



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:21 PM GMT

PDB ID : 2V4E  
Title : A NON-CYTOTOXIC DSRED VARIANT FOR WHOLE-CELL LABELING  
Authors : Strack, R.L.; Strongin, D.E.; Bhattacharyya, D.; Tao, W.; Berman, A.; Broxmeyer, H.E.; Keenan, R.J.; Glick, B.S.  
Deposited on : 2008-09-20  
Resolution : 2.40 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

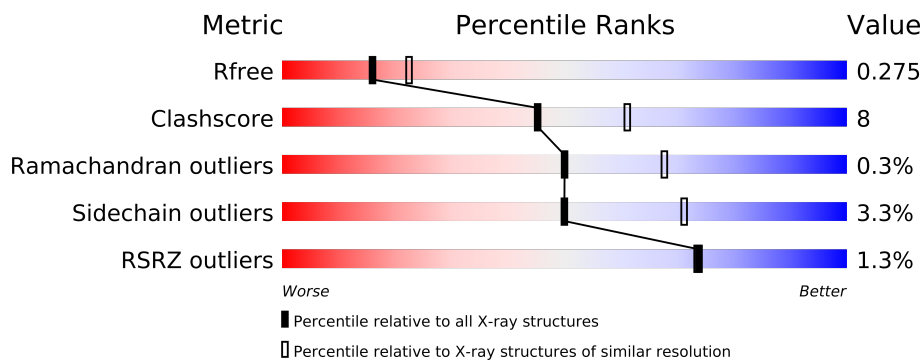
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	218	
2	B	218	
3	C	218	
3	D	218	
3	E	218	
3	F	218	
3	G	218	
3	H	218	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14705 atoms, of which 0 are hydrogen and 0 are deuterium.

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 RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1770	1150	290	323	7			

- Molecule 2 is a protein called RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1779	1154	293	325	7			

- Molecule 3 is a protein called RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	D	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	E	217	Total	C	N	O	S	0	0	0
			1770	1149	290	324	7			
3	F	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	G	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	H	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	78	Total	O	0	0
			78	78		

*Continued on next page...*

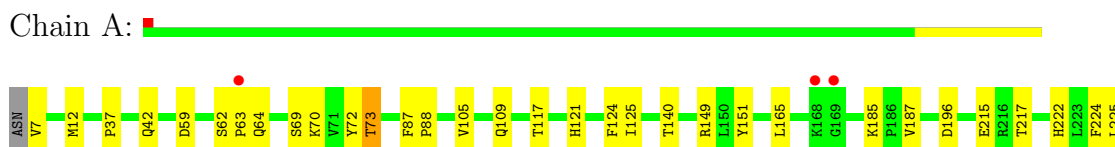
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	70	Total 70	O 70	0	0
4	D	80	Total 80	O 80	0	0
4	E	56	Total 56	O 56	0	0
4	F	73	Total 73	O 73	0	0
4	G	23	Total 23	O 23	0	0
4	H	48	Total 48	O 48	0	0

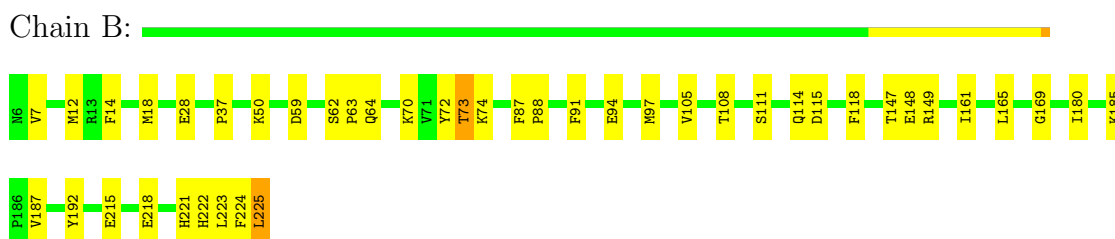
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

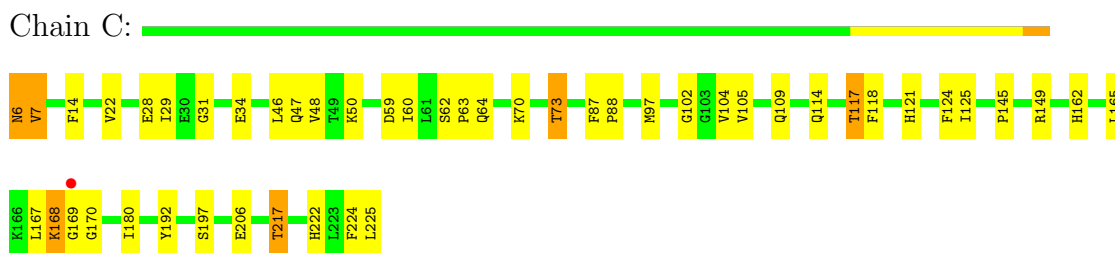
#### • Molecule 1: RED FLUORESCENT PROTEIN DRFP583



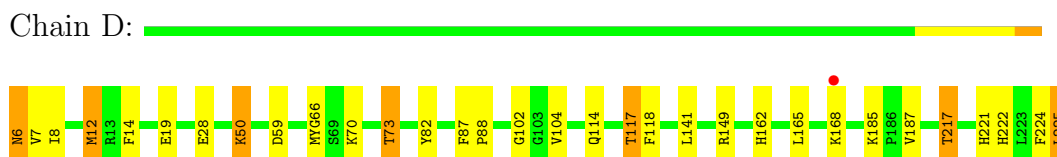
#### • Molecule 2: RED FLUORESCENT PROTEIN DRFP583



