



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 01:32 am BST

PDB ID : 5HZU
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 wwPDB X-ray Structure Validation Summary 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 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 : 2.11
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) : 2.11

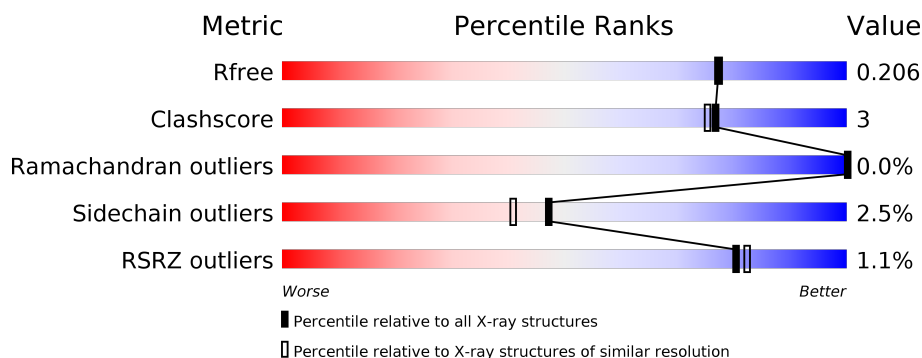
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	<div> <div>2%</div> <div>90%</div> <div>8%</div> <div>..</div> </div>
1	B	215	<div> <div>88%</div> <div>11%</div> </div>
1	C	215	<div> <div>2%</div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	D	215	<div> <div>2%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>
1	E	215	<div> <div>90%</div> <div>9%</div> <div>.</div> </div>
1	F	215	<div> <div>93%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	215	<div><div></div><div>2%</div><div>86%</div><div>13%</div><div></div></div>
1	H	215	<div><div></div><div>%</div><div>90%</div><div>10%</div><div></div></div>
1	I	215	<div><div></div><div></div><div>90%</div><div>8%</div><div></div></div>
1	J	215	<div><div></div><div>%</div><div>92%</div><div>7%</div><div></div></div>
1	K	215	<div><div></div><div>%</div><div>89%</div><div>9%</div><div></div></div>
1	L	215	<div><div></div><div></div><div>90%</div><div>9%</div><div></div></div>

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 (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	2	Total Ni 2 2	0	0
2	J	2	Total Ni 2 2	0	0
2	D	2	Total Ni 2 2	0	0
2	K	3	Total Ni 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	Ni 2	0	0
2	H	2	Total 2	Ni 2	0	0
2	B	2	Total 2	Ni 2	0	0
2	I	2	Total 2	Ni 2	0	0
2	C	2	Total 2	Ni 2	0	0
2	A	2	Total 2	Ni 2	0	0
2	L	2	Total 2	Ni 2	0	0
2	F	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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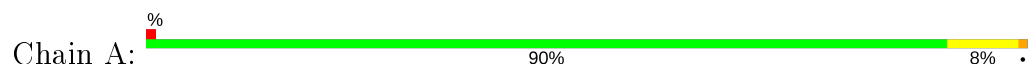
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	184	Total	O	0	0
			184	184		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

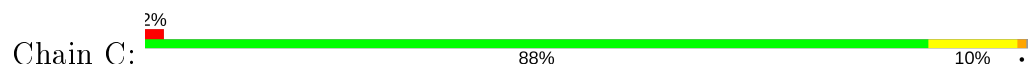
- Molecule 1: Fluorescent protein Dronpa



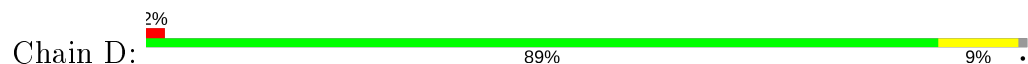
- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa



- Molecule 1: Fluorescent protein Dronpa




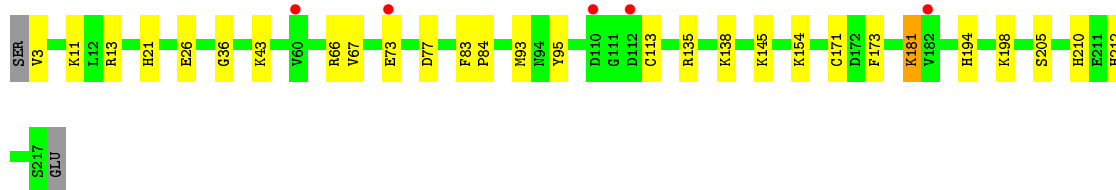
- Molecule 1: Fluorescent protein Dronpa

Chain F:  93% . .




