	1.23
1	E	169	TYR	C-O	5.01	1.29	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	58	THR	N-CA-C	7.78	119.75	111.28
1	B	166	GLY	N-CA-C	-6.27	104.78	112.68
1	L	67	VAL	CB-CA-C	-5.97	102.90	112.16
1	A	67	VAL	CB-CA-C	-5.85	103.09	112.16
1	L	67	VAL	N-CA-CB	5.75	120.49	110.65
1	C	149	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	83	PHE	CB-CA-C	5.47	117.31	109.11
1	E	157	VAL	N-CA-C	5.46	116.52	108.45
1	I	76	VAL	N-CA-CB	5.45	118.62	110.13
1	E	73	GLU	N-CA-C	5.42	117.95	111.71
1	J	129	GLY	CA-C-N	5.32	124.94	119.56
1	J	129	GLY	C-N-CA	5.32	124.94	119.56
1	L	217	SER	N-CA-C	5.23	116.24	108.60
1	G	125	PHE	CA-C-N	-5.20	114.60	119.85
1	G	125	PHE	C-N-CA	-5.20	114.60	119.85
1	F	214	GLU	CB-CG-CD	5.16	121.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	GLU	CA-CB-CG	5.08	124.26	114.10
1	E	58	THR	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

There are no planarity outliers.

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	1721	0	1646	18	0
1	B	1736	0	1658	11	0
1	C	1721	0	1645	9	0
1	D	1721	0	1647	11	0
1	E	1730	0	1653	14	0
1	F	1727	0	1651	9	0
1	G	1721	0	1646	15	0
1	H	1730	0	1652	17	0
1	I	1721	0	1647	14	0
1	J	1727	0	1652	7	0
1	K	1721	0	1646	11	0
1	L	1730	0	1651	10	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
3	A	168	0	0	9	0
3	B	155	0	0	4	0
3	C	166	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	161	0	0	2	0
3	E	173	0	0	3	0
3	F	170	0	0	2	1
3	G	156	0	0	5	1
3	H	164	0	0	3	1
3	I	154	0	0	1	0
3	J	160	0	0	4	1
3	K	193	0	0	1	0
3	L	184	0	0	1	2
All	All	22735	0	19794	139	3

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 3.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:HIS:HE1	3:A:529:HOH:O	1.33	1.08
1:G:21:HIS:HE1	3:G:527:HOH:O	1.36	1.06
1:H:11:LYS:NZ	1:H:113:CYS:SG	2.28	1.06
1:E:164:GLU:OE1	1:K:21:HIS:CE1	2.23	0.91
1:B:133:GLN:OE1	3:B:401:HOH:O	1.90	0.90
1:H:3:VAL:N	3:H:401:HOH:O	2.04	0.89
1:A:65:ASN:OD1	1:A:67:VAL:HG22	1.75	0.86
1:G:11:LYS:NZ	1:G:113:CYS:SG	2.49	0.86
1:E:45:LYS:NZ	3:E:402:HOH:O	2.17	0.76
1:A:210:HIS:HE1	3:A:479:HOH:O	1.71	0.72
1:J:210:HIS:HE1	3:J:403:HOH:O	1.73	0.69
1:A:210:HIS:CE1	3:A:479:HOH:O	2.46	0.68
1:F:21:HIS:CE1	3:F:403:HOH:O	2.47	0.67
1:I:65:ASN:OD1	1:I:67:VAL:HG22	1.97	0.63
1:G:194:HIS:CE1	3:G:414:HOH:O	2.51	0.63
1:D:115:ILE:HD11	3:D:558:HOH:O	1.99	0.61
1:G:3:VAL:HG21	1:G:84:PRO:HB3	1.82	0.61
1:B:21:HIS:CE1	3:B:436:HOH:O	2.53	0.61
1:H:21:HIS:NE2	3:H:402:HOH:O	2.31	0.61
1:E:46:GLU:OE2	3:E:401:HOH:O	2.16	0.60
1:D:65:ASN:CG	1:D:67:VAL:HG22	2.28	0.59
1:H:11:LYS:NZ	1:H:113:CYS:CB	2.66	0.59
1:D:11:LYS:HG2	1:D:113:CYS:SG	2.42	0.59
1:L:65:ASN:OD1	1:L:67:VAL:HG22	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:21:HIS:ND1	3:I:402:HOH:O	2.32	0.58
