



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:26 PM UTC

PDB ID : 3BXB / pdb_00003bxb
Title : Monomeric Far-red Fluorescent Protein mKate Crystallized at pH 7.0
Authors : Pletnev, S.; Pletneva, N.; Pletnev, V.
Deposited on : 2008-01-12
Resolution : 2.60 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

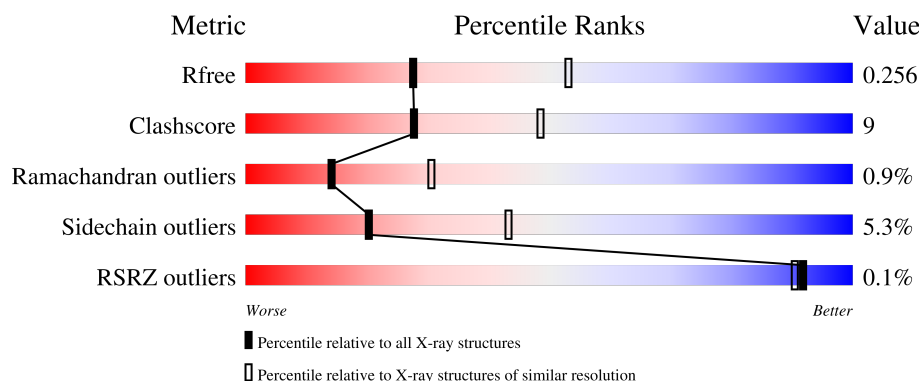
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	243	
1	B	243	
1	C	243	
1	D	243	
1	E	243	

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Mol	Chain	Length	Quality of chain
1	F	243	 70%19%8%
1	G	243	 71%18%8%
1	H	243	 72%18%8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14615 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 Far-red fluorescent protein mKate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1776	1129	300	334	13			
1	B	223	Total	C	N	O	S	0	0	0
			1776	1129	300	334	13			
1	C	223	Total	C	N	O	S	0	1	0
			1787	1135	304	335	13			
1	D	223	Total	C	N	O	S	0	2	0
			1799	1144	305	337	13			
1	E	223	Total	C	N	O	S	0	1	0
			1787	1135	304	335	13			
1	F	223	Total	C	N	O	S	0	1	0
			1787	1135	304	335	13			
1	G	223	Total	C	N	O	S	0	0	0
			1776	1129	300	334	13			
1	H	223	Total	C	N	O	S	0	0	0
			1776	1129	300	334	13			

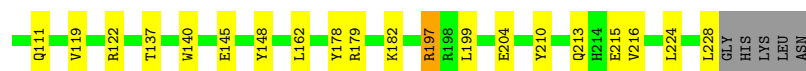
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	48	Total	O	0	0
			48	48		
2	B	51	Total	O	0	0
			51	51		
2	C	42	Total	O	0	0
			42	42		
2	D	60	Total	O	0	0
			60	60		
2	E	51	Total	O	0	0
			51	51		
2	F	45	Total	O	0	0
			45	45		

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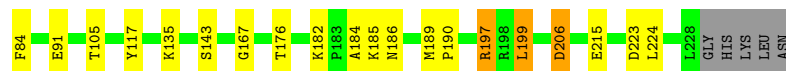
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	25	Total	O	0	0
			25	25		
2	H	29	Total	O	0	0
			29	29		



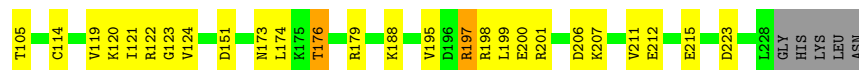
- Molecule 1: Far-red fluorescent protein mKate

Chain E: 73% 16% 8%



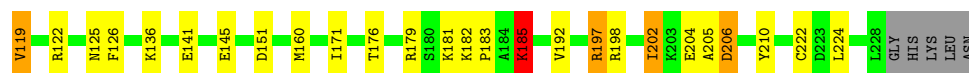
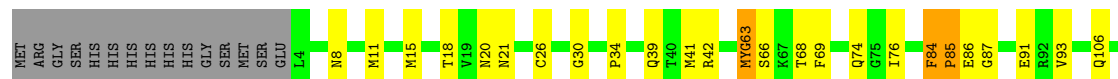
- Molecule 1: Far-red fluorescent protein mKate

Chain F: 70% 19% 8%



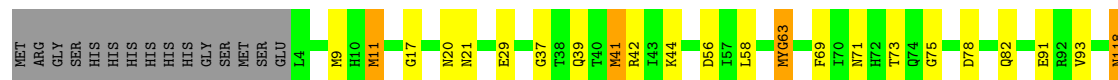
- Molecule 1: Far-red fluorescent protein mKate

Chain G: 71% 18% 8%



- Molecule 1: Far-red fluorescent protein mKate

Chain H: 72% 18% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.18Å 104.97Å 123.03Å 90.00° 105.81° 90.00°	Depositor
Resolution (Å)	29.84 – 2.60 29.84 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.84-2.60) 99.6 (29.84-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.170 , 0.263 0.166 , 0.256	Depositor DCC
R_{free} test set	2814 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14615	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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

