



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:52 PM GMT

PDB ID : 3BXC  
Title : Monomeric Far-red Fluorescent Protein mKate Crystallized at pH 9.0  
Authors : Pletnev, S.; Pletneva, N.; Pletnev, V.  
Deposited on : 2008-01-12  
Resolution : 2.60 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>

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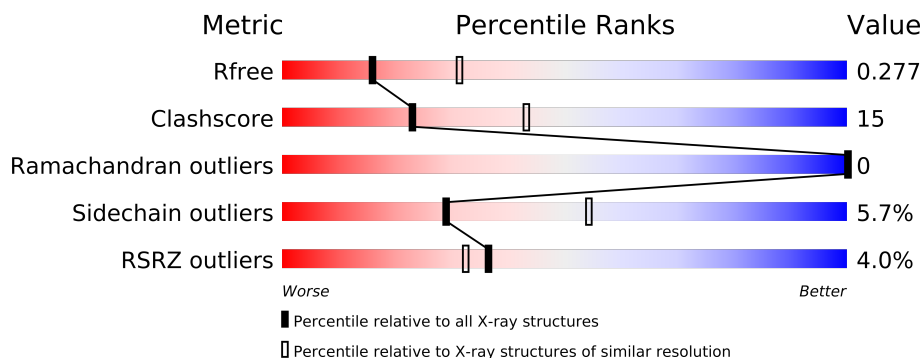
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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))
$R_{free}$	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 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	243	
1	B	243	
1	C	243	
1	D	243	
1	E	243	
1	F	243	
1	G	243	
1	H	243	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14324 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 Far-red fluorescent protein mKate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	B	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	C	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	D	222	Total	C	N	O	S	0	0	0
			1768	1123	299	333	13			
1	E	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	F	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	G	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			
1	H	219	Total	C	N	O	S	0	0	0
			1745	1108	295	329	13			

- Molecule 2 is water.

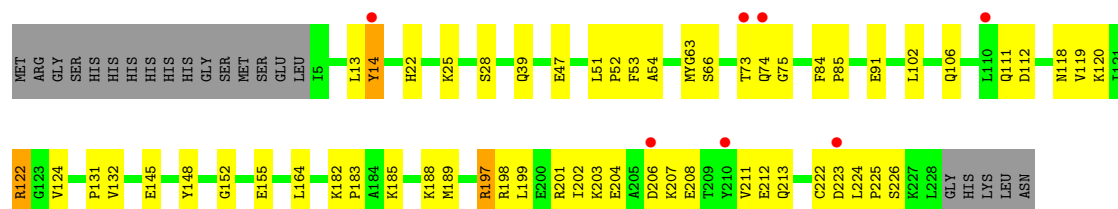
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		
2	B	53	Total	O	0	0
			53	53		
2	C	33	Total	O	0	0
			33	33		
2	D	44	Total	O	0	0
			44	44		
2	E	45	Total	O	0	0
			45	45		
2	F	57	Total	O	0	0
			57	57		

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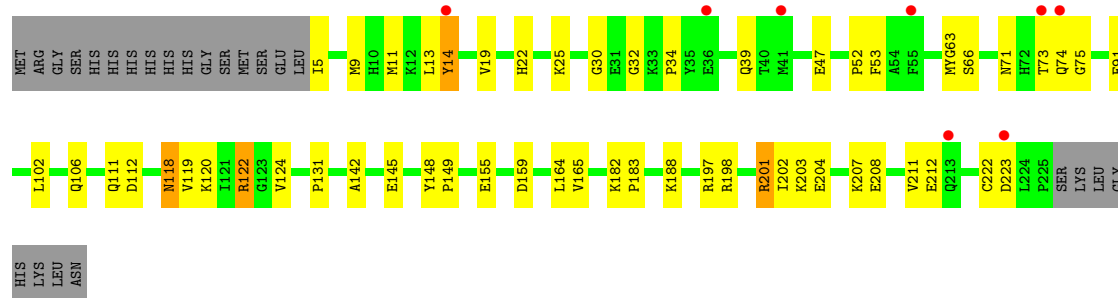
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	28	Total	O	0	0
			28	28		
2	H	35	Total	O	0	0
			35	35		





