



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:24 PM EDT

PDB ID : 3SVS  
Title : Crystal structure of mkate mutant S158A/S143C at pH 4.0  
Authors : Wang, Q.; Bynres, L.; Sondermann, H.  
Deposited on : 2011-07-12  
Resolution : 1.74 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 : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

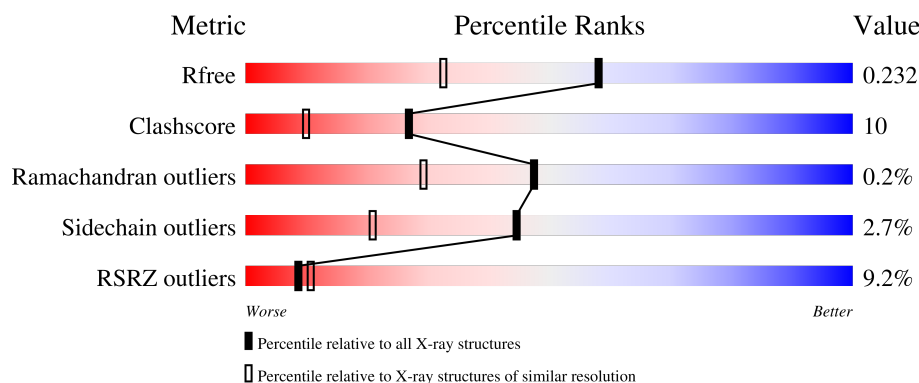
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	233	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	233	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	233	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>
1	D	233	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>• •</div> </div> </div>
1	E	233	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>11%</div> <div>• •</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
1	H	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	H	63[A]	-	-	X	-
1	NRQ	H	63[B]	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16114 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	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			
1	B	226	Total	C	N	O	S	0	2	0
			1816	1156	306	338	16			
1	C	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			
1	D	224	Total	C	N	O	S	0	3	0
			1815	1155	305	339	16			
1	E	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			
1	F	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			
1	G	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			
1	H	223	Total	C	N	O	S	0	2	0
			1801	1147	303	335	16			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	255	Total	O	0	0
			255	255		
2	B	261	Total	O	0	0
			261	261		
2	C	261	Total	O	0	0
			261	261		
2	D	239	Total	O	0	0
			239	239		
2	E	201	Total	O	0	0
			201	201		
2	F	181	Total	O	0	0
			181	181		

*Continued on next page...*

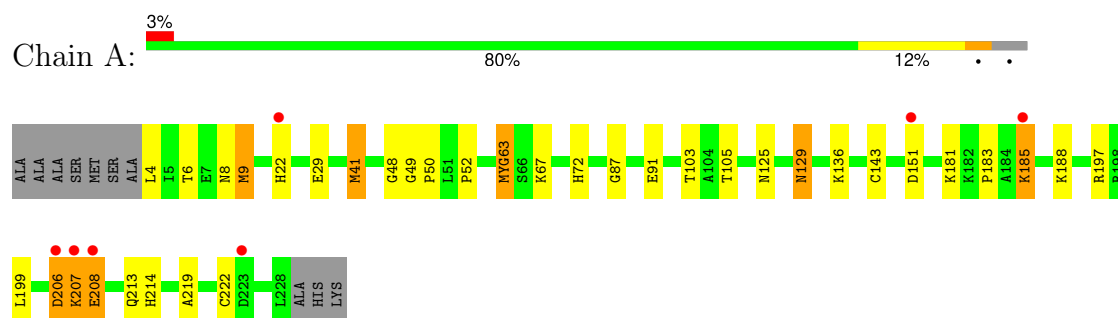
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	143	Total 143	O 143	0	0
2	H	136	Total 136	O 136	0	0

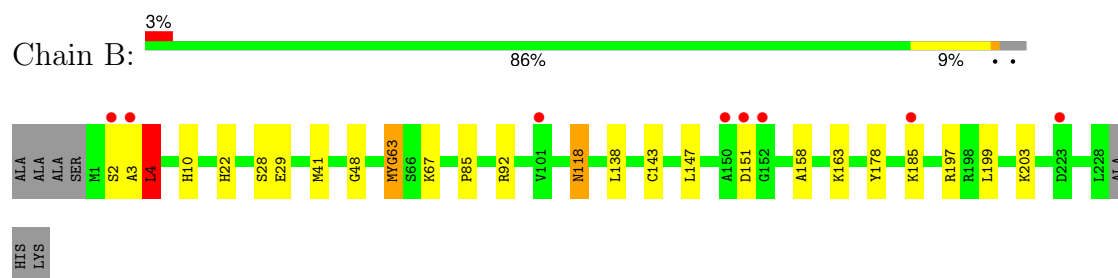
### 3 Residue-property plots

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.

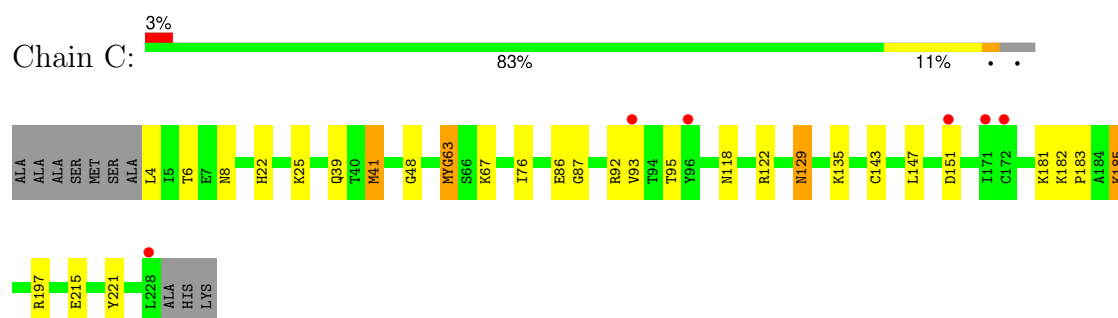
#### • Molecule 1: mKate S158A/S143C



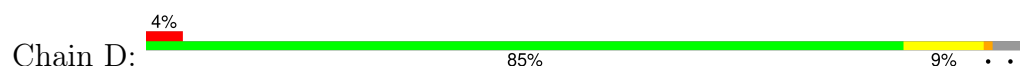
#### • Molecule 1: mKate S158A/S143C



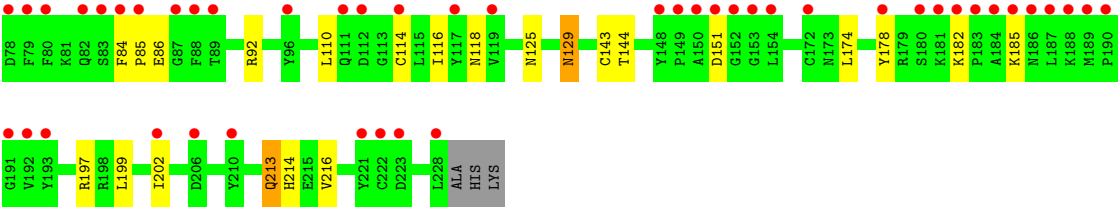
#### • Molecule 1: mKate S158A/S143C



#### • Molecule 1: mKate S158A/S143C









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.71Å 101.97Å 276.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.97 – 1.74 43.97 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.97-1.74) 99.2 (43.97-1.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 1.74Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.199 , 0.236 0.195 , 0.232	Depositor DCC
$R_{free}$ test set	10037 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.8	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	0.95	EDS
Total number of atoms	16114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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: 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	0.42	0/1797	0.60	0/2424
1	B	0.39	0/1812	0.59	0/2445
1	C	0.40	0/1797	0.58	0/2424
1	D	0.36	0/1811	0.56	0/2443
1	E	0.36	0/1797	0.54	0/2424
1	F	0.33	0/1797	0.53	0/2424
1	G	0.33	0/1797	0.50	0/2424
1	H	0.31	0/1797	0.51	0/2424
All	All	0.36	0/14405	0.55	0/19432

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 [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	1801	0	1764	48	0
1	B	1816	0	1776	31	0
1	C	1801	0	1764	32	0
1	D	1815	0	1774	27	0
1	E	1801	0	1764	27	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1801	0	1764	29	0
1	G	1801	0	1764	37	0
1	H	1801	0	1765	66	0
2	A	255	0	0	5	0
2	B	261	0	0	4	0
2	C	261	0	0	6	0
2	D	239	0	0	2	0
2	E	201	0	0	2	0
2	F	181	0	0	3	0
2	G	143	0	0	2	0
2	H	136	0	0	1	0
All	All	16114	0	14135	290	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 10.