1:G:43:LYS:HA	1:G:205:SER:O	2.02	0.58
1:C:11:LYS:HE2	1:C:113:CYS:SG	2.43	0.58
1:G:13:ARG:NH2	1:G:26:GLU:OE1	2.36	0.56
1:C:30:LEU:HD12	1:C:30:LEU:O	2.05	0.56
1:I:65:ASN:CG	1:I:67:VAL:HG22	2.30	0.56
1:I:67:VAL:HG11	1:I:83:PHE:CE2	2.40	0.56
1:D:65:ASN:OD1	1:D:67:VAL:HG22	2.07	0.55
1:E:135:ARG:NE	1:K:48:GLY:O	2.38	0.55
1:A:46:GLU:HG2	3:H:449:HOH:O	2.07	0.54
1:D:81:GLN:HG3	1:D:183:VAL:HB	1.88	0.54
1:E:143:THR:H	1:F:145:LYS:NZ	2.05	0.54
1:D:8:MET:HE2	1:D:114:TYR:CZ	2.42	0.54
1:A:150:ASP:OD1	3:A:401:HOH:O	2.18	0.54
1:I:198:LYS:HE3	1:I:210:HIS:HB2	1.89	0.54
1:C:210:HIS:CD2	3:C:527:HOH:O	2.62	0.53
1:L:7:ASP:OD1	1:L:32:LYS:HE3	2.08	0.53
1:C:210:HIS:HD2	3:C:527:HOH:O	1.92	0.53
1:B:135:ARG:NE	3:B:401:HOH:O	2.29	0.52
1:E:30:LEU:O	1:E:30:LEU:HD12	2.09	0.52
1:A:21:HIS:CE1	3:A:529:HOH:O	2.23	0.52
1:F:202:LYS:H	1:F:202:LYS:CD	2.23	0.51
1:E:128:ASN:HB2	3:E:534:HOH:O	2.11	0.51
1:D:210:HIS:NE2	3:D:401:HOH:O	1.95	0.50
1:H:11:LYS:CE	1:H:113:CYS:SG	2.99	0.50
1:B:85:GLU:OE1	1:B:85:GLU:N	2.41	0.50
1:E:164:GLU:OE1	1:K:21:HIS:ND1	2.44	0.50
1:H:65:ASN:CG	1:H:67:VAL:HG12	2.37	0.50
1:B:218:GLU:O	3:B:403:HOH:O	2.20	0.49
1:D:8:MET:HE2	1:D:114:TYR:CE2	2.47	0.49
1:G:93:MET:HG2	1:G:173:PHE:CD1	2.48	0.49
1:H:11:LYS:HZ3	1:H:113:CYS:CB	2.24	0.49
1:I:198:LYS:HD2	1:I:208:ASN:OD1	2.12	0.49
1:I:67:VAL:HG11	1:I:83:PHE:HE2	1.78	0.48
1:G:83:PHE:HB3	1:G:84:PRO:HA	1.94	0.48
1:L:192:ASP:O	1:L:213:ALA:HA	2.14	0.48
1:H:65:ASN:ND2	1:H:67:VAL:HG12	2.29	0.48
1:I:198:LYS:HE3	1:I:210:HIS:CB	2.43	0.48
1:H:157:VAL:HG13	1:H:173:PHE:HB2	1.95	0.47
1:I:198:LYS:CE	1:I:210:HIS:HB2	2.44	0.47
1:J:3:VAL:HG21	1:J:84:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:36:GLY:O	1:L:212:HIS:HA	2.14	0.47
1:L:210:HIS:NE2	3:L:404:HOH:O	2.31	0.47
1:A:164:GLU:O	3:A:402:HOH:O	2.21	0.46
1:D:67:VAL:HG11	1:D:83:PHE:CE2	2.50	0.46
1:E:143:THR:H	1:F:145:LYS:HZ3	1.62	0.46
1:A:21:HIS:NE2	3:A:404:HOH:O	2.36	0.46
1:F:12:LEU:C	1:F:12:LEU:HD12	2.41	0.46
1:A:8:MET:HE3	1:A:114:TYR:OH	2.17	0.45
1:H:11:LYS:CD	1:H:113:CYS:SG	3.04	0.45
1:H:30:LEU:N	1:H:30:LEU:HD23	2.31	0.45
1:B:78:TYR:CE1	1:B:183:VAL:CG2	2.99	0.45
1:I:30:LEU:O	1:I:30:LEU:HD12	2.16	0.45
1:H:8:MET:HE1	1:H:109:LEU:HD11	1.99	0.45
1:C:144:GLU:HA	1:C:157:VAL:HB	1.99	0.45
1:A:45:LYS:HE2	3:A:498:HOH:O	2.16	0.45
1:B:144:GLU:HA	1:B:157:VAL:HB	1.97	0.45
1:H:198:LYS:HG3	1:H:210:HIS:CD2	2.51	0.44
1:J:134:LYS:NZ	3:J:407:HOH:O	2.48	0.44
1:A:65:ASN:CG	1:A:67:VAL:HG22	2.42	0.44
1:E:11:LYS:HE2	1:E:113:CYS:SG	2.57	0.44
1:A:11:LYS:HG3	1:A:113:CYS:SG	2.57	0.44
1:G:198:LYS:HG3	1:G:210:HIS:CD2	2.52	0.44
1:B:211:GLU:HG2	1:B:212:HIS:N	2.32	0.44
1:A:93:MET:HG2	1:A:173:PHE:CD1	2.52	0.43
1:A:205:SER:HB3	3:A:560:HOH:O	2.17	0.43
