



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:53 PM UTC

PDB ID : 3SVR / pdb_00003svr
Title : Crystal structure of mkate mutant S158A/S143C at pH 7.5
Authors : Wang, Q.; Byrnes, L.; Sondermann, H.
Deposited on : 2011-07-12
Resolution : 1.91 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 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)
Xtriage (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

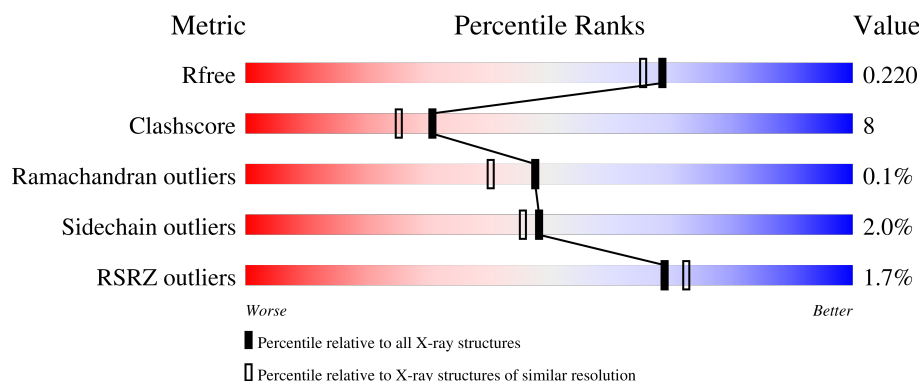
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	233	
1	B	233	
1	C	233	
1	D	233	

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
1	NRQ	A	63[A]	-	-	X	-
1	NRQ	C	63[A]	-	-	X	-
1	NRQ	D	63[A]	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8095 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 S158A/S143C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	2	0
			1789	1141	301	331	16			
1	B	229	Total	C	N	O	S	0	7	0
			1868	1190	316	345	17			
1	C	228	Total	C	N	O	S	0	8	0
			1862	1184	316	346	16			
1	D	225	Total	C	N	O	S	0	2	0
			1811	1153	305	337	16			

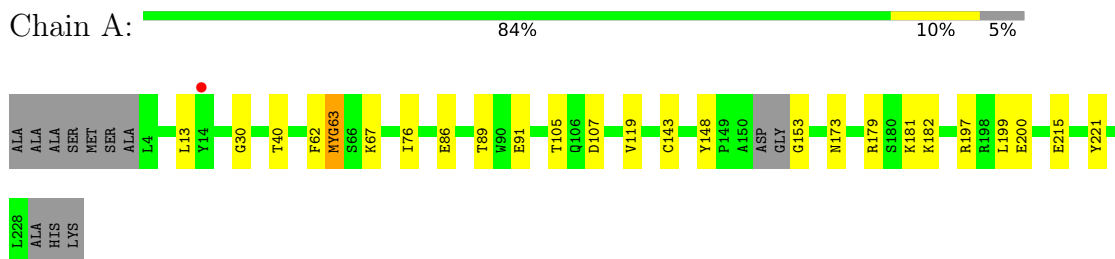
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	201	Total	O	0	0
			201	201		
2	B	219	Total	O	0	0
			219	219		
2	C	191	Total	O	0	0
			191	191		
2	D	154	Total	O	0	0
			154	154		

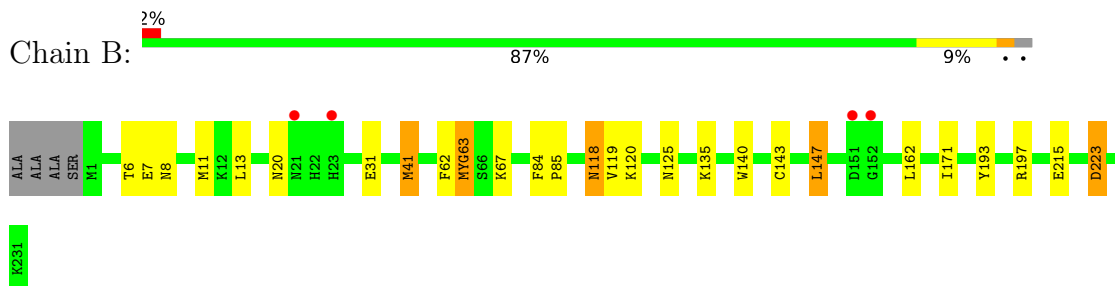
3 Residue-property plots [i](#)

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.