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	0.71	0/1792	0.90	4/2417 (0.2%)
1	B	0.69	0/1792	0.90	2/2417 (0.1%)
1	C	0.70	0/1803	0.88	2/2431 (0.1%)
1	D	0.67	0/1816	0.85	1/2449 (0.0%)
1	E	0.67	0/1803	0.91	2/2431 (0.1%)
1	F	0.67	0/1803	0.91	2/2431 (0.1%)
1	G	0.67	0/1792	0.90	1/2417 (0.0%)
1	H	0.62	0/1792	0.89	3/2417 (0.1%)
All	All	0.67	0/14393	0.89	17/19410 (0.1%)

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	C	0	1
1	F	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLY	N-CA-C	7.30	120.44	110.58
1	B	62	PHE	CA-C-O	-6.97	108.95	120.80
1	A	182	LYS	CA-C-N	6.87	126.91	119.90
1	A	182	LYS	C-N-CA	6.87	126.91	119.90
1	H	224	LEU	CA-C-N	6.42	127.86	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	224	LEU	C-N-CA	6.42	127.86	119.84
1	A	99	GLY	N-CA-C	6.20	120.22	113.58
1	E	33	LYS	CA-C-N	6.00	126.16	119.32
1	E	33	LYS	C-N-CA	6.00	126.16	119.32
1	D	21	ASN	N-CA-C	5.86	119.50	111.54
1	A	121	ILE	CB-CA-C	-5.78	102.01	110.62
1	F	33	LYS	CA-C-N	5.43	125.25	119.28
1	F	33	LYS	C-N-CA	5.43	125.25	119.28
1	C	33	LYS	CA-C-N	5.26	125.32	119.32
1	C	33	LYS	C-N-CA	5.26	125.32	119.32
1	G	74	GLN	N-CA-CB	-5.21	101.69	110.49
1	H	17	GLY	N-CA-C	5.02	116.81	110.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	84	PHE	Peptide
1	F	74	GLN	Peptide
1	G	84	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1776	0	1745	34	0
1	B	1776	0	1745	23	0
1	C	1787	0	1757	41	0
1	D	1799	0	1765	28	0
1	E	1787	0	1757	33	0
1	F	1787	0	1757	41	0
1	G	1776	0	1745	43	0
1	H	1776	0	1745	32	0
2	A	48	0	0	1	0
2	B	51	0	0	0	0
2	C	42	0	0	7	0
2	D	60	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	51	0	0	1	0
2	F	45	0	0	3	0
2	G	25	0	0	5	0
2	H	29	0	0	1	0
All	All	14615	0	14016	255	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 9.