1:E:93:MET:HG2	1:E:173:PHE:CD1	2.53	0.43
1:F:25:ILE:HG12	1:F:44:VAL:HG22	2.00	0.43
1:A:8:MET:HE3	1:A:114:TYR:CZ	2.53	0.43
1:F:21:HIS:ND1	3:F:403:HOH:O	2.37	0.43
1:G:95:TYR:CD2	1:G:171:CYS:HB2	2.54	0.42
1:B:192:ASP:O	1:B:213:ALA:HA	2.19	0.42
1:C:202:LYS:HG3	1:C:203:ASP:N	2.34	0.42
1:E:144:GLU:HA	1:E:157:VAL:HB	2.01	0.42
1:H:14:MET:HE3	1:H:61:PHE:CE1	2.54	0.42
1:F:198:LYS:HG3	1:F:210:HIS:CD2	2.55	0.42
1:L:93:MET:HG2	1:L:173:PHE:CD1	2.54	0.42
1:A:144:GLU:HA	1:A:157:VAL:HB	2.01	0.42
1:G:181:LYS:N	3:G:405:HOH:O	2.50	0.42
1:L:157:VAL:CG1	1:L:173:PHE:HB2	2.50	0.42
1:E:36:GLY:O	1:E:212:HIS:HA	2.19	0.42
1:I:157:VAL:HG13	1:I:173:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:LYS:NZ	3:G:408:HOH:O	2.52	0.42
1:K:12:LEU:C	1:K:12:LEU:HD12	2.45	0.42
1:I:67:VAL:CG1	1:I:83:PHE:HE2	2.33	0.42
1:J:43:LYS:HA	1:J:205:SER:O	2.20	0.42
1:K:36:GLY:O	1:K:212:HIS:HA	2.19	0.42
1:A:85:GLU:CD	1:A:181:LYS:HD3	2.45	0.41
1:D:144:GLU:HA	1:D:157:VAL:HB	2.02	0.41
1:F:201:ASP:HB2	1:F:202:LYS:HE2	2.01	0.41
1:I:93:MET:HG2	1:I:173:PHE:CD1	2.55	0.41
1:K:11:LYS:HE3	1:K:113:CYS:SG	2.61	0.41
1:G:12:LEU:C	1:G:12:LEU:HD12	2.46	0.41
1:K:145:LYS:NZ	1:L:143:THR:H	2.18	0.41
1:B:149:ARG:HH11	1:B:149:ARG:HD2	1.64	0.41
1:C:77:ASP:OD2	1:C:80:LYS:HD2	2.21	0.41
1:C:139:TRP:CZ3	1:C:161:LEU:HG	2.56	0.41
1:K:48:GLY:HA2	1:K:49:PRO:C	2.45	0.41
1:D:139:TRP:CE3	1:D:159:MET:HE3	2.55	0.41
1:G:154:LYS:NZ	3:G:413:HOH:O	2.54	0.41
1:J:21:HIS:NE2	3:J:401:HOH:O	2.12	0.41
1:K:93:MET:HG2	1:K:173:PHE:CD1	2.55	0.41
1:B:31:GLY:HA3	1:B:68:PHE:CE1	2.56	0.40
1:I:143:THR:H	1:J:145:LYS:NZ	2.19	0.40
1:L:157:VAL:HG13	1:L:173:PHE:HB2	2.03	0.40
1:E:67:VAL:HG11	1:E:83:PHE:CE2	2.57	0.40
1:H:11:LYS:HG3	1:H:113:CYS:SG	2.61	0.40
1:J:210:HIS:CE1	3:J:403:HOH:O	2.59	0.40
1:H:203:ASP:CG	1:H:205:SER:HG	2.29	0.40
1:C:8:MET:HE2	1:C:114:TYR:CZ	2.56	0.40
1:G:36:GLY:O	1:G:212:HIS:HA	2.21	0.40
1:H:139:TRP:CZ3	1:H:159:MET:HB3	2.57	0.40
1:K:62:GYS:HE1	1:K:195:ILE:HB	2.03	0.40
1:L:65:ASN:CG	1:L:67:VAL:HG22	2.46	0.40
1:K:154:LYS:NZ	3:K:414:HOH:O	2.54	0.40

All (3) 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)
3:G:544:HOH:O	3:L:543:HOH:O[1_455]	1.96	0.24
3:H:564:HOH:O	3:J:560:HOH:O[1_554]	2.03	0.17
3:F:528:HOH:O	3:L:511:HOH:O[1_455]	2.07	0.13

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	208/215 (97%)	207 (100%)	1 (0%)	0	100	100
1	B	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
1	C	208/215 (97%)	207 (100%)	1 (0%)	0	100	100
1	D	208/215 (97%)	208 (100%)	0	0	100	100
1	E	209/215 (97%)	208 (100%)	1 (0%)	0	100	100
1	F	209/215 (97%)	206 (99%)	3 (1%)	0	100	100
1	G	208/215 (97%)	207 (100%)	1 (0%)	0	100	100
1	H	209/215 (97%)	207 (99%)	1 (0%)	1 (0%)	24	16