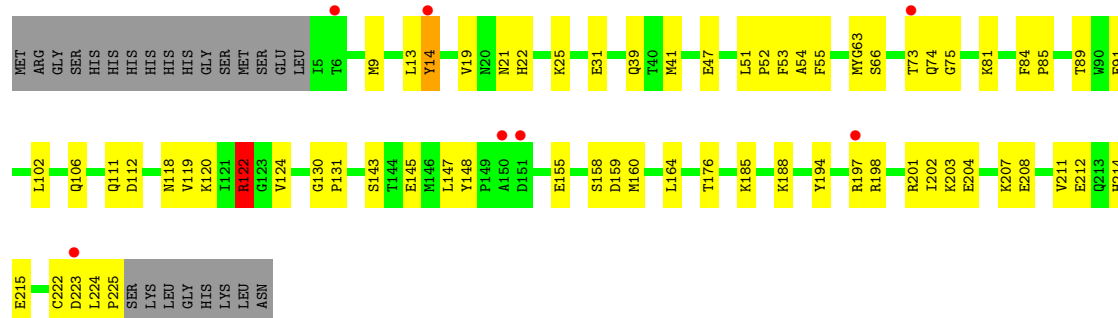
- Molecule 1: Far-red fluorescent protein mKate

Chain E:



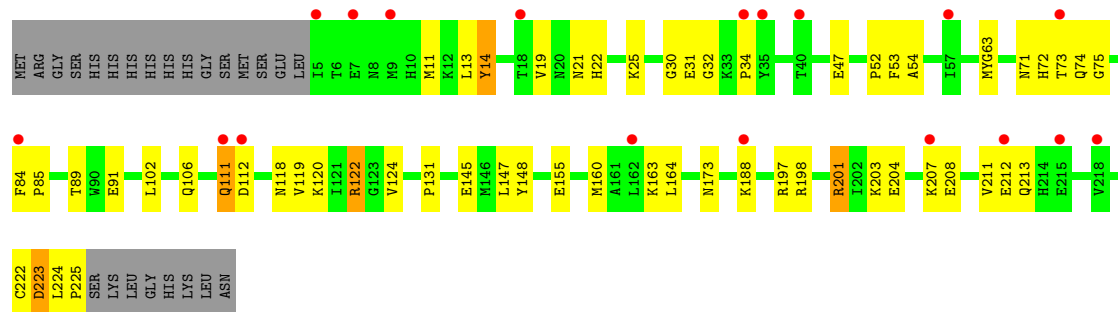
- Molecule 1: Far-red fluorescent protein mKate

Chain F:



- Molecule 1: Far-red fluorescent protein mKate

Chain G:



- Molecule 1: Far-red fluorescent protein mKate

Chain H:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.47Å 104.48Å 123.23Å 90.00° 106.09° 90.00°	Depositor
Resolution (Å)	29.71 – 2.60 29.71 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.7 (29.71-2.60) 83.5 (29.71-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.58 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.235 , 0.282 0.232 , 0.277	Depositor DCC
$R_{free}$ test set	2507 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 30.7	EDS
Estimated twinning fraction	0.094 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 48883 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14324	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% 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	0.54	0/1761	0.63	0/2376
1	B	0.57	0/1761	0.69	2/2376 (0.1%)
1	C	0.52	0/1761	0.65	0/2376
1	D	0.57	0/1784	0.64	0/2406
1	E	0.54	0/1761	0.64	0/2376
1	F	0.57	0/1761	0.68	2/2376 (0.1%)
1	G	0.53	0/1761	0.62	0/2376
1	H	0.54	0/1761	0.67	2/2376 (0.1%)
All	All	0.55	0/14111	0.65	6/19038 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	GLU	CA-CB-CG	9.86	135.09	113.40
1	H	91	GLU	CA-CB-CG	9.33	133.93	113.40
1	F	122	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	F	122	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	91	GLU	CB-CA-C	5.78	121.96	110.40
1	H	91	GLU	CB-CA-C	5.21	120.82	110.40

There are no chirality outliers.

There are no planarity outliers.

### 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	1745	0	1706	50	0
1	B	1745	0	1706	59	1
1	C	1745	0	1706	64	0
1	D	1768	0	1735	56	1
1	E	1745	0	1705	55	3
1	F	1745	0	1706	63	1
1	G	1745	0	1706	50	2
1	H	1745	0	1706	64	2
2	A	46	0	0	6	0
2	B	53	0	0	18	0
2	C	33	0	0	8	0
2	D	44	0	0	7	0
2	E	45	0	0	4	0
2	F	57	0	0	10	0
2	G	28	0	0	8	0
2	H	35	0	0	14	0
All	All	14324	0	13676	403	5

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 15.