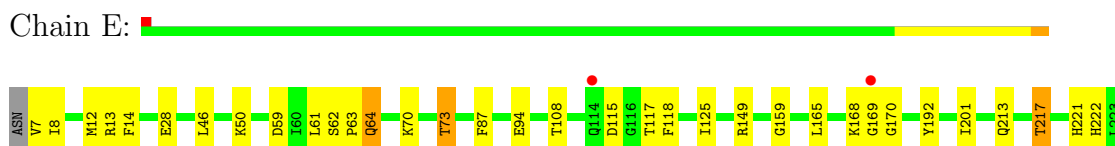
#### • Molecule 3: RED FLUORESCENT PROTEIN DRFP583



#### • Molecule 3: RED FLUORESCENT PROTEIN DRFP583



#### • Molecule 3: RED FLUORESCENT PROTEIN DRFP583



F224  
L225

- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain F: 

N6 V7 I8 M12 M13 R13 H17 E30 E31 E32 D89 S62 P63 Q64 K70 T73 K74 V105 Q114 T117 F118 F124 I125 G126 L141 R149 L165 K168 G169 Y192 L199 T217 E218 H222 L223 F224 L225

- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain G: 

N6 V7 F14 K15 V16 H17 E28 E29 G31 K36 P37 Q42 T43 A44 K45 L46 Q47 V48 T49 K50 A57 I60 L61 Q64 F65 MYG66 S69 K70 V71 Y72 T73 Y82 F87 P88 F99 G102 G103 V104 V105 Q109 S112 L113 Q114 F118 I119

- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain H: 

N6 V7 I8 E28 K50 D59 MYG66 S69 K70 T73 K74 H75 D78 F87 P88 Q114 K139 T140 L141 L150 H162 L165 K168 G169 G170 I180 P186 V187 T217 H221 H222 L223 F224 L225