1	I	208/215 (97%)	206 (99%)	2 (1%)	0	100	100
1	J	209/215 (97%)	209 (100%)	0	0	100	100
1	K	208/215 (97%)	205 (99%)	3 (1%)	0	100	100
1	L	209/215 (97%)	208 (100%)	1 (0%)	0	100	100
All	All	2503/2580 (97%)	2485 (99%)	17 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	165	GLY

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	183/185 (99%)	180 (98%)	3 (2%)	55	54
1	B	185/185 (100%)	178 (96%)	7 (4%)	29	21
1	C	183/185 (99%)	178 (97%)	5 (3%)	39	34
1	D	183/185 (99%)	178 (97%)	5 (3%)	39	34
1	E	184/185 (100%)	182 (99%)	2 (1%)	65	67
1	F	184/185 (100%)	181 (98%)	3 (2%)	55	54
1	G	183/185 (99%)	180 (98%)	3 (2%)	55	54
1	H	184/185 (100%)	180 (98%)	4 (2%)	45	42
1	I	183/185 (99%)	180 (98%)	3 (2%)	55	54
1	J	184/185 (100%)	178 (97%)	6 (3%)	33	26
1	K	183/185 (99%)	181 (99%)	2 (1%)	65	67
1	L	184/185 (100%)	183 (100%)	1 (0%)	81	84
All	All	2203/2220 (99%)	2159 (98%)	44 (2%)	48	46

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	67	VAL
1	A	202	LYS
1	B	8	MET
1	B	67	VAL
1	B	113	CYS
1	B	149	ARG
1	B	181	LYS
1	B	182	VAL
1	B	214	GLU
1	C	3	VAL
1	C	30	LEU
1	C	67	VAL
1	C	113	CYS
1	C	183	VAL
1	D	8	MET
1	D	115	ILE
1	D	157	VAL
1	D	181	LYS
1	D	198	LYS
1	E	76	VAL
1	E	164	GLU

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Mol	Chain	Res	Type
1	F	21	HIS
1	F	202	LYS
1	F	214	GLU
1	G	67	VAL
1	G	73	GLU
1	G	181	LYS
1	H	8	MET
1	H	70	LYS
1	H	73	GLU
1	H	202	LYS
1	I	30	LEU
1	I	76	VAL
1	I	205	SER
1	J	3	VAL
1	J	11	LYS
1	J	67	VAL
1	J	162	SER
1	J	202	LYS
1	J	214	GLU
1	K	3	VAL
1	K	67	VAL
1	L	198	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	210	HIS
1	B	38	GLN
1	B	81	GLN
1	B	133	GLN
1	B	208	ASN
1	B	210	HIS
1	C	158	ASN
1	C	206	ASN
1	C	210	HIS
1	D	158	ASN
1	E	128	ASN
1	E	158	ASN
1	E	206	ASN
1	E	208	ASN
1	F	21	HIS

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Mol	Chain	Res	Type
1	G	21	HIS
1	G	38	GLN
1	G	158	ASN
1	H	158	ASN
1	I	158	ASN
1	K	21	HIS
1	K	158	ASN
1	K	208	ASN
1	L	158	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	GYS	A	62	1	20,22,23	3.25	5 (25%)	25,30,32	2.75	10 (40%)
1	GYS	I	62	1	20,22,23	3.14	6 (30%)	25,30,32	2.30	7 (28%)
1	GYS	D	62	1	20,22,23	3.85	6 (30%)	25,30,32	2.17	7 (28%)
1	GYS	G	62	1	20,22,23	3.59	5 (25%)	25,30,32	3.08	9 (36%)
1	GYS	K	62	1	20,22,23	3.77	7 (35%)	25,30,32	3.93	10 (40%)
1	GYS	J	62	1	20,22,23	3.28	6 (30%)	25,30,32	3.15	6 (24%)
1	GYS	B	62	1	20,22,23	3.13	4 (20%)	25,30,32	2.82	10 (40%)
1	GYS	C	62	1	20,22,23	3.66	5 (25%)	25,30,32	3.41	14 (56%)
1	GYS	E	62	1	20,22,23	3.22	6 (30%)	25,30,32	2.93	12 (48%)
1	GYS	H	62	1	20,22,23	2.96	5 (25%)	25,30,32	2.15	6 (24%)
1	GYS	L	62	1	20,22,23	3.08	5 (25%)	25,30,32	2.25	5 (20%)
1	GYS	F	62	1	20,22,23	3.14	7 (35%)	25,30,32	3.72	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYS	A	62	1	-	2/10/29/30	0/2/2/2