- Molecule 1: Fluorescent protein Dronpa

Chain G:  86% 13% .



- Molecule 1: Fluorescent protein Dronpa

Chain H:  90% 10%




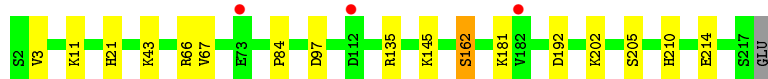
- Molecule 1: Fluorescent protein Dronpa

Chain I:  90% 8% ..




- Molecule 1: Fluorescent protein Dronpa

Chain J:  92% 7%




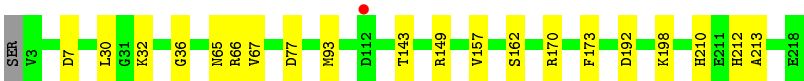
- Molecule 1: Fluorescent protein Dronpa

Chain K:  89% 9% .



- Molecule 1: Fluorescent protein Dronpa

Chain L:  90% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	105.37 Å 109.40 Å 72.09 Å 71.11° 85.97° 61.30°	Depositor
Resolution (Å)	29.03 – 1.89 28.74 – 1.89	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.03-1.89) 94.0 (28.74-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.89 Å)	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 (5.02%)	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 , 42.7	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	0.96	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

5.1 Standard geometry

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	1.02	1/1745 (0.1%)	0.96	2/2355 (0.1%)
1	B	1.00	1/1760 (0.1%)	0.99	3/2375 (0.1%)
1	C	0.99	1/1745 (0.1%)	1.06	9/2355 (0.4%)
1	D	1.01	2/1745 (0.1%)	0.99	4/2355 (0.2%)
1	E	1.05	0/1754	0.98	2/2367 (0.1%)
1	F	1.07	1/1751 (0.1%)	0.99	3/2363 (0.1%)
1	G	0.98	0/1745	0.95	2/2355 (0.1%)
1	H	0.96	0/1754	1.00	4/2367 (0.2%)
1	I	1.00	2/1745 (0.1%)	1.02	6/2355 (0.3%)
1	J	0.99	1/1751 (0.1%)	0.97	3/2363 (0.1%)
1	K	1.09	1/1745 (0.1%)	1.03	7/2355 (0.3%)
1	L	1.04	1/1754 (0.1%)	1.01	3/2367 (0.1%)
All	All	1.02	11/20994 (0.1%)	1.00	48/28332 (0.2%)

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	E	0	1

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	TRP	CB-CG	-7.94	1.35	1.50
1	J	162	SER	CB-OG	-6.35	1.33	1.42
1	L	162	SER	CB-OG	-6.18	1.34	1.42
1	B	170	ARG	C-O	5.63	1.34	1.23
1	D	90	GLU	CG-CD	5.55	1.60	1.51

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	135	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	149	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	K	121	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	H	170	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	K	187	ASP	CB-CG-OD1	6.91	124.52	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	61	PHE	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	1721	0	1650	13	0
1	B	1736	0	1662	11	0
1	C	1721	0	1649	8	0
1	D	1721	0	1651	8	0
1	E	1730	0	1657	13	0
1	F	1727	0	1655	9	0
1	G	1721	0	1650	15	0
1	H	1730	0	1656	14	0
1	I	1721	0	1651	14	0
1	J	1727	0	1656	6	0
1	K	1721	0	1650	9	0
1	L	1730	0	1655	9	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	0
3	B	155	0	0	4	0
3	C	166	0	0	2	0
3	D	161	0	0	2	0
3	E	173	0	0	2	0
3	F	170	0	0	2	1
3	G	156	0	0	6	1
3	H	164	0	0	3	1
3	I	154	0	0	1	0
3	J	160	0	0	3	1
3	K	193	0	0	1	0
3	L	184	0	0	1	2
All	All	22735	0	19842	122	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.

