



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:37 AM UTC

PDB ID : 3BEH / pdb\_00003beh  
Title : Structure of a Bacterial Cyclic Nucleotide Regulated Ion Channel  
Authors : Clayton, G.M.; Morais-Cabral, J.H.  
Deposited on : 2007-11-18  
Resolution : 3.10 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

<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)  
Xtrriage (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

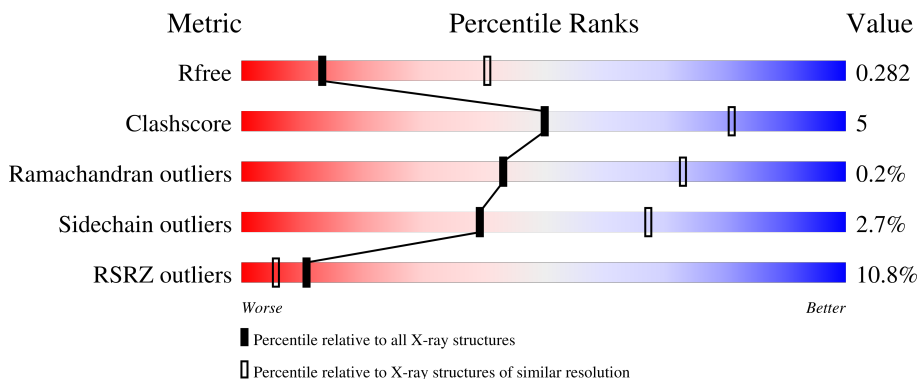
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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  $\geq 3$ , 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	355	 9% 54% 8% 37%
1	B	355	 6% 53% 8% 37%
1	C	355	 5% 55% 8% 36%
1	D	355	 7% 55% 8% 37%

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
2	K	A	360	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6673 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.

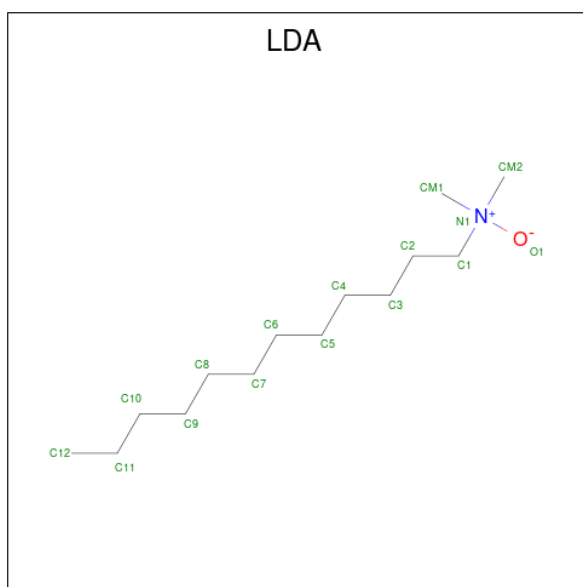
- Molecule 1 is a protein called Mll3241 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	Total 1625	C 1068	N 273	O 279	S 5	0	0	0
1	B	222	Total 1638	C 1075	N 279	O 279	S 5	0	0	0
1	C	226	Total 1663	C 1090	N 283	O 285	S 5	0	0	0
1	D	225	Total 1655	C 1087	N 279	O 284	S 5	0	0	0

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
2	A	4	Total 4	K 4	0	0
2	B	1	Total 1	K 1	0	0