All (290) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MET:HE2	1:A:9:MET:HA	1.18	1.15
1:H:63[B]:NRQ:HD2	1:H:63[B]:NRQ:O2	1.55	1.06
1:H:63[B]:NRQ:HE2A	1:H:213:GLN:HB3	1.41	1.01
1:A:41:MET:HG3	1:A:63[B]:NRQ:HE1A	1.44	0.98
1:B:28:SER:HB2	1:B:41:MET:HE3	1.50	0.94
1:D:41:MET:HG3	1:D:63[A]:NRQ:HE1A	1.54	0.90
1:F:41:MET:HG3	1:F:63[B]:NRQ:HE1A	1.55	0.88
1:B:67:LYS:NZ	1:B:197:ARG:HH22	1.71	0.87
1:A:41:MET:HG3	1:A:63[A]:NRQ:HE1A	1.61	0.83
1:C:63[A]:NRQ:OH	1:C:143[A]:CYS:SG	2.38	0.81
1:F:134:GLN:HG3	2:F:1047:HOH:O	1.80	0.81
1:E:63[B]:NRQ:HD2	1:E:63[B]:NRQ:O2	1.81	0.81
1:A:63[B]:NRQ:HD2	1:A:63[B]:NRQ:O2	1.83	0.78
1:H:63[B]:NRQ:O2	1:H:63[B]:NRQ:CD2	2.30	0.78
1:F:67:LYS:NZ	1:F:197:ARG:HH22	1.82	0.77
1:F:63[B]:NRQ:HD2	1:F:63[B]:NRQ:O2	1.84	0.77
1:H:63[B]:NRQ:C3	1:H:63[B]:NRQ:N1	2.47	0.77
1:D:41:MET:HG3	1:D:63[A]:NRQ:CE	2.15	0.77
1:E:67:LYS:NZ	1:E:197:ARG:HH22	1.83	0.76
1:F:63[B]:NRQ:C3	1:F:63[B]:NRQ:N1	2.47	0.76
1:C:67:LYS:NZ	1:C:197:ARG:HH22	1.82	0.76
1:E:39:GLN:HG3	1:E:63[A]:NRQ:HE2A	1.67	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LYS:NZ	1:D:197:ARG:HH22	1.83	0.76
1:C:63[B]:NRQ:HD2	1:C:63[B]:NRQ:O2	1.86	0.76
1:B:28:SER:HB2	1:B:41:MET:CE	2.17	0.74
1:G:47:GLU:CG	1:H:12:LYS:HD3	2.18	0.74
1:B:3:ALA:O	1:B:4:LEU:HB2	1.86	0.74
1:H:12:LYS:HE2	1:H:116:ILE:HD11	1.68	0.74
1:G:182:LYS:HG3	1:G:183:PRO:HD2	1.69	0.73
1:H:63[A]:NRQ:CD2	1:H:199:LEU:HD12	2.18	0.73
1:F:63[A]:NRQ:N1	1:F:63[A]:NRQ:HA31	2.04	0.73
1:A:63[A]:NRQ:OH	1:A:143[A]:CYS:SG	2.48	0.72
1:H:63[A]:NRQ:CE2	1:H:199:LEU:HD12	2.19	0.72
1:H:67:LYS:NZ	1:H:197:ARG:HH22	1.88	0.71
1:H:67:LYS:HZ1	1:H:197:ARG:HH22	1.38	0.71
1:F:67:LYS:HZ1	1:F:197:ARG:HH22	1.39	0.71
1:H:63[B]:NRQ:CE2	1:H:92:ARG:NH2	2.53	0.70
1:C:129:ASN:HD22	1:C:129:ASN:H	1.38	0.70
1:D:63[A]:NRQ:OH	1:D:143[A]:CYS:SG	2.48	0.70
1:E:63[B]:NRQ:C3	1:E:63[B]:NRQ:N1	2.55	0.70
1:G:63[B]:NRQ:HD2	1:G:63[B]:NRQ:O2	1.91	0.70
1:E:9:MET:HE3	1:E:9:MET:HA	1.73	0.69
1:C:63[B]:NRQ:C3	1:C:63[B]:NRQ:N1	2.55	0.69
1:F:41:MET:HG3	1:F:63[A]:NRQ:HE1A	1.74	0.69
1:D:63[B]:NRQ:N1	1:D:63[B]:NRQ:C3	2.56	0.69
1:H:12:LYS:CE	1:H:116:ILE:HD11	2.24	0.68
1:B:28:SER:CB	1:B:41:MET:HE3	2.21	0.68
1:B:63[B]:NRQ:HD2	1:B:63[B]:NRQ:O2	1.94	0.68
1:A:9:MET:HE2	1:A:9:MET:CA	2.07	0.67
1:A:129:ASN:HD22	1:A:129:ASN:H	1.40	0.67
1:C:67:LYS:HZ2	1:C:197:ARG:HH22	1.40	0.67
1:F:91:GLU:HG2	1:F:105:THR:HG22	1.77	0.67
1:B:67:LYS:HZ2	1:B:197:ARG:HH22	1.42	0.67
1:B:67:LYS:HZ3	1:B:197:ARG:HH22	1.41	0.67
1:B:28:SER:CB	1:B:41:MET:CE	2.74	0.66
1:F:9:MET:HE3	1:F:9:MET:HA	1.78	0.66
1:G:9:MET:HA	1:G:9:MET:HE2	1.77	0.66
1:B:63[B]:NRQ:N1	1:B:63[B]:NRQ:C3	2.59	0.66
1:G:8:ASN:O	1:G:9:MET:HE3	1.97	0.65
1:H:41:MET:HG3	1:H:63[A]:NRQ:HE1A	1.79	0.65
1:G:63[B]:NRQ:N1	1:G:63[B]:NRQ:C3	2.59	0.65
1:H:63[B]:NRQ:HE1	1:H:174:LEU:HD22	1.78	0.65
1:E:67:LYS:HZ2	1:E:197:ARG:HH22	1.42	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:MET:HG3	1:G:63[A]:NRQ:HE2A	1.80	0.65
1:H:41:MET:HG3	1:H:63[A]:NRQ:CE	2.26	0.64
1:A:129:ASN:H	1:A:129:ASN:ND2	1.94	0.64
1:H:63[A]:NRQ:HE2	1:H:199:LEU:HB2	1.79	0.64
1:C:39:GLN:HG3	1:C:63[A]:NRQ:HE2A	1.81	0.63
1:D:63[A]:NRQ:HG11	1:D:215:GLU:OE1	1.98	0.63
1:G:63[A]:NRQ:OH	1:G:143[A]:CYS:SG	2.56	0.63
1:E:63[A]:NRQ:OH	1:E:143[A]:CYS:SG	2.54	0.62
1:B:28:SER:OG	1:B:41:MET:HE1	2.00	0.62
1:B:28:SER:OG	1:B:41:MET:CE	2.48	0.62
1:D:63[B]:NRQ:HD2	1:D:63[B]:NRQ:O2	1.99	0.62
1:G:9:MET:HA	1:G:9:MET:CE	2.29	0.62
1:H:63[B]:NRQ:HE1	1:H:174:LEU:CD2	2.29	0.61
1:H:63[A]:NRQ:HE2	1:H:199:LEU:HD12	1.81	0.61
1:A:67:LYS:NZ	1:A:197:ARG:HH22	1.99	0.61
1:B:63[A]:NRQ:OH	1:B:143[A]:CYS:SG	2.57	0.60
1:F:22:HIS:HE1	1:F:48:GLY:O	1.83	0.60
1:C:135:LYS:HE3	2:C:1486:HOH:O	2.00	0.60
1:H:63[A]:NRQ:HD2	1:H:199:LEU:HD12	1.81	0.60
1:F:63[A]:NRQ:OH	1:F:143[A]:CYS:SG	2.57	0.60
1:G:41:MET:HG3	1:G:63[A]:NRQ:CE	2.32	0.60
1:G:47:GLU:HG2	1:H:12:LYS:HD3	1.82	0.60
1:H:63[B]:NRQ:OH	1:H:174:LEU:HD23	2.02	0.59
1:A:206:ASP:CG	2:A:1475:HOH:O	2.41	0.59
1:C:22:HIS:HE1	1:C:48:GLY:O	1.85	0.58
1:E:214:HIS:HD2	2:E:649:HOH:O	1.85	0.58
1:D:67:LYS:HZ2	1:D:197:ARG:HH22	1.49	0.58
1:F:41:MET:HG3	1:F:63[B]:NRQ:CE	2.30	0.58
1:G:63[A]:NRQ:HG11	1:G:215:GLU:OE1	2.04	0.58
1:D:214:HIS:HD2	2:D:255:HOH:O	1.86	0.58
1:H:4:LEU:HD23	1:H:110:LEU:HD23	1.85	0.58
1:B:2:SER:O	1:B:3:ALA:HB2	2.03	0.58
1:G:67:LYS:NZ	1:G:197:ARG:HH22	2.01	0.58
2:B:275:HOH:O	1:D:105:THR:HG23	2.04	0.57
1:H:22:HIS:HE1	1:H:48:GLY:O	1.87	0.57
1:H:129:ASN:H	1:H:129:ASN:ND2	2.01	0.57
1:A:188:LYS:HG3	2:A:1465:HOH:O	2.04	0.57
1:H:63[B]:NRQ:HE2	1:H:92:ARG:NH2	2.18	0.57
1:B:63[A]:NRQ:HE1	1:B:143[A]:CYS:SG	2.44	0.57
1:G:39:GLN:HE22	1:G:66:SER:HB3	1.69	0.57
1:C:4:LEU:N	2:C:1007:HOH:O	2.38	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63[A]:NRQ:N2	1:F:63[A]:NRQ:HD2	2.20	0.56
1:F:9:MET:HE1	1:F:113:GLY:O	2.06	0.56
1:H:63[B]:NRQ:CE1	1:H:174:LEU:CD2	2.84	0.56
1:H:63[B]:NRQ:HB2	1:H:197:ARG:CD	2.36	0.56
1:A:63[A]:NRQ:HE3	1:A:213:GLN:HE21	1.71	0.56
1:A:63[A]:NRQ:N1	1:A:63[A]:NRQ:HA31	2.21	0.56
1:E:9:MET:HE1	1:E:113:GLY:O	2.06	0.56
1:C:41:MET:HG3	1:C:63[A]:NRQ:HE3	1.87	0.55
1:C:86:GLU:OE2	1:C:182:LYS:HE3	2.07	0.55
1:A:63[B]:NRQ:HE3	1:A:213:GLN:HE21	1.71	0.55
1:H:63[A]:NRQ:N1	1:H:63[A]:NRQ:HA31	2.21	0.55
1:C:41:MET:HG3	1:C:63[A]:NRQ:CE	2.36	0.55
1:E:39:GLN:HG3	1:E:63[B]:NRQ:HE2A	1.88	0.55
1:G:7:GLU:HG2	1:G:8:ASN:ND2	2.21	0.55
1:H:13:LEU:HB3	1:H:28:SER:OG	2.06	0.55
1:D:22:HIS:HE1	1:D:48:GLY:O	1.89	0.55
1:A:105:THR:HG23	2:C:277:HOH:O	2.07	0.55
1:B:63[A]:NRQ:N1	1:B:63[A]:NRQ:HA31	2.21	0.55
1:C:182:LYS:HG3	1:C:183:PRO:HD2	1.87	0.55
1:B:118:ASN:HB2	2:B:970:HOH:O	2.07	0.54
1:G:138:LEU:O	1:G:163:LYS:HE3	2.07	0.54
1:H:63[B]:NRQ:HE2A	1:H:213:GLN:HE21	1.73	0.54
1:H:63[B]:NRQ:CE	1:H:213:GLN:HE21	2.19	0.54
1:A:125:ASN:OD1	1:C:93:VAL:HG12	2.07	0.54
1:C:129:ASN:H	1:C:129:ASN:ND2	2.05	0.54
1:H:63[A]:NRQ:HE3	1:H:213:GLN:HE21	1.74	0.54
1:C:41:MET:HG3	1:C:63[B]:NRQ:CE	2.38	0.53
1:F:13:LEU:HB3	1:F:28:SER:OG	2.08	0.53
2:C:1186:HOH:O	1:E:7:GLU:HG2	2.07	0.53
1:E:140:TRP:CZ3	1:E:162:LEU:HB2	2.44	0.53
1:B:22:HIS:HE1	1:B:48:GLY:O	1.91	0.53
1:A:63[B]:NRQ:HE2A	1:A:213:GLN:HB2	1.91	0.53
1:A:49:GLY:HA2	1:A:50:PRO:C	2.30	0.52
1:A:103:THR:HG21	1:C:122:ARG:HG2	1.90	0.52
1:D:63[A]:NRQ:HE1	1:D:143[A]:CYS:SG	2.50	0.52
1:A:214:HIS:HD2	2:A:258:HOH:O	1.91	0.52
1:C:41:MET:HG3	1:C:63[B]:NRQ:HE3	1.91	0.51
1:F:182:LYS:HG3	1:F:183:PRO:HD2	1.92	0.51
1:A:22:HIS:HE1	1:A:48:GLY:O	1.93	0.51
1:H:37:GLY:O	1:H:216:VAL:HA	2.10	0.51
1:C:95:THR:HG23	2:C:1325:HOH:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:LYS:HZ3	1:D:197:ARG:HH22	1.58	0.51
1:A:199:LEU:HD23	1:A:199:LEU:C	2.32	0.51
1:A:67:LYS:HZ2	1:A:197:ARG:HH22	1.59	0.50
1:E:16:GLU:HG3	1:E:25:LYS:HG2	1.93	0.50