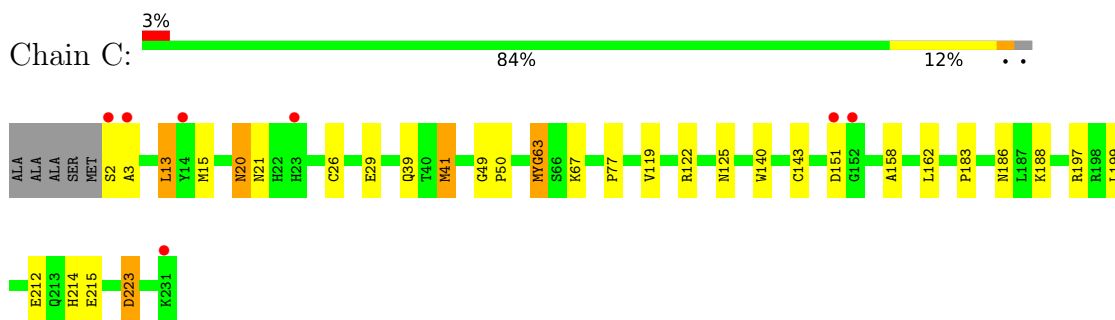
- Molecule 1: mkate S158A/S143C



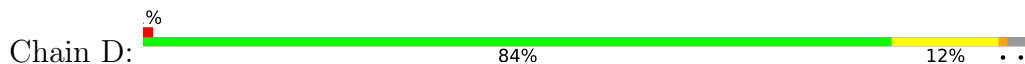
- Molecule 1: mkate S158A/S143C



- Molecule 1: mkate S158A/S143C



- Molecule 1: mkate S158A/S143C





4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	161.31Å 161.31Å 75.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.33 – 1.91 40.33 – 1.91	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.33-1.91) 97.7 (40.33-1.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.180 , 0.227 0.174 , 0.220	Depositor DCC
R_{free} test set	3736 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% 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: 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	0.45	0/1784	0.78	0/2405
1	B	0.44	0/1880	0.74	0/2532
1	C	0.42	0/1878	0.75	1/2535 (0.0%)
1	D	0.42	0/1807	0.76	1/2438 (0.0%)
All	All	0.43	0/7349	0.76	2/9910 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ALA	N-CA-C	-5.75	106.26	113.28
1	D	17	GLY	N-CA-C	5.37	118.10	110.74

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	1789	0	1758	30	0
1	B	1868	0	1841	29	0
1	C	1862	0	1818	35	0
1	D	1811	0	1773	31	0
2	A	201	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	219	0	0	8	0
2	C	191	0	0	6	0
2	D	154	0	0	3	0
All	All	8095	0	7190	120	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 8.

