Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:31 am BST

PDB ID	:	3SVN
Title	:	Crystal structure of mKate S158A mutant at pH 7.5
Authors	:	Wang, Q.; Byrnes, L.; Sondermann, H.
Deposited on	:	2011-07-12
Resolution	:	1.90 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*
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:

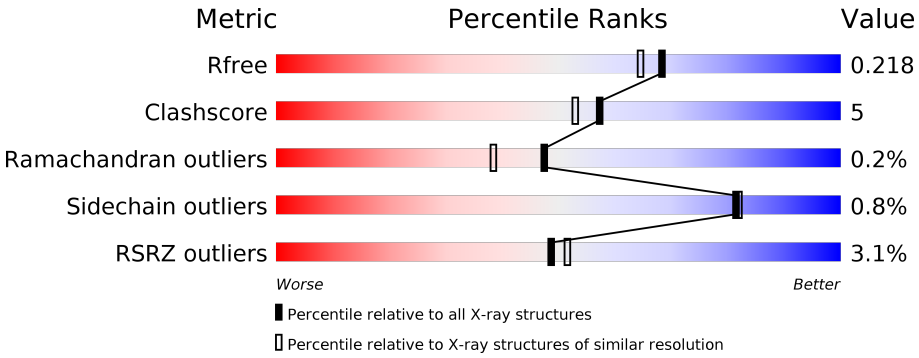
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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 <=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	233	3% 93% 7%
1	B	233	2% 87% 9% 5%
1	C	233	3% 88% 10%
1	D	233	3% 89% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8065 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 mKate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1849	1174	314	346	15			
1	B	222	Total	C	N	O	S	0	1	0
			1775	1131	301	330	13			
1	C	230	Total	C	N	O	S	0	4	0
			1846	1173	313	346	14			
1	D	224	Total	C	N	O	S	0	0	0
			1780	1132	301	334	13			

- Molecule 2 is water.

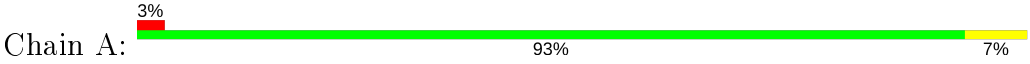
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	226	Total	O	0	0
			226	226		
2	B	216	Total	O	0	0
			216	216		
2	C	208	Total	O	0	0
			208	208		
2	D	165	Total	O	0	0
			165	165		

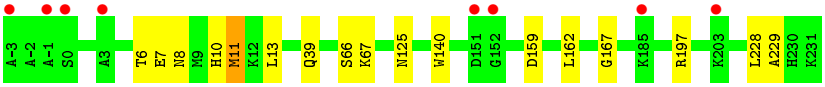
3 Residue-property plots (i)

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: mKate

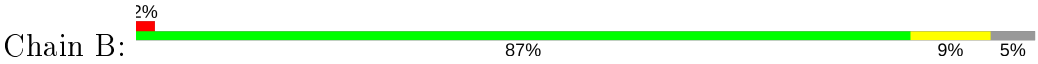
Chain A:

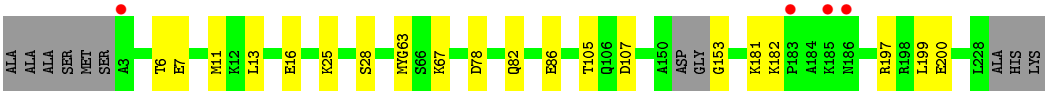




- Molecule 1: mKate

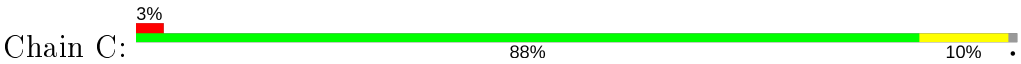
Chain B:





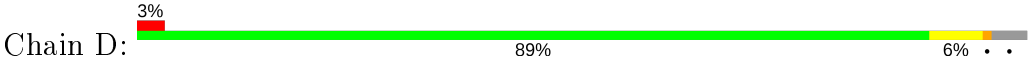
- Molecule 1: mKate

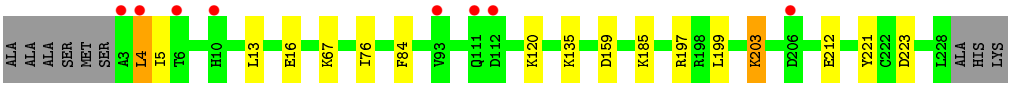
Chain C:



- Molecule 1: mKate

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	161.33Å 161.33Å 76.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.93 – 1.90 43.93 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.93-1.90) 97.8 (43.93-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 1.89Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.172 , 0.221 0.167 , 0.218	Depositor DCC
R_{free} test set	3795 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8065	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NRQ

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	0.38	0/1872	0.54	0/2524
1	B	0.40	0/1794	0.55	0/2419
1	C	0.36	0/1875	0.54	0/2527
1	D	0.36	0/1796	0.53	0/2423
All	All	0.37	0/7337	0.54	0/9893

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1849	0	1828	18	0
1	B	1775	0	1750	19	0
1	C	1846	0	1829	19	0
1	D	1780	0	1751	16	0
2	A	226	0	0	4	0
2	B	216	0	0	1	0
2	C	208	0	0	5	0
2	D	165	0	0	5	0
All	All	8065	0	7158	71	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 (71) 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:223:ASP:HB2	2:D:466:HOH:O	1.75	0.86
1:A:159:ASP:OD2	2:A:447:HOH:O	1.93	0.86
1:C:212:GLU:OE1	2:C:804:HOH:O	1.93	0.85
1:B:67:LYS:NZ	1:B:197:ARG:HH22	1.82	0.77
1:A:125[A]:ASN:ND2	2:A:549:HOH:O	2.08	0.74
1:A:67:LYS:NZ	1:A:197:ARG:HH22	1.86	0.73
1:D:159:ASP:OD2	2:D:462:HOH:O	2.08	0.71
1:D:16:GLU:OE1	1:D:120:LYS:NZ	2.24	0.71
1:C:77:PRO:HG3	1:C:188:LYS:HE3	1.72	0.71
1:D:212:GLU:OE1	2:D:636:HOH:O	2.09	0.70
1:A:167:GLY:O	2:A:448:HOH:O	2.10	0.69
1:A:6:THR:HG22	1:A:8:ASN:H	1.58	0.69
1:D:67:LYS:NZ	1:D:197:ARG:HH22	1.93	0.65
1:B:67:LYS:HZ2	1:B:197:ARG:HH22	1.41	0.65
1:C:2:SER:O	1:C:3:ALA:HB3	1.97	0.65
1:B:6:THR:HG22	1:B:7:GLU:N	2.14	0.62
1:D:4:LEU:HD12	1:D:4:LEU:H	1.66	0.61
1:A:67:LYS:HZ1	1:A:197:ARG:HH22	1.49	0.60
1:B:63:NRQ:HA31	1:B:63:NRQ:N1	2.18	0.58
1:B:16:GLU:HG3	1:B:25:LYS:HG2	1.84	0.57
1:C:67:LYS:NZ	1:C:197:ARG:HH22	2.03	0.57
1:B:86:GLU:OE2	1:B:182:LYS:HE3	2.05	0.56
1:C:2:SER:O	1:C:3:ALA:CB	2.55	0.54
1:A:10:HIS:HA	1:A:11[A]:MET:HE3	1.88	0.54