1:E:41:MET:HG3	1:E:63[A]:NRQ:CE	2.41	0.50
1:F:41:MET:HG3	1:F:63[A]:NRQ:CE	2.34	0.50
1:G:47:GLU:OE1	1:H:10:HIS:HE1	1.94	0.50
1:G:183:PRO:HB2	1:G:186:ASN:HD22	1.76	0.50
1:D:86:GLU:OE2	1:D:182:LYS:HE3	2.11	0.50
1:F:214:HIS:HD2	2:F:933:HOH:O	1.94	0.50
1:G:47:GLU:CD	1:H:12:LYS:HD3	2.32	0.50
1:A:63[A]:NRQ:CE	1:A:213:GLN:HE21	2.26	0.49
1:A:91:GLU:OE2	1:A:105:THR:HG22	2.12	0.49
1:H:63[B]:NRQ:OH	1:H:174:LEU:CD2	2.61	0.49
1:A:9:MET:HE1	2:A:1479:HOH:O	2.12	0.49
1:A:63[B]:NRQ:C3	1:A:63[B]:NRQ:N1	2.76	0.48
1:A:129:ASN:HD22	1:A:129:ASN:N	2.11	0.48
1:E:63[A]:NRQ:N1	1:E:63[A]:NRQ:C3	2.76	0.48
1:A:63[B]:NRQ:CE	1:A:213:GLN:HE21	2.25	0.48
1:B:28:SER:CB	1:B:41:MET:HE1	2.43	0.48
1:H:41:MET:HB2	1:H:63[A]:NRQ:HE2A	1.95	0.48
1:H:67:LYS:NZ	1:H:197:ARG:NH2	2.57	0.48
1:H:202:ILE:HD11	1:H:214:HIS:HB3	1.96	0.48
1:G:29:GLU:OE2	1:G:42:ARG:NH2	2.39	0.48
1:A:207:LYS:O	1:A:208:GLU:HB2	2.14	0.47
1:F:183:PRO:HB2	1:F:186:ASN:ND2	2.29	0.47
1:F:118:ASN:HB2	2:F:1000:HOH:O	2.13	0.47
1:H:63[A]:NRQ:OH	1:H:143[A]:CYS:SG	2.65	0.47
1:H:84:PHE:HB3	1:H:85:PRO:HA	1.97	0.47
1:G:72:HIS:HA	1:G:219:ALA:HB3	1.97	0.47
1:B:10:HIS:HD2	2:B:1357:HOH:O	1.98	0.47
1:H:63[B]:NRQ:HB2	1:H:197:ARG:NE	2.30	0.47
1:B:63[A]:NRQ:HD2	1:B:63[A]:NRQ:N2	2.31	0.46
1:C:63[B]:NRQ:SD	1:C:215:GLU:HB2	2.55	0.46
1:H:63[B]:NRQ:HB2	1:H:197:ARG:HD3	1.96	0.46
1:A:22:HIS:CE1	1:A:48:GLY:O	2.68	0.46
1:G:206:ASP:HB2	1:G:209:THR:OG1	2.15	0.46
1:A:207:LYS:O	1:A:208:GLU:CB	2.63	0.46
1:E:22:HIS:HE1	1:E:48:GLY:O	1.98	0.46
1:A:9:MET:HA	1:A:9:MET:CE	2.13	0.46
1:A:206:ASP:O	1:A:208:GLU:N	2.49	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:HD23	1:B:85:PRO:HB3	1.98	0.46
1:B:138:LEU:O	1:B:163:LYS:HE3	2.14	0.46
1:B:147:LEU:HD12	1:B:147:LEU:N	2.30	0.46
1:F:62:PHE:HB2	1:F:63[B]:NRQ:HB11	1.98	0.46
1:G:63[B]:NRQ:CZ	1:G:174:LEU:HD22	2.46	0.46
1:G:140:TRP:CZ3	1:G:162:LEU:HB2	2.51	0.46
1:C:6:THR:OG1	1:C:8:ASN:O	2.34	0.45
1:G:86:GLU:OE2	1:G:182:LYS:HE2	2.16	0.45
1:A:136:LYS:HD2	2:A:963:HOH:O	2.15	0.45
1:A:63[A]:NRQ:HE3	1:A:213:GLN:NE2	2.31	0.45
1:F:9:MET:HE3	1:F:9:MET:CA	2.46	0.45
1:G:97:GLU:HG3	1:G:171:ILE:O	2.17	0.45
1:A:206:ASP:O	1:A:207:LYS:C	2.55	0.45
1:E:37:GLY:O	1:E:216:VAL:HA	2.16	0.45
1:H:4:LEU:N	2:H:399:HOH:O	2.49	0.45
1:H:34:PRO:HA	1:H:69:PHE:HA	1.98	0.45
1:A:72:HIS:HA	1:A:219:ALA:HB3	1.99	0.45
1:D:3:ALA:O	1:D:4:LEU:CB	2.65	0.45
1:E:41:MET:HG3	1:E:63[B]:NRQ:HE3	1.99	0.44
1:G:13:LEU:HB3	1:G:28:SER:OG	2.18	0.44
1:B:67:LYS:HE2	1:B:178:TYR:CE1	2.52	0.44
1:B:118:ASN:ND2	2:B:970:HOH:O	2.49	0.44
1:H:39:GLN:NE2	1:H:69:PHE:HB2	2.32	0.44
1:D:22:HIS:HD2	2:D:1420:HOH:O	2.00	0.44
1:D:136:LYS:HE2	1:D:136:LYS:HB3	1.76	0.44
1:E:11:MET:N	1:E:11:MET:HE3	2.33	0.44
1:E:22:HIS:HD2	2:E:1664:HOH:O	2.01	0.43
1:F:34:PRO:HA	1:F:69:PHE:HA	2.00	0.43
1:C:4:LEU:N	1:C:4:LEU:HD12	2.33	0.43
1:D:125:ASN:N	1:D:125:ASN:HD22	2.15	0.43
1:G:37:GLY:HA2	1:G:69:PHE:O	2.17	0.43
1:H:63[A]:NRQ:HE3	1:H:213:GLN:NE2	2.32	0.43
1:G:63[A]:NRQ:HE1	1:G:143[A]:CYS:SG	2.58	0.43
1:G:76:ILE:HG12	1:G:221:TYR:CZ	2.54	0.43
1:B:143[B]:CYS:SG	1:B:158:ALA:HB1	2.58	0.43
1:E:63[B]:NRQ:HD2	1:E:92:ARG:NH2	2.33	0.43
1:H:63[B]:NRQ:CZ	1:H:174:LEU:HD23	2.49	0.43
1:H:86:GLU:OE2	1:H:182:LYS:HE3	2.19	0.43
1:C:185:LYS:H	1:C:185:LYS:HG3	1.71	0.43
1:D:3:ALA:C	1:D:5:ILE:H	2.22	0.43
1:G:162:LEU:HB3	2:G:1129:HOH:O	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:143[B]:CYS:SG	1:H:144:THR:N	2.92	0.43
1:A:129:ASN:ND2	1:A:129:ASN:N	2.65	0.43
1:H:16:GLU:HG2	1:H:17:GLY:N	2.34	0.42
1:A:41:MET:HE2	1:A:41:MET:HB3	1.81	0.42
1:E:41:MET:HG3	1:E:63[B]:NRQ:CE	2.48	0.42
1:F:4:LEU:HD12	1:F:4:LEU:HA	1.83	0.42
1:G:33:LYS:HD3	1:G:36:GLU:CD	2.39	0.42
1:C:25:LYS:HE2	2:C:1521:HOH:O	2.19	0.42
1:C:67:LYS:HZ3	1:C:197:ARG:HH22	1.63	0.42
1:C:87:GLY:C	1:C:181:LYS:HE3	2.40	0.42
1:A:63[A]:NRQ:N2	1:A:63[A]:NRQ:HD2	2.35	0.42
1:H:41:MET:HE2	1:H:41:MET:HB3	1.94	0.42
1:H:63[A]:NRQ:HD2	1:H:63[A]:NRQ:N2	2.35	0.42
1:A:6:THR:OG1	1:A:8:ASN:O	2.35	0.42
1:H:12:LYS:HB2	1:H:116:ILE:HD13	2.00	0.42
1:C:76:ILE:HG12	1:C:221:TYR:CZ	2.55	0.42
1:H:63[A]:NRQ:HE1	1:H:143[A]:CYS:SG	2.60	0.42
1:E:4:LEU:HD12	1:E:4:LEU:HA	1.92	0.42
1:F:13:LEU:C	1:F:13:LEU:HD23	2.40	0.42
1:G:204:GLU:HA	1:G:210:TYR:O	2.19	0.42
1:C:63[B]:NRQ:HD2	1:C:92:ARG:NH2	2.35	0.42
1:D:185:LYS:H	1:D:185:LYS:HG3	1.59	0.41
1:E:67:LYS:HZ3	1:E:197:ARG:HH22	1.62	0.41
1:G:67:LYS:HZ2	1:G:197:ARG:HH22	1.67	0.41
1:E:49:GLY:HA2	1:E:50:PRO:C	2.41	0.41
1:F:63[A]:NRQ:HE1	1:F:143[A]:CYS:SG	2.60	0.41
1:H:18:THR:HA	1:H:22:HIS:O	2.20	0.41
1:A:206:ASP:C	1:A:208:GLU:N	2.69	0.41
1:B:2:SER:O	1:B:3:ALA:CB	2.67	0.41
1:D:41:MET:HE2	1:D:41:MET:HB3	1.91	0.41
1:D:72:HIS:HA	1:D:219:ALA:HB3	2.02	0.41
1:G:90:TRP:CE2	1:G:106:GLN:CB	3.03	0.41
1:A:91:GLU:OE2	1:A:105:THR:CG2	2.68	0.41
1:H:129:ASN:ND2	1:H:129:ASN:N	2.68	0.41
1:A:63[A]:NRQ:HE1	1:A:143[A]:CYS:SG	2.61	0.41
1:G:47:GLU:CB	1:H:12:LYS:HD3	2.50	0.41
1:H:63[B]:NRQ:HE2	1:H:178:TYR:OH	2.19	0.41
1:A:87:GLY:C	1:A:181:LYS:HE3	2.41	0.41
1:A:183:PRO:HB2	1:A:185:LYS:HG3	2.03	0.41
1:B:63[B]:NRQ:HD2	1:B:92:ARG:NH2	2.36	0.41
1:E:129:ASN:HA	1:E:134:GLN:HE21	1.85	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:LYS:HG3	1:H:114:CYS:SG	2.61	0.41
1:D:4:LEU:HD21	1:D:85:PRO:HB3	2.02	0.41
1:D:147:LEU:N	1:D:147:LEU:HD12	2.34	0.41
1:C:39:GLN:HG3	1:C:63[A]:NRQ:CE	2.50	0.41
1:C:63[A]:NRQ:N1	1:C:63[A]:NRQ:HA31	2.36	0.41
1:D:41:MET:HG3	1:D:63[B]:NRQ:CE	2.50	0.41
1:D:137:THR:HG21	1:D:162:LEU:HD21	2.03	0.41
1:F:76:ILE:HG12	1:F:221:TYR:CZ	2.55	0.41
1:A:22:HIS:CD2	1:A:52:PRO:HG3	2.57	0.40
1:B:199:LEU:C	1:B:199:LEU:HD23	2.41	0.40
1:H:12:LYS:HB2	1:H:116:ILE:CD1	2.51	0.40
1:D:185:LYS:HB2	1:D:185:LYS:HE2	1.85	0.40
1:E:39:GLN:HE22	1:E:66:SER:HB3	1.85	0.40
1:H:39:GLN:HE22	1:H:66:SER:HB3	1.87	0.40
1:H:41:MET:HG3	1:H:63[A]:NRQ:HE2A	2.02	0.40
1:B:203:LYS:HE2	1:B:203:LYS:HB3	1.85	0.40
1:F:138:LEU:O	1:F:163:LYS:HE3	2.21	0.40
1:G:9:MET:HE2	2:G:248:HOH:O	2.21	0.40
1:H:62:PHE:HB2	1:H:63[B]:NRQ:HB11	2.03	0.40
1:H:182:LYS:HE3	1:H:182:LYS:HB2	1.82	0.40
1:C:147:LEU:HD12	1:C:147:LEU:N	2.36	0.40
1:H:41:MET:HG3	1:H:63[B]:NRQ:HE1A	2.03	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	219/233 (94%)	212 (97%)	4 (2%)	3 (1%)	11	2
1	B	222/233 (95%)	218 (98%)	3 (1%)	1 (0%)	29	12
1	C	219/233 (94%)	217 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	221/233 (95%)	219 (99%)	2 (1%)	0	100	100
1	E	219/233 (94%)	218 (100%)	1 (0%)	0	100	100
1	F	219/233 (94%)	215 (98%)	4 (2%)	0	100	100
1	G	219/233 (94%)	216 (99%)	3 (1%)	0	100	100
1	H	219/233 (94%)	215 (98%)	4 (2%)	0	100	100
All	All	1757/1864 (94%)	1730 (98%)	23 (1%)	4 (0%)	47	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	208	GLU
1	B	4	LEU
1	A	206	ASP