All (255) 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:41:MET:HG3	1:A:63:NRQ:CE	1.85	1.06
1:C:73:THR:HA	2:C:266:HOH:O	1.55	1.05
1:A:41:MET:HG3	1:A:63:NRQ:HE2A	1.36	1.04
1:E:67:LYS:NZ	1:E:197[B]:ARG:HH22	1.59	1.00
1:H:78:ASP:O	1:H:82:GLN:HB2	1.62	0.98
1:D:91:GLU:OE2	1:D:179:ARG:NH1	1.99	0.94
1:B:197:ARG:HH11	1:B:197:ARG:HG2	1.37	0.90
1:E:67:LYS:HZ2	1:E:197[B]:ARG:HH22	1.17	0.87
1:H:44:LYS:HE3	1:H:210:TYR:HD2	1.39	0.87
1:E:41:MET:HG3	1:E:63:NRQ:HE2A	1.58	0.86
1:F:28:SER:OG	1:F:41:MET:HG2	1.80	0.82
1:H:91:GLU:CD	1:H:179:ARG:HH12	1.88	0.80
1:G:11:MET:HG3	1:G:41:MET:HE3	1.66	0.78
1:H:71:ASN:OD1	1:H:73:THR:HG23	1.84	0.77
1:G:125:ASN:HB2	2:G:247:HOH:O	1.84	0.77
1:G:197:ARG:CG	1:G:197:ARG:HH11	1.98	0.76
1:E:67:LYS:NZ	1:E:197[B]:ARG:NH2	2.33	0.75
1:C:41:MET:CE	1:C:62:PHE:HB3	2.17	0.75
1:G:85:PRO:HD2	1:G:86:GLU:OE2	1.87	0.74
1:B:197:ARG:HH11	1:B:197:ARG:CG	2.01	0.74
1:C:82:GLN:O	1:C:182:LYS:HE2	1.88	0.73
1:F:197[A]:ARG:HG2	1:F:197[A]:ARG:HH11	1.53	0.72
1:F:67:LYS:HZ1	1:F:197[B]:ARG:HH12	1.36	0.71
1:G:197:ARG:HH11	1:G:197:ARG:HG2	1.55	0.70
1:H:118:ASN:HD22	1:H:118:ASN:N	1.89	0.70
1:F:25:LYS:HB2	1:F:25:LYS:NZ	2.07	0.70
1:F:91:GLU:OE2	1:F:179:ARG:NH1	2.25	0.70
1:G:91:GLU:CD	1:G:179:ARG:HH12	2.00	0.70
1:E:67:LYS:HZ2	1:E:197[B]:ARG:NH2	1.88	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:HG3	1:A:63:NRQ:HE1A	1.76	0.67
1:B:73:THR:OG1	1:B:219:ALA:O	2.13	0.66
1:E:197[B]:ARG:HD3	1:E:215:GLU:OE2	1.96	0.66
1:E:67:LYS:HZ1	1:E:197[B]:ARG:HH22	1.44	0.66
1:H:44:LYS:HE3	1:H:210:TYR:CD2	2.27	0.65
1:A:18:THR:HB	1:A:122:ARG:NH1	2.12	0.65
1:D:13:LEU:HB3	1:D:28:SER:OG	1.97	0.64
1:G:205:ALA:HB3	1:G:210:TYR:HB3	1.78	0.64
1:F:92:ARG:HD3	1:F:174:LEU:HD23	1.80	0.64
1:C:41:MET:HE1	1:C:62:PHE:HB3	1.79	0.64
1:F:25:LYS:HB2	1:F:25:LYS:HZ3	1.63	0.64
1:E:77:PRO:HG2	1:E:190:PRO:HA	1.78	0.63
1:C:151:ASP:HB3	2:C:260:HOH:O	1.97	0.63
1:F:41:MET:HB2	1:F:63:NRQ:HE2A	1.81	0.63
1:E:22:HIS:HE1	1:E:48:GLY:O	1.80	0.63
1:H:39:GLN:HG3	1:H:63:NRQ:HE3	1.81	0.63
1:E:39:GLN:HG3	1:E:63:NRQ:HE3	1.79	0.63
1:F:12:LYS:HD2	1:F:114:CYS:SG	2.39	0.63
1:G:15:MET:HB3	1:G:26:CYS:HB2	1.80	0.63
1:A:122:ARG:HD3	1:C:105:THR:HG23	1.80	0.62
1:H:118:ASN:N	1:H:118:ASN:ND2	2.48	0.62
1:H:41:MET:HG3	1:H:63:NRQ:HE2A	1.81	0.62
1:B:41:MET:HE3	1:B:62:PHE:O	1.99	0.61
1:H:227:LYS:HG2	2:H:246:HOH:O	2.00	0.61
1:H:136:LYS:HB3	1:H:165:VAL:HB	1.83	0.61
1:C:63:NRQ:CE1	1:C:197[A]:ARG:HE	2.14	0.60
1:A:41:MET:CG	1:A:63:NRQ:HE2A	2.23	0.60
1:F:197[A]:ARG:HH11	1:F:197[A]:ARG:CG	2.14	0.60
1:G:87:GLY:O	1:G:181:LYS:HB2	2.02	0.60
1:A:118:ASN:HB2	2:A:267:HOH:O	2.02	0.60
1:F:63:NRQ:HE2	1:F:199:LEU:HB2	1.84	0.59
1:A:37:GLY:HA2	1:A:69:PHE:O	2.02	0.59
1:D:197[B]:ARG:NH1	2:D:240:HOH:O	2.35	0.58
1:D:11:MET:SD	1:D:41:MET:HE3	2.43	0.58
1:G:20:ASN:HD21	1:G:126:PHE:HB2	1.69	0.58
1:E:63:NRQ:CE2	1:E:197[B]:ARG:HD2	2.34	0.57
1:B:34:PRO:HA	1:B:69:PHE:HA	1.87	0.57
1:C:63:NRQ:HE2	1:C:199:LEU:HB2	1.85	0.57
1:E:39:GLN:HE22	1:E:66:SER:HB3	1.69	0.57
1:H:37:GLY:O	1:H:216:VAL:HA	2.05	0.57
1:F:16:GLU:HG3	1:F:25:LYS:HZ2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TRP:CZ3	1:A:162:LEU:HB2	2.40	0.56
1:D:39:GLN:NE2	1:D:69:PHE:HB2	2.20	0.56
1:E:73:THR:HA	2:E:266:HOH:O	2.04	0.56
1:B:145:GLU:HB2	1:B:197:ARG:NH2	2.19	0.55
1:G:145:GLU:HB2	1:G:197:ARG:NH2	2.21	0.55
1:C:67:LYS:NZ	1:C:197[B]:ARG:HH22	2.04	0.55
1:D:44:LYS:HE3	1:D:210:TYR:HE1	1.71	0.55
1:G:63:NRQ:N1	1:G:63:NRQ:HA31	2.21	0.55
1:G:185:LYS:HE3	1:G:185:LYS:H	1.71	0.55
1:B:203:LYS:H	1:B:212:GLU:HB3	1.71	0.55
1:G:106:GLN:CG	1:G:119:VAL:HG22	2.37	0.54
1:F:212:GLU:HB3	2:F:254:HOH:O	2.07	0.54
1:A:74:GLN:C	1:A:76:ILE:H	2.15	0.54
1:C:12:LYS:HG2	1:C:29:GLU:OE1	2.08	0.53
1:A:63:NRQ:HE2	1:A:199:LEU:HB2	1.89	0.53
1:B:93:VAL:HG23	1:B:103:THR:HG22	1.90	0.53
1:A:22:HIS:HE1	1:A:48:GLY:O	1.91	0.53
1:F:201:ARG:HD3	1:F:211:VAL:HG13	1.91	0.53
1:H:41:MET:CG	1:H:63:NRQ:HE2A	2.38	0.53
1:H:29:GLU:OE2	1:H:42:ARG:NE	2.39	0.52