1	GYS	I	62	1	-	2/10/29/30	0/2/2/2
1	GYS	D	62	1	-	3/10/29/30	0/2/2/2
1	GYS	G	62	1	-	2/10/29/30	0/2/2/2
1	GYS	K	62	1	-	2/10/29/30	0/2/2/2
1	GYS	J	62	1	-	2/10/29/30	0/2/2/2
1	GYS	B	62	1	-	1/10/29/30	0/2/2/2
1	GYS	C	62	1	-	1/10/29/30	0/2/2/2
1	GYS	E	62	1	-	3/10/29/30	0/2/2/2
1	GYS	H	62	1	-	2/10/29/30	0/2/2/2
1	GYS	L	62	1	-	3/10/29/30	0/2/2/2
1	GYS	F	62	1	-	3/10/29/30	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	GYS	CB2-CA2	14.83	1.49	1.35
1	C	62	GYS	CB2-CA2	13.99	1.48	1.35
1	G	62	GYS	CB2-CA2	13.50	1.48	1.35
1	K	62	GYS	CB2-CA2	13.35	1.48	1.35
1	A	62	GYS	CB2-CA2	12.17	1.46	1.35
1	F	62	GYS	CB2-CA2	11.80	1.46	1.35
1	J	62	GYS	CB2-CA2	11.55	1.46	1.35
1	H	62	GYS	CB2-CA2	11.41	1.46	1.35
1	B	62	GYS	CB2-CA2	11.40	1.46	1.35
1	I	62	GYS	CB2-CA2	10.90	1.45	1.35
1	L	62	GYS	CB2-CA2	10.22	1.45	1.35
1	E	62	GYS	CB2-CA2	9.15	1.44	1.35
1	E	62	GYS	CA2-C2	-9.02	1.38	1.48
1	K	62	GYS	CA2-C2	-7.06	1.40	1.48
1	B	62	GYS	CA2-C2	-6.60	1.41	1.48
1	L	62	GYS	CA2-C2	-6.28	1.41	1.48
1	G	62	GYS	C1-N2	5.90	1.40	1.32
1	C	62	GYS	C1-N2	5.26	1.39	1.32
1	J	62	GYS	C1-N2	5.18	1.39	1.32
1	J	62	GYS	C2-N3	-4.75	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	62	GYS	CA2-C2	-4.68	1.43	1.48
1	A	62	GYS	CA2-C2	-4.61	1.43	1.48
1	I	62	GYS	C2-N3	-4.32	1.30	1.40
1	K	62	GYS	C2-N3	-4.22	1.30	1.40
1	D	62	GYS	C1-N2	4.06	1.38	1.32
1	D	62	GYS	O2-C2	4.02	1.31	1.23
1	G	62	GYS	C2-N3	-3.87	1.31	1.40
1	C	62	GYS	O2-C2	3.86	1.30	1.23
1	A	62	GYS	C1-N2	3.70	1.37	1.32
1	F	62	GYS	C2-N3	-3.70	1.31	1.40
1	J	62	GYS	CA2-C2	-3.69	1.44	1.48
1	D	62	GYS	CA2-C2	-3.68	1.44	1.48
1	K	62	GYS	C1-N2	3.66	1.37	1.32
1	L	62	GYS	C2-N3	-3.63	1.31	1.40
1	D	62	GYS	C2-N3	-3.44	1.32	1.40
1	I	62	GYS	C1-N2	3.41	1.37	1.32
1	L	62	GYS	C1-N2	3.40	1.37	1.32
1	H	62	GYS	C1-N2	3.40	1.37	1.32
1	G	62	GYS	CA2-C2	-3.36	1.44	1.48
1	F	62	GYS	C1-N2	3.30	1.37	1.32
1	I	62	GYS	O2-C2	3.23	1.29	1.23
1	A	62	GYS	C2-N3	-3.14	1.32	1.40
1	H	62	GYS	O2-C2	3.00	1.29	1.23
1	H	62	GYS	C2-N3	-2.98	1.33	1.40
1	E	62	GYS	C1-N2	2.89	1.36	1.32
1	E	62	GYS	C2-N3	-2.89	1.33	1.40
1	A	62	GYS	O2-C2	2.88	1.28	1.23
1	F	62	GYS	CA2-C2	-2.86	1.45	1.48
1	D	62	GYS	CA3-N3	-2.72	1.42	1.47
1	E	62	GYS	O2-C2	2.61	1.28	1.23
1	H	62	GYS	C1-N3	2.60	1.41	1.37
1	F	62	GYS	CA2-N2	-2.59	1.33	1.38
1	F	62	GYS	CA3-N3	-2.56	1.42	1.47
1	C	62	GYS	CA2-C2	-2.54	1.45	1.48
1	G	62	GYS	O2-C2	2.48	1.28	1.23
1	L	62	GYS	CE2-CD2	2.47	1.42	1.38
1	C	62	GYS	C2-N3	-2.37	1.34	1.40
1	K	62	GYS	CE1-CD1	2.31	1.42	1.38
1	K	62	GYS	C1-N3	2.26	1.41	1.37
1	B	62	GYS	C2-N3	-2.24	1.34	1.40
1	J	62	GYS	O2-C2	2.22	1.27	1.23
1	I	62	GYS	C1-N3	2.20	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	GYS	CG2-CB2	-2.07	1.43	1.46