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.53Å 122.62Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 34.89 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.40) 98.1 (34.89-2.39)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, $R_{free}$	0.220 , 0.271 0.224 , 0.275	Depositor DCC
$R_{free}$ test set	4542 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.7	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 29.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 91099 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14705	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.57	0/1799	0.68	0/2425
2	B	0.62	0/1808	0.71	2/2439 (0.1%)
3	C	0.59	0/1808	0.67	0/2439
3	D	0.62	0/1808	0.70	1/2439 (0.0%)
3	E	0.52	0/1799	0.68	1/2426 (0.0%)
3	F	0.59	0/1808	0.72	4/2439 (0.2%)
3	G	0.57	0/1808	0.64	0/2439
3	H	0.57	0/1808	0.68	0/2439
All	All	0.58	0/14446	0.69	8/19485 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	1
3	D	0	1
3	G	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	64	GLN	C-N-CA	-7.17	103.78	121.70
3	F	13	ARG	NE-CZ-NH1	7.01	123.80	120.30
3	D	225	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	169	GLY	N-CA-C	-6.02	98.05	113.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	64	GLN	O-C-N	5.93	132.19	122.70
3	E	64	GLN	O-C-N	5.52	131.53	122.70
2	B	225	LEU	CA-CB-CG	5.36	127.62	115.30
3	F	64	GLN	CA-C-N	-5.00	106.19	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	GLN	Mainchain
3	C	64	GLN	Mainchain
3	D	6	ASN	Peptide
3	G	64	GLN	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1770	0	1727	20	0
2	B	1779	0	1731	34	0
3	C	1779	0	1729	39	0
3	D	1779	0	1729	29	0
3	E	1770	0	1722	29	0
3	F	1779	0	1729	25	0
3	G	1779	0	1729	45	0
3	H	1779	0	1729	24	0
4	A	63	0	0	2	0
4	B	78	0	0	1	0
4	C	70	0	0	2	0
4	D	80	0	0	3	0
4	E	56	0	0	3	0
4	F	73	0	0	4	0
4	G	23	0	0	0	0
4	H	48	0	0	4	0
All	All	14705	0	13825	236	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (236) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:6:ASN:O	3:C:7:VAL:CG2	1.94	1.15
3:H:217:THR:HG21	4:H:2045:HOH:O	1.55	1.03
3:C:6:ASN:O	3:C:7:VAL:HG22	1.53	1.02
3:C:6:ASN:C	3:C:7:VAL:HG23	1.88	0.92
3:C:6:ASN:O	3:C:7:VAL:HG23	1.68	0.90
3:F:13:ARG:HH11	3:F:13:ARG:HG2	1.37	0.88
3:H:222:HIS:H	3:H:225:LEU:HD12	1.38	0.88
3:C:70:LYS:O	3:C:73:THR:HG22	1.75	0.85
3:E:70:LYS:O	3:E:73:THR:CG2	2.25	0.84
3:H:168:LYS:NZ	4:H:2038:HOH:O	2.09	0.83
3:D:117:THR:HG23	4:D:2037:HOH:O	1.80	0.80
1:A:70:LYS:O	1:A:73:THR:HG22	1.80	0.79
3:D:70:LYS:O	3:D:73:THR:HG23	1.84	0.78
3:C:6:ASN:C	3:C:7:VAL:CG2	2.43	0.77
3:F:73:THR:HG21	4:F:2023:HOH:O	1.85	0.76
3:D:12:MET:HE2	3:D:118:PHE:CZ	2.21	0.76
2:B:70:LYS:O	2:B:73:THR:CG2	2.33	0.76
3:C:70:LYS:O	3:C:73:THR:CG2	2.34	0.74
3:H:70:LYS:O	3:H:73:THR:HG22	1.86	0.74
3:F:70:LYS:O	3:F:73:THR:CG2	2.36	0.73
3:H:70:LYS:O	3:H:73:THR:CG2	2.37	0.73
3:E:217:THR:HG21	4:E:2052:HOH:O	1.86	0.72
1:A:73:THR:HG21	4:A:2019:HOH:O	1.88	0.72
3:F:222:HIS:HD2	3:F:224:PHE:H	1.39	0.70
2:B:222:HIS:H	2:B:225:LEU:HD12	1.56	0.69
3:D:12:MET:CE	3:D:118:PHE:CZ	2.77	0.68
3:G:70:LYS:O	3:G:73:THR:HG23	1.92	0.68
3:F:70:LYS:O	3:F:73:THR:HG23	1.93	0.67
3:E:70:LYS:O	3:E:73:THR:HG23	1.94	0.67
3:F:141:LEU:HD11	3:F:168:LYS:HA	1.77	0.66
2:B:70:LYS:O	2:B:73:THR:HG23	1.95	0.65
3:F:17:HIS:HB2	4:F:2007:HOH:O	1.96	0.65
1:A:70:LYS:O	1:A:73:THR:CG2	2.45	0.65
3:C:168:LYS:O	3:C:170:GLY:N	2.30	0.64
3:H:222:HIS:N	3:H:225:LEU:HD12	2.10	0.63
3:D:6:ASN:N	3:D:7:VAL:CA	2.62	0.63
3:C:28:GLU:HB2	3:C:50:LYS:HB2	1.81	0.62
3:H:78:ASP:N	3:H:78:ASP:OD1	2.30	0.62
3:E:12:MET:HE3	3:E:118:PHE:CZ	2.35	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:E:7:VAL:CA	4:E:2001:HOH:O	2.47	0.61
3:E:70:LYS:O	3:E:73:THR:HG22	2.00	0.60
2:B:59:ASP:HB3	2:B:165:LEU:HD21	1.83	0.60
3:E:8:ILE:HA	3:E:12:MET:HE1	1.83	0.60
2:B:74:LYS:HB3	2:B:218:GLU:HG2	1.84	0.60
3:G:109:GLN:HG3	3:G:122:VAL:HG22	1.84	0.60
3:D:6:ASN:N	3:D:7:VAL:C	2.56	0.59
3:D:222:HIS:CD2	3:D:224:PHE:H	2.19	0.59
2:B:222:HIS:N	2:B:225:LEU:HD12	2.17	0.59
3:G:162:HIS:CE1	3:H:162:HIS:CE1	2.91	0.59
2:B:221:HIS:HB3	2:B:225:LEU:HD12	1.84	0.59
3:G:29:ILE:HG12	3:G:48:VAL:HG22	1.86	0.58
3:E:62:SER:OG	3:E:63:PRO:HD3	2.04	0.58
3:F:105:VAL:HG11	3:F:124:PHE:CE2	2.38	0.57