1:D:140:TRP:CZ3	1:D:162:LEU:HB2	2.44	0.52
1:D:63:NRQ:CZ	1:D:197[A]:ARG:HG3	2.39	0.52
1:F:67:LYS:NZ	1:F:197[B]:ARG:HH12	2.08	0.52
1:C:63:NRQ:CD2	1:C:197[B]:ARG:HD2	2.40	0.52
1:G:41:MET:HG3	1:G:63:NRQ:HE2A	1.91	0.52
1:F:105:THR:HG23	1:G:122:ARG:HD3	1.92	0.52
1:C:34:PRO:HA	1:C:69:PHE:HA	1.92	0.51
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.75	0.51
1:E:11:MET:HE3	1:E:69:PHE:CZ	2.46	0.51
1:F:42:ARG:HG2	1:F:212:GLU:HG2	1.93	0.51
1:G:197:ARG:CG	1:G:197:ARG:NH1	2.67	0.51
1:D:84:PHE:HB3	1:D:85:PRO:HA	1.93	0.51
1:A:11:MET:HG3	1:A:41:MET:HE3	1.92	0.51
1:D:63:NRQ:HE2	1:D:199:LEU:HB2	1.92	0.51
1:E:22:HIS:CE1	1:E:48:GLY:O	2.63	0.51
1:F:13:LEU:HD22	1:F:28:SER:HB3	1.93	0.51
1:A:223:ASP:OD1	1:A:223:ASP:N	2.37	0.50
1:A:63:NRQ:HG11	1:A:215:GLU:OE1	2.10	0.50
1:G:106:GLN:HG3	1:G:119:VAL:HG22	1.93	0.50
1:E:25:LYS:HB2	1:E:47:GLU:HB2	1.92	0.50
1:C:207:LYS:O	1:C:208:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:NRQ:CE2	1:C:197[B]:ARG:HD2	2.41	0.50
1:A:91:GLU:HG3	1:C:124:VAL:HB	1.94	0.50
1:G:224:LEU:O	1:H:198:ARG:NH2	2.41	0.50
1:D:145:GLU:OE2	1:D:178:TYR:OH	2.29	0.49
1:G:198:ARG:NH2	1:H:222:CYS:SG	2.85	0.49
1:F:85:PRO:HG2	2:F:269:HOH:O	2.11	0.49
1:C:29:GLU:HB2	2:C:265:HOH:O	2.12	0.49
1:C:129:ASN:HA	1:C:134:GLN:OE1	2.12	0.49
1:F:49:GLY:HA2	1:F:50:PRO:C	2.36	0.49
1:C:67:LYS:HZ1	1:C:197[B]:ARG:HH22	1.61	0.49
1:G:151:ASP:N	2:G:256:HOH:O	2.44	0.49
1:C:33:LYS:HD3	1:C:36:GLU:OE2	2.13	0.49
1:E:67:LYS:HZ1	1:E:197[B]:ARG:NH2	2.04	0.49
1:B:105:THR:HG23	1:D:122:ARG:HD3	1.95	0.48
1:C:165:VAL:O	1:C:166:GLY:C	2.55	0.48
1:F:92:ARG:HB2	1:F:176:THR:HG23	1.95	0.48
1:H:164:LEU:HD21	1:H:170:LEU:HB2	1.94	0.48
1:H:56:ASP:OD1	1:H:137:THR:OG1	2.31	0.48
1:G:18:THR:HB	1:G:122:ARG:NH1	2.29	0.48
1:C:75:GLY:HA2	2:C:268:HOH:O	2.14	0.48
1:C:102:LEU:HD21	1:C:121:ILE:HG23	1.96	0.47
1:H:140:TRP:CZ3	1:H:162:LEU:HB2	2.49	0.47
1:F:91:GLU:HG2	2:G:248:HOH:O	2.15	0.47
1:B:85:PRO:HD2	1:B:86:GLU:OE2	2.14	0.47
1:F:63:NRQ:CE1	1:F:197[B]:ARG:HD3	2.44	0.47
1:B:77:PRO:HG3	1:B:188:LYS:HE3	1.96	0.47
1:C:216:VAL:HG13	1:D:224:LEU:HD13	1.97	0.47
1:G:39:GLN:HG3	1:G:63:NRQ:HE3	1.96	0.47
1:A:105:THR:OG1	1:C:122:ARG:NH1	2.48	0.47
1:C:63:NRQ:N1	1:C:63:NRQ:HA31	2.30	0.47
1:B:197:ARG:CG	1:B:197:ARG:NH1	2.67	0.47
1:C:207:LYS:HE3	2:C:258:HOH:O	2.14	0.46
1:F:15:MET:HB3	1:F:26:CYS:HB2	1.96	0.46
1:H:145:GLU:HB2	1:H:197:ARG:NH2	2.30	0.46
1:A:11:MET:HE1	1:A:39:GLN:HB2	1.96	0.46
1:E:5:ILE:HD11	1:E:84:PHE:CD1	2.51	0.46
1:F:98:ASP:C	1:F:98:ASP:OD1	2.59	0.46
1:B:49:GLY:HA2	1:B:50:PRO:C	2.40	0.46
1:C:63:NRQ:CD1	1:C:197[A]:ARG:HE	2.29	0.46
1:G:106:GLN:HG2	1:G:119:VAL:HG22	1.98	0.46
1:D:137:THR:HB	1:D:162:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:VAL:HG12	1:F:197[B]:ARG:HG2	1.97	0.46
1:H:58:LEU:HD22	1:H:121:ILE:HD12	1.98	0.46
1:E:105:THR:HG23	1:H:122:ARG:HD3	1.98	0.46
1:D:197[B]:ARG:HD3	1:D:215:GLU:OE2	2.15	0.46
1:D:74:GLN:O	1:D:75:GLY:C	2.56	0.46
1:A:20:ASN:O	1:A:21:ASN:HB3	2.16	0.45
1:A:14:TYR:HD2	1:A:118:ASN:HD21	1.64	0.45
1:A:15:MET:HB3	1:A:26:CYS:HB2	1.99	0.45
1:E:19:VAL:HB	1:E:53:PHE:CE2	2.52	0.45
1:E:91:GLU:OE1	1:H:20:ASN:HA	2.17	0.45
1:G:21:ASN:N	2:G:248:HOH:O	2.41	0.45
1:E:13:LEU:HD12	1:E:117:TYR:HD2	1.81	0.45
1:E:189:MET:HE3	1:E:190:PRO:HD2	1.98	0.45
1:H:148:TYR:HA	1:H:149:PRO:HD3	1.78	0.45
1:B:63:NRQ:HD2	1:B:215:GLU:OE1	2.17	0.45
1:F:198:ARG:O	1:F:215:GLU:HA	2.17	0.45
1:G:39:GLN:HE22	1:G:66:SER:HB3	1.82	0.45
1:C:195:VAL:O	1:C:197[A]:ARG:NH1	2.49	0.45
1:F:197[A]:ARG:CG	1:F:197[A]:ARG:NH1	2.77	0.45
1:A:14:TYR:HD2	1:A:118:ASN:ND2	2.15	0.45
1:G:141:GLU:HG3	1:H:192:VAL:HG21	1.99	0.45
1:A:171:ILE:HG13	1:B:148:TYR:OH	2.17	0.45
1:E:143:SER:OG	1:E:197[A]:ARG:NH1	2.50	0.45
1:F:18:THR:CB	1:F:122:ARG:HH22	2.30	0.45
1:G:222:CYS:SG	1:G:224:LEU:HB2	2.57	0.45
1:A:63:NRQ:CZ	1:A:197:ARG:HG3	2.47	0.44
1:B:74:GLN:O	1:B:75:GLY:C	2.59	0.44
1:B:42:ARG:HG2	1:B:212:GLU:HG3	2.00	0.44
1:E:10:HIS:ND1	1:E:31:GLU:HB3	2.32	0.44
