



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 09:23 AM EDT

PDB ID : 2OWM
Title : Motor domain of Neurospora crassa kinesin-3 (NcKin3)
Authors : Marx, A.; Muller, J.; Mandelkow, E.-M.; Woehlke, G.; Mandelkow, E.
Deposited on : unknown
Resolution : 3.25 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

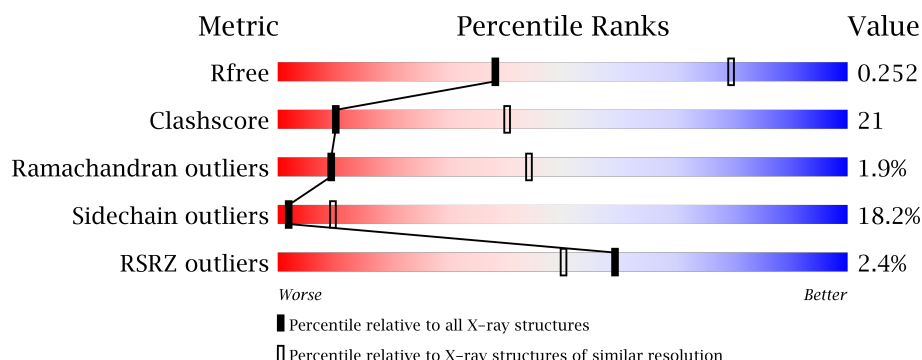
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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. 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	443	<div> <div>44%</div> <div>23%</div> <div>6%</div> <div>26%</div> </div>
1	B	443	<div> <div>45%</div> <div>22%</div> <div>7%</div> <div>26%</div> </div>
1	C	443	<div> <div>43%</div> <div>24%</div> <div>7%</div> <div>26%</div> </div>
1	D	443	<div> <div>45%</div> <div>21%</div> <div>6%</div> <div>27%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10338 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 Related to KINESIN-LIKE PROTEIN KIF1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2560	1609	445	495	11			
1	B	327	Total	C	N	O	S	0	0	0
			2561	1609	449	492	11			
1	C	328	Total	C	N	O	S	0	0	0
			2560	1609	445	495	11			
1	D	325	Total	C	N	O	S	0	0	0
			2545	1600	444	490	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	GLU	LYS	CONFLICT	UNP Q9C2M3
A	83	ASP	ASN	CONFLICT	UNP Q9C2M3
A	252	GLY	ARG	CONFLICT	UNP Q9C2M3
B	59	GLU	LYS	CONFLICT	UNP Q9C2M3
B	83	ASP	ASN	CONFLICT	UNP Q9C2M3
B	252	GLY	ARG	CONFLICT	UNP Q9C2M3
C	59	GLU	LYS	CONFLICT	UNP Q9C2M3
C	83	ASP	ASN	CONFLICT	UNP Q9C2M3
C	252	GLY	ARG	CONFLICT	UNP Q9C2M3
D	59	GLU	LYS	CONFLICT	UNP Q9C2M3
D	83	ASP	ASN	CONFLICT	UNP Q9C2M3
D	252	GLY	ARG	CONFLICT	UNP Q9C2M3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