1:D:4:LEU:N	1:D:4:LEU:HD12	2.23	0.54
1:D:13:LEU:C	1:D:13:LEU:HD23	2.28	0.54
1:B:199:LEU:C	1:B:199:LEU:HD23	2.28	0.53
1:B:6:THR:HG22	1:B:7:GLU:H	1.72	0.52
1:B:153:GLY:HA2	2:B:789:HOH:O	2.08	0.52
1:A:228:LEU:O	1:A:229:ALA:HB3	2.11	0.51
1:C:159:ASP:HB2	2:C:463:HOH:O	2.10	0.50
1:A:10:HIS:CA	1:A:11[A]:MET:HE3	2.42	0.50
1:A:67:LYS:HZ2	1:A:197:ARG:HH22	1.59	0.50
1:A:13:LEU:HD23	1:A:13:LEU:C	2.32	0.50
1:B:105:THR:HG23	1:C:122:ARG:HD3	1.93	0.50
1:D:67:LYS:HZ2	1:D:197:ARG:HH22	1.60	0.49
1:A:10:HIS:C	1:A:11[A]:MET:HE3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:NRQ:CA3	1:B:63:NRQ:N1	2.76	0.48
1:D:135:LYS:HE3	2:D:469:HOH:O	2.14	0.48
1:D:159:ASP:HB2	2:D:462:HOH:O	2.13	0.47
1:A:39:GLN:HE22	1:A:66:SER:HB3	1.79	0.47
1:A:140:TRP:CZ3	1:A:162:LEU:HB2	2.50	0.47
1:B:13:LEU:HD23	1:B:13:LEU:C	2.33	0.47
1:B:199:LEU:HD23	1:B:200:GLU:N	2.30	0.47
1:B:67:LYS:HZ3	1:B:197:ARG:HH22	1.59	0.47
1:D:76:ILE:HG12	1:D:221:TYR:CZ	2.51	0.46
1:A:229:ALA:HB1	2:A:258:HOH:O	2.16	0.46
1:D:67:LYS:HZ1	1:D:197:ARG:HH22	1.63	0.46
1:A:6:THR:HG22	1:A:7:GLU:N	2.31	0.44
1:C:6:THR:HG22	1:C:8:ASN:H	1.83	0.44
1:A:6:THR:CG2	1:A:7:GLU:N	2.80	0.44
1:D:5:ILE:HD11	1:D:84:PHE:CD1	2.51	0.44
1:C:228:LEU:O	1:C:229:ALA:HB3	2.17	0.44
1:B:107:ASP:OD2	1:B:181:LYS:NZ	2.31	0.43
1:D:203:LYS:HB3	1:D:203:LYS:HE2	1.65	0.43
1:B:78:ASP:O	1:B:82:GLN:HG3	2.19	0.43
1:C:18:THR:HG22	2:C:461:HOH:O	2.18	0.43
1:B:6:THR:CG2	1:B:7:GLU:N	2.81	0.43
1:C:184:ALA:O	2:C:652:HOH:O	2.21	0.43
1:C:13:LEU:HB3	1:C:28:SER:OG	2.18	0.43
1:C:136[A]:LYS:HE2	1:C:136[A]:LYS:HB3	1.77	0.42
1:C:67:LYS:HZ2	1:C:197:ARG:HH22	1.66	0.42
1:D:199:LEU:HD23	1:D:199:LEU:C	2.40	0.42
1:C:101:VAL:O	1:C:123:GLY:HA2	2.20	0.41
1:B:63:NRQ:HE2	1:B:199:LEU:HB2	2.03	0.41
1:B:13:LEU:HB3	1:B:28:SER:OG	2.22	0.40
1:C:125[A]:ASN:ND2	2:C:583:HOH:O	2.02	0.40
1:C:39:GLN:HE22	1:C:66:SER:HB3	1.86	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	230/233 (99%)	227 (99%)	3 (1%)	0	100 100
1	B	216/233 (93%)	214 (99%)	2 (1%)	0	100 100
1	C	229/233 (98%)	225 (98%)	2 (1%)	2 (1%)	17 7
1	D	219/233 (94%)	217 (99%)	2 (1%)	0	100 100
All	All	894/932 (96%)	883 (99%)	9 (1%)	2 (0%)	47 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	ALA
1	C	20	ASN