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0

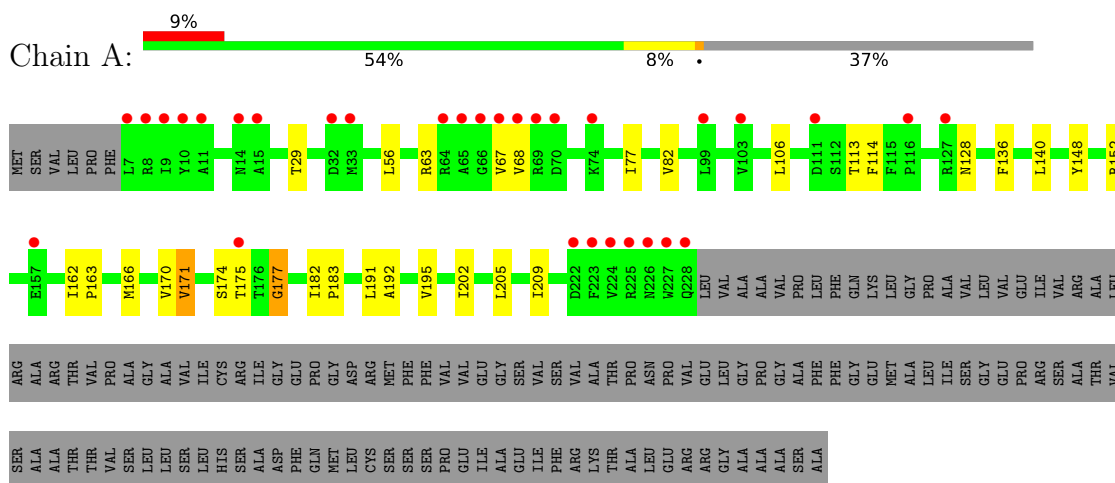
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total 4	O 4	0	0
4	B	4	Total 4	O 4	0	0
4	C	8	Total 8	O 8	0	0
4	D	7	Total 7	O 7	0	0

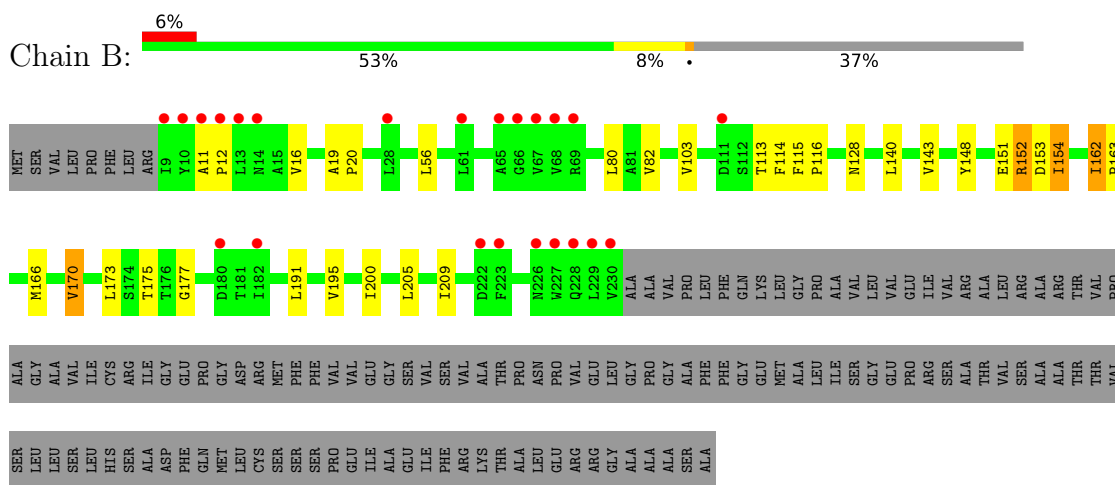
### 3 Residue-property plots [i](#)

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.

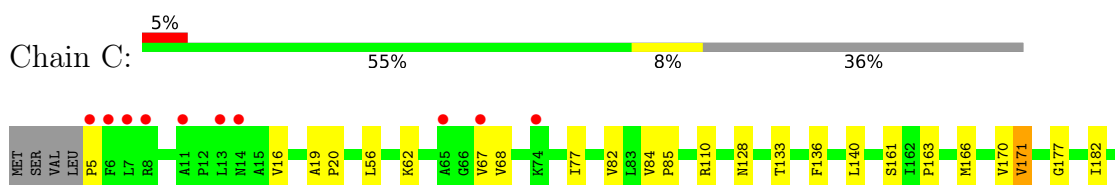
- Molecule 1: Mll3241 protein



- Molecule 1: Mll3241 protein



- Molecule 1: Mll3241 protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	282.73Å 282.73Å 105.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.10 48.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.45-3.10) 99.3 (48.45-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 3.12Å)	Xtrriage
Refinement program	REFMAC refmac_5.2.0019 24/04/2001	Depositor
R, $R_{free}$	0.276 , 0.286 0.273 , 0.282	Depositor DCC
$R_{free}$ test set	1970 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	96.2	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 93.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6673	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: K, LDA