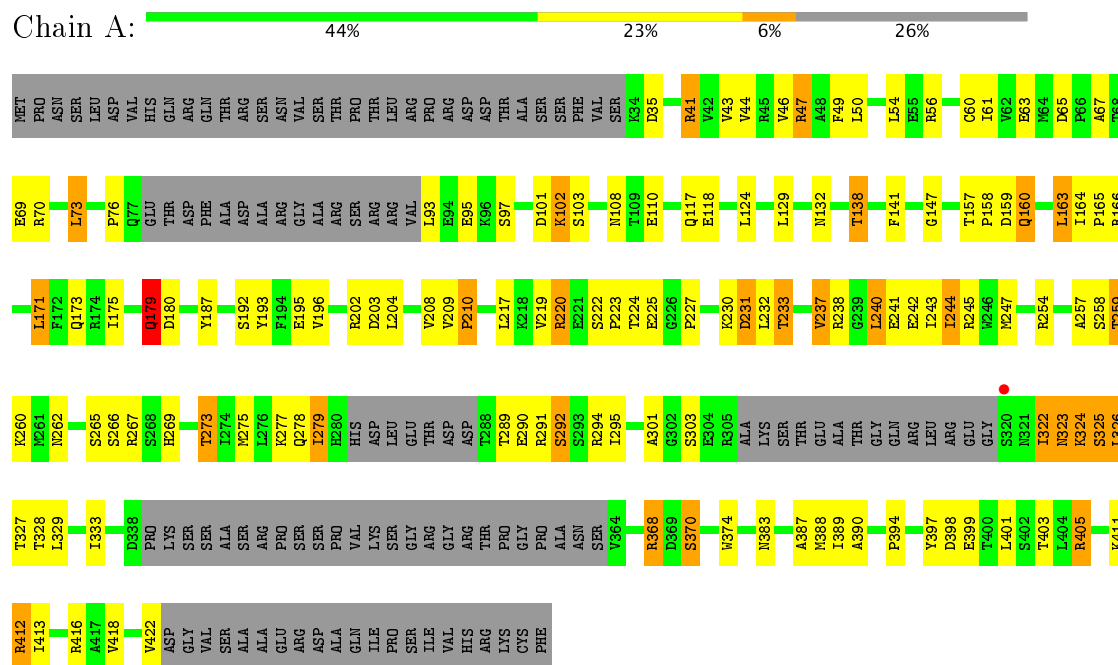
-
- The diagram illustrates the chemical structure of Adenosine Diphosphate (ADP). It consists of three main components: an adenine base, a ribose sugar, and two phosphate groups. The adenine base is a purine ring system with atoms labeled N1, N3, N7, and N9. The ribose sugar is a five-membered ring with carbons labeled C2, C4, C5, C6, and C8. The two phosphate groups are linked by a pyrophosphate bridge, with phosphorus atoms labeled P(4S) and P(5S). The terminal phosphate group is further labeled with oxygen atoms O1A, O1B, O2B, O3B, O4A, O4B, O5A, and O5B. The structure is shown in a 3D representation with wedges and dashes indicating stereochemistry.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0