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	197/195 (101%)	195 (99%)	2 (1%)	76 76
1	B	190/195 (97%)	189 (100%)	1 (0%)	88 89
1	C	199/195 (102%)	198 (100%)	1 (0%)	88 89
1	D	190/195 (97%)	187 (98%)	3 (2%)	62 60
All	All	776/780 (100%)	769 (99%)	7 (1%)	81 79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11[A]	MET
1	A	11[B]	MET
1	B	11	MET
1	C	11	MET
1	D	4	LEU
1	D	185	LYS

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Mol	Chain	Res	Type
1	D	203	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	NRQ	A	63	1	23,24,25	5.79	7 (30%)	23,32,34	3.90	8 (34%)
1	NRQ	D	63	1	23,24,25	5.89	7 (30%)	23,32,34	4.20	6 (26%)
1	NRQ	B	63	1	23,24,25	5.71	8 (34%)	23,32,34	3.84	9 (39%)
1	NRQ	C	63	1	23,24,25	5.82	7 (30%)	23,32,34	3.83	7 (30%)

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	NRQ	A	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	B	63	1	-	2/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	1/9/31/32	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	CB2-CA2	21.32	1.52	1.35
1	D	63	NRQ	CB2-CA2	21.24	1.52	1.35
1	B	63	NRQ	CB2-CA2	21.15	1.52	1.35
1	C	63	NRQ	CB2-CA2	20.64	1.52	1.35
1	C	63	NRQ	CA2-C2	-13.71	1.35	1.48
1	D	63	NRQ	CA2-C2	-13.39	1.35	1.48
1	A	63	NRQ	CA2-C2	-12.42	1.36	1.48
1	B	63	NRQ	CA2-C2	-12.19	1.36	1.48
1	C	63	NRQ	O2-C2	7.53	1.39	1.23
1	D	63	NRQ	O2-C2	7.50	1.38	1.23
1	C	63	NRQ	CA1-N1	7.43	1.45	1.27
1	A	63	NRQ	O2-C2	7.34	1.38	1.23
1	D	63	NRQ	CA1-N1	7.33	1.45	1.27
1	A	63	NRQ	CA1-N1	7.10	1.44	1.27
1	B	63	NRQ	O2-C2	7.07	1.38	1.23
1	B	63	NRQ	CA1-N1	7.03	1.44	1.27
1	B	63	NRQ	CD2-CG2	5.02	1.49	1.39
1	D	63	NRQ	CD2-CG2	4.90	1.49	1.39
1	C	63	NRQ	CD2-CG2	4.87	1.48	1.39
1	A	63	NRQ	CD2-CG2	4.87	1.48	1.39
1	B	63	NRQ	CG2-CB2	3.23	1.53	1.46
1	A	63	NRQ	CG2-CB2	3.19	1.53	1.46
1	D	63	NRQ	CG2-CB2	2.99	1.52	1.46
1	C	63	NRQ	CG2-CB2	2.81	1.52	1.46
1	D	63	NRQ	CE1-CZ	2.45	1.43	1.38
1	A	63	NRQ	CE1-CZ	2.44	1.43	1.38
1	C	63	NRQ	CE1-CZ	2.26	1.43	1.38
1	B	63	NRQ	CE1-CZ	2.20	1.43	1.38
1	B	63	NRQ	C2-N3	-2.08	1.35	1.39

