W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2024 – 09:02 AM EDT

PDB ID	:	5K4L
Title	:	Crystal structure of KDM5A in complex with a naphthyridone inhibitor
Authors	:	Kiefer, J.R.; Vinogradova, M.V.
Deposited on	:	2016-05-20
Resolution	:	3.18 Å(reported)

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

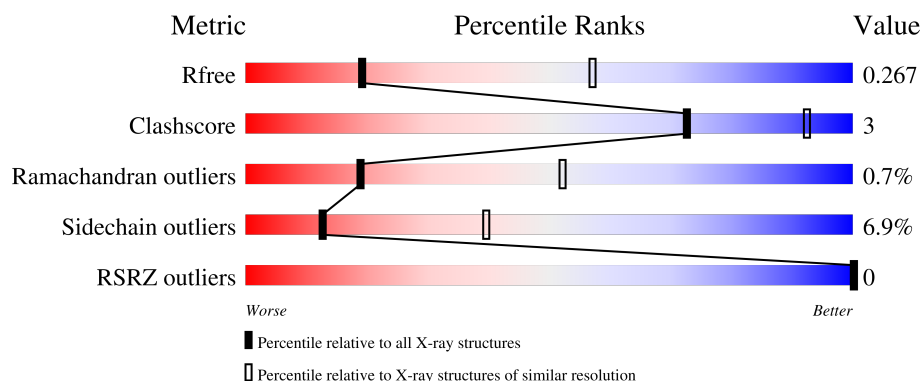|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.18 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		3
Ramachandran outliers		0.7%
Sidechain outliers		6.9%
RSRZ outliers		0

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1851 (3.20-3.16)
Clashscore	180529	1999 (3.20-3.16)
Ramachandran outliers	177936	1961 (3.20-3.16)
Sidechain outliers	177891	1960 (3.20-3.16)
RSRZ outliers	164620	1852 (3.20-3.16)

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 <=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	790	63% 9% 27%
1	B	790	64% 8% • 27%
2	F	10	90% 10%
2	G	10	70% 30%

2   Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18192 atoms, of which 8844 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 Lysine-specific demethylase 5A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	577	Total	C	H	N	O	S	0	0	0
			8998	2952	4407	755	846	38			
1	B	577	Total	C	H	N	O	S	0	0	0
			9012	2955	4415	758	846	38			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	SER	-	expression tag	UNP P29375
A	798	GLY	-	expression tag	UNP P29375
A	799	ASN	-	expression tag	UNP P29375
A	800	SER	-	expression tag	UNP P29375
B	11	SER	-	expression tag	UNP P29375
B	798	GLY	-	expression tag	UNP P29375
B	799	ASN	-	expression tag	UNP P29375
B	800	SER	-	expression tag	UNP P29375

- Molecule 2 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			50	30	10	10			
2	G	10	Total	C	N	O	0	0	0
			50	30	10	10			

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ni	0	0
			1	1		
3	B	1	Total	Ni	0	0
			1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total Zn 2 2		0	0
4	B	2	Total Zn 2 2		0	0

- Molecule 5 is {N}-ethyl-4-oxidanyl-2-oxidanylidene-1 {H}-1,7-naphthyridine-3-carboxamide (three-letter code: 6QN) (formula: $C_{11}H_{11}N_3O_3$).
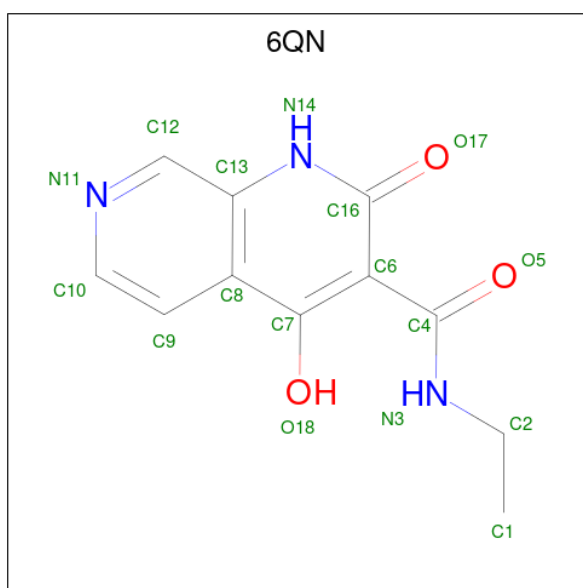
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
5	A	1	28	11	11	3	3	0	0
			Total	C	H	N	O		
5	B	1	28	11	11	3	3	0	0

- Molecule 6 is water.