1:D:145:GLU:HB2	1:D:197[A]:ARG:CZ	2.48	0.44
1:A:28:SER:OG	1:A:41:MET:HE2	2.16	0.44
1:C:11:MET:HE3	1:C:41:MET:SD	2.57	0.44
1:D:14[A]:TYR:OH	1:D:25:LYS:HE3	2.17	0.44
1:A:63:NRQ:HA31	1:A:63:NRQ:N1	2.31	0.44
1:C:140:TRP:CZ3	1:C:162:LEU:HB2	2.52	0.44
1:G:85:PRO:CD	1:G:86:GLU:OE2	2.63	0.44
1:E:51:LEU:O	1:E:135:LYS:NZ	2.40	0.44
1:C:42:ARG:HG2	1:C:212:GLU:HG3	2.00	0.44
1:C:63:NRQ:CE1	1:C:197[A]:ARG:NE	2.80	0.44
1:F:63:NRQ:HA31	1:F:63:NRQ:N1	2.33	0.43
1:F:198:ARG:HD2	1:F:200:GLU:OE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:NRQ:CZ	1:E:197[A]:ARG:HG3	2.48	0.43
1:D:59:ALA:HA	1:D:213:GLN:HE22	1.84	0.43
1:E:184:ALA:O	1:E:186:ASN:N	2.51	0.43
1:F:25:LYS:HZ3	1:F:25:LYS:CB	2.31	0.43
1:G:30:GLY:HA2	1:G:42:ARG:NH2	2.33	0.43
1:G:91:GLU:OE2	1:G:179:ARG:NH1	2.49	0.43
1:H:9:MET:HE2	1:H:9:MET:HB3	1.75	0.43
1:D:67:LYS:HE3	1:D:70:ILE:HD11	2.01	0.43
1:G:125:ASN:CB	2:G:247:HOH:O	2.53	0.43
1:G:202:ILE:HD12	1:G:202:ILE:HA	1.69	0.43
1:D:11:MET:HE1	1:D:39:GLN:HB2	1.99	0.43
1:G:11:MET:HE1	1:G:39:GLN:HB2	1.99	0.43
1:G:192:VAL:HG21	1:H:141:GLU:HG3	1.99	0.43
1:D:41:MET:HB2	1:D:63:NRQ:CE	2.49	0.43
1:F:101:VAL:O	1:F:123:GLY:HA2	2.19	0.43
1:A:74:GLN:H	1:A:74:GLN:HG3	1.62	0.43
1:A:101:VAL:O	1:A:123:GLY:HA2	2.19	0.43
1:A:206:ASP:HB2	1:A:209:THR:OG1	2.19	0.43
1:C:41:MET:HE2	1:C:63:NRQ:HE2A	2.01	0.43
1:E:63:NRQ:CZ	1:E:197[B]:ARG:HD2	2.48	0.43
1:G:222:CYS:SG	1:H:198:ARG:NH2	2.92	0.43
1:C:173:ASN:C	1:C:174:LEU:HD12	2.44	0.42
1:F:84:PHE:HB3	1:F:85:PRO:HA	2.01	0.42
1:H:20:ASN:O	1:H:21:ASN:CB	2.67	0.42
1:F:25:LYS:HB2	1:F:25:LYS:HZ2	1.83	0.42
1:A:9:MET:HG3	1:A:34:PRO:HG2	2.00	0.42
1:A:106:GLN:HG3	1:A:119:VAL:HG22	2.01	0.42
1:C:86:GLU:OE2	1:C:182:LYS:NZ	2.45	0.42
1:D:82:GLN:O	1:D:182:LYS:HE3	2.20	0.42
1:G:63:NRQ:HE1	1:G:160:MET:SD	2.59	0.42
1:B:111:GLN:O	1:B:112:ASP:C	2.62	0.42
1:G:39:GLN:NE2	1:G:69:PHE:HB2	2.33	0.42
1:A:157:ARG:HG3	1:B:171:ILE:HG21	2.01	0.42
1:E:21:ASN:O	1:E:21:ASN:CG	2.63	0.42
1:E:8:ASN:OD1	1:E:33:LYS:NZ	2.52	0.42
1:F:92:ARG:HD2	2:F:278:HOH:O	2.19	0.42
1:B:140:TRP:CE3	1:B:160:MET:HE2	2.56	0.41
1:C:171:ILE:HG13	1:D:148:TYR:OH	2.20	0.41
1:D:41:MET:HB2	1:D:63:NRQ:HE1A	2.02	0.41
1:B:73:THR:HB	1:B:74:GLN:H	1.68	0.41
1:H:63:NRQ:CD1	1:H:197:ARG:HE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:HB2	1:C:116:ILE:HD13	2.02	0.41
1:C:60:THR:HG23	2:C:240:HOH:O	2.19	0.41
1:D:78:ASP:OD2	1:D:81:LYS:HD2	2.20	0.41
1:E:63:NRQ:HE2	1:E:199:LEU:HB2	2.01	0.41
1:F:54:ALA:O	1:F:57:ILE:HG12	2.21	0.41
1:G:84:PHE:HB3	1:G:85:PRO:HA	2.03	0.41
1:B:9:MET:HG3	1:B:34:PRO:HG2	2.02	0.41
1:E:224:LEU:O	1:F:198:ARG:NH2	2.48	0.41
1:F:13:LEU:HB3	1:F:28:SER:HB3	2.01	0.41
1:F:206:ASP:O	1:F:207:LYS:C	2.64	0.41
1:G:20:ASN:ND2	1:G:126:PHE:HB2	2.34	0.41
1:C:200:GLU:HG2	1:D:228:LEU:HD12	2.03	0.41
1:C:126:PHE:HA	1:C:127:PRO:HD3	1.97	0.41
1:A:91:GLU:HB2	1:A:105:THR:HG22	2.03	0.40
1:G:182:LYS:HA	1:G:183:PRO:HD3	1.97	0.40
1:G:171:ILE:HG13	1:H:148:TYR:OH	2.20	0.40
1:C:18:THR:HG21	2:C:256:HOH:O	2.22	0.40
1:D:44:LYS:HG2	1:D:210:TYR:CE1	2.57	0.40
1:H:11:MET:HE3	1:H:69:PHE:CZ	2.56	0.40
1:A:28:SER:OG	1:A:41:MET:CE	2.70	0.40
1:F:124:VAL:HG21	1:G:93:VAL:HB	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	218/243 (90%)	211 (97%)	6 (3%)	1 (0%)	24	46
1	B	218/243 (90%)	209 (96%)	7 (3%)	2 (1%)	14	30
1	C	219/243 (90%)	209 (95%)	9 (4%)	1 (0%)	24	46
1	D	220/243 (90%)	211 (96%)	8 (4%)	1 (0%)	24	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	219/243 (90%)	204 (93%)	10 (5%)	5 (2%)	5	9
1	F	219/243 (90%)	211 (96%)	8 (4%)	0	100	100
1	G	218/243 (90%)	200 (92%)	14 (6%)	4 (2%)	6	14
1	H	218/243 (90%)	205 (94%)	11 (5%)	2 (1%)	14	30
All	All	1749/1944 (90%)	1660 (95%)	73 (4%)	16 (1%)	14	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	THR
1	E	73	THR
1	E	74	GLN
1	G	206	ASP
1	E	185	LYS
1	D	73	THR
1	E	167	GLY
1	G	185	LYS
1	H	225	PRO
1	A	74	GLN
1	C	73	THR
1	E	206	ASP
1	H	75	GLY
1	B	75	GLY
1	G	34	PRO
1	G	85	PRO