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	0.45	0/1660	0.85	0/2276
1	B	0.44	1/1674 (0.1%)	0.83	0/2290
1	C	0.45	0/1699	0.85	1/2326 (0.0%)
1	D	0.44	0/1691	0.85	1/2316 (0.0%)
All	All	0.44	1/6724 (0.0%)	0.84	2/9208 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	ILE	CA-CB	5.17	1.57	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	PRO	N-CA-CB	6.77	110.45	103.00
1	D	5	PRO	N-CA-CB	6.67	110.33	103.00

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	1625	0	1655	21	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1638	0	1686	18	0
1	C	1663	0	1698	20	0
1	D	1655	0	1694	17	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	31	0	0
3	C	16	0	31	0	0
3	D	32	0	62	0	0
4	A	4	0	0	2	0
4	B	4	0	0	0	0
4	C	8	0	0	2	0
4	D	7	0	0	2	0
All	All	6673	0	6857	72	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 5.

All (72) 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:D:171:VAL:HG11	4:D:364:HOH:O	1.46	1.13
1:C:219:ARG:NH2	4:C:358:HOH:O	1.92	1.00
1:A:171:VAL:HG13	1:A:177:GLY:HA2	1.55	0.88
1:D:56:LEU:HD22	1:D:82:VAL:HG21	1.69	0.75
1:B:140:LEU:HD11	1:B:170:VAL:HG22	1.72	0.70
1:A:56:LEU:HD22	1:A:82:VAL:HG21	1.75	0.67
1:D:155:GLN:NE2	4:D:362:HOH:O	2.27	0.61
1:A:191:LEU:O	1:A:195:VAL:HG23	2.00	0.60
1:C:140:LEU:HD11	1:C:170:VAL:HG22	1.82	0.60
1:A:171:VAL:HG11	4:A:364:HOH:O	2.05	0.56
1:D:11:ALA:HB3	1:D:12:PRO:HD3	1.87	0.56
1:C:56:LEU:HD22	1:C:82:VAL:HG21	1.86	0.56
1:A:140:LEU:HD11	1:A:170:VAL:HG22	1.89	0.55
1:C:171:VAL:HG13	1:C:177:GLY:HA2	1.88	0.55
1:B:12:PRO:HB2	1:B:16:VAL:HG23	1.87	0.55
1:D:171:VAL:CG1	1:D:177:GLY:HA2	2.37	0.55
1:D:171:VAL:HG13	1:D:177:GLY:HA2	1.88	0.54
1:A:171:VAL:HG13	1:A:177:GLY:CA	2.34	0.54
1:B:19:ALA:HB3	1:B:20:PRO:HD3	1.90	0.54
1:B:56:LEU:HD22	1:B:82:VAL:HG21	1.89	0.53
1:C:205:LEU:O	1:C:209:ILE:HG12	2.09	0.53