All (120) 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:223:ASP:OD2	2:B:757:HOH:O	1.83	0.95
1:B:20:ASN:O	2:B:761:HOH:O	1.85	0.94
1:C:63[B]:NRQ:HD2	1:C:63[B]:NRQ:O2	1.66	0.94
1:B:41:MET:HG3	1:B:63[A]:NRQ:HE2A	1.49	0.93
1:D:159:ASP:OD1	2:D:417:HOH:O	1.89	0.89
1:C:41:MET:HG3	1:C:63[A]:NRQ:HE2A	1.56	0.87
1:C:212:GLU:OE1	2:C:411:HOH:O	1.92	0.87
1:C:63[A]:NRQ:OH	1:C:143[A]:CYS:SG	2.32	0.86
1:D:63[B]:NRQ:O2	1:D:63[B]:NRQ:HD2	1.74	0.85
1:A:91:GLU:CD	1:A:179:ARG:HH12	1.85	0.84
1:A:63[A]:NRQ:HOH	1:A:143[A]:CYS:HG	1.20	0.84
1:B:63[A]:NRQ:OH	1:B:143[A]:CYS:SG	2.24	0.82
1:D:67:LYS:HZ2	1:D:197:ARG:HH22	1.28	0.81
1:D:134:GLN:HB3	1:D:136:LYS:HD3	1.61	0.80
1:B:41:MET:HG3	1:B:63[B]:NRQ:HE2A	1.65	0.78
1:C:63[A]:NRQ:HOH	1:C:143[A]:CYS:HG	1.19	0.77
1:D:67:LYS:NZ	1:D:197:ARG:HH22	1.84	0.76
1:A:173:ASN:ND2	2:A:398:HOH:O	2.01	0.76
1:B:63[B]:NRQ:HD2	1:B:63[B]:NRQ:O2	1.88	0.73
1:A:153:GLY:N	2:A:549:HOH:O	2.22	0.72
1:C:223:ASP:HB3	2:C:412:HOH:O	1.92	0.69
1:C:77:PRO:HG3	1:C:188:LYS:HE3	1.76	0.68
1:A:63[B]:NRQ:HD2	1:A:63[B]:NRQ:O2	1.94	0.68
1:B:67:LYS:NZ	1:B:197:ARG:HH22	1.91	0.68
1:D:63[A]:NRQ:HA31	1:D:63[A]:NRQ:N1	2.11	0.65
1:A:197:ARG:HG2	2:A:753:HOH:O	1.97	0.64
1:D:63[A]:NRQ:OH	1:D:143[A]:CYS:SG	2.40	0.64
1:A:63[A]:NRQ:OH	1:A:143[A]:CYS:SG	2.39	0.63
1:B:13:LEU:C	1:B:13:LEU:HD23	2.24	0.62
1:B:118:ASN:ND2	2:B:616:HOH:O	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:GLU:OE2	1:D:179:ARG:NH1	2.28	0.62
1:A:63[A]:NRQ:HE1	1:A:143[A]:CYS:SG	2.40	0.61
1:C:41:MET:HG3	1:C:63[B]:NRQ:HE2A	1.83	0.60
1:C:63[A]:NRQ:HE1	1:C:143[A]:CYS:SG	2.41	0.60
1:D:134:GLN:CB	1:D:136:LYS:HD3	2.31	0.60
1:A:63[A]:NRQ:HA31	1:A:63[A]:NRQ:N1	2.17	0.59
1:A:67:LYS:NZ	1:A:197:ARG:HH22	2.01	0.59
1:B:223:ASP:CG	2:B:757:HOH:O	2.40	0.59
1:C:67:LYS:NZ	1:C:197:ARG:HH22	2.00	0.58
1:B:6:THR:HG22	1:B:7:GLU:N	2.18	0.58
1:D:41:MET:HB2	1:D:63[A]:NRQ:HE1A	1.86	0.57
1:D:41:MET:HG3	1:D:63[A]:NRQ:HE3	1.87	0.56
1:A:67:LYS:HZ1	1:A:197:ARG:HH22	1.54	0.55
1:A:63[A]:NRQ:HG11	1:A:215:GLU:OE1	2.07	0.55
1:D:13:LEU:C	1:D:13:LEU:HD23	2.32	0.54
1:D:173:ASN:ND2	2:D:255:HOH:O	1.89	0.54
1:A:13:LEU:C	1:A:13:LEU:HD23	2.32	0.54
1:D:63[A]:NRQ:HE1	1:D:143[A]:CYS:SG	2.48	0.53
1:B:67:LYS:HZ2	1:B:197:ARG:HH22	1.53	0.53
1:B:6:THR:HG22	1:B:8:ASN:H	1.74	0.53
1:B:63[B]:NRQ:C3	1:B:63[B]:NRQ:N1	2.72	0.53
1:C:63[B]:NRQ:C3	1:C:63[B]:NRQ:N1	2.72	0.53
1:D:63[A]:NRQ:OH	1:D:160:MET:HE3	2.10	0.52
1:C:223:ASP:CB	2:C:412:HOH:O	2.53	0.52
1:A:89:THR:HG21	1:C:21[B]:ASN:ND2	2.25	0.52
1:C:214:HIS:CE1	1:D:227:LYS:HE2	2.46	0.51
1:D:199:LEU:C	1:D:199:LEU:HD23	2.36	0.50
1:C:13:LEU:C	1:C:13:LEU:HD23	2.37	0.50
1:B:125[B]:ASN:ND2	2:B:399:HOH:O	2.23	0.50
1:B:140:TRP:CZ3	1:B:162:LEU:HB2	2.47	0.50
1:A:107:ASP:OD2	1:A:181:LYS:HE2	2.12	0.49
1:C:2:SER:N	2:C:547:HOH:O	2.46	0.49
1:B:6:THR:CG2	1:B:7:GLU:N	2.76	0.49
1:A:76:ILE:HG12	1:A:221:TYR:CZ	2.48	0.49
1:B:223:ASP:CB	2:B:757:HOH:O	2.60	0.49
1:D:147:LEU:HD12	1:D:147:LEU:N	2.27	0.48
1:B:63[A]:NRQ:HE1	1:B:143[A]:CYS:SG	2.53	0.48
1:C:214:HIS:HD2	2:C:301:HOH:O	1.95	0.48
1:A:105:THR:HG23	1:C:122:ARG:HD3	1.96	0.47
1:C:49:GLY:HA2	1:C:50:PRO:C	2.40	0.47
1:C:63[B]:NRQ:HG11	1:C:215:GLU:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:GLN:HG3	1:C:63[A]:NRQ:HE3	1.97	0.47
1:A:63[A]:NRQ:CZ	1:A:143[A]:CYS:HG	2.27	0.46
1:D:212:GLU:OE1	2:D:418:HOH:O	2.21	0.46
1:A:63[A]:NRQ:CE1	1:A:143[A]:CYS:SG	3.04	0.46
1:C:63[A]:NRQ:CE1	1:C:143[A]:CYS:SG	3.03	0.45
1:A:197:ARG:CG	2:A:753:HOH:O	2.59	0.45
1:A:63[A]:NRQ:N1	1:A:63[A]:NRQ:CA3	2.78	0.45
1:D:5:ILE:HD11	1:D:84:PHE:CD1	2.50	0.45
1:C:63[A]:NRQ:HG11	1:C:215:GLU:OE1	2.17	0.45
1:D:11:MET:HE1	1:D:39:GLN:OE1	2.16	0.45
1:C:125[B]:ASN:ND2	2:C:567:HOH:O	2.07	0.45
2:B:761:HOH:O	1:D:105:THR:HG22	2.17	0.45
1:C:63[A]:NRQ:HE2	1:C:199:LEU:HD12	1.98	0.45
1:A:91:GLU:OE2	1:C:20:ASN:O	2.35	0.44
1:B:84:PHE:HB3	1:B:85:PRO:HA	1.99	0.44
1:C:143[B]:CYS:SG	1:C:158:ALA:HB1	2.56	0.44
1:A:199:LEU:C	1:A:199:LEU:HD23	2.43	0.44
1:B:62:PHE:HB2	1:B:63[B]:NRQ:HB11	1.99	0.44
1:D:41:MET:CG	1:D:63[A]:NRQ:HE3	2.47	0.44
1:C:29:GLU:C	1:C:41:MET:HE3	2.42	0.44
1:B:120:LYS:HD3	2:B:277:HOH:O	2.18	0.44
1:D:60:THR:O	1:D:63[B]:NRQ:C1	2.67	0.43
1:D:134:GLN:HB3	1:D:136:LYS:CD	2.40	0.43
1:C:63[A]:NRQ:CE2	1:C:199:LEU:HD12	2.49	0.43
1:B:41:MET:HG3	1:B:63[A]:NRQ:CE	2.34	0.43
1:B:63[A]:NRQ:CZ	1:B:143[A]:CYS:SG	3.06	0.43
1:C:67:LYS:HZ2	1:C:197:ARG:HH22	1.64	0.43
1:D:11:MET:HE1	1:D:39:GLN:HB2	2.00	0.43
1:A:63[A]:NRQ:CZ	1:A:197:ARG:HD2	2.49	0.43
1:D:63[B]:NRQ:OH	1:D:158:ALA:HB3	2.18	0.43
1:A:86:GLU:OE2	1:A:182:LYS:HE3	2.18	0.42
1:D:30:GLY:HA3	1:D:40:THR:O	2.20	0.42
1:C:183:PRO:HG2	1:C:186:ASN:ND2	2.35	0.42
1:B:63[A]:NRQ:HG11	1:B:215:GLU:OE1	2.19	0.42
1:D:63[A]:NRQ:N1	1:D:63[A]:NRQ:CA3	2.79	0.42
1:D:41:MET:HG3	1:D:63[A]:NRQ:CE	2.50	0.42
1:A:30:GLY:HA3	1:A:40:THR:O	2.20	0.42
1:B:147:LEU:HD23	1:B:193:TYR:CZ	2.55	0.42
1:A:63[A]:NRQ:CE1	1:A:197:ARG:HD2	2.51	0.41
1:A:62:PHE:HB2	1:A:63[B]:NRQ:HB11	2.02	0.41
1:A:199:LEU:HD23	1:A:200:GLU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:HZ3	1:B:197:ARG:HH22	1.66	0.41
1:C:15:MET:HB3	1:C:26:CYS:HB2	2.01	0.41
1:A:148:TYR:OH	1:B:171:ILE:HG13	2.20	0.40
1:B:11:MET:HE3	1:B:31:GLU:N	2.37	0.40
1:C:63[A]:NRQ:N1	1:C:63[A]:NRQ:C3	2.84	0.40
1:C:140:TRP:CZ3	1:C:162:LEU:HB2	2.56	0.40
1:D:63[A]:NRQ:CE1	1:D:143[A]:CYS:SG	3.08	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	215/233 (92%)	213 (99%)	2 (1%)	0	100	100
1	B	229/233 (98%)	226 (99%)	3 (1%)	0	100	100
1	C	230/233 (99%)	224 (97%)	5 (2%)	1 (0%)	30	22
1	D	221/233 (95%)	218 (99%)	3 (1%)	0	100	100
All	All	895/932 (96%)	881 (98%)	13 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	190/195 (97%)	189 (100%)	1 (0%)	81	84
1	B	199/195 (102%)	193 (97%)	6 (3%)	36	30
1	C	198/195 (102%)	194 (98%)	4 (2%)	48	46
1	D	191/195 (98%)	187 (98%)	4 (2%)	47	44
All	All	778/780 (100%)	763 (98%)	15 (2%)	48	47