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	NRQ	CA2-C2-N3	14.19	110.08	103.37
1	D	63	NRQ	CA2-C2-N3	13.66	109.83	103.37
1	B	63	NRQ	CA2-C2-N3	13.66	109.83	103.37
1	C	63	NRQ	CA2-C2-N3	12.44	109.25	103.37
1	D	63	NRQ	O2-C2-CA2	-11.45	124.53	130.96
1	C	63	NRQ	O2-C2-CA2	-9.03	125.89	130.96
1	A	63	NRQ	O2-C2-CA2	-8.49	126.19	130.96
1	B	63	NRQ	CG2-CB2-CA2	-7.83	120.34	129.94
1	C	63	NRQ	CG2-CB2-CA2	-7.42	120.86	129.94
1	B	63	NRQ	O2-C2-CA2	-7.05	127.00	130.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	NRQ	CG2-CB2-CA2	-6.94	121.44	129.94
1	A	63	NRQ	CG2-CB2-CA2	-5.52	123.17	129.94
1	C	63	NRQ	N3-C1-N2	-3.04	109.27	113.28
1	A	63	NRQ	C2-CA2-N2	-2.84	106.94	108.93
1	A	63	NRQ	CE-SD-CG1	2.80	110.03	100.40
1	D	63	NRQ	N3-C1-N2	-2.64	109.79	113.28
1	C	63	NRQ	O3-C3-CA3	-2.56	118.66	126.39
1	A	63	NRQ	N3-C1-N2	-2.55	109.91	113.28
1	B	63	NRQ	O3-C3-CA3	-2.53	118.75	126.39
1	D	63	NRQ	CE-SD-CG1	2.52	109.06	100.40
1	B	63	NRQ	C2-CA2-N2	-2.44	107.22	108.93
1	A	63	NRQ	O3-C3-CA3	-2.42	119.07	126.39
1	C	63	NRQ	CE-SD-CG1	2.39	108.62	100.40
1	B	63	NRQ	CE-SD-CG1	2.30	108.30	100.40
1	B	63	NRQ	N3-C1-N2	-2.28	110.27	113.28
1	C	63	NRQ	CE2-CD2-CG2	-2.18	118.41	121.25
1	D	63	NRQ	CB2-CA2-N2	2.11	131.75	128.83
1	B	63	NRQ	CD1-CG2-CB2	-2.09	114.10	121.22
1	B	63	NRQ	CE2-CD2-CG2	-2.05	118.58	121.25
1	A	63	NRQ	CD1-CG2-CB2	-2.04	114.28	121.22

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	63	NRQ	CA1-CB1-CG1-SD
1	A	63	NRQ	CA1-CB1-CG1-SD
1	D	63	NRQ	CA1-CB1-CG1-SD
1	B	63	NRQ	CA1-CB1-CG1-SD
1	B	63	NRQ	CB1-CG1-SD-CE

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRQ	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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^{th} 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	232/233 (99%)	0.00	8 (3%) 45 48	14, 21, 39, 56	0
1	B	221/233 (94%)	0.01	4 (1%) 68 71	14, 21, 36, 56	0
1	C	229/233 (98%)	0.02	8 (3%) 44 47	16, 24, 38, 49	0
1	D	223/233 (95%)	0.08	8 (3%) 42 45	17, 27, 43, 59	0
All	All	905/932 (97%)	0.03	28 (3%) 49 51	14, 23, 40, 59	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-1	ALA	6.6
1	C	2	SER	4.5
1	C	3	ALA	4.1
1	B	185	LYS	3.9
1	D	6	THR	3.6
1	C	152	GLY	3.6
1	A	151	ASP	3.5
1	A	0	SER	3.3
1	A	-3	ALA	3.2
1	A	152	GLY	3.1
1	C	206	ASP	3.1
1	C	0	SER	3.0
1	A	185	LYS	2.9
1	D	112	ASP	2.9
1	C	1	MET	2.9
1	C	151	ASP	2.7
1	B	186	ASN	2.6
1	B	183	PRO	2.5
1	B	3	ALA	2.5
1	D	3	ALA	2.3
1	D	4	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	93	VAL	2.2
1	D	10	HIS	2.2
1	C	207	LYS	2.2
1	D	206	ASP	2.1
1	D	111	GLN	2.1
1	A	3	ALA	2.1
1	A	203	LYS	2.1

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, 95^{th} 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	NRQ	D	63	23/24	0.96	0.09	20,24,27,33	0
1	NRQ	B	63	23/24	0.96	0.09	15,19,24,29	0
1	NRQ	A	63	23/24	0.97	0.09	15,18,26,28	0
1	NRQ	C	63	23/24	0.97	0.09	17,20,26,35	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.