3:D:59:ASP:HB3	3:D:165:LEU:HD21	1.86	0.57
3:C:73:THR:HG23	4:C:2019:HOH:O	2.04	0.57
3:E:222:HIS:H	3:E:225:LEU:HD22	1.70	0.56
3:C:62:SER:OG	3:C:63:PRO:HD3	2.05	0.56
3:G:109:GLN:CG	3:G:122:VAL:HG22	2.35	0.56
3:C:168:LYS:C	3:C:170:GLY:H	2.08	0.56
3:G:141:LEU:HD11	3:G:168:LYS:HA	1.88	0.56
1:A:87:PHE:HB3	1:A:88:PRO:HA	1.88	0.55
2:B:225:LEU:CD1	4:B:2064:HOH:O	2.54	0.55
3:D:222:HIS:H	3:D:225:LEU:HD12	1.71	0.55
3:D:66:NRQ:HA31	3:D:66:NRQ:N1	2.22	0.55
3:G:180:ILE:N	3:G:180:ILE:HD12	2.21	0.55
3:C:31:GLY:HA3	3:C:46:LEU:HD13	1.89	0.54
3:E:61:LEU:O	3:E:64:GLN:HG2	2.08	0.54
3:D:217:THR:CG2	4:D:2012:HOH:O	2.57	0.53
3:C:167:LEU:O	3:C:168:LYS:C	2.44	0.53
3:G:29:ILE:CG1	3:G:48:VAL:HG22	2.39	0.53
1:A:222:HIS:H	1:A:225:LEU:HD12	1.74	0.53
2:B:12:MET:CE	2:B:118:PHE:CZ	2.92	0.53
1:A:185:LYS:O	1:A:187:VAL:HG13	2.09	0.52
3:G:57:ALA:HB2	3:G:138:LYS:HA	1.90	0.52
3:E:222:HIS:CD2	3:E:224:PHE:H	2.27	0.52
3:G:16:VAL:HG23	3:G:120:TYR:CB	2.39	0.52
3:G:16:VAL:HG23	3:G:120:TYR:HB2	1.92	0.52
3:C:197:SER:OG	3:C:217:THR:HG23	2.10	0.52
3:D:222:HIS:N	3:D:225:LEU:HD12	2.24	0.52
3:C:222:HIS:H	3:C:225:LEU:HD12	1.76	0.51
3:H:139:LYS:HD2	3:H:168:LYS:HD2	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:180:ILE:HD12	2:B:180:ILE:N	2.25	0.51
3:F:8:ILE:HD12	3:F:8:ILE:N	2.25	0.51
3:F:141:LEU:CD1	3:F:168:LYS:HA	2.41	0.51
2:B:147:THR:O	2:B:161:ILE:HG23	2.09	0.51
2:B:221:HIS:HB3	2:B:225:LEU:CD1	2.41	0.50
1:A:222:HIS:CD2	1:A:224:PHE:H	2.29	0.50
1:A:37:PRO:HA	1:A:72:TYR:HA	1.93	0.50
3:D:82:TYR:CD1	3:D:187:VAL:CG2	2.94	0.50
3:C:162:HIS:CE1	3:D:162:HIS:CE1	2.99	0.50
3:G:82:TYR:CD1	3:G:187:VAL:CG2	2.94	0.50
3:E:222:HIS:HD2	3:E:224:PHE:H	1.59	0.50
1:A:125:ILE:HD12	3:C:125:ILE:HD12	1.94	0.50
3:F:13:ARG:HG2	3:F:13:ARG:NH1	2.14	0.50
3:C:167:LEU:O	3:C:168:LYS:O	2.30	0.49
3:D:102:GLY:O	3:D:104:VAL:HG23	2.12	0.49
1:A:105:VAL:HG11	1:A:124:PHE:CE2	2.47	0.49
3:G:14:PHE:CB	3:G:118:PHE:HB2	2.42	0.49
1:A:59:ASP:HB3	1:A:165:LEU:HD21	1.93	0.49
3:G:147:THR:O	3:G:161:ILE:HG23	2.12	0.49
3:F:74:LYS:HB3	3:F:218:GLU:HG2	1.94	0.49
3:H:87:PHE:HB3	3:H:88:PRO:HA	1.94	0.49
2:B:28:GLU:HB2	2:B:50:LYS:HB2	1.95	0.49
3:F:12:MET:HE2	3:F:118:PHE:CE2	2.47	0.49
2:B:12:MET:HE3	2:B:118:PHE:CZ	2.48	0.49
3:C:14:PHE:HB3	3:C:118:PHE:HB2	1.95	0.49
3:E:12:MET:CE	3:E:118:PHE:CZ	2.95	0.49
3:H:225:LEU:HD13	4:H:2046:HOH:O	2.11	0.49
3:F:222:HIS:CD2	3:F:224:PHE:H	2.27	0.49
3:F:222:HIS:HB3	3:F:225:LEU:HG	1.94	0.49
3:D:6:ASN:N	3:D:7:VAL:HA	2.28	0.48
3:D:149:ARG:C	3:D:149:ARG:HD2	2.33	0.48
3:D:6:ASN:N	3:D:8:ILE:N	2.61	0.48
3:C:222:HIS:CD2	3:C:224:PHE:H	2.31	0.48
3:G:87:PHE:HB3	3:G:88:PRO:HA	1.96	0.48
2:B:37:PRO:HA	2:B:72:TYR:HA	1.96	0.48
3:G:72:TYR:O	3:G:217:THR:HG23	2.13	0.48
3:G:222:HIS:CD2	3:G:224:PHE:H	2.31	0.48
3:E:125:ILE:HD12	3:G:125:ILE:HD12	1.96	0.48
2:B:222:HIS:CD2	2:B:224:PHE:H	2.31	0.47
3:H:28:GLU:HB2	3:H:50:LYS:HB2	1.95	0.47
3:G:222:HIS:H	3:G:225:LEU:HD12	1.80	0.47
2:B:148:GLU:HG3	2:B:161:ILE:HG12	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:140:THR:HG21	3:G:165:LEU:HD13	1.96	0.47
3:F:217:THR:CG2	4:F:2068:HOH:O	2.63	0.47
3:H:73:THR:HB	3:H:217:THR:OG1	2.15	0.46
3:E:8:ILE:HD11	3:E:87:PHE:HB2	1.97	0.46
3:G:147:THR:HG22	3:G:194:TYR:HD2	1.79	0.46
3:E:149:ARG:HD3	3:E:192:TYR:CZ	2.51	0.46
3:E:221:HIS:HB3	3:E:225:LEU:HD23	1.98	0.46
3:D:12:MET:HE3	3:D:118:PHE:CZ	2.49	0.46
3:H:8:ILE:HD11	3:H:87:PHE:HB2	1.96	0.46
3:G:61:LEU:O	3:G:64:GLN:HG2	2.15	0.46
3:G:82:TYR:CD1	3:G:187:VAL:HG22	2.51	0.46
3:E:168:LYS:C	3:E:170:GLY:H	2.18	0.46
3:E:94:GLU:HG2	3:E:108:THR:HA	1.98	0.46
3:E:14:PHE:HB3	3:E:118:PHE:HB2	1.98	0.46
2:B:14:PHE:CB	2:B:118:PHE:HB2	2.45	0.46
3:D:82:TYR:CD1	3:D:187:VAL:HG23	2.50	0.46
2:B:12:MET:HE2	2:B:118:PHE:CZ	2.51	0.46
3:C:145:PRO:HB2	3:D:222:HIS:CD2	2.51	0.45
3:E:46:LEU:N	3:E:46:LEU:HD22	2.31	0.45
3:H:186:PRO:O	3:H:187:VAL:HG12	2.16	0.45
3:C:149:ARG:HD3	3:C:192:TYR:CZ	2.52	0.45
2:B:70:LYS:NZ	2:B:215:GLU:OE2	2.43	0.45
2:B:149:ARG:HD3	2:B:192:TYR:CZ	2.51	0.45
3:G:149:ARG:C	3:G:149:ARG:HD2	2.36	0.45
2:B:18:MET:CE	2:B:64:GLN:HB2	2.46	0.45
3:F:105:VAL:HG11	3:F:124:PHE:CZ	2.51	0.45
2:B:94:GLU:HG2	2:B:108:THR:HA	1.98	0.45
3:D:73:THR:HG21	4:D:2029:HOH:O	2.17	0.45
1:A:140:THR:HG21	1:A:165:LEU:HD13	1.99	0.45