The worst 5 of 122 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

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	210/215 (98%)	209 (100%)	1 (0%)	0	100	100
1	B	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
1	C	210/215 (98%)	208 (99%)	2 (1%)	0	100	100
1	D	210/215 (98%)	210 (100%)	0	0	100	100
1	E	211/215 (98%)	209 (99%)	2 (1%)	0	100	100
1	F	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
1	G	210/215 (98%)	209 (100%)	1 (0%)	0	100	100
1	H	211/215 (98%)	208 (99%)	2 (1%)	1 (0%)	29	18
1	I	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
1	J	211/215 (98%)	210 (100%)	1 (0%)	0	100	100
1	K	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
1	L	211/215 (98%)	210 (100%)	1 (0%)	0	100	100
All	All	2527/2580 (98%)	2502 (99%)	24 (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%)	62	60
1	B	185/185 (100%)	177 (96%)	8 (4%)	29	19
1	C	183/185 (99%)	178 (97%)	5 (3%)	44	38
1	D	183/185 (99%)	178 (97%)	5 (3%)	44	38
1	E	184/185 (100%)	180 (98%)	4 (2%)	52	47
1	F	184/185 (100%)	180 (98%)	4 (2%)	52	47
1	G	183/185 (99%)	178 (97%)	5 (3%)	44	38
1	H	184/185 (100%)	181 (98%)	3 (2%)	62	60
1	I	183/185 (99%)	179 (98%)	4 (2%)	52	47
1	J	184/185 (100%)	177 (96%)	7 (4%)	33	24
1	K	183/185 (99%)	179 (98%)	4 (2%)	52	47
1	L	184/185 (100%)	181 (98%)	3 (2%)	62	60
All	All	2203/2220 (99%)	2148 (98%)	55 (2%)	47	41

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	164	GLU
1	G	67	VAL
1	K	67	VAL
1	F	21	HIS
1	F	202	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	206	ASN
1	C	210	HIS
1	G	21	HIS
1	C	38	GLN
1	F	21	HIS

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	I	62	1	22,22,23	3.32	6 (27%)	27,30,32	2.71	7 (25%)
1	GYS	F	62	1	22,22,23	3.33	7 (31%)	27,30,32	4.45	9 (33%)
1	GYS	D	62	1	22,22,23	4.11	6 (27%)	27,30,32	2.89	7 (25%)
1	GYS	J	62	1	22,22,23	3.45	5 (22%)	27,30,32	4.06	8 (29%)
1	GYS	H	62	1	22,22,23	3.15	5 (22%)	27,30,32	2.74	7 (25%)
1	GYS	L	62	1	22,22,23	3.26	5 (22%)	27,30,32	3.10	5 (18%)
1	GYS	E	62	1	22,22,23	3.39	5 (22%)	27,30,32	3.28	12 (44%)
1	GYS	C	62	1	22,22,23	3.93	6 (27%)	27,30,32	4.04	13 (48%)
1	GYS	G	62	1	22,22,23	3.84	5 (22%)	27,30,32	3.78	9 (33%)
1	GYS	K	62	1	22,22,23	4.00	6 (27%)	27,30,32	4.86	11 (40%)
1	GYS	A	62	1	22,22,23	3.48	5 (22%)	27,30,32	3.54	9 (33%)
1	GYS	B	62	1	22,22,23	3.38	3 (13%)	27,30,32	3.34	10 (37%)

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	I	62	1	-	2/9/29/30	0/2/2/2
1	GYS	F	62	1	-	2/9/29/30	0/2/2/2
1	GYS	D	62	1	-	3/9/29/30	0/2/2/2
1	GYS	J	62	1	-	1/9/29/30	0/2/2/2
1	GYS	H	62	1	-	1/9/29/30	0/2/2/2
1	GYS	L	62	1	-	3/9/29/30	0/2/2/2
1	GYS	E	62	1	-	3/9/29/30	0/2/2/2
1	GYS	C	62	1	-	1/9/29/30	0/2/2/2
1	GYS	G	62	1	-	1/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GYS	K	62	1	-	1/9/29/30	0/2/2/2
1	GYS	A	62	1	-	3/9/29/30	0/2/2/2
1	GYS	B	62	1	-	1/9/29/30	0/2/2/2

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	62	GYS	CB2-CA2	17.11	1.49	1.35
1	C	62	GYS	CB2-CA2	16.15	1.48	1.35
1	G	62	GYS	CB2-CA2	15.58	1.48	1.35
1	K	62	GYS	CB2-CA2	15.41	1.48	1.35
1	A	62	GYS	CB2-CA2	14.06	1.46	1.35

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	62	GYS	O2-C2-CA2	-17.94	120.89	130.96
1	F	62	GYS	O2-C2-CA2	-17.40	121.19	130.96
1	J	62	GYS	CA2-C2-N3	14.91	110.42	103.37
1	K	62	GYS	CA2-C2-N3	14.81	110.38	103.37
1	A	62	GYS	CA2-C2-N3	13.43	109.72	103.37

