



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 24, 2017 – 08:26 PM EDT

PDB ID : 5JM5  
Title : Crystal structure of AKR1C3 complexed with a pro-drug  
Authors : Wang, C.; Wang, C.; Li, Q.; Wang, Z.; Xie, W.  
Deposited on : 2016-04-28  
Resolution : 1.99 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](mailto: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.

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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-20029077  
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-20029077

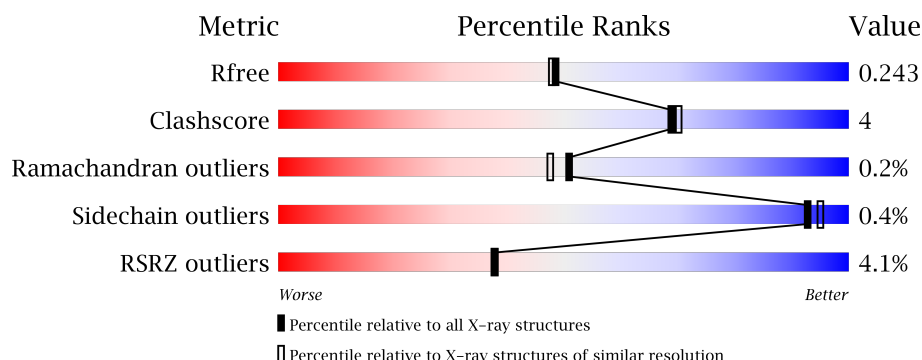
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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  $\geq 3$ , 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	332	<div> <div>3%</div> <div>89%</div> <div>6%</div> <div>•</div> </div>
1	B	332	<div> <div>5%</div> <div>84%</div> <div>10%</div> <div>• 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	6LG	B	403	-	-	-	X
4	6NY	A	403	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5749 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.

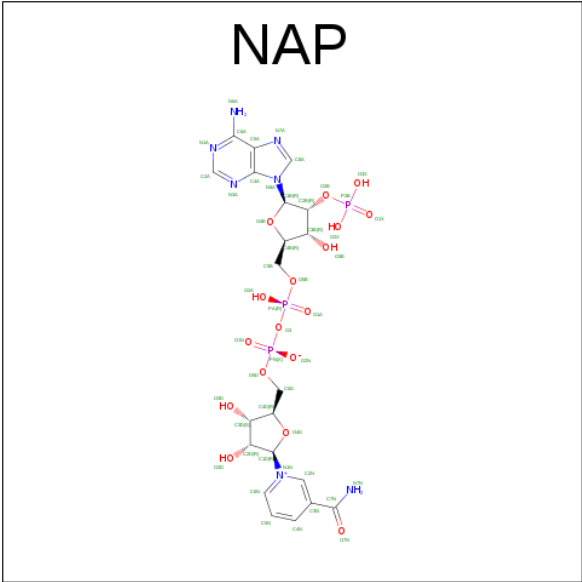
- Molecule 1 is a protein called Aldo-keto reductase family 1 member C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	S	0	0	0
			2519	1605	441	461	12			
1	B	312	Total	C	N	O	S	0	0	0
			2483	1583	436	452	12			

There are 20 discrepancies between the modelled and reference sequences:

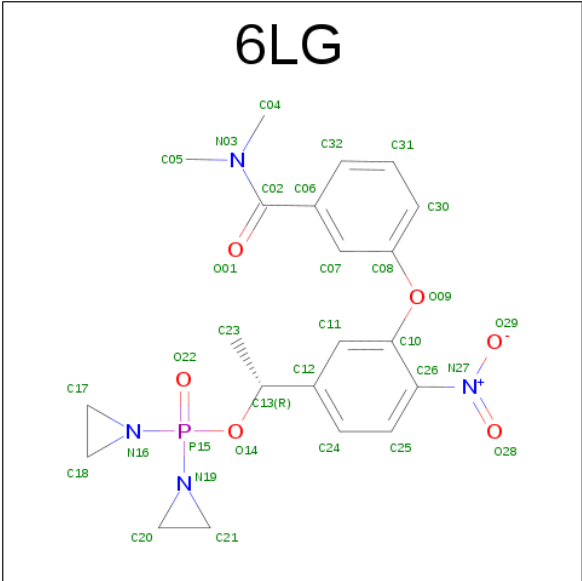
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLN	HIS	engineered mutation	UNP P42330
A	324	TYR	-	expression tag	UNP P42330
A	325	LEU	-	expression tag	UNP P42330
A	326	GLU	-	expression tag	UNP P42330
A	327	HIS	-	expression tag	UNP P42330
A	328	HIS	-	expression tag	UNP P42330
A	329	HIS	-	expression tag	UNP P42330
A	330	HIS	-	expression tag	UNP P42330
A	331	HIS	-	expression tag	UNP P42330
A	332	HIS	-	expression tag	UNP P42330
B	5	GLN	HIS	engineered mutation	UNP P42330
B	324	TYR	-	expression tag	UNP P42330
B	325	LEU	-	expression tag	UNP P42330
B	326	GLU	-	expression tag	UNP P42330
B	327	HIS	-	expression tag	UNP P42330
B	328	HIS	-	expression tag	UNP P42330
B	329	HIS	-	expression tag	UNP P42330
B	330	HIS	-	expression tag	UNP P42330
B	331	HIS	-	expression tag	UNP P42330
B	332	HIS	-	expression tag	UNP P42330

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (1R)-1-{3-[3-(dimethylcarbamoyl)phenoxy]-4-nitrophenyl}ethyl bis[(aziridin-1-yl)]phosphate (three-letter code: 6LG) (formula: C<sub>21</sub>H<sub>25</sub>N<sub>4</sub>O<sub>6</sub>P).



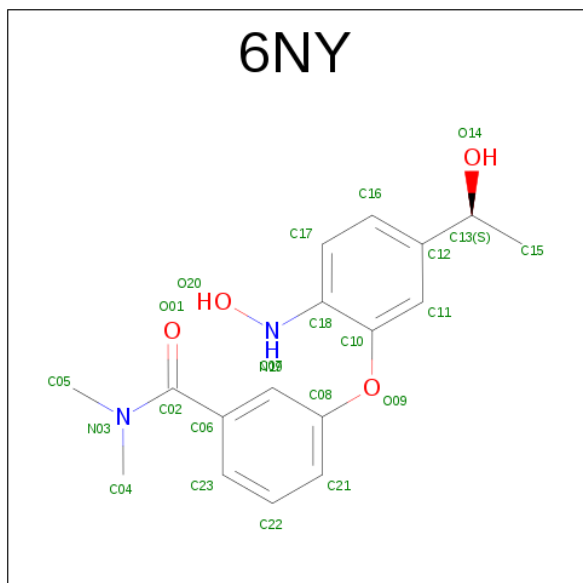
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	21	4	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			32	21	4	6	1		
3	B	1	Total	C	N	O	P	0	0
			32	21	4	6	1		

- Molecule 4 is 3-{2-(hydroxyamino)-5-[(1S)-1-hydroxyethyl]phenoxy}-N,N-dimethylbenzamide (three-letter code: 6NY) (formula: C<sub>17</sub>H<sub>20</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	17	2	4		

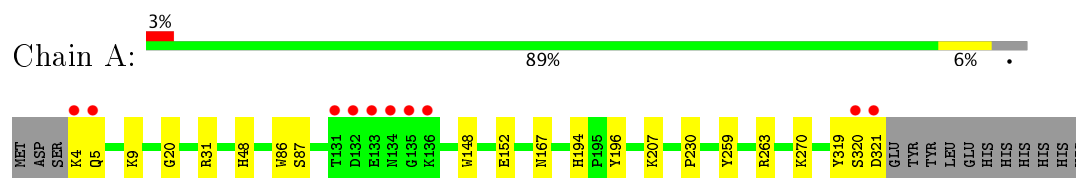
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	277	Total	O	0	0
			277	277		
5	B	255	Total	O	0	0
			255	255		