3:G:66:NRQ:HA31	3:G:66:NRQ:N1	2.32	0.45
3:F:70:LYS:O	3:F:73:THR:HG22	2.14	0.45
3:G:102:GLY:O	3:G:104:VAL:HG23	2.17	0.45
3:H:180:ILE:HD12	3:H:180:ILE:N	2.31	0.45
2:B:185:LYS:O	2:B:187:VAL:HG13	2.16	0.45
3:H:222:HIS:CD2	3:H:224:PHE:H	2.35	0.45
3:H:141:LEU:HD11	3:H:168:LYS:HA	1.98	0.45
3:F:217:THR:HG22	4:F:2068:HOH:O	2.17	0.45
3:C:114:GLN:O	3:C:117:THR:HG23	2.17	0.45
2:B:12:MET:HE3	2:B:118:PHE:CE2	2.52	0.45
3:G:42:GLN:HG3	3:G:66:NRQ:CE	2.47	0.44
3:G:28:GLU:HB2	3:G:50:LYS:HB3	1.98	0.44
3:H:78:ASP:OD2	3:H:221:HIS:NE2	2.42	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:221:HIS:HB3	3:D:225:LEU:HD12	1.99	0.44
2:B:149:ARG:HD2	2:B:149:ARG:C	2.37	0.44
3:F:59:ASP:HB3	3:F:165:LEU:HD21	1.98	0.44
1:A:196:ASP:OD2	2:B:223:LEU:HD12	2.17	0.44
3:G:143:TRP:CE3	3:G:163:LYS:HE3	2.52	0.44
3:E:168:LYS:O	3:E:170:GLY:N	2.51	0.44
3:G:43:THR:HA	3:G:213:GLN:O	2.18	0.44
1:A:215:GLU:OE2	1:A:217:THR:OG1	2.34	0.44
1:A:109:GLN:HA	1:A:121:HIS:O	2.18	0.44
1:A:62:SER:N	1:A:63:PRO:CD	2.81	0.44
1:A:42:GLN:HE22	1:A:69:SER:HB3	1.82	0.44
3:C:180:ILE:HD12	3:C:180:ILE:N	2.33	0.44
2:B:91:PHE:O	2:B:111:SER:HB2	2.18	0.44
3:C:97:MET:HB2	3:C:105:VAL:HB	1.98	0.44
3:E:28:GLU:HB2	3:E:50:LYS:HB2	2.00	0.43
3:H:7:VAL:HG23	3:H:8:ILE:HD12	1.99	0.43
3:G:143:TRP:CE2	3:G:165:LEU:HD21	2.53	0.43
3:C:222:HIS:HD2	3:C:224:PHE:H	1.65	0.43
3:C:222:HIS:HB3	3:C:225:LEU:HG	2.00	0.43
3:G:196:ASP:OD2	3:H:223:LEU:HD12	2.18	0.43
3:H:66:NRQ:CB2	3:H:70:LYS:HE2	2.48	0.43
1:A:7:VAL:CA	4:A:2001:HOH:O	2.66	0.43
2:B:222:HIS:HD2	2:B:224:PHE:H	1.66	0.43
3:C:87:PHE:HB3	3:C:88:PRO:HA	2.01	0.43
3:C:14:PHE:CB	3:C:118:PHE:HB2	2.49	0.43
3:G:112:SER:O	3:G:119:ILE:N	2.45	0.43
3:D:141:LEU:HD11	3:D:168:LYS:HA	2.00	0.43
1:A:151:TYR:N	1:A:151:TYR:CD1	2.86	0.43
3:C:109:GLN:HA	3:C:121:HIS:O	2.19	0.43
3:C:225:LEU:CD1	4:C:2057:HOH:O	2.67	0.42
3:C:168:LYS:C	3:C:170:GLY:N	2.72	0.42
3:G:82:TYR:CE1	3:G:187:VAL:HG22	2.55	0.42
3:C:29:ILE:HG12	3:C:48:VAL:HG22	2.00	0.42
1:A:149:ARG:HD2	1:A:149:ARG:C	2.40	0.42
3:G:31:GLY:HA3	3:G:46:LEU:HD13	2.00	0.42
3:E:217:THR:CG2	4:E:2051:HOH:O	2.67	0.42
3:C:102:GLY:O	3:C:104:VAL:HG23	2.20	0.42
2:B:97:MET:HB2	2:B:105:VAL:HB	2.01	0.42
3:E:149:ARG:O	3:E:159:GLY:HA2	2.20	0.42
3:G:42:GLN:HG3	3:G:66:NRQ:HE1A	2.02	0.42
3:G:99:PHE:CD2	3:G:173:TYR:CE2	3.08	0.42
3:E:201:ILE:HD13	3:E:213:GLN:HG2	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:70:LYS:O	2:B:73:THR:HG22	2.14	0.42
3:C:22:VAL:HG21	3:C:60:ILE:HD11	2.02	0.42
3:H:59:ASP:HB3	3:H:165:LEU:HD21	2.02	0.42
3:G:36:LYS:HA	3:G:37:PRO:HD3	1.93	0.42
2:B:62:SER:OG	2:B:63:PRO:HD3	2.20	0.42
3:E:125:ILE:CD1	3:G:125:ILE:HD12	2.49	0.42
3:D:14:PHE:HB3	3:D:118:PHE:HB2	2.02	0.41
3:F:199:LEU:C	3:F:199:LEU:HD23	2.40	0.41
3:G:44:ALA:O	3:G:212:GLU:HA	2.20	0.41
3:G:143:TRP:CD2	3:G:165:LEU:HD21	2.55	0.41
3:F:105:VAL:HG22	3:F:126:GLY:HA2	2.02	0.41
3:D:87:PHE:HB3	3:D:88:PRO:HA	2.02	0.41
3:F:62:SER:N	3:F:63:PRO:CD	2.84	0.41
2:B:14:PHE:HB3	2:B:118:PHE:HB2	2.03	0.41
3:F:12:MET:CE	3:F:118:PHE:CZ	3.04	0.41
3:E:125:ILE:HG13	3:G:125:ILE:HD12	2.03	0.41
3:D:28:GLU:HB2	3:D:50:LYS:HB2	2.02	0.41
3:H:225:LEU:CD1	4:H:2046:HOH:O	2.68	0.41
3:C:105:VAL:HG11	3:C:124:PHE:CE2	2.56	0.41
3:E:59:ASP:HB3	3:E:165:LEU:HD21	2.03	0.41
3:G:14:PHE:HB3	3:G:118:PHE:HB2	2.03	0.40
3:G:148:GLU:O	3:G:150:LEU:HD12	2.21	0.40
3:G:66:NRQ:HE2	3:G:199:LEU:HB2	2.03	0.40
3:D:222:HIS:HD2	3:D:224:PHE:H	1.67	0.40
3:C:59:ASP:HB3	3:C:165:LEU:HD21	2.03	0.40
3:C:62:SER:N	3:C:63:PRO:CD	2.85	0.40
3:D:19:GLU:HG2	3:D:28:GLU:HG2	2.03	0.40
3:F:149:ARG:HD3	3:F:192:TYR:CZ	2.57	0.40
2:B:87:PHE:HB3	2:B:88:PRO:HA	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	212/218 (97%)	207 (98%)	5 (2%)	0	100	100
2	B	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
3	C	213/218 (98%)	206 (97%)	4 (2%)	3 (1%)	16	22
3	D	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
3	E	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	38	53
3	F	213/218 (98%)	209 (98%)	4 (2%)	0	100	100
3	G	213/218 (98%)	206 (97%)	6 (3%)	1 (0%)	38	53
3	H	213/218 (98%)	205 (96%)	8 (4%)	0	100	100
All	All	1702/1744 (98%)	1658 (97%)	39 (2%)	5 (0%)	50	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	7	VAL
3	C	168	LYS
3	C	169	GLY
3	E	169	GLY
3	G	186	PRO