### 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	191/195 (98%)	183 (96%)	8 (4%)	30	9
1	B	191/195 (98%)	186 (97%)	5 (3%)	46	22
1	C	191/195 (98%)	186 (97%)	5 (3%)	46	22
1	D	192/195 (98%)	189 (98%)	3 (2%)	62	44
1	E	191/195 (98%)	185 (97%)	6 (3%)	40	16
1	F	191/195 (98%)	187 (98%)	4 (2%)	53	30
1	G	191/195 (98%)	188 (98%)	3 (2%)	62	44
1	H	191/195 (98%)	184 (96%)	7 (4%)	34	11
All	All	1529/1560 (98%)	1488 (97%)	41 (3%)	44	21

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	9	MET
1	A	29	GLU
1	A	41	MET
1	A	129	ASN
1	A	151	ASP
1	A	185	LYS
1	A	222	CYS
1	B	4	LEU
1	B	29	GLU
1	B	118	ASN
1	B	151	ASP
1	B	185	LYS
1	C	41	MET
1	C	118	ASN
1	C	129	ASN
1	C	151	ASP
1	C	185	LYS
1	D	41	MET
1	D	118	ASN
1	D	185	LYS
1	E	4	LEU
1	E	11	MET
1	E	29	GLU
1	E	41	MET
1	E	118	ASN
1	E	135	LYS
1	F	41	MET
1	F	118	ASN
1	F	125	ASN
1	F	185	LYS
1	G	9	MET
1	G	41	MET
1	G	185	LYS
1	H	29	GLU
1	H	118	ASN
1	H	125	ASN
1	H	129	ASN
1	H	151	ASP
1	H	185	LYS
1	H	213	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	111	GLN
1	A	213	GLN
1	A	214	HIS
1	B	22	HIS
1	B	118	ASN
1	B	125	ASN
1	C	22	HIS
1	C	129	ASN
1	D	21	ASN
1	D	22	HIS
1	D	125	ASN
1	D	213	GLN
1	D	214	HIS
1	E	10	HIS
1	E	22	HIS
1	E	214	HIS
1	F	22	HIS
1	F	125	ASN
1	F	214	HIS
1	G	22	HIS
1	G	186	ASN
1	G	214	HIS
1	H	10	HIS
1	H	22	HIS
1	H	23	HIS
1	H	213	GLN
1	H	214	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 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[A]	1	24,24,25	3.26	4 (16%)	24,32,34	3.01	11 (45%)
1	NRQ	C	63[A]	1	24,24,25	3.34	4 (16%)	24,32,34	2.84	11 (45%)
1	NRQ	C	63[B]	1	24,24,25	3.36	4 (16%)	24,32,34	2.39	11 (45%)
1	NRQ	H	63[B]	1	24,24,25	5.40	8 (33%)	24,32,34	4.25	6 (25%)
1	NRQ	D	63[A]	1	24,24,25	3.36	4 (16%)	24,32,34	3.17	13 (54%)
1	NRQ	B	63[B]	1	24,24,25	3.39	4 (16%)	24,32,34	2.40	10 (41%)
1	NRQ	A	63[B]	1	24,24,25	3.37	4 (16%)	24,32,34	2.52	11 (45%)
1	NRQ	E	63[A]	1	24,24,25	3.43	4 (16%)	24,32,34	3.18	12 (50%)
1	NRQ	D	63[B]	1	24,24,25	3.48	4 (16%)	24,32,34	2.59	12 (50%)
1	NRQ	E	63[B]	1	24,24,25	3.43	4 (16%)	24,32,34	2.47	10 (41%)
1	NRQ	F	63[A]	1	24,24,25	3.39	4 (16%)	24,32,34	3.02	9 (37%)
1	NRQ	G	63[A]	1	24,24,25	3.37	4 (16%)	24,32,34	3.28	13 (54%)
1	NRQ	F	63[B]	1	24,24,25	3.41	4 (16%)	24,32,34	2.46	10 (41%)
1	NRQ	H	63[A]	1	24,24,25	3.26	4 (16%)	24,32,34	3.02	12 (50%)
1	NRQ	G	63[B]	1	24,24,25	3.47	4 (16%)	24,32,34	2.44	10 (41%)
1	NRQ	B	63[A]	1	24,24,25	3.27	4 (16%)	24,32,34	2.96	10 (41%)