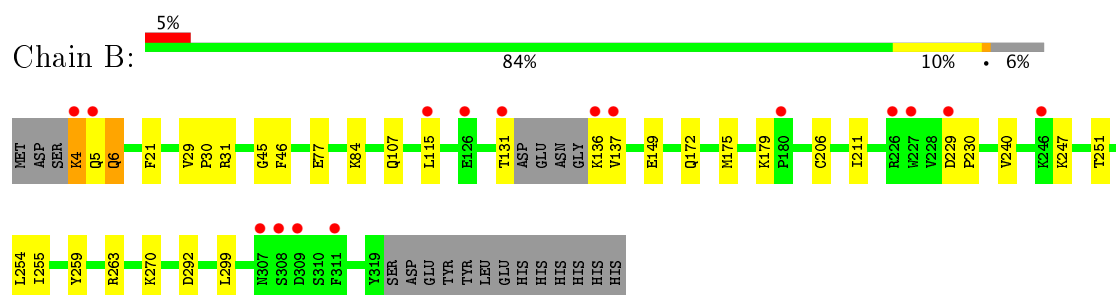
### 3 Residue-property plots [i](#)

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: Aldo-keto reductase family 1 member C3



- Molecule 1: Aldo-keto reductase family 1 member C3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.77Å 106.42Å 74.94Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	25.32 – 1.99 25.32 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.32-1.99) 94.3 (25.32-1.99)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.195 , 0.245 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	2411 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.5	Xtriage
Anisotropy	0.914	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAP, 6LG, 6NY

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	0.36	0/2577	0.51	0/3493
1	B	0.36	0/2539	0.53	0/3437
All	All	0.36	0/5116	0.52	0/6930

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	4	LYS	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	2519	0	2498	17	0
1	B	2483	0	2475	22	0
2	A	48	0	23	6	0
2	B	48	0	23	4	0
3	A	32	0	0	0	0
3	B	64	0	0	0	0
4	A	23	0	0	0	0
5	A	277	0	0	6	1
5	B	255	0	0	1	1
All	All	5749	0	5019	44	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 4.

All (44) 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:4:LYS:HB2	1:B:5:GLN:HG2	1.70	0.73
1:A:167:ASN:HD21	2:A:401:NAP:H72N	1.34	0.73
1:A:31:ARG:NH2	5:A:502:HOH:O	2.25	0.70
1:B:5:GLN:HG3	1:B:6:GLN:H	1.56	0.69
1:A:270:LYS:O	2:A:401:NAP:H8A	2.00	0.62
2:A:401:NAP:H51N	2:A:401:NAP:H6N	1.81	0.62
1:A:4:LYS:N	5:A:508:HOH:O	2.32	0.62
1:B:149:GLU:HG3	1:B:179:LYS:HE3	1.83	0.59
1:B:270:LYS:O	2:B:401:NAP:H8A	2.02	0.59
2:A:401:NAP:H51N	2:A:401:NAP:C6N	2.34	0.57
1:A:259:TYR:O	1:A:263:ARG:HG3	2.05	0.56
2:B:401:NAP:H6N	2:B:401:NAP:H51N	1.87	0.56
1:B:4:LYS:HE3	1:B:45:GLY:HA3	1.89	0.53
1:A:230:PRO:HG3	1:B:77:GLU:HB2	1.91	0.53
1:A:167:ASN:ND2	2:A:401:NAP:H72N	2.07	0.52
1:B:131:THR:HA	1:B:137:VAL:HA	1.92	0.52
1:B:259:TYR:O	1:B:263:ARG:HG3	2.10	0.52
1:A:4:LYS:N	5:A:515:HOH:O	2.43	0.50
2:B:401:NAP:H3D	2:B:401:NAP:H6N	1.94	0.48
1:B:172:GLN:O	1:B:175:MET:HB3	2.12	0.48
1:B:206:CYS:HB3	1:B:211:ILE:O	2.13	0.48
2:B:401:NAP:C6N	2:B:401:NAP:H51N	2.44	0.47
1:B:31:ARG:HD2	1:B:31:ARG:N	2.28	0.47
1:B:259:TYR:CZ	1:B:263:ARG:HD2	2.50	0.46
1:A:9:LYS:NZ	5:A:504:HOH:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLN:HG2	5:A:707:HOH:O	2.15	0.46
1:B:21:PHE:HB2	1:B:46:PHE:CD2	2.50	0.46
2:A:401:NAP:H3D	2:A:401:NAP:H6N	1.97	0.46
1:A:31:ARG:HA	1:A:31:ARG:HD3	1.61	0.45
1:B:136:LYS:NZ	5:B:508:HOH:O	2.38	0.45
1:B:29:VAL:HA	1:B:30:PRO:HD2	1.83	0.44
1:B:29:VAL:O	1:B:31:ARG:NH1	2.47	0.43
1:A:86:TRP:CG	1:A:87:SER:N	2.86	0.43
1:B:240:VAL:HG21	1:B:299:LEU:HD21	2.01	0.43
1:B:251:THR:O	1:B:255:ILE:HG12	2.19	0.43
1:A:319:TYR:O	1:A:321:ASP:N	2.52	0.42
1:A:20:GLY:HA2	1:A:48:HIS:HB3	2.01	0.42
1:A:148:TRP:O	1:A:152:GLU:HG3	2.21	0.41
1:A:207:LYS:NZ	5:A:507:HOH:O	2.31	0.41
1:B:247:LYS:NZ	1:B:292:ASP:OD1	2.49	0.41
1:B:254:LEU:HA	1:B:254:LEU:HD23	1.96	0.41
1:A:194:HIS:CE1	1:A:196:TYR:HB2	2.56	0.41
1:B:84:LYS:HG2	1:B:115:LEU:HB2	2.02	0.41
1:B:229:ASP:HA	1:B:230:PRO:HD2	1.86	0.40