1	J	62	GYS	CG2-CB2	-2.07	1.43	1.46
1	E	62	GYS	CG2-CB2	-2.06	1.43	1.46
1	F	62	GYS	CE2-CZ	2.04	1.42	1.39
1	K	62	GYS	CA3-N3	-2.01	1.43	1.47

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	62	GYS	O2-C2-CA2	-15.87	120.89	131.02
1	F	62	GYS	O2-C2-CA2	-15.40	121.19	131.02
1	J	62	GYS	O2-C2-CA2	-10.54	124.30	131.02
1	C	62	GYS	O2-C2-CA2	-9.92	124.69	131.02
1	E	62	GYS	O2-C2-CA2	-9.71	124.82	131.02
1	J	62	GYS	CA2-C2-N3	8.24	110.42	103.50
1	K	62	GYS	CA2-C2-N3	8.19	110.38	103.50
1	G	62	GYS	O2-C2-CA2	-8.18	125.80	131.02
1	I	62	GYS	O2-C2-CA2	-7.96	125.94	131.02
1	A	62	GYS	CA2-C2-N3	7.41	109.72	103.50
1	G	62	GYS	CA2-C2-N3	7.40	109.71	103.50
1	B	62	GYS	O2-C2-CA2	-7.36	126.32	131.02
1	C	62	GYS	C2-N3-C1	-7.25	104.71	108.07
1	C	62	GYS	CA2-C2-N3	7.19	109.54	103.50
1	A	62	GYS	O2-C2-CA2	-7.11	126.48	131.02
1	G	62	GYS	C2-N3-C1	-6.99	104.83	108.07
1	L	62	GYS	CA2-C2-N3	6.99	109.37	103.50
1	D	62	GYS	O2-C2-CA2	-6.83	126.66	131.02
1	H	62	GYS	O2-C2-CA2	-6.51	126.86	131.02
1	B	62	GYS	CA2-C2-N3	6.24	108.74	103.50
1	F	62	GYS	CA2-C2-N3	6.22	108.72	103.50
1	L	62	GYS	O2-C2-CA2	-6.10	127.13	131.02
1	B	62	GYS	C2-N3-C1	-5.22	105.65	108.07
1	A	62	GYS	C2-N3-C1	-5.19	105.66	108.07
1	J	62	GYS	C2-N3-C1	-5.18	105.67	108.07
1	H	62	GYS	CA2-C2-N3	4.86	107.59	103.50
1	D	62	GYS	CA2-C2-N3	4.85	107.58	103.50
1	E	62	GYS	CA2-N2-C1	-4.16	102.55	105.80
1	E	62	GYS	CD1-CE1-CZ	4.11	124.23	119.88
1	B	62	GYS	C2-CA2-N2	-4.04	106.06	108.95
1	G	62	GYS	CA2-N2-C1	-4.03	102.65	105.80
1	I	62	GYS	CA2-C2-N3	3.95	106.82	103.50
1	F	62	GYS	C2-CA2-N2	-3.89	106.17	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	62	GYS	C2-CA2-N2	-3.88	106.17	108.95
1	E	62	GYS	CA2-C2-N3	3.75	106.65	103.50
1	C	62	GYS	CD2-CE2-CZ	-3.71	115.95	119.88
1	G	62	GYS	C3-CA3-N3	3.62	120.66	112.43
1	I	62	GYS	CA2-N2-C1	-3.48	103.08	105.80
1	B	62	GYS	C3-CA3-N3	3.43	120.23	112.43
1	E	62	GYS	C3-CA3-N3	3.42	120.22	112.43
1	H	62	GYS	C2-N3-C1	-3.27	106.55	108.07
1	B	62	GYS	CD1-CE1-CZ	3.22	123.29	119.88
1	E	62	GYS	CE1-CD1-CG2	-3.19	117.10	121.22
1	B	62	GYS	CE1-CD1-CG2	-3.12	117.19	121.22
1	A	62	GYS	C3-CA3-N3	3.09	119.47	112.43
1	G	62	GYS	O3-C3-CA3	-3.05	111.74	125.47
1	I	62	GYS	C3-CA3-N3	3.03	119.31	112.43
1	D	62	GYS	O3-C3-CA3	-2.95	112.21	125.47
1	C	62	GYS	N3-C1-N2	2.93	113.79	111.48
1	K	62	GYS	O3-C3-CA3	-2.92	112.31	125.47
1	C	62	GYS	CE1-CD1-CG2	-2.91	117.47	121.22
1	F	62	GYS	O3-C3-CA3	-2.88	112.51	125.47
1	L	62	GYS	C3-CA3-N3	2.86	118.93	112.43
1	D	62	GYS	CA1-C1-N3	-2.85	121.12	124.84
1	C	62	GYS	O3-C3-CA3	-2.84	112.69	125.47
1	E	62	GYS	CD2-CG2-CB2	-2.75	111.76	121.22
1	K	62	GYS	N3-C1-N2	-2.75	109.32	111.48
1	K	62	GYS	C2-N3-C1	-2.70	106.82	108.07