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[A]	1	-	1/9/31/32	0/2/2/2
1	NRQ	C	63[A]	1	-	0/9/31/32	0/2/2/2
1	NRQ	C	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	H	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	D	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	A	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	E	63[A]	1	-	3/9/31/32	0/2/2/2
1	NRQ	D	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	E	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	F	63[A]	1	-	3/9/31/32	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	G	63[A]	1	-	2/9/31/32	0/2/2/2
1	NRQ	F	63[B]	1	-	5/9/31/32	0/2/2/2
1	NRQ	H	63[A]	1	-	1/9/31/32	0/2/2/2
1	NRQ	G	63[B]	1	-	4/9/31/32	0/2/2/2
1	NRQ	B	63[A]	1	-	1/9/31/32	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	63[B]	NRQ	CB2-CA2	18.73	1.53	1.35
1	D	63[B]	NRQ	CB2-CA2	12.06	1.46	1.35
1	H	63[B]	NRQ	CA2-C2	-11.85	1.35	1.48
1	E	63[B]	NRQ	CB2-CA2	11.74	1.46	1.35
1	F	63[B]	NRQ	CB2-CA2	11.74	1.46	1.35
1	A	63[B]	NRQ	CB2-CA2	11.67	1.46	1.35
1	G	63[B]	NRQ	CB2-CA2	11.62	1.46	1.35
1	B	63[B]	NRQ	CB2-CA2	11.60	1.46	1.35
1	C	63[B]	NRQ	CB2-CA2	11.33	1.46	1.35
1	F	63[A]	NRQ	CB2-CA2	11.28	1.46	1.35
1	E	63[A]	NRQ	CB2-CA2	10.81	1.45	1.35
1	G	63[A]	NRQ	CB2-CA2	10.80	1.45	1.35
1	C	63[A]	NRQ	CB2-CA2	10.71	1.45	1.35
1	D	63[A]	NRQ	CB2-CA2	10.57	1.45	1.35
1	B	63[A]	NRQ	CB2-CA2	10.47	1.45	1.35
1	H	63[A]	NRQ	CB2-CA2	10.25	1.45	1.35
1	A	63[A]	NRQ	CB2-CA2	10.23	1.45	1.35
1	E	63[A]	NRQ	CA2-C2	-8.77	1.39	1.48
1	D	63[A]	NRQ	CA2-C2	-8.60	1.39	1.48
1	H	63[B]	NRQ	O2-C2	8.53	1.40	1.23
1	G	63[A]	NRQ	CA2-C2	-8.14	1.39	1.48
1	H	63[A]	NRQ	CA2-C2	-8.08	1.39	1.48
1	A	63[A]	NRQ	CA2-C2	-8.06	1.39	1.48
1	C	63[A]	NRQ	CA2-C2	-8.06	1.39	1.48
1	H	63[B]	NRQ	CA1-N1	8.04	1.45	1.27
1	B	63[A]	NRQ	CA2-C2	-7.96	1.39	1.48
1	G	63[B]	NRQ	CA2-C2	-7.75	1.40	1.48
1	F	63[A]	NRQ	CA1-N1	7.75	1.44	1.27
1	G	63[B]	NRQ	CA1-N1	7.68	1.44	1.27
1	D	63[B]	NRQ	CA1-N1	7.62	1.44	1.27
1	E	63[B]	NRQ	CA1-N1	7.61	1.44	1.27
1	D	63[A]	NRQ	CA1-N1	7.60	1.44	1.27
1	F	63[B]	NRQ	CA1-N1	7.60	1.44	1.27

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	63[A]	NRQ	CA1-N1	7.59	1.44	1.27
1	B	63[B]	NRQ	CA1-N1	7.57	1.44	1.27
1	F	63[A]	NRQ	CA2-C2	-7.56	1.40	1.48
1	C	63[B]	NRQ	CA1-N1	7.55	1.44	1.27
1	A	63[B]	NRQ	CA1-N1	7.53	1.44	1.27
1	G	63[A]	NRQ	CA1-N1	7.53	1.44	1.27
1	C	63[A]	NRQ	CA1-N1	7.51	1.44	1.27
1	H	63[A]	NRQ	CA1-N1	7.51	1.44	1.27
1	A	63[A]	NRQ	CA1-N1	7.50	1.44	1.27
1	B	63[A]	NRQ	CA1-N1	7.43	1.44	1.27
1	E	63[B]	NRQ	CA2-C2	-7.37	1.40	1.48
1	D	63[B]	NRQ	CA2-C2	-7.35	1.40	1.48
1	C	63[B]	NRQ	CA2-C2	-7.25	1.40	1.48
1	F	63[B]	NRQ	CA2-C2	-7.17	1.40	1.48
1	B	63[B]	NRQ	CA2-C2	-7.15	1.40	1.48
1	A	63[B]	NRQ	CA2-C2	-6.95	1.41	1.48
1	B	63[B]	NRQ	O2-C2	4.79	1.32	1.23
1	H	63[B]	NRQ	CD2-CG2	4.64	1.48	1.39
1	C	63[B]	NRQ	O2-C2	4.63	1.32	1.23
1	G	63[B]	NRQ	O2-C2	4.61	1.32	1.23
1	F	63[A]	NRQ	O2-C2	4.60	1.32	1.23
1	A	63[B]	NRQ	O2-C2	4.60	1.32	1.23
1	E	63[B]	NRQ	O2-C2	4.51	1.32	1.23
1	B	63[A]	NRQ	O2-C2	4.51	1.32	1.23
1	D	63[B]	NRQ	O2-C2	4.49	1.32	1.23
1	C	63[A]	NRQ	O2-C2	4.47	1.32	1.23
1	G	63[A]	NRQ	O2-C2	4.45	1.32	1.23
1	A	63[A]	NRQ	O2-C2	4.43	1.32	1.23
1	F	63[B]	NRQ	O2-C2	4.42	1.32	1.23
1	H	63[A]	NRQ	O2-C2	4.40	1.32	1.23
1	E	63[A]	NRQ	O2-C2	4.27	1.31	1.23
1	D	63[A]	NRQ	O2-C2	4.07	1.31	1.23
1	H	63[B]	NRQ	C1-CA1	3.58	1.53	1.48
1	H	63[B]	NRQ	CG2-CB2	3.41	1.53	1.46
1	H	63[B]	NRQ	CE1-CZ	2.74	1.44	1.39