### 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	188/190 (99%)	185 (98%)	3 (2%)	75	89
2	B	190/190 (100%)	186 (98%)	4 (2%)	66	84
3	C	190/190 (100%)	183 (96%)	7 (4%)	45	66
3	D	190/190 (100%)	183 (96%)	7 (4%)	45	66
3	E	188/190 (99%)	182 (97%)	6 (3%)	51	72
3	F	190/190 (100%)	180 (95%)	10 (5%)	32	48
3	G	190/190 (100%)	183 (96%)	7 (4%)	45	66
3	H	190/190 (100%)	184 (97%)	6 (3%)	51	72
All	All	1516/1520 (100%)	1466 (97%)	50 (3%)	50	71



All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	73	THR
1	A	117	THR
2	B	7	VAL
2	B	73	THR
2	B	114	GLN
2	B	115	ASP
3	C	6	ASN
3	C	34	GLU
3	C	47	GLN
3	C	73	THR
3	C	117	THR
3	C	206	GLU
3	C	217	THR
3	D	12	MET
3	D	50	LYS
3	D	73	THR
3	D	114	GLN
3	D	117	THR
3	D	185	LYS
3	D	217	THR
3	E	13	ARG
3	E	73	THR
3	E	115	ASP
3	E	117	THR
3	E	217	THR
3	E	225	LEU
3	F	6	ASN
3	F	7	VAL
3	F	12	MET
3	F	13	ARG
3	F	30	GLU
3	F	32	GLU
3	F	73	THR
3	F	114	GLN
3	F	117	THR
3	F	217	THR
3	G	47	GLN
3	G	60	ILE
3	G	73	THR
3	G	187	VAL
3	G	209	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	G	211	VAL
3	G	217	THR
3	H	73	THR
3	H	75	HIS
3	H	78	ASP
3	H	114	GLN
3	H	150	LEU
3	H	217	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
2	B	47	GLN
2	B	222	HIS
3	C	6	ASN
3	C	222	HIS
3	D	222	HIS
3	E	121	HIS
3	E	222	HIS
3	F	222	HIS
3	G	121	HIS
3	G	222	HIS
3	H	47	GLN
3	H	162	HIS
3	H	222	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	A	66	1	24,24,25	4.85	9 (37%)	30,32,34	2.76	7 (23%)
2	NRQ	B	66	2	24,24,25	4.83	9 (37%)	30,32,34	3.14	9 (30%)
3	NRQ	C	66	3	24,24,25	5.01	10 (41%)	30,32,34	2.72	8 (26%)
3	NRQ	D	66	3	24,24,25	5.17	9 (37%)	30,32,34	3.20	8 (26%)
3	NRQ	E	66	3	24,24,25	5.21	10 (41%)	30,32,34	3.03	7 (23%)
3	NRQ	F	66	3	24,24,25	4.69	9 (37%)	30,32,34	2.85	9 (30%)
3	NRQ	G	66	3	24,24,25	5.08	9 (37%)	30,32,34	2.95	8 (26%)
3	NRQ	H	66	3	24,24,25	5.33	11 (45%)	30,32,34	3.10	8 (26%)