All (403) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:120:LYS:HE2	2:B:252:HOH:O	1.49	1.12
1:F:185:LYS:HD3	2:F:254:HOH:O	1.50	1.10
1:A:125:ASN:HB2	2:A:253:HOH:O	1.52	1.10
1:B:197:ARG:HH11	1:B:197:ARG:HG2	1.14	1.07
1:B:197:ARG:HH11	1:B:197:ARG:CG	1.68	1.02
1:F:122:ARG:HH12	1:G:120:LYS:HB3	1.21	1.00
1:B:173:ASN:HB3	2:B:250:HOH:O	1.63	0.99
1:B:170:LEU:HD11	2:B:276:HOH:O	1.64	0.97
1:F:122:ARG:NH1	1:G:120:LYS:HB3	1.82	0.93
1:F:120:LYS:HB3	1:G:122:ARG:HH12	1.33	0.93
1:C:170:LEU:HD12	2:C:242:HOH:O	1.69	0.93
1:F:120:LYS:HB3	1:G:122:ARG:NH1	1.83	0.91
1:E:39:GLN:HG3	1:E:63:NRQ:HE1A	1.52	0.91
1:E:198:ARG:NH2	1:F:222:CYS:HB3	1.88	0.87
1:C:18:THR:HG22	2:C:246:HOH:O	1.73	0.87
1:E:39:GLN:HG3	1:E:63:NRQ:CE	2.07	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:ARG:NH2	1:B:222:CYS:HB3	1.95	0.81
1:C:97:GLU:HB2	2:C:242:HOH:O	1.81	0.81
1:E:39:GLN:CG	1:E:63:NRQ:HE1A	2.12	0.79
1:H:163:LYS:HB3	2:H:267:HOH:O	1.82	0.79
1:A:118:ASN:HB2	2:A:258:HOH:O	1.80	0.79
1:A:198:ARG:HH22	1:B:222:CYS:HB3	1.48	0.79
1:C:41:MET:HB2	1:C:63:NRQ:HE3	1.62	0.78
1:A:124:VAL:HG12	1:C:91:GLU:HG2	1.65	0.78
1:C:63:NRQ:N1	1:C:63:NRQ:HA31	1.99	0.77
1:B:92:ARG:NH1	2:B:288:HOH:O	2.16	0.75
1:E:198:ARG:HH22	1:F:222:CYS:HB3	1.49	0.75
1:A:63:NRQ:HD1	1:A:197:ARG:HH21	1.52	0.74
1:F:22:HIS:CD2	1:F:52:PRO:HG2	2.23	0.74
1:B:207:LYS:HG2	2:B:247:HOH:O	1.85	0.73
1:F:41:MET:HB2	1:F:63:NRQ:HE3	1.71	0.72
1:F:197:ARG:NH2	2:F:282:HOH:O	2.22	0.72
1:C:199:LEU:C	1:C:199:LEU:HD23	2.09	0.72
1:E:222:CYS:HB3	1:F:198:ARG:HH22	1.55	0.72
1:D:22:HIS:CD2	1:D:52:PRO:HG2	2.24	0.72
1:F:9:MET:HE3	2:F:255:HOH:O	1.91	0.70
1:G:63:NRQ:CG2	1:G:197:ARG:HE	2.04	0.70
1:A:91:GLU:HG2	1:C:124:VAL:HG12	1.73	0.70
1:D:145:GLU:HB2	1:D:197:ARG:HH22	1.57	0.70
1:B:22:HIS:CD2	1:B:52:PRO:HG2	2.27	0.70
1:A:63:NRQ:CD1	1:A:197:ARG:HE	2.04	0.70
1:E:5:ILE:N	2:E:264:HOH:O	2.23	0.70
1:H:63:NRQ:CD1	1:H:197:ARG:HH21	2.05	0.69
1:E:124:VAL:HG12	1:H:91:GLU:HG3	1.74	0.69
1:C:22:HIS:CD2	1:C:52:PRO:HG2	2.27	0.69
1:B:96:TYR:HB2	2:B:254:HOH:O	1.93	0.69
1:H:201:ARG:HD3	1:H:211:VAL:HG13	1.74	0.69
1:A:201:ARG:HD3	1:A:211:VAL:HG13	1.75	0.69
1:A:22:HIS:CD2	1:A:52:PRO:HG2	2.28	0.68
1:H:63:NRQ:HD1	1:H:197:ARG:HH21	1.58	0.68