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)
5:A:732:HOH:O	5:B:686:HOH:O[2_646]	2.15	0.05

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	316/332 (95%)	309 (98%)	6 (2%)	1 (0%)	44 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	308/332 (93%)	304 (99%)	4 (1%)	0	100	100
All	All	624/664 (94%)	613 (98%)	10 (2%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	320	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/296 (93%)	274 (100%)	0	100	100
1	B	270/296 (91%)	268 (99%)	2 (1%)	87	90
All	All	544/592 (92%)	542 (100%)	2 (0%)	93	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	GLN
1	B	107	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands 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	$\# Z  > 2$
2	NAP	A	401	-	44,52,52	4.43	13 (29%)	51,80,80	2.18	10 (19%)
3	6LG	A	402	-	30,35,35	2.36	4 (13%)	42,52,52	3.80	10 (23%)
4	6NY	A	403	-	23,24,24	2.49	5 (21%)	31,33,33	1.30	4 (12%)
2	NAP	B	401	-	44,52,52	4.48	14 (31%)	51,80,80	2.19	8 (15%)
3	6LG	B	402	-	30,35,35	2.37	5 (16%)	42,52,52	3.79	7 (16%)
3	6LG	B	403	-	30,35,35	2.36	5 (16%)	42,52,52	4.08	7 (16%)