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	VAL
1	B	41	MET
1	B	118	ASN
1	B	119	VAL
1	B	135	LYS
1	B	147	LEU
1	B	223	ASP
1	C	13	LEU
1	C	41	MET
1	C	119	VAL
1	C	223	ASP
1	D	13	LEU
1	D	119	VAL
1	D	213	GLN
1	D	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	214	HIS
1	D	10	HIS
1	D	111	GLN
1	D	186	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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	B	63[A]	1	24,24,25	5.25	8 (33%)	24,32,34	3.03	7 (29%)
1	NRQ	A	63[B]	1	24,24,25	5.52	9 (37%)	24,32,34	2.97	7 (29%)
1	NRQ	D	63[B]	1	24,24,25	5.32	8 (33%)	24,32,34	3.14	8 (33%)
1	NRQ	C	63[B]	1	24,24,25	5.56	8 (33%)	24,32,34	3.38	9 (37%)
1	NRQ	D	63[A]	1	24,24,25	5.33	8 (33%)	24,32,34	3.21	5 (20%)
1	NRQ	A	63[A]	1	24,24,25	5.42	9 (37%)	24,32,34	2.52	6 (25%)
1	NRQ	B	63[B]	1	24,24,25	5.55	8 (33%)	24,32,34	3.59	10 (41%)
1	NRQ	C	63[A]	1	24,24,25	5.37	8 (33%)	24,32,34	2.72	6 (25%)