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PHE:N	1:B:116:PRO:HD2	2.25	0.52
1:C:19:ALA:HB3	1:C:20:PRO:HD3	1.91	0.52
1:C:191:LEU:O	1:C:195:VAL:HG23	2.10	0.52
1:D:19:ALA:HB3	1:D:20:PRO:HD3	1.91	0.51
1:B:166:MET:O	1:B:170:VAL:HG23	2.11	0.51
1:B:113:THR:O	1:B:114:PHE:HB3	2.11	0.51
1:B:191:LEU:O	1:B:195:VAL:HG23	2.12	0.49
1:D:148:TYR:CZ	1:D:152:ARG:HD3	2.47	0.49
1:C:136:PHE:O	1:C:140:LEU:HB2	2.12	0.49
1:A:205:LEU:O	1:A:209:ILE:HG12	2.12	0.48
1:C:171:VAL:HG11	4:C:365:HOH:O	2.13	0.48
1:C:77:ILE:CD1	1:C:110:ARG:HB2	2.44	0.47
1:C:166:MET:O	1:C:170:VAL:HG23	2.14	0.47
1:A:162:ILE:N	1:A:163:PRO:HD2	2.30	0.47
1:A:29:THR:HG21	1:B:162:ILE:HG12	1.97	0.47
1:D:136:PHE:O	1:D:140:LEU:HB2	2.15	0.47
1:A:67:VAL:HG12	1:A:68:VAL:HG23	1.97	0.46
1:A:77:ILE:HG12	1:A:106:LEU:HB3	1.97	0.46
1:A:128:ASN:HD22	1:D:114:PHE:HD1	1.62	0.46
1:A:171:VAL:CG1	1:A:177:GLY:HA2	2.37	0.46
1:A:182:ILE:O	4:A:361:HOH:O	2.21	0.46
1:A:136:PHE:O	1:A:140:LEU:HB2	2.17	0.45
1:B:80:LEU:HB3	1:B:103:VAL:HG11	1.99	0.44
1:D:191:LEU:O	1:D:195:VAL:HG23	2.16	0.44
1:C:193:GLY:HA2	1:C:196:MET:HE3	1.99	0.44
1:A:166:MET:O	1:A:170:VAL:HG23	2.17	0.44
1:C:133:THR:HG23	1:D:197:MET:HE1	1.98	0.44
1:A:148:TYR:O	1:A:152:ARG:HB3	2.17	0.44
1:C:67:VAL:HG12	1:C:68:VAL:HG23	2.00	0.44
1:B:11:ALA:H	1:B:12:PRO:HD2	1.83	0.43
1:C:84:VAL:HB	1:C:85:PRO:HD3	2.00	0.43
1:C:171:VAL:HG13	1:C:177:GLY:CA	2.48	0.43
1:D:154:ILE:HD13	1:D:185:SER:HB3	1.99	0.43
1:B:151:GLU:HA	1:B:154:ILE:HD12	2.00	0.43
1:B:162:ILE:HB	1:B:163:PRO:HD3	2.00	0.43
1:A:136:PHE:HD1	1:A:202:ILE:HG21	1.84	0.43
1:C:171:VAL:CG1	1:C:177:GLY:HA2	2.49	0.43
1:C:128:ASN:HB3	1:C:209:ILE:HD12	2.01	0.43
1:B:128:ASN:HB3	1:B:209:ILE:HD12	2.01	0.42
1:B:152:ARG:HG2	1:B:153:ASP:N	2.35	0.42
1:C:77:ILE:HD12	1:C:110:ARG:HB2	2.00	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:THR:N	1:D:73:PRO:HD2	2.35	0.42
1:A:174:SER:HA	1:B:200:ILE:HD11	2.02	0.41
1:A:183:PRO:HG2	1:A:192:ALA:HB2	2.02	0.41
1:D:140:LEU:HD11	1:D:170:VAL:HG13	2.02	0.41
1:D:128:ASN:HB3	1:D:209:ILE:HD12	2.02	0.41
1:D:155:GLN:HG2	1:D:158:LYS:HB2	2.01	0.41
1:B:148:TYR:O	1:B:152:ARG:HB3	2.21	0.40
1:B:173:LEU:C	1:B:175:THR:H	2.29	0.40
1:C:161:SER:HB2	1:C:163:PRO:HD2	2.03	0.40
1:A:113:THR:O	1:A:114:PHE:HB3	2.20	0.40

There are no symmetry-related clashes.

## 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	220/355 (62%)	210 (96%)	9 (4%)	1 (0%)	24	57
1	B	220/355 (62%)	210 (96%)	9 (4%)	1 (0%)	24	57
1	C	224/355 (63%)	210 (94%)	14 (6%)	0	100	100
1	D	223/355 (63%)	215 (96%)	8 (4%)	0	100	100
All	All	887/1420 (62%)	845 (95%)	40 (4%)	2 (0%)	43	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLY
1	B	177	GLY