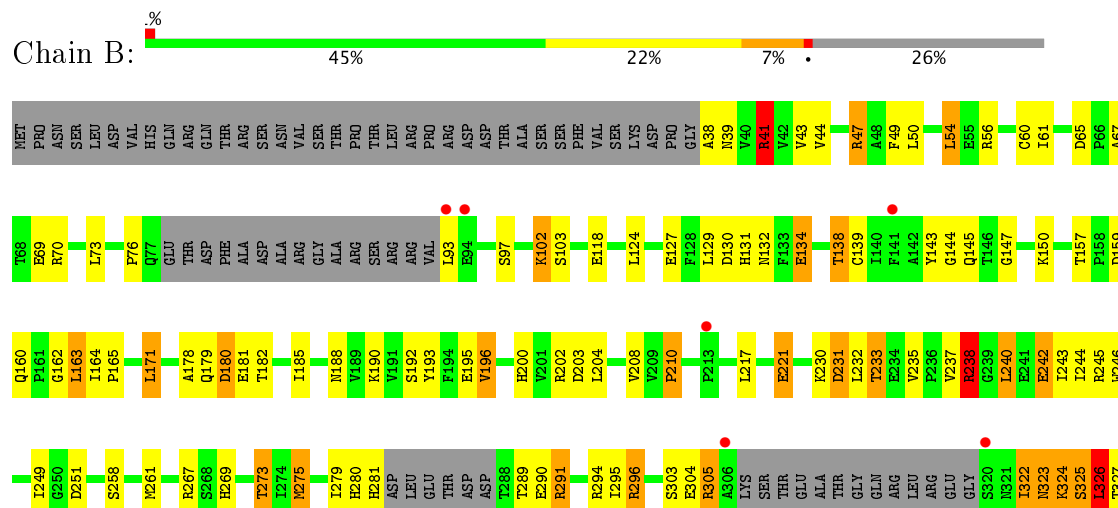
3 Residue-property plots

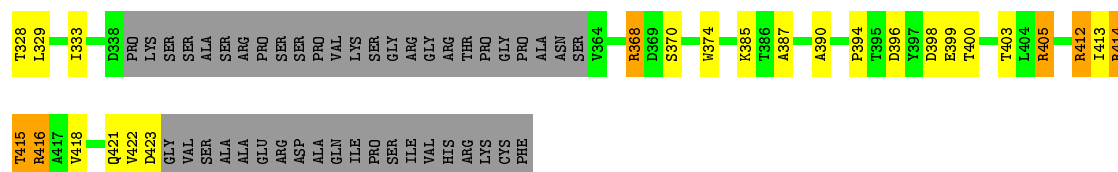
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Related to KINESIN-LIKE PROTEIN KIF1C

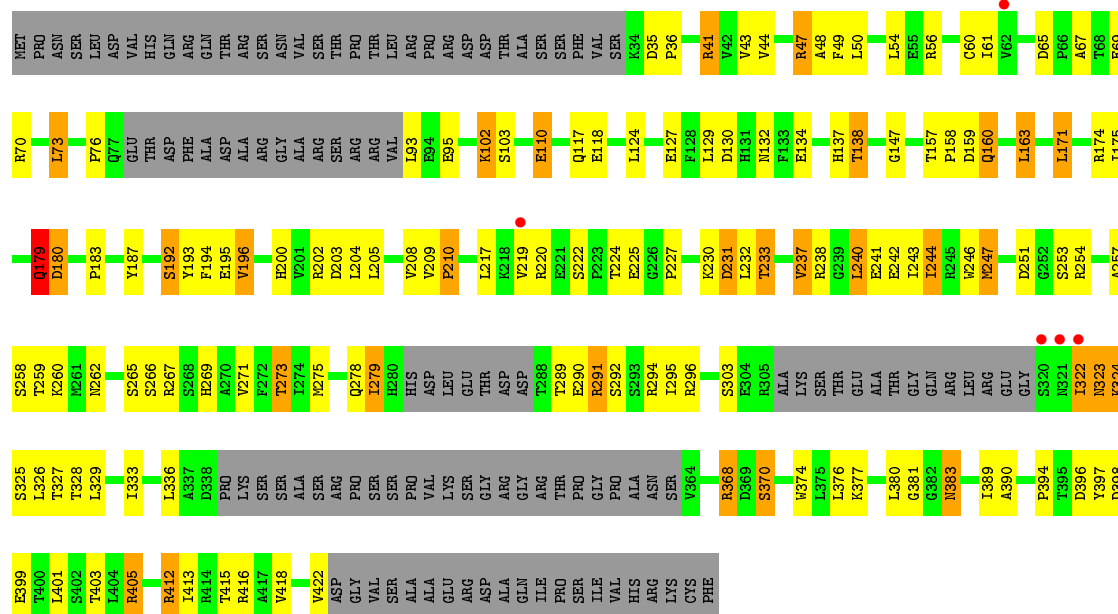
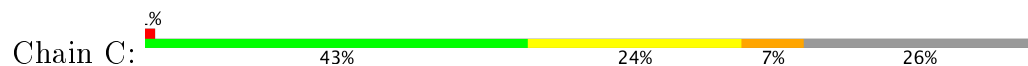