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	63[B]	NRQ	CG2-CB2-CA2	-17.19	109.44	129.87
1	F	63[A]	NRQ	CG2-CB2-CA2	-9.58	118.48	129.87
1	H	63[A]	NRQ	CG2-CB2-CA2	-8.36	119.93	129.87

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63[A]	NRQ	CG2-CB2-CA2	-8.36	119.93	129.87
1	B	63[A]	NRQ	CG2-CB2-CA2	-8.26	120.05	129.87
1	H	63[B]	NRQ	O2-C2-CA2	-7.83	126.02	131.02
1	D	63[A]	NRQ	CG2-CB2-CA2	-7.81	120.58	129.87
1	G	63[A]	NRQ	CG2-CB2-CA2	-7.31	121.17	129.87
1	F	63[B]	NRQ	CA2-C2-N3	7.12	109.48	103.50
1	E	63[A]	NRQ	CA2-C2-N3	7.06	109.43	103.50
1	D	63[A]	NRQ	CA2-C2-N3	6.82	109.22	103.50
1	G	63[B]	NRQ	CA2-C2-N3	6.74	109.16	103.50
1	A	63[B]	NRQ	CA2-C2-N3	6.65	109.08	103.50
1	D	63[B]	NRQ	CA2-C2-N3	6.64	109.08	103.50
1	G	63[A]	NRQ	CA2-C2-N3	6.63	109.07	103.50
1	E	63[B]	NRQ	CA2-C2-N3	6.49	108.95	103.50
1	C	63[A]	NRQ	CG2-CB2-CA2	-6.48	122.16	129.87
1	F	63[A]	NRQ	C3-CA3-N3	6.28	126.71	112.43
1	C	63[B]	NRQ	CA2-C2-N3	6.24	108.74	103.50
1	E	63[A]	NRQ	CG2-CB2-CA2	-6.10	122.61	129.87
1	B	63[B]	NRQ	CA2-C2-N3	6.08	108.60	103.50
1	C	63[A]	NRQ	CA2-C2-N3	6.04	108.57	103.50
1	A	63[A]	NRQ	CA2-C2-N3	5.84	108.41	103.50
1	H	63[A]	NRQ	CA2-C2-N3	5.82	108.39	103.50
1	B	63[A]	NRQ	CA2-C2-N3	5.73	108.31	103.50
1	B	63[A]	NRQ	C3-CA3-N3	5.72	125.45	112.43
1	G	63[A]	NRQ	C3-CA3-N3	5.62	125.21	112.43
1	H	63[B]	NRQ	CA2-C2-N3	5.44	108.07	103.50
1	D	63[A]	NRQ	C3-CA3-N3	5.39	124.70	112.43
1	F	63[A]	NRQ	CA2-C2-N3	5.38	108.02	103.50
1	G	63[A]	NRQ	CA3-N3-C1	5.10	138.45	128.39
1	E	63[A]	NRQ	CA3-N3-C1	4.95	138.16	128.39
1	E	63[A]	NRQ	C3-CA3-N3	4.94	123.66	112.43
1	D	63[B]	NRQ	C3-CA3-N3	4.88	123.53	112.43
1	A	63[B]	NRQ	C3-CA3-N3	4.84	123.44	112.43
1	C	63[A]	NRQ	C3-CA3-N3	4.67	123.06	112.43
1	A	63[A]	NRQ	C3-CA3-N3	4.63	122.95	112.43
1	H	63[A]	NRQ	C3-CA3-N3	4.61	122.92	112.43
1	E	63[A]	NRQ	CB2-CA2-C2	-4.50	116.90	122.36
1	C	63[A]	NRQ	CB2-CA2-C2	-4.44	116.97	122.36
1	G	63[B]	NRQ	CA3-N3-C1	4.43	137.13	128.39
1	C	63[B]	NRQ	C3-CA3-N3	4.35	122.33	112.43
1	D	63[B]	NRQ	CA3-N3-C1	4.33	136.92	128.39
1	E	63[A]	NRQ	CB2-CA2-N2	4.29	134.59	128.76
1	E	63[B]	NRQ	C3-CA3-N3	4.29	122.19	112.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	63[A]	NRQ	CA3-N3-C1	4.26	136.78	128.39
1	B	63[B]	NRQ	C3-CA3-N3	4.22	122.02	112.43
1	H	63[A]	NRQ	CB2-CA2-C2	-4.16	117.31	122.36
1	A	63[A]	NRQ	CB2-CA2-C2	-4.15	117.33	122.36
1	F	63[B]	NRQ	CA3-N3-C1	4.09	136.45	128.39
1	E	63[B]	NRQ	CA3-N3-C1	4.08	136.44	128.39
1	G	63[B]	NRQ	C3-CA3-N3	4.08	121.72	112.43
1	C	63[B]	NRQ	CA3-N3-C1	4.05	136.37	128.39
1	B	63[A]	NRQ	CB2-CA2-C2	-4.04	117.46	122.36
1	C	63[A]	NRQ	CB2-CA2-N2	4.03	134.23	128.76
1	H	63[A]	NRQ	CD1-CE1-CZ	-3.85	115.81	119.88
1	A	63[A]	NRQ	CD1-CE1-CZ	-3.84	115.82	119.88
1	D	63[A]	NRQ	CB2-CA2-C2	-3.82	117.72	122.36
1	G	63[A]	NRQ	CB2-CA2-C2	-3.82	117.72	122.36
1	H	63[B]	NRQ	N3-C1-N2	-3.76	108.15	112.62
1	G	63[A]	NRQ	O2-C2-CA2	3.73	133.40	131.02
1	B	63[B]	NRQ	CD1-CE1-CZ	-3.67	116.00	119.88
1	A	63[B]	NRQ	CD1-CE1-CZ	-3.66	116.00	119.88
1	B	63[B]	NRQ	CA3-N3-C1	3.66	135.60	128.39
1	F	63[B]	NRQ	C3-CA3-N3	3.62	120.67	112.43
1	D	63[A]	NRQ	CB2-CA2-N2	3.60	133.65	128.76
1	A	63[B]	NRQ	CA3-N3-C1	3.60	135.49	128.39
1	D	63[B]	NRQ	CD1-CE1-CZ	-3.55	116.13	119.88
1	H	63[A]	NRQ	CB2-CA2-N2	3.54	133.56	128.76
1	A	63[A]	NRQ	CB2-CA2-N2	3.53	133.56	128.76
1	E	63[A]	NRQ	CD1-CE1-CZ	-3.47	116.20	119.88
1	C	63[A]	NRQ	CD1-CE1-CZ	-3.47	116.21	119.88
1	G	63[A]	NRQ	CB2-CA2-N2	3.46	133.46	128.76
1	F	63[A]	NRQ	CD1-CE1-CZ	-3.45	116.22	119.88
1	D	63[A]	NRQ	CD1-CE1-CZ	-3.42	116.26	119.88
1	G	63[A]	NRQ	O2-C2-N3	-3.28	117.48	124.31
1	G	63[A]	NRQ	CA3-N3-C2	-3.28	116.47	123.67
1	E	63[B]	NRQ	CD1-CE1-CZ	-3.27	116.42	119.88
1	G	63[B]	NRQ	CD1-CE1-CZ	-3.26	116.43	119.88
1	H	63[A]	NRQ	CD1-CG2-CD2	3.25	122.47	117.65
1	B	63[A]	NRQ	CB2-CA2-N2	3.24	133.16	128.76
1	A	63[A]	NRQ	CD1-CG2-CD2	3.24	122.45	117.65
1	C	63[B]	NRQ	CD1-CE1-CZ	-3.19	116.50	119.88
1	B	63[B]	NRQ	CD1-CG2-CB2	-3.17	110.33	121.22
1	B	63[A]	NRQ	CD1-CE1-CZ	-3.16	116.53	119.88
1	F	63[B]	NRQ	O2-C2-N3	-3.13	117.79	124.31
1	G	63[A]	NRQ	CD1-CE1-CZ	-3.09	116.61	119.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63[B]	NRQ	CD1-CG2-CB2	-3.08	110.62	121.22
1	H	63[B]	NRQ	CB2-CA2-C2	3.08	126.09	122.36
1	E	63[B]	NRQ	CD1-CG2-CB2	-3.04	110.78	121.22
1	A	63[B]	NRQ	O2-C2-N3	-3.04	117.98	124.31
1	D	63[B]	NRQ	CD1-CG2-CB2	-3.01	110.89	121.22
1	F	63[B]	NRQ	CD1-CE1-CZ	-2.98	116.73	119.88
1	G	63[B]	NRQ	CD1-CG2-CB2	-2.97	111.02	121.22
1	F	63[B]	NRQ	CD1-CG2-CB2	-2.97	111.03	121.22
1	A	63[B]	NRQ	O2-C2-CA2	2.95	132.91	131.02
1	E	63[A]	NRQ	CA3-N3-C2	-2.94	117.21	123.67
1	D	63[B]	NRQ	O2-C2-N3	-2.94	118.19	124.31
1	E	63[B]	NRQ	O2-C2-N3	-2.91	118.24	124.31
1	E	63[A]	NRQ	CD1-CG2-CD2	2.91	121.97	117.65
1	D	63[A]	NRQ	CD1-CG2-CD2	2.91	121.96	117.65
1	D	63[A]	NRQ	CD1-CG2-CB2	-2.89	111.28	121.22
1	G	63[A]	NRQ	CD1-CG2-CB2	-2.89	111.29	121.22
1	B	63[A]	NRQ	CD1-CG2-CD2	2.88	121.92	117.65
1	H	63[A]	NRQ	CD1-CG2-CB2	-2.87	111.36	121.22
1	A	63[A]	NRQ	CD1-CG2-CB2	-2.86	111.38	121.22
1	E	63[A]	NRQ	CD1-CG2-CB2	-2.85	111.44	121.22
1	A	63[B]	NRQ	CD1-CG2-CB2	-2.84	111.46	121.22
1	C	63[A]	NRQ	CA3-N3-C1	2.82	133.94	128.39
1	E	63[A]	NRQ	O2-C2-N3	-2.81	118.47	124.31
1	G	63[A]	NRQ	CD1-CG2-CD2	2.80	121.80	117.65
1	E	63[B]	NRQ	O2-C2-CA2	2.76	132.78	131.02
1	H	63[A]	NRQ	CE1-CZ-CE2	2.74	124.12	119.77
1	C	63[B]	NRQ	O2-C2-N3	-2.73	118.63	124.31
1	A	63[A]	NRQ	CE1-CZ-CE2	2.73	124.10	119.77
1	C	63[A]	NRQ	CD1-CG2-CD2	2.71	121.67	117.65
1	B	63[A]	NRQ	CD1-CG2-CB2	-2.67	112.03	121.22
1	A	63[B]	NRQ	CD1-CG2-CD2	2.67	121.62	117.65
1	B	63[B]	NRQ	O2-C2-N3	-2.64	118.82	124.31
1	F	63[B]	NRQ	O2-C2-CA2	2.63	132.70	131.02
1	D	63[B]	NRQ	O2-C2-CA2	2.61	132.69	131.02
1	E	63[A]	NRQ	CE1-CZ-CE2	2.60	123.91	119.77
1	D	63[A]	NRQ	CE1-CZ-CE2	2.59	123.89	119.77
1	C	63[A]	NRQ	CD1-CG2-CB2	-2.59	112.32	121.22
1	F	63[A]	NRQ	CE1-CZ-CE2	2.56	123.84	119.77
1	G	63[B]	NRQ	O2-C2-N3	-2.54	119.03	124.31
1	C	63[A]	NRQ	CE1-CZ-CE2	2.54	123.80	119.77
1	F	63[A]	NRQ	CD1-CG2-CD2	2.50	121.36	117.65
1	D	63[A]	NRQ	CA3-N3-C2	-2.49	118.20	123.67