1:B:91:GLU:HG3	1:D:124:VAL:HG12	1.75	0.68
1:F:63:NRQ:CG2	1:F:197:ARG:HE	2.06	0.68
1:C:201:ARG:HD3	1:C:211:VAL:HG13	1.74	0.68
1:G:224:LEU:HB2	2:H:290:HOH:O	1.94	0.68
1:A:63:NRQ:HE2	1:A:199:LEU:HB2	1.75	0.67
1:E:201:ARG:HD3	1:E:211:VAL:HG13	1.77	0.67
1:A:222:CYS:HB3	1:B:198:ARG:NH2	2.10	0.67
1:G:208:GLU:OE1	2:G:257:HOH:O	2.10	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:201:ARG:HD3	1:F:211:VAL:HG13	1.77	0.67
1:F:222:CYS:SG	2:F:267:HOH:O	2.52	0.67
1:D:63:NRQ:HG11	1:D:199:LEU:HD12	1.78	0.66
1:H:22:HIS:CD2	1:H:52:PRO:HG2	2.30	0.66
1:C:166:GLY:O	1:H:203:LYS:HE2	1.96	0.66
1:G:145:GLU:HB3	1:G:197:ARG:HH12	1.61	0.66
1:A:222:CYS:HB3	1:B:198:ARG:HH22	1.61	0.66
1:H:63:NRQ:CD1	1:H:197:ARG:HE	2.09	0.65
1:B:201:ARG:HD3	1:B:211:VAL:HG13	1.78	0.65
1:H:133:MET:HB2	2:H:283:HOH:O	1.95	0.65
1:G:22:HIS:CD2	1:G:52:PRO:HG2	2.31	0.65
1:B:16:GLU:OE1	2:B:252:HOH:O	2.14	0.65
1:C:197:ARG:HH11	1:C:197:ARG:HG2	1.61	0.65
1:H:41:MET:HB2	1:H:63:NRQ:CE	2.27	0.65
1:G:31:GLU:OE2	2:G:260:HOH:O	2.15	0.65
1:A:145:GLU:CB	1:A:197:ARG:HH12	2.11	0.64
1:G:201:ARG:HD3	1:G:211:VAL:HG13	1.80	0.64
1:B:170:LEU:CD1	2:B:276:HOH:O	2.31	0.64
1:C:211:VAL:HG22	2:C:252:HOH:O	1.97	0.64
1:E:165:VAL:HG11	2:E:256:HOH:O	1.96	0.64
1:H:9:MET:HE3	2:H:285:HOH:O	1.98	0.63
1:F:145:GLU:CB	1:F:197:ARG:HH12	2.11	0.63
1:C:134:GLN:NE2	1:H:138:LEU:HD21	2.14	0.63
1:E:222:CYS:HB3	1:F:198:ARG:NH2	2.12	0.63
1:B:120:LYS:HB3	1:D:122:ARG:NH1	2.13	0.62
1:F:145:GLU:HB3	1:F:197:ARG:HH12	1.64	0.62
1:B:122:ARG:NH1	1:D:120:LYS:HB3	2.14	0.62
1:G:145:GLU:CB	1:G:197:ARG:HH12	2.12	0.62
1:H:63:NRQ:CG2	1:H:197:ARG:HE	2.12	0.62
1:H:145:GLU:HB3	1:H:197:ARG:HH12	1.64	0.62
1:E:145:GLU:HB3	1:E:197:ARG:HH12	1.64	0.62
1:B:97:GLU:N	2:B:276:HOH:O	2.33	0.61
1:B:98:ASP:OD1	2:B:254:HOH:O	2.16	0.61
1:B:197:ARG:CG	1:B:197:ARG:NH1	2.37	0.61
1:D:145:GLU:CB	1:D:197:ARG:HH22	2.14	0.61
1:H:21:ASN:ND2	2:H:261:HOH:O	2.34	0.61
1:D:63:NRQ:CE2	1:D:197:ARG:HD2	2.30	0.61
1:D:152:GLY:O	1:D:189:MET:CE	2.49	0.61
1:D:201:ARG:HD3	1:D:211:VAL:HG13	1.81	0.61
1:D:145:GLU:OE1	1:D:197:ARG:NH2	2.34	0.60
1:E:22:HIS:CD2	1:E:52:PRO:HG2	2.36	0.60