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
2	NAP	A	401	-	-	0/27/67/67	0/5/5/5
3	6LG	A	402	-	-	0/31/41/41	0/2/4/4
4	6NY	A	403	-	-	0/16/18/18	0/2/2/2
2	NAP	B	401	-	-	0/27/67/67	0/5/5/5
3	6LG	B	402	-	-	0/31/41/41	0/2/4/4
3	6LG	B	403	-	-	0/31/41/41	0/2/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	C2D-C1D	-14.53	1.30	1.53
2	B	401	NAP	C2D-C1D	-14.41	1.30	1.53
2	B	401	NAP	O4B-C4B	-7.48	1.28	1.45
2	A	401	NAP	O4B-C4B	-7.27	1.28	1.45
2	B	401	NAP	O4D-C4D	-6.73	1.29	1.45
2	A	401	NAP	O4D-C4D	-6.33	1.30	1.45
3	B	403	6LG	O14-C13	-3.89	1.41	1.45
3	A	402	6LG	O14-C13	-3.72	1.41	1.45
2	B	401	NAP	O3D-C3D	-3.28	1.35	1.43
2	A	401	NAP	O3B-C3B	-3.08	1.35	1.43
2	B	401	NAP	O3B-C3B	-3.05	1.35	1.43
2	A	401	NAP	O3D-C3D	-2.81	1.36	1.43
3	B	402	6LG	O14-C13	-2.80	1.42	1.45
3	B	403	6LG	C06-C02	2.02	1.53	1.50
3	B	402	6LG	C06-C02	2.03	1.53	1.50
3	A	402	6LG	P15-O22	2.03	1.49	1.46
2	B	401	NAP	C2A-N1A	2.07	1.37	1.33
2	A	401	NAP	C2A-N1A	2.24	1.38	1.33
2	A	401	NAP	C3N-C7N	2.30	1.54	1.50
2	B	401	NAP	O2B-C2B	2.36	1.53	1.44
2	B	401	NAP	C3N-C7N	2.83	1.54	1.50
2	A	401	NAP	C6A-N6A	3.00	1.46	1.34
3	B	402	6LG	P15-O22	3.01	1.51	1.46
2	B	401	NAP	C6A-N6A	3.18	1.47	1.34
4	A	403	6NY	O09-C08	3.27	1.46	1.39
2	A	401	NAP	C2A-N3A	3.50	1.38	1.32
2	A	401	NAP	O2D-C2D	3.64	1.51	1.43
2	A	401	NAP	C7N-N7N	3.65	1.40	1.33
2	B	401	NAP	O2D-C2D	3.73	1.51	1.43
3	B	403	6LG	P15-O22	3.83	1.52	1.46
2	B	401	NAP	C2A-N3A	3.88	1.38	1.32
4	A	403	6NY	C07-C06	3.96	1.45	1.39
2	B	401	NAP	C7N-N7N	4.16	1.41	1.33
4	A	403	6NY	C22-C21	4.82	1.48	1.38
4	A	403	6NY	C06-C02	6.26	1.59	1.50
3	B	403	6LG	C02-N03	6.46	1.43	1.34
4	A	403	6NY	C02-N03	6.60	1.43	1.34
3	A	402	6LG	C02-N03	7.21	1.44	1.34
3	B	402	6LG	C02-N03	7.51	1.45	1.34
3	B	402	6LG	O28-N27	8.37	1.38	1.22
3	B	403	6LG	O28-N27	8.41	1.38	1.22
3	A	402	6LG	O28-N27	8.93	1.39	1.22
2	B	401	NAP	O4D-C1D	14.79	1.61	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	NAP	O4B-C1B	15.09	1.62	1.41
2	A	401	NAP	O4D-C1D	15.11	1.62	1.41
2	B	401	NAP	O4B-C1B	15.37	1.62	1.41