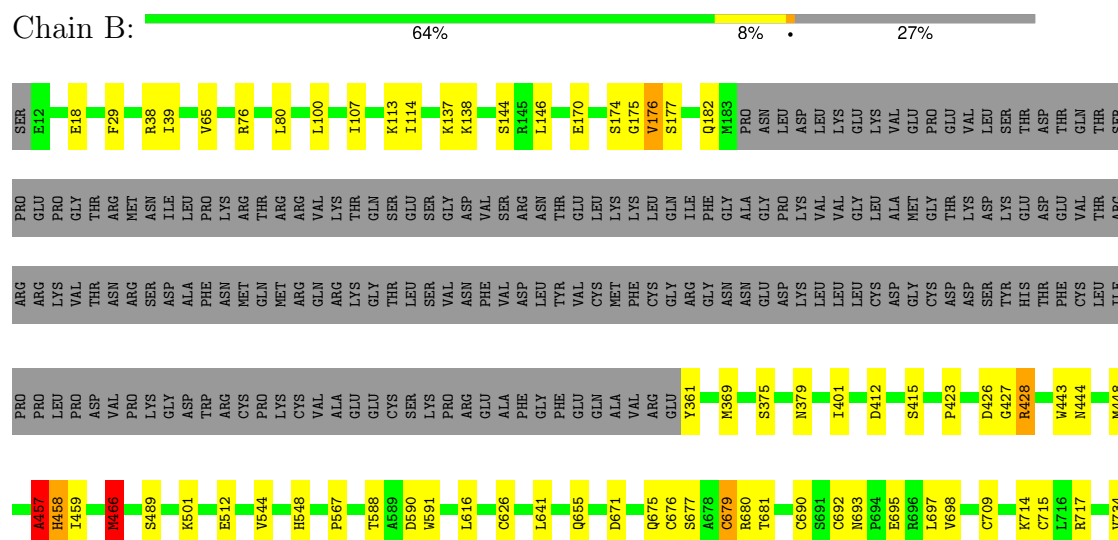| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total O 7 7		0	0
6	B	13	Total O 13 13		0	0

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: Lysine-specific demethylase 5A
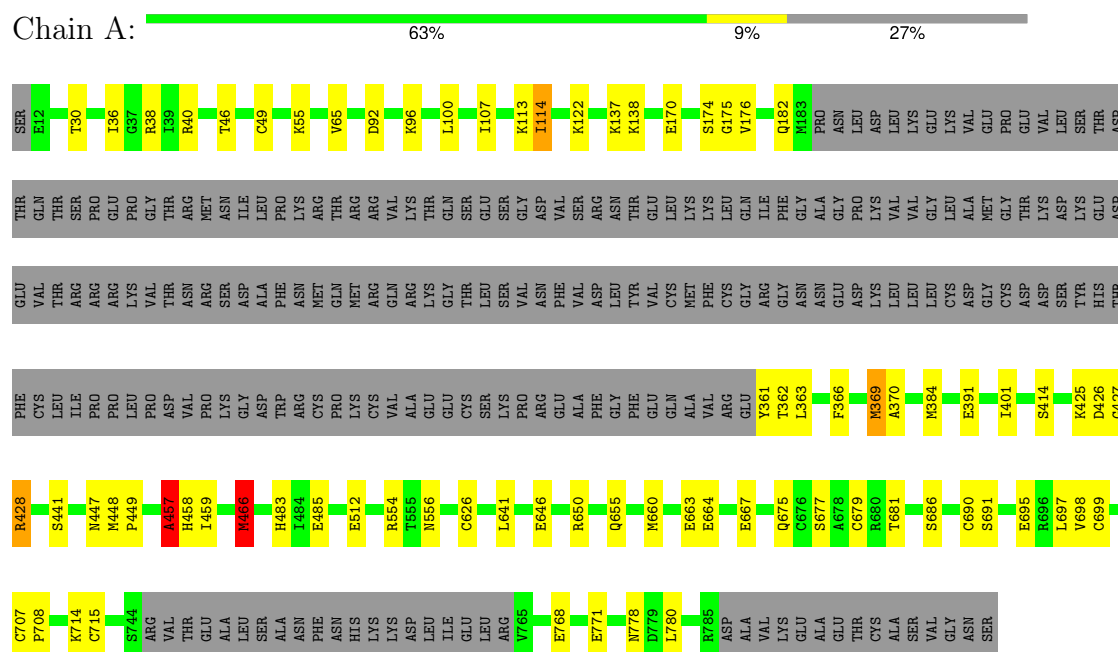
Chain A:

- Molecule 1: Lysine-specific demethylase 5A

Chain B:

S738 S744 ARG VAL THR GLU ALA LEU SER ALA ASN PHE ASN HIS LYS LYS ASP LEU ILE GLU LEU ARG V765 N778 D779 L780 R785 ASP ALA VAL LYS GLU ALA GLU THR CYS ALA SER VAL GLY ASN SER

• Molecule 2: Unknown Peptide

Chain F:

90%   10%

X219 X223 X228

• Molecule 2: Unknown Peptide

Chain G:

70%   30%

X219 X220 X221 X224 X227 X228
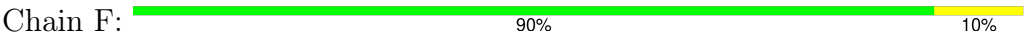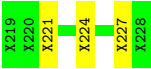
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	159.14Å 159.14Å 92.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.50 – 3.18 34.50 – 3.18	Depositor EDS
% Data completeness (in resolution range)	92.9 (34.50-3.18) 88.9 (34.50-3.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.222 , 0.257 0.232 , 0.267	Depositor DCC
R_{free} test set	1969 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	64.8	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.7	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.068 for -h,-k,l 0.429 for h,-h-k,-l 0.075 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for k,h,-l	Depositor
Outliers	0 of 40747 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18192	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 6QN, ZN, NI

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	0.25	0/4719	0.47	0/6415
1	B	0.25	0/4725	0.47	0/6422
All	All	0.25	0/9444	0.47	0/12837

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	A	0	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	425	LYS	Peptide
1	A	457	ALA	Peptide
1	A	466	MET	Peptide
1	A	778	ASN	Peptide
1	B	457	ALA	Peptide
1	B	466	MET	Peptide
1	B	778	ASN	Peptide

5.2 Too-close contacts (i)

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	4591	4407	4391	30	0
1	B	4597	4415	4401	26	0
2	F	50	0	13	1	0
2	G	50	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	17	11	0	2	0
5	B	17	11	0	0	0
6	A	7	0	0	0	0
6	B	13	0	0	0	0
All	All	9348	8844	8817	57	0