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	191/208 (92%)	181 (95%)	10 (5%)	21	44
1	B	191/208 (92%)	180 (94%)	11 (6%)	18	39
1	C	192/208 (92%)	183 (95%)	9 (5%)	23	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	193/208 (93%)	184 (95%)	9 (5%)	23	48
1	E	192/208 (92%)	181 (94%)	11 (6%)	18	40
1	F	192/208 (92%)	177 (92%)	15 (8%)	11	26
1	G	191/208 (92%)	180 (94%)	11 (6%)	18	39
1	H	191/208 (92%)	183 (96%)	8 (4%)	26	52
All	All	1533/1664 (92%)	1449 (94%)	84 (6%)	20	41

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	9	MET
1	A	18	THR
1	A	29	GLU
1	A	74	GLN
1	A	86	GLU
1	A	102	LEU
1	A	185	LYS
1	A	207	LYS
1	A	223	ASP
1	B	11	MET
1	B	18	THR
1	B	31	GLU
1	B	73	THR
1	B	111	GLN
1	B	118	ASN
1	B	119	VAL
1	B	197	ARG
1	B	207	LYS
1	B	223	ASP
1	B	228	LEU
1	C	11	MET
1	C	21	ASN
1	C	41	MET
1	C	47	GLU
1	C	119	VAL
1	C	120	LYS
1	C	158	SER
1	C	187	LEU
1	C	223	ASP