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	B	63[A]	1	-	2/9/31/32	0/2/2/2
1	NRQ	A	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	D	63[B]	1	-	2/9/31/32	0/2/2/2
1	NRQ	C	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	D	63[A]	1	-	1/9/31/32	0/2/2/2
1	NRQ	A	63[A]	1	-	2/9/31/32	0/2/2/2
1	NRQ	B	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	C	63[A]	1	-	2/9/31/32	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[A]	NRQ	CB2-CA2	20.03	1.54	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63[B]	NRQ	CB2-CA2	19.98	1.54	1.35
1	C	63[B]	NRQ	CB2-CA2	19.86	1.54	1.35
1	A	63[B]	NRQ	CB2-CA2	19.68	1.54	1.35
1	C	63[A]	NRQ	CB2-CA2	19.20	1.53	1.35
1	D	63[B]	NRQ	CB2-CA2	19.13	1.53	1.35
1	D	63[A]	NRQ	CB2-CA2	19.04	1.53	1.35
1	B	63[A]	NRQ	CB2-CA2	18.73	1.53	1.35
1	C	63[A]	NRQ	CA2-C2	-11.77	1.35	1.48
1	D	63[A]	NRQ	CA2-C2	-11.75	1.35	1.48
1	C	63[B]	NRQ	CA2-C2	-11.56	1.36	1.48
1	B	63[A]	NRQ	CA2-C2	-11.46	1.36	1.48
1	B	63[B]	NRQ	CA2-C2	-11.41	1.36	1.48
1	A	63[B]	NRQ	CA2-C2	-11.32	1.36	1.48
1	A	63[A]	NRQ	CA2-C2	-10.54	1.37	1.48
1	D	63[B]	NRQ	CA2-C2	-10.35	1.37	1.48
1	D	63[B]	NRQ	O2-C2	8.56	1.40	1.23
1	A	63[B]	NRQ	O2-C2	8.33	1.40	1.23
1	A	63[B]	NRQ	CA1-N1	8.22	1.46	1.27
1	C	63[B]	NRQ	O2-C2	8.16	1.39	1.23
1	C	63[B]	NRQ	CA1-N1	8.14	1.45	1.27
1	B	63[B]	NRQ	O2-C2	8.11	1.39	1.23
1	B	63[B]	NRQ	CA1-N1	8.10	1.45	1.27
1	D	63[B]	NRQ	CA1-N1	8.04	1.45	1.27
1	C	63[A]	NRQ	CA1-N1	7.82	1.45	1.27
1	A	63[A]	NRQ	CA1-N1	7.75	1.44	1.27
1	B	63[A]	NRQ	CA1-N1	7.73	1.44	1.27
1	D	63[A]	NRQ	CA1-N1	7.73	1.44	1.27
1	D	63[A]	NRQ	O2-C2	7.73	1.38	1.23
1	C	63[A]	NRQ	O2-C2	7.70	1.38	1.23
1	A	63[A]	NRQ	O2-C2	7.65	1.38	1.23
1	B	63[A]	NRQ	O2-C2	7.55	1.38	1.23
1	C	63[B]	NRQ	CD2-CG2	4.92	1.49	1.39
1	A	63[B]	NRQ	CD2-CG2	4.88	1.49	1.39
1	A	63[A]	NRQ	CD2-CG2	4.86	1.49	1.39
1	B	63[B]	NRQ	CD2-CG2	4.77	1.49	1.39
1	D	63[A]	NRQ	CD2-CG2	4.71	1.49	1.39
1	C	63[A]	NRQ	CD2-CG2	4.67	1.48	1.39
1	D	63[B]	NRQ	CD2-CG2	4.66	1.48	1.39
1	B	63[A]	NRQ	CD2-CG2	4.62	1.48	1.39
1	A	63[B]	NRQ	CG2-CB2	4.29	1.54	1.46
1	B	63[B]	NRQ	C1-CA1	4.11	1.54	1.48
1	C	63[B]	NRQ	C1-CA1	4.06	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63[A]	NRQ	CG2-CB2	3.90	1.54	1.46
1	B	63[B]	NRQ	CG2-CB2	3.70	1.53	1.46
1	C	63[B]	NRQ	CG2-CB2	3.66	1.53	1.46
1	D	63[B]	NRQ	CG2-CB2	3.63	1.53	1.46
1	D	63[B]	NRQ	C1-CA1	3.42	1.53	1.48
1	C	63[A]	NRQ	CG2-CB2	3.37	1.53	1.46
1	A	63[A]	NRQ	C1-CA1	3.36	1.52	1.48
1	D	63[A]	NRQ	CG2-CB2	3.14	1.52	1.46
1	C	63[A]	NRQ	C1-CA1	3.09	1.52	1.48
1	A	63[B]	NRQ	C1-CA1	3.04	1.52	1.48
1	A	63[B]	NRQ	CE1-CZ	2.98	1.44	1.39
1	D	63[A]	NRQ	C1-CA1	2.93	1.52	1.48
1	B	63[A]	NRQ	CG2-CB2	2.85	1.52	1.46
1	B	63[A]	NRQ	C1-CA1	2.77	1.52	1.48
1	B	63[A]	NRQ	CE1-CZ	2.69	1.44	1.39
1	C	63[B]	NRQ	CE1-CZ	2.66	1.44	1.39
1	B	63[B]	NRQ	CE1-CZ	2.62	1.43	1.39
1	D	63[B]	NRQ	CE1-CZ	2.60	1.43	1.39
1	D	63[A]	NRQ	CE1-CZ	2.50	1.43	1.39
1	A	63[A]	NRQ	CE1-CZ	2.40	1.43	1.39
1	C	63[A]	NRQ	CE1-CZ	2.33	1.43	1.39
1	A	63[B]	NRQ	CD1-CE1	2.14	1.42	1.38
1	A	63[A]	NRQ	C2-N3	-2.07	1.35	1.40