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 (57) 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:B:457:ALA:O	1:B:459:ILE:N	2.16	0.78
1:A:457:ALA:O	1:A:459:ILE:N	2.23	0.70
1:A:426:ASP:O	1:A:428:ARG:N	2.29	0.66
1:B:170:GLU:O	1:B:174:SER:N	2.28	0.64
1:B:426:ASP:O	1:B:428:ARG:N	2.30	0.64
1:A:677:SER:N	1:A:697:LEU:O	2.34	0.60
1:A:483:HIS:CD2	1:A:485:GLU:OE2	2.56	0.59
1:A:714:LYS:CB	1:A:715:CYS:HA	2.31	0.58
1:A:714:LYS:CB	1:A:715:CYS:CA	2.82	0.57
1:B:714:LYS:CB	1:B:715:CYS:HA	2.34	0.56
1:B:677:SER:N	1:B:697:LEU:O	2.39	0.55
1:A:664:GLU:HG3	2:G:227:UNK:HA	1.87	0.55
1:B:714:LYS:CB	1:B:715:CYS:CA	2.83	0.55
1:A:426:ASP:N	1:A:426:ASP:OD1	2.40	0.55
1:A:646:GLU:OE2	1:A:686:SER:OG	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ASP:N	1:B:426:ASP:OD1	2.42	0.52
1:A:690:CYS:SG	1:A:691:SER:N	2.83	0.51
1:A:92:ASP:OD2	1:A:96:LYS:NZ	2.36	0.51
1:B:679:CYS:HB3	1:B:681:THR:N	2.26	0.49
1:A:391:GLU:OE2	1:A:554:ARG:NH1	2.47	0.48
1:B:679:CYS:CB	1:B:680:ARG:HA	2.44	0.48
1:B:466:MET:SD	1:B:466:MET:N	2.85	0.48
1:B:544:VAL:O	1:B:548:HIS:ND1	2.44	0.47
1:B:717:ARG:NH1	2:F:223:UNK:O	2.47	0.47
1:A:466:MET:SD	1:A:466:MET:N	2.87	0.46
1:A:170:GLU:O	1:A:174:SER:N	2.42	0.46
1:B:734:VAL:O	1:B:738:SER:N	2.49	0.46
1:A:554:ARG:NH2	1:A:556:ASN:OD1	2.49	0.46
1:B:489:SER:O	1:B:567:PRO:HA	2.16	0.46
1:A:362:THR:O	1:A:366:PHE:N	2.48	0.46
1:B:679:CYS:HB3	1:B:680:ARG:CA	2.45	0.46
1:B:489:SER:HA	1:B:591:TRP:CD1	2.52	0.44
1:A:667:GLU:OE1	1:A:667:GLU:N	2.43	0.44
1:A:441:SER:O	1:A:447:ASN:ND2	2.50	0.44
1:A:707:CYS:SG	1:A:708:PRO:HD2	2.58	0.44
1:A:448:MET:HB2	1:A:449:PRO:HD3	1.98	0.44
1:A:646:GLU:O	1:A:650:ARG:N	2.51	0.44
1:B:29:PHE:O	1:B:443:TRP:NE1	2.40	0.43
1:A:768:GLU:O	1:A:771:GLU:N	2.51	0.43
1:B:174:SER:OG	1:B:175:GLY:N	2.52	0.43
1:A:114:ILE:HD13	1:A:114:ILE:H	1.83	0.42
1:A:483:HIS:CE1	5:A:904:6QN:C12	3.02	0.42
1:B:176:VAL:HG13	1:B:177:SER:N	2.34	0.42
1:A:174:SER:OG	1:A:175:GLY:N	2.51	0.42
1:B:423:PRO:O	1:B:444:ASN:ND2	2.53	0.42
1:B:692:CYS:SG	1:B:709:CYS:HB2	2.59	0.42
1:B:76:ARG:O	1:B:80:LEU:N	2.53	0.42
1:B:588:THR:OG1	1:B:590:ASP:OD1	2.29	0.41
1:B:375:SER:O	1:B:379:ASN:N	2.51	0.41
1:A:36:ILE:O	1:A:40:ARG:N	2.52	0.41
1:A:483:HIS:CE1	5:A:904:6QN:N11	2.88	0.41
1:B:176:VAL:HG13	1:B:177:SER:H	1.85	0.41
1:B:176:VAL:HG22	1:B:177:SER:H	1.86	0.41
1:A:660:MET:HB2	1:A:714:LYS:CB	2.51	0.40
1:A:679:CYS:HB3	1:A:681:THR:N	2.36	0.40
1:A:369:MET:HG3	1:A:370:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:221:UNK:O	2:G:224:UNK:N	2.54	0.40

There are no symmetry-related clashes.