• Molecule 1: Related to KINESIN-LIKE PROTEIN KIF1C

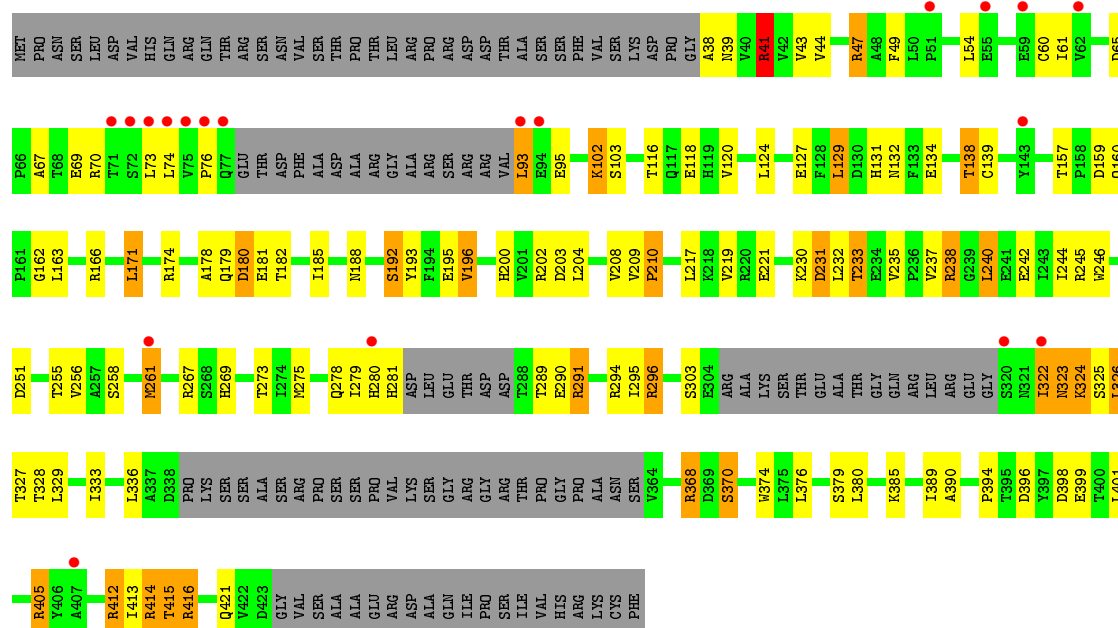
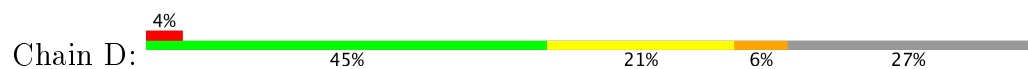




• Molecule 1: Related to KINESIN-LIKE PROTEIN KIF1C



• Molecule 1: Related to KINESIN-LIKE PROTEIN KIF1C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.94Å 98.41Å 111.76Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	111.80 – 3.25 111.71 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (111.80-3.25) 100.0 (111.71-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 3.26Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0005	Depositor
R, R_{free}	0.210 , 0.256 0.209 , 0.252	Depositor DCC
R_{free} test set	1329 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	10338	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: MG, ADP

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	0.92	0/2610	0.94	3/3546 (0.1%)
1	B	0.88	1/2611 (0.0%)	0.93	4/3546 (0.1%)
1	C	0.86	0/2610	0.92	2/3546 (0.1%)
1	D	0.78	1/2595 (0.0%)	0.87	3/3525 (0.1%)
All	All	0.86	2/10426 (0.0%)	0.92	12/14163 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	134	GLU	CG-CD	5.84	1.60	1.51
1	B	134	GLU	CG-CD	5.43	1.60	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	ARG	NE-CZ-NH1	-8.83	115.89	120.30
1	A	166	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	D	41	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	41	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	254	ARG	NE-CZ-NH1	-6.07	117.26	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2560	0	2475	115	1
1	B	2561	0	2482	116	0
1	C	2560	0	2475	117	0
1	D	2545	0	2464	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	1	0
3	C	27	0	12	1	0
3	D	27	0	12	0	0
All	All	10338	0	9944	426	1

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 21.

The worst 5 of 426 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:157:THR:HG23	1:A:158:PRO:HD2	1.32	1.10
1:B:305:ARG:HG3	1:B:305:ARG:HH11	1.02	1.07
1:B:412:ARG:HH11	1:B:412:ARG:HG2	1.17	1.05
1:A:132:ASN:HD21	1:A:138:THR:HB	1.22	1.04
1:C:157:THR:HG23	1:C:158:PRO:HD2	1.39	1.04

All (1) 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:A:63:GLU:OE2	1:A:220:ARG:NH1[2_646]	1.97	0.23