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	63[B]	NRQ	CA3-N3-C2	-2.48	118.22	123.67
1	A	63[A]	NRQ	CE2-CD2-CG2	-2.45	118.06	121.22
1	H	63[A]	NRQ	CE2-CD2-CG2	-2.45	118.06	121.22
1	D	63[B]	NRQ	CA3-N3-C2	-2.44	118.31	123.67
1	E	63[B]	NRQ	CD1-CG2-CD2	2.37	121.16	117.65
1	B	63[A]	NRQ	CE1-CZ-CE2	2.36	123.53	119.77
1	C	63[B]	NRQ	O2-C2-CA2	2.32	132.50	131.02
1	D	63[A]	NRQ	O2-C2-N3	-2.30	119.52	124.31
1	G	63[A]	NRQ	CE1-CZ-CE2	2.30	123.42	119.77
1	A	63[B]	NRQ	CE1-CZ-CE2	2.27	123.38	119.77
1	B	63[B]	NRQ	O2-C2-CA2	2.27	132.47	131.02
1	F	63[A]	NRQ	CD1-CG2-CB2	-2.26	113.45	121.22
1	F	63[B]	NRQ	CD1-CG2-CD2	2.26	121.00	117.65
1	G	63[B]	NRQ	CD1-CG2-CD2	2.23	120.96	117.65
1	B	63[B]	NRQ	CD2-CG2-CB2	2.22	128.85	121.22
1	F	63[B]	NRQ	C2-CA2-N2	-2.22	107.36	108.95
1	H	63[A]	NRQ	CA3-N3-C1	2.21	132.75	128.39
1	A	63[A]	NRQ	CA3-N3-C1	2.20	132.73	128.39
1	D	63[B]	NRQ	C2-CA2-N2	-2.19	107.38	108.95
1	F	63[A]	NRQ	CB2-CA2-C2	-2.17	119.72	122.36
1	F	63[A]	NRQ	O2-C2-N3	-2.17	119.80	124.31
1	C	63[B]	NRQ	CD1-CG2-CD2	2.16	120.85	117.65
1	E	63[B]	NRQ	CA3-N3-C2	-2.15	118.96	123.67
1	C	63[A]	NRQ	O2-C2-N3	-2.14	119.85	124.31
1	C	63[B]	NRQ	CA3-N3-C2	-2.14	118.97	123.67
1	B	63[B]	NRQ	CD1-CG2-CD2	2.13	120.81	117.65
1	C	63[B]	NRQ	CD2-CG2-CB2	2.12	128.50	121.22
1	D	63[B]	NRQ	CD1-CG2-CD2	2.10	120.77	117.65
1	B	63[A]	NRQ	CA3-N3-C1	2.09	132.51	128.39
1	H	63[B]	NRQ	CA2-N2-C1	2.09	107.93	104.09
1	E	63[B]	NRQ	CE1-CZ-CE2	2.08	123.07	119.77
1	D	63[B]	NRQ	CD2-CG2-CB2	2.07	128.33	121.22
1	A	63[B]	NRQ	C2-CA2-N2	-2.05	107.48	108.95
1	G	63[B]	NRQ	C2-CA2-N2	-2.05	107.48	108.95
1	D	63[A]	NRQ	CE2-CD2-CG2	-2.04	118.59	121.22
1	C	63[B]	NRQ	CE1-CZ-CE2	2.04	123.01	119.77
1	B	63[B]	NRQ	CE1-CZ-CE2	2.03	122.99	119.77
1	A	63[B]	NRQ	CE2-CD2-CG2	-2.02	118.61	121.22
1	F	63[B]	NRQ	CE1-CZ-CE2	2.02	122.98	119.77
1	G	63[B]	NRQ	CE1-CZ-CE2	2.02	122.98	119.77
1	D	63[B]	NRQ	CE1-CZ-CE2	2.01	122.97	119.77
1	H	63[A]	NRQ	O2-C2-N3	-2.01	120.13	124.31

There are no chirality outliers.

All (50) 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	A	63[B]	NRQ	C3-CA3-N3-C1
1	A	63[B]	NRQ	C3-CA3-N3-C2
1	B	63[B]	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[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[B]	NRQ	N2-CA2-CB2-CG2
1	D	63[B]	NRQ	C2-CA2-CB2-CG2
1	D	63[B]	NRQ	C3-CA3-N3-C1
1	D	63[B]	NRQ	C3-CA3-N3-C2
1	E	63[A]	NRQ	C3-CA3-N3-C1
1	E	63[A]	NRQ	C3-CA3-N3-C2
1	E	63[B]	NRQ	C2-CA2-CB2-CG2
1	E	63[B]	NRQ	C3-CA3-N3-C1
1	E	63[B]	NRQ	C3-CA3-N3-C2
1	F	63[A]	NRQ	C1-CA1-CB1-CG1
1	F	63[B]	NRQ	N2-CA2-CB2-CG2
1	F	63[B]	NRQ	C2-CA2-CB2-CG2
1	F	63[B]	NRQ	C3-CA3-N3-C1
1	F	63[B]	NRQ	C3-CA3-N3-C2
1	G	63[A]	NRQ	C3-CA3-N3-C1
1	G	63[A]	NRQ	C3-CA3-N3-C2
1	G	63[B]	NRQ	N2-CA2-CB2-CG2
1	G	63[B]	NRQ	C2-CA2-CB2-CG2
1	G	63[B]	NRQ	C3-CA3-N3-C1
1	G	63[B]	NRQ	C3-CA3-N3-C2
1	H	63[A]	NRQ	CA1-CB1-CG1-SD
1	H	63[B]	NRQ	N2-CA2-CB2-CG2
1	H	63[B]	NRQ	C2-CA2-CB2-CG2
1	E	63[B]	NRQ	N2-CA2-CB2-CG2
1	D	63[A]	NRQ	C3-CA3-N3-C2
1	F	63[A]	NRQ	CB1-CG1-SD-CE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	B	63[A]	NRQ	CB1-CG1-SD-CE
1	E	63[B]	NRQ	CB1-CG1-SD-CE
1	C	63[B]	NRQ	CB1-CG1-SD-CE
1	F	63[B]	NRQ	CB1-CG1-SD-CE
1	F	63[A]	NRQ	C3-CA3-N3-C2
1	E	63[A]	NRQ	CB1-CG1-SD-CE
1	H	63[B]	NRQ	CA2-CB2-CG2-CD1
1	D	63[A]	NRQ	C3-CA3-N3-C1
1	H	63[B]	NRQ	C3-CA3-N3-C1
1	H	63[B]	NRQ	CA2-CB2-CG2-CD2

There are no ring outliers.