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	571/790 (72%)	527 (92%)	40 (7%)	4 (1%)	19	52
1	B	571/790 (72%)	523 (92%)	44 (8%)	4 (1%)	19	52
All	All	1142/1580 (72%)	1050 (92%)	84 (7%)	8 (1%)	19	52

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	HIS
1	B	458	HIS
1	A	427	GLY
1	B	427	GLY
1	A	457	ALA
1	B	457	ALA
1	A	176	VAL
1	B	176	VAL

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	498/710 (70%)	466 (94%)	32 (6%)	14	42
1	B	499/710 (70%)	462 (93%)	37 (7%)	11	37
All	All	997/1420 (70%)	928 (93%)	69 (7%)	13	39

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	38	ARG
1	A	46	THR
1	A	49	CYS
1	A	55	LYS
1	A	65	VAL
1	A	100	LEU
1	A	107	ILE
1	A	113	LYS
1	A	114	ILE
1	A	122	LYS
1	A	137	LYS
1	A	138	LYS
1	A	182	GLN
1	A	361	TYR
1	A	363	LEU
1	A	369	MET
1	A	384	MET
1	A	401	ILE
1	A	414	SER
1	A	428	ARG
1	A	466	MET
1	A	512	GLU
1	A	626	CYS
1	A	641	LEU
1	A	655	GLN
1	A	663	GLU
1	A	675	GLN
1	A	695	GLU
1	A	698	VAL
1	A	699	CYS
1	A	780	LEU
1	B	18	GLU
1	B	38	ARG
1	B	39	ILE

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Mol	Chain	Res	Type
1	B	65	VAL
1	B	100	LEU
1	B	107	ILE
1	B	113	LYS
1	B	114	ILE
1	B	137	LYS
1	B	138	LYS
1	B	144	SER
1	B	146	LEU
1	B	182	GLN
1	B	361	TYR
1	B	369	MET
1	B	401	ILE
1	B	412	ASP
1	B	415	SER
1	B	428	ARG
1	B	448	MET
1	B	458	HIS
1	B	466	MET
1	B	501	LYS
1	B	512	GLU
1	B	616	LEU
1	B	626	CYS
1	B	641	LEU
1	B	655	GLN
1	B	671	ASP
1	B	675	GLN
1	B	676	CYS
1	B	679	CYS
1	B	690	CYS
1	B	693	ASN
1	B	695	GLU
1	B	698	VAL
1	B	780	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	493	ASN
1	B	556	ASN
1	B	613	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	#$|Z| > 2$
5	6QN	B	904	3	18,18,18	0.24	0	23,25,25	0.84	1 (4%)
5	6QN	A	904	3	18,18,18	0.19	0	23,25,25	0.84	1 (4%)

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
5	6QN	B	904	3	-	0/7/7/7	0/2/2/2
5	6QN	A	904	3	-	0/7/7/7	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	904	6QN	C12-C13-N14	2.64	124.37	120.20
5	B	904	6QN	C12-C13-N14	2.34	123.90	120.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	904	6QN	2	0

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	577/790 (73%)	-1.37	0	100	100	48, 123, 180, 221	0
1	B	577/790 (73%)	-1.46	0	100	100	40, 103, 175, 212	0
2	F	0/10	-		-		-	-
2	G	0/10	-		-		-	-
All	All	1154/1600 (72%)	-1.41	0	100	100	40, 114, 178, 221	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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
3	NI	A	901	1/1	1.00	0.01	66,66,66,66	0
3	NI	B	901	1/1	1.00	0.01	78,78,78,78	0
4	ZN	A	902	1/1	1.00	0.02	192,192,192,192	0
4	ZN	A	903	1/1	1.00	0.01	64,64,64,64	0
4	ZN	B	902	1/1	1.00	0.01	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ZN	B	903	1/1	1.00	0.02	202,202,202,202	0
5	6QN	A	904	17/17	1.00	0.04	53,108,132,143	0
5	6QN	B	904	17/17	1.00	0.03	48,87,107,108	0

6.5 Other polymers (i)

There are no such residues in this entry.