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	318/443 (72%)	286 (90%)	26 (8%)	6 (2%)	9	44
1	B	317/443 (72%)	282 (89%)	29 (9%)	6 (2%)	9	44
1	C	318/443 (72%)	288 (91%)	24 (8%)	6 (2%)	9	44
1	D	315/443 (71%)	284 (90%)	25 (8%)	6 (2%)	9	44
All	All	1268/1772 (72%)	1140 (90%)	104 (8%)	24 (2%)	9	44

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ALA
1	A	210	PRO
1	A	324	LYS
1	B	304	GLU
1	B	324	LYS

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	278/389 (72%)	225 (81%)	53 (19%)	2	8
1	B	278/389 (72%)	229 (82%)	49 (18%)	2	10
1	C	278/389 (72%)	227 (82%)	51 (18%)	2	9
1	D	277/389 (71%)	228 (82%)	49 (18%)	2	10
All	All	1111/1556 (71%)	909 (82%)	202 (18%)	2	10

5 of 202 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	326	LEU
1	C	129	LEU
1	D	289	THR

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Mol	Chain	Res	Type
1	B	368	ARG
1	C	35	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	280	HIS
1	C	160	GLN
1	D	173	GLN
1	B	173	GLN
1	C	179	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	ADP	A	1002	-	25,29,29	1.13	3 (12%)	24,45,45	1.79	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	B	1002	2	25,29,29	1.07	2 (8%)	24,45,45	1.85	4 (16%)
3	ADP	C	1002	2	25,29,29	1.10	2 (8%)	24,45,45	2.07	4 (16%)
3	ADP	D	1002	2	25,29,29	1.23	2 (8%)	24,45,45	1.75	3 (12%)

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
3	ADP	A	1002	-	-	0/12/32/32	0/3/3/3
3	ADP	B	1002	2	-	0/12/32/32	0/3/3/3
3	ADP	C	1002	2	-	0/12/32/32	0/3/3/3
3	ADP	D	1002	2	-	0/12/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	ADP	C5-N7	-2.31	1.31	1.39
3	A	1002	ADP	C2-N3	2.28	1.36	1.32
3	A	1002	ADP	C5-C4	2.38	1.45	1.40
3	B	1002	ADP	C5-C4	2.42	1.46	1.40
3	C	1002	ADP	C5-C4	2.60	1.46	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1002	ADP	N3-C2-N1	-7.18	122.61	128.86
3	D	1002	ADP	N3-C2-N1	-6.20	123.45	128.86
3	B	1002	ADP	N3-C2-N1	-6.12	123.53	128.86
3	A	1002	ADP	N3-C2-N1	-5.29	124.25	128.86
3	A	1002	ADP	C5-C6-N6	-3.20	113.94	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	ADP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1002	ADP	1	0
3	C	1002	ADP	1	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	328/443 (74%)	0.14	1 (0%) 93 92	70, 76, 79, 83	0
1	B	327/443 (73%)	0.21	6 (1%) 69 60	68, 76, 79, 90	0
1	C	328/443 (74%)	0.29	5 (1%) 74 65	70, 76, 79, 83	0
1	D	325/443 (73%)	0.40	19 (5%) 24 18	67, 76, 79, 82	0
All	All	1308/1772 (73%)	0.26	31 (2%) 59 50	67, 76, 79, 90	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	320	SER	8.9
1	A	320	SER	5.5
1	D	320	SER	5.3
1	B	306	ALA	4.1
1	D	77	GLN	4.0

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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	ADP	A	1002	27/27	0.95	0.24	0.13	72,75,77,77	0
3	ADP	C	1002	27/27	0.94	0.23	-0.09	72,75,77,77	0
3	ADP	D	1002	27/27	0.94	0.22	-0.19	72,75,76,77	0
3	ADP	B	1002	27/27	0.96	0.20	-0.81	72,75,77,77	0
2	MG	A	1001	1/1	0.95	0.40	-	61,61,61,61	0
2	MG	D	1001	1/1	0.88	0.26	-	61,61,61,61	0
2	MG	C	1001	1/1	0.82	0.35	-	60,60,60,60	0
2	MG	B	1001	1/1	0.92	0.23	-	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.