1	C	62	GYS	CA3-N3-C2	2.68	129.56	123.67
1	F	62	GYS	O2-C2-N3	2.68	129.90	124.31
1	G	62	GYS	N3-C1-N2	2.67	113.59	111.48
1	B	62	GYS	CB2-CA2-C2	2.67	125.59	122.36
1	E	62	GYS	CG2-CB2-CA2	-2.66	126.70	129.87
1	K	62	GYS	C3-CA3-N3	2.66	118.48	112.43
1	J	62	GYS	CE2-CD2-CG2	-2.65	117.80	121.22
1	E	62	GYS	O3-C3-CA3	-2.63	113.62	125.47
1	F	62	GYS	CA2-N2-C1	2.62	107.85	105.80
1	J	62	GYS	C3-CA3-N3	2.60	118.34	112.43
1	A	62	GYS	C2-CA2-N2	-2.59	107.10	108.95
1	J	62	GYS	O3-C3-CA3	-2.56	113.95	125.47
1	H	62	GYS	O3-C3-CA3	-2.52	114.12	125.47
1	F	62	GYS	C2-N3-C1	-2.52	106.90	108.07
1	C	62	GYS	CD2-CG2-CB2	-2.51	112.61	121.22
1	K	62	GYS	CE1-CD1-CG2	-2.47	118.03	121.22
1	C	62	GYS	C3-CA3-N3	2.46	118.03	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	62	GYS	CG2-CB2-CA2	-2.46	126.94	129.87
1	I	62	GYS	O3-C3-CA3	-2.43	114.54	125.47
1	B	62	GYS	CA2-N2-C1	2.43	107.70	105.80
1	K	62	GYS	C2-CA2-N2	-2.42	107.21	108.95
1	A	62	GYS	CD2-CE2-CZ	2.42	122.44	119.88
1	I	62	GYS	CB2-CA2-C2	-2.40	119.44	122.36
1	G	62	GYS	CD2-CG2-CB2	-2.37	113.07	121.22
1	H	62	GYS	CD2-CE2-CZ	2.34	122.35	119.88
1	A	62	GYS	O3-C3-CA3	-2.34	114.96	125.47
1	A	62	GYS	CB2-CA2-N2	2.32	131.91	128.76
1	C	62	GYS	C2-CA2-N2	-2.27	107.33	108.95
1	H	62	GYS	CA1-C1-N3	-2.25	121.92	124.84
1	E	62	GYS	CD2-CG2-CD1	2.24	120.98	117.65
1	D	62	GYS	CD2-CG2-CB2	-2.24	113.52	121.22
1	L	62	GYS	O3-C3-CA3	-2.24	115.40	125.47
1	D	62	GYS	C3-CA3-N3	2.19	117.41	112.43
1	C	62	GYS	CD2-CG2-CD1	2.18	120.89	117.65
1	B	62	GYS	O3-C3-CA3	-2.18	115.67	125.47
1	E	62	GYS	C2-CA2-N2	2.16	110.50	108.95
1	E	62	GYS	CB2-CA2-C2	-2.14	119.77	122.36
1	D	62	GYS	C2-N3-C1	-2.10	107.10	108.07
1	A	62	GYS	CD1-CE1-CZ	-2.07	117.69	119.88
1	I	62	GYS	C2-CA2-N2	2.06	110.43	108.95
1	K	62	GYS	O2-C2-N3	2.06	128.61	124.31
1	C	62	GYS	CB2-CA2-C2	2.05	124.84	122.36
1	C	62	GYS	CE2-CZ-CE1	2.04	123.01	119.77
1	A	62	GYS	CD2-CG2-CB2	-2.01	114.33	121.22
1	G	62	GYS	CA1-C1-N3	-2.00	122.23	124.84

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	62	GYS	N1-CA1-CB1-OG1
1	D	62	GYS	C1-CA1-CB1-OG1
1	D	62	GYS	C3-CA3-N3-C2
1	E	62	GYS	N1-CA1-CB1-OG1
1	F	62	GYS	C3-CA3-N3-C2
1	G	62	GYS	C3-CA3-N3-C2
1	H	62	GYS	C3-CA3-N3-C2
1	I	62	GYS	C3-CA3-N3-C2
1	J	62	GYS	C3-CA3-N3-C2

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Mol	Chain	Res	Type	Atoms
1	L	62	GYS	N1-CA1-CB1-OG1
1	L	62	GYS	C3-CA3-N3-C2
1	B	62	GYS	C3-CA3-N3-C2
1	A	62	GYS	C3-CA3-N3-C2
1	C	62	GYS	C3-CA3-N3-C2
1	E	62	GYS	C3-CA3-N3-C2
1	K	62	GYS	C3-CA3-N3-C2
1	L	62	GYS	C1-CA1-CB1-OG1
1	E	62	GYS	C1-CA1-CB1-OG1
1	A	62	GYS	N1-CA1-CB1-OG1
1	I	62	GYS	N1-CA1-CB1-OG1
1	F	62	GYS	C3-CA3-N3-C1
1	F	62	GYS	N1-CA1-CB1-OG1
1	G	62	GYS	N1-CA1-CB1-OG1
1	H	62	GYS	N1-CA1-CB1-OG1
1	J	62	GYS	N1-CA1-CB1-OG1