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	NRQ	O2-C2-CA2	-9.47	124.98	131.02
1	B	63[A]	NRQ	O2-C2-CA2	-9.14	125.19	131.02
1	A	63[B]	NRQ	O2-C2-CA2	-8.67	125.49	131.02
1	D	63[A]	NRQ	CG2-CB2-CA2	-8.57	119.67	129.87
1	B	63[B]	NRQ	CB2-CA2-C2	8.08	132.15	122.36
1	D	63[B]	NRQ	CB2-CA2-C2	8.06	132.13	122.36
1	C	63[B]	NRQ	CB2-CA2-C2	7.54	131.49	122.36
1	A	63[A]	NRQ	CA2-C2-N3	7.43	109.74	103.50
1	B	63[B]	NRQ	CA2-C2-N3	7.36	109.68	103.50
1	B	63[A]	NRQ	CA2-C2-N3	7.35	109.67	103.50
1	B	63[B]	NRQ	O2-C2-CA2	-7.30	126.36	131.02
1	C	63[B]	NRQ	CA2-C2-N3	7.23	109.57	103.50
1	C	63[A]	NRQ	CA2-C2-N3	7.19	109.53	103.50
1	D	63[A]	NRQ	CA2-C2-N3	7.07	109.44	103.50
1	C	63[A]	NRQ	O2-C2-CA2	-7.04	126.53	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[B]	NRQ	CG2-CB2-CA2	-6.75	121.85	129.87
1	B	63[A]	NRQ	CG2-CB2-CA2	-6.62	121.99	129.87
1	C	63[B]	NRQ	CG2-CB2-CA2	-6.49	122.15	129.87
1	D	63[B]	NRQ	CB2-CA2-N2	-6.32	120.17	128.76
1	A	63[A]	NRQ	CG2-CB2-CA2	-6.30	122.38	129.87
1	B	63[B]	NRQ	CG2-CB2-CA2	-6.26	122.42	129.87
1	A	63[B]	NRQ	CB2-CA2-C2	6.02	129.65	122.36
1	C	63[A]	NRQ	CG2-CB2-CA2	-5.92	122.83	129.87
1	C	63[B]	NRQ	O2-C2-CA2	-5.70	127.38	131.02
1	A	63[B]	NRQ	CA2-C2-N3	5.51	108.13	103.50
1	D	63[B]	NRQ	CA2-C2-N3	5.19	107.86	103.50
1	D	63[B]	NRQ	O2-C2-CA2	-5.16	127.72	131.02
1	B	63[B]	NRQ	CB2-CA2-N2	-5.10	121.83	128.76
1	C	63[B]	NRQ	CB2-CA2-N2	-4.75	122.31	128.76
1	C	63[B]	NRQ	N3-C1-N2	-4.63	107.12	112.62
1	A	63[B]	NRQ	CB2-CA2-N2	-4.61	122.51	128.76
1	B	63[B]	NRQ	N3-C1-N2	-4.55	107.22	112.62
1	B	63[B]	NRQ	C2-CA2-N2	-4.18	105.95	108.95
1	C	63[B]	NRQ	C2-CA2-N2	-3.94	106.12	108.95
1	A	63[B]	NRQ	CG2-CB2-CA2	-3.92	125.21	129.87
1	A	63[B]	NRQ	N3-C1-N2	-3.50	108.47	112.62
1	A	63[A]	NRQ	C2-CA2-N2	-3.34	106.56	108.95
1	D	63[B]	NRQ	N3-C1-N2	-3.31	108.69	112.62
1	C	63[A]	NRQ	N3-C1-N2	-3.18	108.84	112.62
1	B	63[B]	NRQ	CA2-N2-C1	3.15	109.89	104.09
1	A	63[A]	NRQ	N3-C1-N2	-3.05	109.00	112.62
1	B	63[B]	NRQ	C3-CA3-N3	3.05	119.36	112.43
1	C	63[B]	NRQ	CA2-N2-C1	2.95	109.52	104.09
1	A	63[A]	NRQ	O2-C2-CA2	-2.79	129.24	131.02
1	C	63[B]	NRQ	C3-CA3-N3	2.67	118.49	112.43
1	B	63[A]	NRQ	N3-C1-N2	-2.63	109.50	112.62
1	A	63[A]	NRQ	C3-CA3-N3	2.53	118.19	112.43
1	D	63[A]	NRQ	N3-C1-N2	-2.47	109.69	112.62
1	D	63[B]	NRQ	CA2-N2-C1	2.45	108.59	104.09
1	C	63[A]	NRQ	C2-CA2-N2	-2.39	107.24	108.95
1	A	63[B]	NRQ	CA2-N2-C1	2.30	108.32	104.09
1	B	63[A]	NRQ	CD1-CG2-CD2	2.21	120.94	117.65
1	C	63[A]	NRQ	CE2-CD2-CG2	-2.18	118.41	121.22
1	B	63[A]	NRQ	C2-CA2-N2	-2.13	107.43	108.95
1	D	63[B]	NRQ	C2-CA2-N2	-2.08	107.46	108.95
1	D	63[A]	NRQ	CE2-CD2-CG2	-2.07	118.54	121.22
1	B	63[B]	NRQ	CE-SD-CG1	2.05	110.91	100.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63[A]	NRQ	CB2-CA2-N2	2.03	131.51	128.76