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Mol	Chain	Res	Type
1	D	7	GLU
1	D	40	THR
1	D	47	GLU
1	D	111	GLN
1	D	119	VAL
1	D	197[A]	ARG
1	D	197[B]	ARG
1	D	204	GLU
1	D	216	VAL
1	E	7	GLU
1	E	11	MET
1	E	18	THR
1	E	21	ASN
1	E	176	THR
1	E	182	LYS
1	E	197[A]	ARG
1	E	197[B]	ARG
1	E	199	LEU
1	E	206	ASP
1	E	223	ASP
1	F	11	MET
1	F	12	LYS
1	F	25	LYS
1	F	41	MET
1	F	102	LEU
1	F	119	VAL
1	F	120	LYS
1	F	121	ILE
1	F	151	ASP
1	F	173	ASN
1	F	176	THR
1	F	188	LYS
1	F	197[A]	ARG
1	F	197[B]	ARG
1	F	223	ASP
1	G	8	ASN
1	G	68	THR
1	G	76	ILE
1	G	119	VAL
1	G	136	LYS
1	G	176	THR
1	G	185	LYS

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Mol	Chain	Res	Type
1	G	197	ARG
1	G	202	ILE
1	G	204	GLU
1	G	206	ASP
1	H	11	MET
1	H	41	MET
1	H	93	VAL
1	H	118	ASN
1	H	124	VAL
1	H	137	THR
1	H	185	LYS
1	H	223	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	169	HIS
1	B	22	HIS
1	D	22	HIS
1	D	74	GLN
1	D	173	ASN
1	D	213	GLN
1	E	22	HIS
1	E	23	HIS
1	E	118	ASN
1	F	10	HIS
1	F	22	HIS
1	F	39	GLN
1	G	8	ASN
1	G	21	ASN
1	G	22	HIS
1	G	74	GLN
1	G	169	HIS
1	H	74	GLN
1	H	118	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	F	63	1	24,24,25	1.00	1 (4%)	24,32,34	1.11	1 (4%)
1	NRQ	G	63	1	24,24,25	1.27	2 (8%)	24,32,34	1.02	2 (8%)
1	NRQ	D	63	1	24,24,25	0.91	1 (4%)	24,32,34	1.02	1 (4%)
1	NRQ	E	63	1	24,24,25	1.23	2 (8%)	24,32,34	1.35	2 (8%)
1	NRQ	A	63	1	24,24,25	1.09	2 (8%)	24,32,34	1.08	1 (4%)
1	NRQ	B	63	1	24,24,25	1.11	2 (8%)	24,32,34	1.33	1 (4%)
1	NRQ	C	63	1	24,24,25	1.03	1 (4%)	24,32,34	1.14	2 (8%)
1	NRQ	H	63	1	24,24,25	0.77	0	24,32,34	0.91	1 (4%)