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	62	GYS	C-CA3-N3-C2
1	F	62	GYS	C-CA3-N3-C2
1	D	62	GYS	N-CA1-CB1-OG1
1	D	62	GYS	C1-CA1-CB1-OG1
1	D	62	GYS	C-CA3-N3-C2

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.18	2 (0%) 84 85	14, 22, 40, 56	0
1	B	214/215 (99%)	-0.22	1 (0%) 91 92	14, 21, 38, 70	0
1	C	212/215 (98%)	-0.22	4 (1%) 66 69	14, 20, 37, 52	0
1	D	212/215 (98%)	-0.22	4 (1%) 66 69	14, 22, 40, 52	0
1	E	213/215 (99%)	-0.27	0 100 100	13, 21, 39, 61	0
1	F	213/215 (99%)	-0.33	1 (0%) 91 92	13, 19, 33, 49	0
1	G	212/215 (98%)	-0.10	5 (2%) 59 62	15, 25, 43, 59	0
1	H	213/215 (99%)	-0.21	3 (1%) 75 77	13, 22, 40, 66	0
1	I	212/215 (98%)	-0.20	1 (0%) 91 92	13, 23, 43, 58	0
1	J	213/215 (99%)	-0.08	3 (1%) 75 77	13, 24, 42, 55	0
1	K	212/215 (98%)	-0.26	2 (0%) 84 85	13, 19, 31, 49	0
1	L	213/215 (99%)	-0.36	1 (0%) 91 92	13, 20, 36, 49	0
All	All	2551/2580 (98%)	-0.22	27 (1%) 80 82	13, 21, 39, 70	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	SER	4.2
1	G	112	ASP	3.4
1	C	60	VAL	3.4
1	J	73	GLU	2.9
1	G	73	GLU	2.9

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	GYS	H	62	21/22	0.96	0.13	15,19,21,29	0
1	GYS	C	62	21/22	0.96	0.17	14,16,20,30	0
1	GYS	J	62	21/22	0.97	0.20	16,19,23,31	0
1	GYS	I	62	21/22	0.97	0.10	14,19,21,29	0
1	GYS	D	62	21/22	0.97	0.14	14,21,24,39	0
1	GYS	G	62	21/22	0.97	0.16	18,21,23,26	0
1	GYS	A	62	21/22	0.97	0.15	16,19,21,29	0
1	GYS	B	62	21/22	0.97	0.15	13,17,20,39	0
1	GYS	K	62	21/22	0.98	0.18	13,15,16,18	0
1	GYS	L	62	21/22	0.98	0.10	13,16,19,24	0
1	GYS	E	62	21/22	0.98	0.13	15,18,19,26	0
1	GYS	F	62	21/22	0.99	0.14	13,15,17,23	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	0.95	0.04	45,45,45,45	0
2	NI	D	301	1/1	0.98	0.03	41,41,41,41	0
2	NI	H	301	1/1	0.98	0.05	38,38,38,38	0
2	NI	G	301	1/1	0.98	0.03	40,40,40,40	0
2	NI	A	302	1/1	0.99	0.04	42,42,42,42	0
2	NI	L	302	1/1	0.99	0.04	28,28,28,28	0
2	NI	A	301	1/1	0.99	0.03	36,36,36,36	0
2	NI	J	302	1/1	0.99	0.03	43,43,43,43	0
2	NI	K	303	1/1	0.99	0.06	32,32,32,32	0
2	NI	J	301	1/1	0.99	0.03	39,39,39,39	0
2	NI	C	301	1/1	0.99	0.04	36,36,36,36	0
2	NI	D	302	1/1	0.99	0.03	35,35,35,35	0
2	NI	L	301	1/1	0.99	0.03	32,32,32,32	0
2	NI	I	301	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NI	E	301	1/1	0.99	0.05	37,37,37,37	0
2	NI	C	302	1/1	0.99	0.02	38,38,38,38	0
2	NI	F	301	1/1	0.99	0.03	28,28,28,28	0
2	NI	K	302	1/1	0.99	0.02	30,30,30,30	0
2	NI	I	302	1/1	1.00	0.02	38,38,38,38	0
2	NI	B	301	1/1	1.00	0.02	32,32,32,32	0
2	NI	E	302	1/1	1.00	0.04	31,31,31,31	0
2	NI	H	302	1/1	1.00	0.02	37,37,37,37	0
2	NI	F	302	1/1	1.00	0.04	32,32,32,32	0
2	NI	B	302	1/1	1.00	0.03	34,34,34,34	0
2	NI	K	301	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.