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	63[A]	NRQ	CA1-CB1-CG1-SD
1	A	63[B]	NRQ	N2-CA2-CB2-CG2
1	A	63[B]	NRQ	C2-CA2-CB2-CG2
1	B	63[A]	NRQ	CA1-CB1-CG1-SD
1	B	63[B]	NRQ	N2-CA2-CB2-CG2
1	B	63[B]	NRQ	C2-CA2-CB2-CG2
1	B	63[B]	NRQ	C3-CA3-N3-C1
1	B	63[B]	NRQ	C3-CA3-N3-C2
1	C	63[A]	NRQ	CA1-CB1-CG1-SD
1	C	63[B]	NRQ	N2-CA2-CB2-CG2
1	C	63[B]	NRQ	C2-CA2-CB2-CG2
1	C	63[B]	NRQ	C3-CA3-N3-C1
1	C	63[B]	NRQ	C3-CA3-N3-C2
1	D	63[A]	NRQ	CA1-CB1-CG1-SD
1	D	63[B]	NRQ	N2-CA2-CB2-CG2
1	D	63[B]	NRQ	C2-CA2-CB2-CG2
1	B	63[A]	NRQ	CB1-CG1-SD-CE
1	B	63[B]	NRQ	CB1-CG1-SD-CE
1	C	63[A]	NRQ	CB1-CG1-SD-CE
1	A	63[B]	NRQ	CA1-CB1-CG1-SD
1	A	63[A]	NRQ	CB1-CG1-SD-CE
1	A	63[B]	NRQ	CB1-CG1-SD-CE