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	F	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	G	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	E	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	A	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	B	63	1	-	2/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	H	63	1	-	1/9/31/32	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	NRQ	C1-CA1	-4.68	1.41	1.48
1	E	63	NRQ	C1-CA1	-4.16	1.41	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	CA1-N1	3.94	1.36	1.27
1	F	63	NRQ	CA1-N1	3.50	1.35	1.27
1	C	63	NRQ	C1-CA1	-3.03	1.43	1.48
1	B	63	NRQ	C1-CA1	-2.97	1.43	1.48
1	D	63	NRQ	OH-CZ	-2.30	1.31	1.37
1	A	63	NRQ	C1-CA1	-2.23	1.44	1.48
1	B	63	NRQ	CA1-N1	2.16	1.32	1.27
1	G	63	NRQ	OH-CZ	-2.09	1.32	1.37
1	E	63	NRQ	OH-CZ	-2.02	1.32	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	NRQ	C3-CA3-N3	4.57	122.84	112.43
1	F	63	NRQ	C3-CA3-N3	3.81	121.09	112.43
1	C	63	NRQ	C3-CA3-N3	3.02	119.30	112.43
1	D	63	NRQ	C3-CA3-N3	2.96	119.17	112.43
1	E	63	NRQ	C3-CA3-N3	2.86	118.94	112.43
1	E	63	NRQ	CD1-CG2-CD2	2.80	121.81	117.65
1	A	63	NRQ	C3-CA3-N3	2.80	118.79	112.43
1	H	63	NRQ	C3-CA3-N3	2.51	118.14	112.43
1	C	63	NRQ	CE1-CD1-CG2	-2.47	118.03	121.22
1	G	63	NRQ	C3-CA3-N3	2.33	117.73	112.43
1	G	63	NRQ	N3-C1-N2	2.08	115.09	112.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	63	NRQ	C1-CA1-CB1-CG1
1	C	63	NRQ	CB1-CG1-SD-CE
1	D	63	NRQ	CB1-CG1-SD-CE
1	A	63	NRQ	CB1-CG1-SD-CE
1	B	63	NRQ	CB1-CG1-SD-CE
1	E	63	NRQ	CB1-CG1-SD-CE
1	B	63	NRQ	C1-CA1-CB1-CG1
1	G	63	NRQ	C1-CA1-CB1-CG1
1	H	63	NRQ	CB1-CG1-SD-CE

There are no ring outliers.

8 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	63	NRQ	4	0
1	G	63	NRQ	4	0
1	D	63	NRQ	4	0
1	E	63	NRQ	6	0
1	A	63	NRQ	8	0
1	B	63	NRQ	1	0
1	C	63	NRQ	8	0
1	H	63	NRQ	4	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	222/243 (91%)	-0.68	0	100 100	23, 39, 62, 85	0
1	B	222/243 (91%)	-0.74	0	100 100	23, 36, 64, 88	0
1	C	222/243 (91%)	-0.60	0	100 100	18, 42, 66, 82	1 (0%)
1	D	222/243 (91%)	-0.65	1 (0%)	87 85	16, 39, 68, 94	2 (0%)
1	E	222/243 (91%)	-0.67	0	100 100	18, 39, 68, 88	1 (0%)
1	F	222/243 (91%)	-0.64	0	100 100	18, 40, 68, 91	1 (0%)
1	G	222/243 (91%)	-0.39	0	100 100	26, 49, 78, 90	0
1	H	222/243 (91%)	-0.31	0	100 100	28, 52, 73, 97	0
All	All	1776/1944 (91%)	-0.59	1 (0%)	92 90	16, 42, 71, 97	5 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	THR	3.2

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(Å ²)	Q<0.9
1	NRQ	B	63	23/24	0.93	0.10	17,40,61,73	0
1	NRQ	G	63	23/24	0.93	0.11	32,51,86,107	0
1	NRQ	H	63	23/24	0.93	0.13	30,62,100,111	0
1	NRQ	C	63	23/24	0.94	0.09	30,46,57,97	0
1	NRQ	E	63	23/24	0.94	0.09	23,42,59,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NRQ	F	63	23/24	0.96	0.08	20,33,69,71	0
1	NRQ	D	63	23/24	0.97	0.09	28,36,61,89	0
1	NRQ	A	63	23/24	0.98	0.06	25,36,64,79	0

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.