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAP	N3A-C2A-N1A	-9.89	120.25	128.86
2	B	401	NAP	N3A-C2A-N1A	-9.54	120.55	128.86
2	B	401	NAP	N6A-C6A-N1A	-5.11	108.64	118.77
2	A	401	NAP	N6A-C6A-N1A	-4.90	109.05	118.77
2	B	401	NAP	C1B-N9A-C4A	-4.76	118.42	126.64
2	A	401	NAP	C1B-N9A-C4A	-4.20	119.38	126.64
2	B	401	NAP	O4D-C4D-C5D	-3.77	96.67	109.40
4	A	403	6NY	C07-C06-C02	-3.68	112.22	120.20
2	A	401	NAP	O4D-C4D-C5D	-3.62	97.18	109.40
2	B	401	NAP	C4B-O4B-C1B	-3.62	105.92	109.77
2	A	401	NAP	C4B-O4B-C1B	-3.61	105.93	109.77
3	B	402	6LG	O14-P15-O22	-3.15	106.58	113.94
3	B	403	6LG	C24-C12-C13	-2.91	115.75	120.60
3	A	402	6LG	O22-P15-N16	-2.82	104.62	115.42
3	B	402	6LG	C11-C12-C13	-2.80	117.27	120.36
3	A	402	6LG	C11-C12-C13	-2.40	117.71	120.36
3	A	402	6LG	C10-O09-C08	-2.31	111.94	117.97
3	A	402	6LG	O14-P15-O22	-2.19	108.83	113.94
3	A	402	6LG	O14-C13-C12	-2.05	106.35	109.73
2	A	401	NAP	C4D-O4D-C1D	-2.03	107.60	109.77
4	A	403	6NY	C11-C10-C18	-2.00	118.16	120.44
2	A	401	NAP	O3D-C3D-C4D	2.05	117.09	111.09
2	B	401	NAP	C3B-C2B-C1B	2.12	106.90	102.75
4	A	403	6NY	C05-N03-C04	2.14	122.23	115.73
3	B	403	6LG	C24-C12-C11	2.14	121.29	118.79
2	A	401	NAP	C3B-C2B-C1B	2.34	107.33	102.75
3	B	403	6LG	C11-C12-C13	2.36	122.96	120.36
2	B	401	NAP	C2N-C3N-C4N	2.95	121.63	118.26
4	A	403	6NY	C23-C06-C02	2.96	127.69	120.27
3	B	402	6LG	O14-P15-N16	3.43	120.25	103.25
2	A	401	NAP	C2N-C3N-C4N	3.44	122.18	118.26
3	A	402	6LG	O14-P15-N16	3.52	120.72	103.25
2	A	401	NAP	C5A-C6A-N6A	5.06	130.79	120.47
2	B	401	NAP	C5A-C6A-N6A	5.43	131.54	120.47
3	A	402	6LG	P15-N16-C17	9.79	143.06	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	6LG	P15-N16-C17	10.57	144.91	119.68
3	A	402	6LG	P15-N19-C21	11.27	146.58	119.68
3	B	402	6LG	P15-N19-C21	11.42	146.94	119.68
3	B	402	6LG	P15-N16-C18	12.02	148.39	119.68
3	B	403	6LG	P15-N16-C17	12.06	148.47	119.68
3	A	402	6LG	P15-N16-C18	12.17	148.74	119.68
3	B	402	6LG	P15-N19-C20	12.29	149.01	119.68
3	B	403	6LG	P15-N19-C20	12.38	149.24	119.68
3	B	403	6LG	P15-N19-C21	12.84	150.34	119.68
3	A	402	6LG	P15-N19-C20	13.06	150.87	119.68
3	B	403	6LG	P15-N16-C18	13.48	151.86	119.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NAP	6	0
2	B	401	NAP	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	318/332 (95%)	0.18	10 (3%) 49 49	11, 19, 32, 52	0
1	B	312/332 (93%)	0.34	16 (5%) 29 29	12, 20, 40, 53	0
All	All	630/664 (94%)	0.26	26 (4%) 38 38	11, 19, 36, 53	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	ASP	3.9
1	A	134	ASN	3.5
1	A	320	SER	3.5
1	B	137	VAL	3.5
1	B	5	GLN	3.4
1	A	5	GLN	3.3
1	B	307	ASN	3.3
1	B	227	TRP	3.2
1	A	4	LYS	3.1
1	A	135	GLY	3.0
1	B	308	SER	2.8
1	B	131	THR	2.8
1	A	321	ASP	2.8
1	B	311	PHE	2.8
1	B	136	LYS	2.6
1	A	133	GLU	2.5
1	A	131	THR	2.5
1	B	180	PRO	2.4
1	B	4	LYS	2.4
1	B	115	LEU	2.3
1	B	226	ARG	2.3
1	B	246	LYS	2.3
1	A	132	ASP	2.1
1	B	126	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	136	LYS	2.0
1	B	229	ASP	2.0

## 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	6LG	B	403	32/32	0.79	0.25	4.13	22,34,49,60	0
4	6NY	A	403	23/23	0.87	0.20	2.61	20,27,33,38	0
3	6LG	A	402	32/32	0.84	0.17	1.73	18,29,48,50	0
3	6LG	B	402	32/32	0.76	0.22	1.51	19,33,43,57	0
2	NAP	B	401	48/48	0.94	0.12	0.09	12,17,22,27	0
2	NAP	A	401	48/48	0.95	0.10	-0.72	8,15,21,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.