### 5.3.2 Protein sidechains [i](#)

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	156/273 (57%)	153 (98%)	3 (2%)	50	73
1	B	159/273 (58%)	154 (97%)	5 (3%)	35	64
1	C	160/273 (59%)	156 (98%)	4 (2%)	42	69
1	D	160/273 (59%)	155 (97%)	5 (3%)	35	64
All	All	635/1092 (58%)	618 (97%)	17 (3%)	39	67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ARG
1	A	171	VAL
1	A	175	THR
1	B	143	VAL
1	B	152	ARG
1	B	154	ILE
1	B	170	VAL
1	B	205	LEU
1	C	16	VAL
1	C	62	LYS
1	C	171	VAL
1	C	182	ILE
1	D	14	ASN
1	D	54	LEU
1	D	113	THR
1	D	143	VAL
1	D	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	128	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	164	GLN
1	B	55	GLN
1	B	128	ASN
1	B	216	GLN
1	C	128	ASN
1	C	184	GLN
1	C	216	GLN
1	D	55	GLN
1	D	216	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 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	LDA	A	359	-	13,15,15	2.26	2 (15%)	14,17,17	0.55	0
3	LDA	C	357	-	13,15,15	2.27	2 (15%)	14,17,17	0.54	0
3	LDA	D	356	-	13,15,15	2.24	2 (15%)	14,17,17	0.61	0
3	LDA	D	357	-	13,15,15	2.26	2 (15%)	14,17,17	0.65	0

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	LDA	A	359	-	-	12/13/13/13	-
3	LDA	C	357	-	-	5/13/13/13	-
3	LDA	D	356	-	-	5/13/13/13	-
3	LDA	D	357	-	-	12/13/13/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	359	LDA	O1-N1	-6.69	1.25	1.42
3	C	357	LDA	O1-N1	-6.63	1.25	1.42
3	D	357	LDA	O1-N1	-6.56	1.26	1.42
3	D	356	LDA	O1-N1	-6.51	1.26	1.42
3	D	357	LDA	C1-N1	-4.76	1.46	1.51
3	C	357	LDA	C1-N1	-4.73	1.46	1.51
3	D	356	LDA	C1-N1	-4.70	1.46	1.51
3	A	359	LDA	C1-N1	-4.59	1.46	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	359	LDA	C2-C1-N1-CM1
3	D	357	LDA	C2-C1-N1-CM1
3	D	357	LDA	C3-C4-C5-C6
3	D	356	LDA	C3-C4-C5-C6
3	D	357	LDA	C4-C5-C6-C7
3	D	357	LDA	C7-C8-C9-C10
3	A	359	LDA	C3-C4-C5-C6
3	A	359	LDA	C4-C5-C6-C7
3	A	359	LDA	C11-C10-C9-C8
3	A	359	LDA	C7-C8-C9-C10
3	C	357	LDA	C1-C2-C3-C4
3	A	359	LDA	C5-C6-C7-C8
3	C	357	LDA	C3-C4-C5-C6
3	A	359	LDA	C6-C7-C8-C9
3	D	356	LDA	C1-C2-C3-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	357	LDA	C1-C2-C3-C4
3	D	356	LDA	C9-C10-C11-C12
3	D	357	LDA	C6-C7-C8-C9
3	D	357	LDA	C9-C10-C11-C12
3	D	357	LDA	C11-C10-C9-C8
3	C	357	LDA	C9-C10-C11-C12
3	A	359	LDA	C9-C10-C11-C12
3	A	359	LDA	C2-C1-N1-CM2
3	D	357	LDA	C2-C1-N1-CM2
3	A	359	LDA	N1-C1-C2-C3
3	C	357	LDA	C6-C7-C8-C9
3	D	356	LDA	C2-C3-C4-C5
3	A	359	LDA	C1-C2-C3-C4
3	D	357	LDA	C5-C6-C7-C8
3	D	357	LDA	N1-C1-C2-C3
3	D	356	LDA	C11-C10-C9-C8
3	C	357	LDA	C2-C3-C4-C5
3	A	359	LDA	C2-C1-N1-O1
3	D	357	LDA	C2-C1-N1-O1