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	66	1	-	0/9/31/32	0/2/2/2
2	NRQ	B	66	2	-	0/9/31/32	0/2/2/2
3	NRQ	C	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	D	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	E	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	F	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	G	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	H	66	3	-	0/9/31/32	0/2/2/2

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	66	NRQ	O3-C3	20.31	1.25	1.11
3	E	66	NRQ	O3-C3	19.94	1.25	1.11
3	H	66	NRQ	O3-C3	19.76	1.25	1.11
3	G	66	NRQ	O3-C3	19.74	1.25	1.11
3	C	66	NRQ	O3-C3	19.31	1.24	1.11
1	A	66	NRQ	O3-C3	19.17	1.24	1.11
2	B	66	NRQ	O3-C3	18.39	1.24	1.11
3	F	66	NRQ	O3-C3	18.18	1.23	1.11
3	D	66	NRQ	CB2-CA2	10.00	1.42	1.35
2	B	66	NRQ	CB2-CA2	9.11	1.41	1.35
1	A	66	NRQ	CB2-CA2	8.98	1.41	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	66	NRQ	CB2-CA2	8.78	1.41	1.35
3	E	66	NRQ	CA2-C2	-8.54	1.39	1.48
3	C	66	NRQ	CB2-CA2	8.43	1.40	1.35
3	H	66	NRQ	C1-CA1	8.17	1.59	1.48
3	F	66	NRQ	CA2-C2	-8.09	1.39	1.48
3	G	66	NRQ	CB2-CA2	8.03	1.40	1.35
3	H	66	NRQ	CA2-C2	-7.98	1.39	1.48
3	C	66	NRQ	CA2-C2	-7.83	1.40	1.48
2	B	66	NRQ	CA2-C2	-7.75	1.40	1.48
3	E	66	NRQ	CB2-CA2	7.62	1.40	1.35
3	G	66	NRQ	CA2-C2	-7.21	1.40	1.48
3	F	66	NRQ	CB2-CA2	6.85	1.39	1.35
3	D	66	NRQ	CA2-C2	-6.76	1.41	1.48
1	A	66	NRQ	CA2-C2	-6.69	1.41	1.48
3	E	66	NRQ	C1-CA1	6.18	1.56	1.48
2	B	66	NRQ	OH-CZ	-5.51	1.23	1.37
3	G	66	NRQ	CA3-C3	5.47	1.55	1.48
3	G	66	NRQ	OH-CZ	-5.44	1.23	1.37
3	C	66	NRQ	OH-CZ	-5.43	1.23	1.37
3	H	66	NRQ	OH-CZ	-5.39	1.23	1.37
3	E	66	NRQ	OH-CZ	-5.32	1.23	1.37
3	F	66	NRQ	OH-CZ	-5.15	1.24	1.37
1	A	66	NRQ	OH-CZ	-5.05	1.24	1.37
3	D	66	NRQ	OH-CZ	-4.64	1.25	1.37
3	C	66	NRQ	C1-CA1	4.51	1.54	1.48
3	D	66	NRQ	C1-CA1	4.25	1.53	1.48
3	F	66	NRQ	C1-CA1	4.16	1.53	1.48
3	E	66	NRQ	CA3-C3	4.13	1.53	1.48
2	B	66	NRQ	C1-CA1	4.13	1.53	1.48
3	G	66	NRQ	CA3-N3	4.12	1.50	1.47
3	H	66	NRQ	C2-N3	-3.82	1.31	1.39
3	D	66	NRQ	CA3-C3	3.77	1.53	1.48
3	C	66	NRQ	CA3-C3	3.68	1.53	1.48
3	H	66	NRQ	CA3-C3	3.58	1.53	1.48
1	A	66	NRQ	CA3-C3	3.40	1.52	1.48
3	G	66	NRQ	C1-CA1	-3.32	1.43	1.48
3	F	66	NRQ	CG2-CB2	-3.28	1.40	1.46
3	E	66	NRQ	CG2-CB2	-3.16	1.40	1.46
3	C	66	NRQ	C2-N3	-3.13	1.33	1.39
1	A	66	NRQ	C2-N3	-3.08	1.33	1.39
3	E	66	NRQ	C2-N3	-3.05	1.33	1.39
3	F	66	NRQ	C2-N3	-2.96	1.33	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	NRQ	CA3-C3	2.93	1.52	1.48
3	F	66	NRQ	CA3-C3	2.81	1.52	1.48
3	D	66	NRQ	C2-N3	-2.69	1.34	1.39
3	G	66	NRQ	CG2-CB2	-2.67	1.41	1.46
3	C	66	NRQ	C1-N3	-2.65	1.33	1.38
2	B	66	NRQ	CG2-CB2	-2.57	1.41	1.46
3	D	66	NRQ	C1-N3	-2.57	1.33	1.38
3	C	66	NRQ	CG2-CB2	-2.51	1.41	1.46
3	H	66	NRQ	C1-N3	-2.49	1.33	1.38
3	E	66	NRQ	C1-N3	-2.43	1.33	1.38
3	H	66	NRQ	CG2-CB2	-2.43	1.42	1.46
3	D	66	NRQ	CG2-CB2	-2.30	1.42	1.46
1	A	66	NRQ	CG2-CB2	-2.22	1.42	1.46
3	G	66	NRQ	C2-N3	-2.20	1.35	1.39
3	H	66	NRQ	CA2-N2	-2.18	1.33	1.38
3	F	66	NRQ	CA2-N2	-2.16	1.33	1.38
2	B	66	NRQ	C1-N3	-2.14	1.34	1.38
1	A	66	NRQ	C1-N3	-2.14	1.34	1.38
1	A	66	NRQ	C1-CA1	2.11	1.51	1.48
3	H	66	NRQ	CA1-N1	2.09	1.32	1.27
3	C	66	NRQ	CA2-N2	-2.08	1.33	1.38
2	B	66	NRQ	C2-N3	-2.02	1.35	1.39
3	E	66	NRQ	CA2-N2	-2.02	1.33	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	66	NRQ	CA2-C2-N3	10.40	109.37	103.44
3	D	66	NRQ	CA2-C2-N3	9.58	108.89	103.44
2	B	66	NRQ	O2-C2-CA2	-9.34	125.56	130.96
3	E	66	NRQ	CA2-C2-N3	9.33	108.76	103.44
3	G	66	NRQ	O2-C2-CA2	-8.95	125.78	130.96
1	A	66	NRQ	CA2-C2-N3	8.62	108.35	103.44
3	G	66	NRQ	CA2-C2-N3	8.36	108.20	103.44
3	E	66	NRQ	O2-C2-CA2	-8.10	126.27	130.96
3	F	66	NRQ	N3-C1-N2	-7.80	107.16	113.24
2	B	66	NRQ	CA2-C2-N3	7.76	107.86	103.44
2	B	66	NRQ	N3-C1-N2	-7.72	107.22	113.24
3	C	66	NRQ	CA2-C2-N3	7.56	107.75	103.44
3	D	66	NRQ	O2-C2-CA2	-7.53	126.61	130.96
1	A	66	NRQ	N3-C1-N2	-7.19	107.63	113.24
3	H	66	NRQ	N3-C1-N2	-7.14	107.67	113.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	66	NRQ	CA2-C2-N3	6.97	107.41	103.44
3	E	66	NRQ	N3-C1-N2	-6.70	108.02	113.24
3	C	66	NRQ	N3-C1-N2	-6.62	108.08	113.24
3	D	66	NRQ	N3-C1-N2	-6.60	108.09	113.24
3	C	66	NRQ	O2-C2-CA2	-6.47	127.22	130.96
3	H	66	NRQ	C2-CA2-N2	-6.46	104.04	108.91
3	D	66	NRQ	C2-CA2-N2	-6.21	104.23	108.91
3	H	66	NRQ	O2-C2-CA2	-6.05	127.46	130.96
3	F	66	NRQ	O2-C2-CA2	-6.01	127.48	130.96
3	D	66	NRQ	CA3-N3-C2	5.96	127.17	123.46
1	A	66	NRQ	C2-CA2-N2	-5.87	104.49	108.91
3	G	66	NRQ	N3-C1-N2	-5.73	108.77	113.24
2	B	66	NRQ	C2-CA2-N2	-5.32	104.91	108.91
3	C	66	NRQ	C2-CA2-N2	-5.14	105.04	108.91
3	E	66	NRQ	C2-CA2-N2	-4.96	105.18	108.91
3	G	66	NRQ	CA3-N3-C2	4.59	126.32	123.46
3	G	66	NRQ	C2-CA2-N2	-4.47	105.55	108.91
3	F	66	NRQ	C2-CA2-N2	-4.40	105.60	108.91
3	F	66	NRQ	CA1-C1-N3	4.36	130.89	124.78
1	A	66	NRQ	O2-C2-CA2	-4.32	128.46	130.96
3	C	66	NRQ	CA3-N3-C2	3.87	125.87	123.46
2	B	66	NRQ	CA1-C1-N3	3.57	129.79	124.78
2	B	66	NRQ	CA2-N2-C1	3.52	110.93	104.22
3	F	66	NRQ	CA3-N3-C1	3.47	129.26	124.10
1	A	66	NRQ	CA2-N2-C1	3.43	110.75	104.22
3	F	66	NRQ	CA2-N2-C1	3.37	110.65	104.22
3	E	66	NRQ	CB2-CA2-N2	3.35	134.78	128.59
3	H	66	NRQ	CA2-N2-C1	3.34	110.59	104.22
3	D	66	NRQ	CA2-N2-C1	3.24	110.38	104.22
3	F	66	NRQ	CA3-N3-C2	-3.22	121.46	123.46
3	H	66	NRQ	CA1-C1-N3	3.19	129.25	124.78
3	C	66	NRQ	CA2-N2-C1	3.18	110.28	104.22
2	B	66	NRQ	CB2-CA2-N2	3.04	134.21	128.59
2	B	66	NRQ	CA3-N3-C2	3.04	125.35	123.46
3	G	66	NRQ	CA2-N2-C1	2.95	109.85	104.22
3	E	66	NRQ	CA2-N2-C1	2.92	109.79	104.22
3	C	66	NRQ	CA1-C1-N3	2.91	128.85	124.78
3	H	66	NRQ	CB2-CA2-N2	2.81	133.78	128.59
3	E	66	NRQ	CA1-C1-N3	2.66	128.50	124.78
3	F	66	NRQ	CB2-CA2-N2	2.51	133.23	128.59
1	A	66	NRQ	CA1-C1-N3	2.49	128.28	124.78
3	D	66	NRQ	CB2-CA2-N2	2.47	133.16	128.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	66	NRQ	CB2-CA2-N2	2.47	133.16	128.59
3	H	66	NRQ	CA3-N3-C1	2.39	127.66	124.10
2	B	66	NRQ	CB1-CG1-SD	-2.35	106.41	112.84
3	G	66	NRQ	CB2-CA2-N2	2.33	132.90	128.59
3	D	66	NRQ	CD1-CE1-CZ	2.26	122.59	119.87
3	G	66	NRQ	CA1-C1-N3	2.16	127.81	124.78
1	A	66	NRQ	CB2-CA2-N2	2.08	132.43	128.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