There are no ring outliers.

8 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63[A]	NRQ	6	0
1	A	63[B]	NRQ	2	0
1	D	63[B]	NRQ	3	0
1	C	63[B]	NRQ	4	0
1	D	63[A]	NRQ	10	0
1	A	63[A]	NRQ	10	0
1	B	63[B]	NRQ	4	0
1	C	63[A]	NRQ	10	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	220/233 (94%)	-0.19	1 (0%) 87 89	14, 24, 41, 60	1 (0%)
1	B	228/233 (97%)	-0.15	4 (1%) 67 71	13, 24, 38, 56	6 (2%)
1	C	227/233 (97%)	-0.07	7 (3%) 51 55	15, 26, 40, 47	7 (3%)
1	D	224/233 (96%)	0.02	3 (1%) 75 78	15, 28, 44, 60	1 (0%)
All	All	899/932 (96%)	-0.10	15 (1%) 69 72	13, 26, 41, 60	15 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	GLY	3.2
1	C	3	ALA	3.0
1	D	2	SER	2.8
1	C	2	SER	2.8
1	D	3	ALA	2.7
1	C	151[A]	ASP	2.5
1	C	231	LYS	2.5
1	D	6	THR	2.4
1	C	23[A]	HIS	2.4
1	B	152	GLY	2.4
1	B	21	ASN	2.3
1	B	151[A]	ASP	2.2
1	B	23[A]	HIS	2.2
1	A	14	TYR	2.1
1	C	14	TYR	2.0

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, 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($\text{\AA}^2$)	Q<0.9
1	NRQ	A	63[A]	23/24	0.93	0.08	17,22,24,31	23
1	NRQ	A	63[B]	23/24	0.93	0.08	15,21,24,30	23
1	NRQ	D	63[A]	23/24	0.94	0.08	21,23,27,32	23
1	NRQ	D	63[B]	23/24	0.94	0.08	20,24,27,29	23
1	NRQ	C	63[A]	23/24	0.95	0.07	18,22,25,32	23
1	NRQ	C	63[B]	23/24	0.95	0.07	18,21,24,29	23
1	NRQ	B	63[A]	23/24	0.95	0.08	17,20,25,30	23
1	NRQ	B	63[B]	23/24	0.95	0.08	18,20,24,29	23

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.