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, 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	222/355 (62%)	0.64	31 (13%) <b>6</b> <b>4</b>	53, 62, 63, 64	0
1	B	222/355 (62%)	0.80	23 (10%) <b>11</b> <b>6</b>	57, 61, 63, 64	0
1	C	226/355 (63%)	0.66	17 (7%) <b>20</b> <b>11</b>	57, 61, 64, 65	0
1	D	225/355 (63%)	0.60	26 (11%) <b>9</b> <b>5</b>	56, 61, 63, 64	0
All	All	895/1420 (63%)	0.68	97 (10%) <b>11</b> <b>6</b>	53, 61, 63, 65	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ASN	13.4
1	B	9	ILE	11.1
1	B	13	LEU	10.8
1	B	12	PRO	10.3
1	C	14	ASN	8.0
1	C	13	LEU	7.8
1	C	5	PRO	7.1
1	A	68	VAL	6.9
1	B	68	VAL	6.8
1	D	5	PRO	6.5
1	A	7	LEU	6.4
1	B	10	TYR	6.0
1	A	10	TYR	5.9
1	B	222	ASP	5.5
1	A	15	ALA	5.3
1	A	14	ASN	5.1
1	D	9	ILE	4.8
1	D	215	TYR	4.8
1	A	228	GLN	4.8
1	A	67	VAL	4.7
1	C	230	VAL	4.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	12	PRO	4.6
1	A	226	ASN	4.6
1	A	227	TRP	4.6
1	C	6	PHE	4.5
1	C	11	ALA	4.4
1	D	223	PHE	4.4
1	B	67	VAL	4.3
1	C	74	LYS	4.3
1	D	68	VAL	4.2
1	B	223	PHE	4.2
1	A	69	ARG	4.1
1	A	111	ASP	4.1
1	A	225	ARG	4.1
1	A	65	ALA	4.1
1	C	65	ALA	4.0
1	D	6	PHE	3.8
1	B	11	ALA	3.8
1	A	9	ILE	3.8
1	A	11	ALA	3.7
1	B	229	LEU	3.7
1	B	230	VAL	3.6
1	C	215	TYR	3.6
1	D	13	LEU	3.5
1	D	10	TYR	3.4
1	B	180	ASP	3.4
1	A	224	VAL	3.4
1	C	7	LEU	3.4
1	C	226	ASN	3.3
1	B	111	ASP	3.2
1	D	67	VAL	3.2
1	C	67	VAL	3.2
1	A	64	ARG	3.1
1	D	219	ARG	3.1
1	B	66	GLY	3.1
1	D	8	ARG	3.1
1	D	128	ASN	3.1
1	A	222	ASP	3.1
1	A	66	GLY	3.0
1	C	228	GLN	3.0
1	D	216	GLN	2.9
1	D	228	GLN	2.9
1	B	228	GLN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	224	VAL	2.9
1	D	213	GLY	2.8
1	C	8	ARG	2.8
1	C	224	VAL	2.7
1	D	132	VAL	2.7
1	A	157	GLU	2.7
1	D	65	ALA	2.7
1	B	65	ALA	2.6
1	B	182	ILE	2.6
1	A	8	ARG	2.6
1	D	222	ASP	2.5
1	A	116	PRO	2.5
1	A	74	LYS	2.5
1	D	11	ALA	2.5
1	B	28	LEU	2.4
1	D	66	GLY	2.4
1	A	223	PHE	2.4
1	A	99	LEU	2.4
1	B	61	LEU	2.3
1	D	157	GLU	2.3
1	A	70	ASP	2.3
1	A	103	VAL	2.3
1	B	226	ASN	2.3
1	A	127	ARG	2.2
1	B	69	ARG	2.2
1	D	156	PRO	2.2
1	C	206	TRP	2.2
1	B	227	TRP	2.2
1	D	178	TYR	2.1
1	C	202	ILE	2.1
1	A	175	THR	2.1
1	D	227	TRP	2.0
1	A	33	MET	2.0
1	A	32	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	K	A	360	1/1	0.67	0.76	110,110,110,110	1
2	K	A	356	1/1	0.74	0.26	136,136,136,136	1
3	LDA	D	356	16/16	0.87	0.24	76,77,82,83	0
3	LDA	A	359	16/16	0.90	0.23	77,79,83,84	0
3	LDA	C	357	16/16	0.91	0.24	87,88,90,90	0
3	LDA	D	357	16/16	0.94	0.18	75,77,84,84	0
2	K	B	356	1/1	0.97	0.07	76,76,76,76	0
2	K	A	357	1/1	0.99	0.05	70,70,70,70	0
2	K	A	358	1/1	1.00	0.07	51,51,51,51	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.