16 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63[A]	NRQ	8	0
1	C	63[A]	NRQ	6	0
1	C	63[B]	NRQ	6	0
1	H	63[B]	NRQ	20	0
1	D	63[A]	NRQ	5	0
1	B	63[B]	NRQ	3	0
1	A	63[B]	NRQ	6	0
1	E	63[A]	NRQ	4	0
1	D	63[B]	NRQ	3	0
1	E	63[B]	NRQ	6	0
1	F	63[A]	NRQ	6	0
1	G	63[A]	NRQ	5	0
1	F	63[B]	NRQ	5	0
1	H	63[A]	NRQ	15	0
1	G	63[B]	NRQ	3	0
1	B	63[A]	NRQ	4	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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 ⓘ

### 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	222/233 (95%)	0.13	7 (3%) 47 53	8, 16, 32, 47	0
1	B	225/233 (96%)	0.21	8 (3%) 42 48	9, 16, 29, 52	0
1	C	222/233 (95%)	0.29	6 (2%) 54 60	8, 14, 26, 42	0
1	D	223/233 (95%)	0.30	9 (4%) 38 43	9, 19, 33, 49	0
1	E	222/233 (95%)	0.47	12 (5%) 25 30	11, 21, 35, 45	0
1	F	222/233 (95%)	0.62	15 (6%) 17 21	12, 22, 39, 58	0
1	G	222/233 (95%)	1.12	36 (16%) 1 2	12, 26, 44, 53	0
1	H	222/233 (95%)	1.64	70 (31%) 0 0	12, 29, 46, 63	0
All	All	1780/1864 (95%)	0.60	163 (9%) 9 11	8, 20, 38, 63	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	4	LEU	8.0
1	H	84	PHE	7.5
1	H	152	GLY	6.8
1	H	151	ASP	6.7
1	D	3	ALA	5.7
1	H	189	MET	5.6
1	H	184	ALA	5.6
1	H	185	LYS	5.4
1	G	167	GLY	5.4
1	H	186	ASN	5.4
1	H	187	LEU	5.3
1	G	185	LYS	5.1
1	H	79	PHE	5.0
1	G	183	PRO	4.9
1	H	75	GLY	4.7
1	H	183	PRO	4.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	150	ALA	4.7
1	H	73	THR	4.6
1	H	85	PRO	4.6
1	G	210	TYR	4.4
1	H	69	PHE	4.4
1	H	76	ILE	4.4
1	H	149	PRO	4.4
1	H	112	ASP	4.4
1	G	166	GLY	4.2
1	G	205	ALA	4.2
1	F	228	LEU	4.2
1	H	87	GLY	4.2
1	G	112	ASP	4.1
1	A	223	ASP	4.1
1	G	14	TYR	4.0
1	H	190	PRO	4.0
1	A	207	LYS	4.0
1	B	3	ALA	4.0
1	G	202	ILE	4.0
1	F	185	LYS	3.9
1	F	152	GLY	3.8
1	H	5	ILE	3.8
1	G	111	GLN	3.6
1	G	4	LEU	3.6
1	G	116	ILE	3.5
1	B	185	LYS	3.5
1	F	151	ASP	3.5
1	D	4	LEU	3.5
1	H	70	ILE	3.5
1	H	188	LYS	3.5
1	H	80	PHE	3.4
1	F	87	GLY	3.4
1	D	112	ASP	3.4
1	E	151	ASP	3.4
1	A	151	ASP	3.3
1	C	151	ASP	3.3
1	H	111	GLN	3.3
1	F	14	TYR	3.3
1	H	221	TYR	3.2
1	G	129	ASN	3.2
1	F	6	THR	3.2
1	H	178	TYR	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	185	LYS	3.1
1	G	186	ASN	3.1
1	G	138	LEU	3.1
1	H	210	TYR	3.1
1	H	228	LEU	3.1
1	H	77	PRO	3.0
1	H	153	GLY	3.0
1	H	14	TYR	3.0
1	E	186	ASN	3.0
1	H	182	LYS	3.0
1	H	6	THR	3.0
1	A	185	LYS	3.0
1	H	83	SER	2.9
1	H	88	PHE	2.9
1	F	75	GLY	2.9
1	H	38	THR	2.9
1	F	184	ALA	2.9
1	E	46	VAL	2.9
1	E	93	VAL	2.9
1	H	74	GLN	2.9
1	H	89	THR	2.9
1	H	206	ASP	2.8
1	B	2	SER	2.8
1	H	45	VAL	2.8
1	G	134	GLN	2.8
1	H	114	CYS	2.8
1	E	152	GLY	2.8
1	F	188	LYS	2.8
1	H	12	LYS	2.7
1	H	36	GLU	2.7
1	C	172	CYS	2.7
1	G	168	GLY	2.7
1	H	35	TYR	2.7
1	G	223	ASP	2.7
1	G	204	GLU	2.7
1	B	151	ASP	2.7
1	E	112	ASP	2.7
1	H	8	ASN	2.7
1	H	191	GLY	2.6
1	G	206	ASP	2.6
1	H	9	MET	2.6
1	A	208	GLU	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	6	THR	2.6
1	E	206	ASP	2.6
1	F	114	CYS	2.6
1	C	171	ILE	2.6
1	H	117	TYR	2.6
1	H	66	SER	2.6
1	H	78	ASP	2.5
1	H	193	TYR	2.5
1	G	137	THR	2.5
1	H	119	VAL	2.5
1	H	192	VAL	2.5
1	G	151	ASP	2.5
1	E	53	PHE	2.5
1	C	96	TYR	2.4
1	H	32	GLY	2.4
1	H	7	GLU	2.4
1	F	113	GLY	2.4
1	G	130	GLY	2.4
1	B	101	VAL	2.4
1	B	150	ALA	2.4
1	F	69	PHE	2.4
1	H	50	PRO	2.3
1	E	188	LYS	2.3
1	G	203	LYS	2.3
1	C	228	LEU	2.3
1	H	181	LYS	2.3
1	G	158	ALA	2.3
1	D	101	VAL	2.3
1	H	26	CYS	2.3
1	F	183	PRO	2.3
1	C	93	VAL	2.3
1	F	186	ASN	2.3
1	B	223	ASP	2.3
1	H	223	ASP	2.3
1	G	51	LEU	2.2
1	D	151	ASP	2.2
1	G	226	SER	2.2
1	H	154	LEU	2.2
1	G	53	PHE	2.2
1	H	222	CYS	2.2
1	D	93	VAL	2.2
1	H	202	ILE	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	152	GLY	2.2
1	H	82	GLN	2.1
1	H	96	TYR	2.1
1	H	148	TYR	2.1
1	A	22	HIS	2.1
1	G	136	LYS	2.1
1	G	165	VAL	2.1
1	H	180	SER	2.1
1	G	12	LYS	2.1
1	A	206	ASP	2.1
1	E	129	ASN	2.1
1	G	6	THR	2.1
1	H	10	HIS	2.1
1	D	174	LEU	2.1
1	H	172	CYS	2.1
1	D	124	VAL	2.0
1	G	50	PRO	2.0
1	G	184	ALA	2.0
1	E	174	LEU	2.0
1	G	24	PHE	2.0
1	G	228	LEU	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, 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
1	NRQ	H	63[A]	23/24	0.84	0.29	11,13,21,23	23
1	NRQ	H	63[B]	23/24	0.84	0.29	11,14,17,22	23
1	NRQ	G	63[A]	23/24	0.91	0.16	19,24,31,35	23
1	NRQ	G	63[B]	23/24	0.91	0.16	19,23,29,34	23
1	NRQ	F	63[A]	23/24	0.91	0.16	17,20,25,28	23
1	NRQ	F	63[B]	23/24	0.91	0.16	18,20,25,28	23
1	NRQ	D	63[A]	23/24	0.93	0.14	14,18,20,24	23
1	NRQ	D	63[B]	23/24	0.93	0.14	15,18,19,22	23
1	NRQ	B	63[A]	23/24	0.94	0.15	12,16,17,21	23
1	NRQ	B	63[B]	23/24	0.94	0.15	11,15,17,18	23
1	NRQ	C	63[A]	23/24	0.95	0.17	11,13,17,23	23
1	NRQ	C	63[B]	23/24	0.95	0.17	11,13,15,21	23

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	NRQ	A	63[A]	23/24	0.95	0.13	11,13,21,23	23
1	NRQ	A	63[B]	23/24	0.95	0.13	11,14,17,22	23
1	NRQ	E	63[A]	23/24	0.95	0.13	16,19,22,29	23
1	NRQ	E	63[B]	23/24	0.95	0.13	14,19,22,28	23

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.