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<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	217/218 (99%)	-0.16	3 (1%) 72 71	28, 40, 48, 53	0
2	B	218/218 (100%)	-0.46	0 100 100	27, 38, 47, 53	0
3	C	218/218 (100%)	-0.33	1 (0%) 88 88	28, 40, 48, 66	0
3	D	218/218 (100%)	-0.40	1 (0%) 88 88	26, 35, 43, 51	0
3	E	217/218 (99%)	-0.16	2 (0%) 81 81	31, 47, 56, 60	0
3	F	218/218 (100%)	-0.27	2 (0%) 81 81	29, 37, 47, 55	0
3	G	218/218 (100%)	0.59	11 (5%) 28 25	41, 57, 65, 72	0
3	H	218/218 (100%)	-0.19	3 (1%) 72 71	31, 43, 56, 62	0
All	All	1742/1744 (99%)	-0.17	23 (1%) 74 73	26, 41, 59, 72	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	169	GLY	5.9
3	F	169	GLY	3.4
1	A	169	GLY	3.3
3	G	170	GLY	3.1
3	G	168	LYS	3.0
3	G	7	VAL	3.0
3	H	168	LYS	2.9
3	E	114	GLN	2.7
1	A	168	LYS	2.7
3	G	6	ASN	2.6
3	G	114	GLN	2.6
3	G	219	ALA	2.5
3	G	105	VAL	2.4
3	C	169	GLY	2.3
3	D	168	LYS	2.3
3	F	168	LYS	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	H	170	GLY	2.2
3	H	169	GLY	2.2
3	G	47	GLN	2.2
3	G	17	HIS	2.2
1	A	63	PRO	2.2
3	G	225	LEU	2.0
3	G	210	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NRQ	G	66	23/24	0.24	1.15	59,60,62,66	0
1	NRQ	A	66	23/24	0.20	0.79	37,41,43,44	0
2	NRQ	B	66	23/24	0.13	0.73	38,41,42,46	0
3	NRQ	H	66	23/24	0.15	0.62	40,44,47,48	0
3	NRQ	D	66	23/24	0.14	0.25	29,34,36,39	0
3	NRQ	F	66	23/24	0.15	0.14	33,37,39,39	0
3	NRQ	C	66	23/24	0.13	-0.07	35,40,43,44	0
3	NRQ	E	66	23/24	0.13	-0.14	39,44,48,49	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.