1	K	62	GYS	N1-CA1-CB1-OG1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	K	62	GYS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	212/215 (98%)	-0.37	0 100 100	14, 22, 40, 56	0
1	B	214/215 (99%)	-0.43	0 100 100	14, 21, 38, 70	0
1	C	212/215 (98%)	-0.40	1 (0%) 87 89	14, 20, 37, 52	0
1	D	212/215 (98%)	-0.35	1 (0%) 87 89	14, 22, 40, 52	0
1	E	213/215 (99%)	-0.40	1 (0%) 87 89	13, 21, 39, 61	0
1	F	213/215 (99%)	-0.54	0 100 100	12, 19, 33, 49	0
1	G	212/215 (98%)	-0.24	0 100 100	15, 25, 43, 59	0
1	H	213/215 (99%)	-0.40	0 100 100	13, 22, 40, 66	0
1	I	212/215 (98%)	-0.31	1 (0%) 87 89	13, 23, 43, 58	0
1	J	213/215 (99%)	-0.28	0 100 100	13, 24, 42, 55	0
1	K	212/215 (98%)	-0.51	0 100 100	13, 19, 31, 49	0
1	L	213/215 (99%)	-0.47	1 (0%) 87 89	13, 20, 36, 49	0
All	All	2551/2580 (98%)	-0.39	5 (0%) 91 92	12, 21, 39, 70	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	VAL	4.6
1	I	3	VAL	2.8
1	L	3	VAL	2.4
1	E	3	VAL	2.2
1	D	3	VAL	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. 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	GYS	C	62	21/22	0.95	0.06	14,16,20,30	0
1	GYS	D	62	21/22	0.96	0.06	14,21,24,39	0
1	GYS	G	62	21/22	0.96	0.05	18,21,23,26	0
1	GYS	H	62	21/22	0.96	0.06	15,19,21,29	0
1	GYS	B	62	21/22	0.96	0.05	13,17,20,39	0
1	GYS	E	62	21/22	0.97	0.04	15,18,19,26	0
1	GYS	I	62	21/22	0.97	0.06	14,19,21,29	0
1	GYS	J	62	21/22	0.97	0.05	16,19,23,31	0
1	GYS	L	62	21/22	0.97	0.05	13,16,19,24	0
1	GYS	A	62	21/22	0.97	0.05	16,19,21,29	0
1	GYS	F	62	21/22	0.98	0.04	13,15,17,23	0
1	GYS	K	62	21/22	0.98	0.04	13,15,16,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
2	NI	G	302	1/1	0.97	0.04	45,45,45,45	0
2	NI	C	301	1/1	0.99	0.04	36,36,36,36	0
2	NI	C	302	1/1	0.99	0.02	38,38,38,38	0
2	NI	D	301	1/1	0.99	0.02	41,41,41,41	0
2	NI	D	302	1/1	0.99	0.03	35,35,35,35	0
2	NI	E	301	1/1	0.99	0.05	37,37,37,37	0
2	NI	F	301	1/1	0.99	0.04	28,28,28,28	0
2	NI	G	301	1/1	0.99	0.03	40,40,40,40	0
2	NI	A	301	1/1	0.99	0.02	36,36,36,36	0
2	NI	H	301	1/1	0.99	0.04	38,38,38,38	0
2	NI	I	301	1/1	0.99	0.04	45,45,45,45	0
2	NI	I	302	1/1	0.99	0.02	38,38,38,38	0
2	NI	J	301	1/1	0.99	0.03	39,39,39,39	0
2	NI	J	302	1/1	0.99	0.03	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	K	302	1/1	0.99	0.02	30,30,30,30	0
2	NI	K	303	1/1	0.99	0.05	32,32,32,32	0
2	NI	L	301	1/1	0.99	0.04	32,32,32,32	0
2	NI	L	302	1/1	0.99	0.02	28,28,28,28	0
2	NI	A	302	1/1	1.00	0.02	42,42,42,42	0
2	NI	B	301	1/1	1.00	0.01	32,32,32,32	0
2	NI	K	301	1/1	1.00	0.02	26,26,26,26	0
2	NI	E	302	1/1	1.00	0.02	31,31,31,31	0
2	NI	H	302	1/1	1.00	0.02	37,37,37,37	0
2	NI	B	302	1/1	1.00	0.03	34,34,34,34	0
2	NI	F	302	1/1	1.00	0.05	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.