1:B:197:ARG:NH1	1:B:197:ARG:HG2	1.97	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:145:GLU:HB3	1:A:197:ARG:HH12	1.65	0.60
1:C:134:GLN:HE22	1:H:138:LEU:HD21	1.65	0.60
1:B:145:GLU:HB2	1:B:197:ARG:HH22	1.66	0.60
1:B:22:HIS:CE1	2:B:268:HOH:O	2.54	0.59
1:B:145:GLU:HB2	1:B:197:ARG:NH2	2.17	0.59
1:E:145:GLU:CB	1:E:197:ARG:HH12	2.14	0.59
1:E:13:LEU:HG	1:E:14:TYR:H	1.68	0.59
1:C:198:ARG:NH2	1:D:222:CYS:HB3	2.18	0.59
1:G:222:CYS:HB3	1:H:198:ARG:NH2	2.17	0.59
1:E:39:GLN:CD	1:E:63:NRQ:HE1A	2.23	0.58
1:H:18:THR:HG22	2:H:263:HOH:O	2.02	0.58
1:C:222:CYS:HB3	1:D:198:ARG:NH2	2.18	0.58
1:E:63:NRQ:CG2	1:E:197:ARG:HE	2.16	0.58
1:H:204:GLU:HG2	2:H:281:HOH:O	2.04	0.58
1:C:199:LEU:HD23	1:C:199:LEU:O	2.03	0.58
1:G:223:ASP:OD2	2:G:235:HOH:O	2.17	0.58
1:F:120:LYS:CB	1:G:122:ARG:NH1	2.61	0.58
1:F:63:NRQ:CD1	1:F:197:ARG:HE	2.17	0.58
1:A:21:ASN:ND2	1:C:89:THR:OG1	2.37	0.57
1:D:197:ARG:HH11	1:D:197:ARG:HG3	1.69	0.57
1:H:145:GLU:CB	1:H:197:ARG:HH12	2.15	0.57
1:F:122:ARG:NH1	1:G:120:LYS:CB	2.63	0.57
1:B:98:ASP:N	2:B:276:HOH:O	2.38	0.57
1:F:106:GLN:HG2	1:F:119:VAL:HG22	1.86	0.57
1:A:73:THR:HA	2:A:238:HOH:O	2.04	0.57
1:F:41:MET:HB2	1:F:63:NRQ:CE	2.34	0.57
1:F:63:NRQ:HD1	1:F:197:ARG:HH21	1.70	0.56
1:E:106:GLN:HG2	1:E:119:VAL:HG22	1.87	0.56
1:F:63:NRQ:CD1	1:F:197:ARG:HH21	2.19	0.55
1:B:122:ARG:HH12	1:D:120:LYS:HB3	1.70	0.55
1:E:202:ILE:O	1:E:202:ILE:HG22	2.06	0.55
1:D:25:LYS:HB2	1:D:47:GLU:HB2	1.86	0.55
1:B:120:LYS:HB3	1:D:122:ARG:HH12	1.72	0.55
1:C:222:CYS:HB3	1:D:198:ARG:HH22	1.71	0.55
1:C:134:GLN:OE1	1:H:138:LEU:CD2	2.54	0.55
1:C:62:PHE:C	1:C:63:NRQ:HA31	2.26	0.55
1:D:22:HIS:CD2	1:D:52:PRO:CG	2.89	0.54
1:G:173:ASN:HB2	2:G:250:HOH:O	2.05	0.54
1:E:63:NRQ:CD1	1:E:197:ARG:HE	2.19	0.54
1:E:63:NRQ:HA31	1:E:63:NRQ:N1	2.21	0.54
1:H:63:NRQ:HB12	1:H:199:LEU:HD11	1.90	0.54
1:A:39:GLN:HE22	1:A:66:SER:HB3	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:25:LYS:HB2	1:F:47:GLU:HB2	1.90	0.53
1:E:91:GLU:HG3	2:H:261:HOH:O	2.09	0.53
1:H:13:LEU:HG	1:H:14:TYR:H	1.73	0.53
1:G:106:GLN:HG2	1:G:119:VAL:HG22	1.91	0.53
1:C:198:ARG:HH22	1:D:222:CYS:HB3	1.73	0.53
1:D:183:PRO:HB2	2:D:264:HOH:O	2.08	0.53
1:A:63:NRQ:CD1	1:A:197:ARG:HH21	2.22	0.53
1:F:63:NRQ:HE1	1:F:143:SER:OG	2.08	0.53
1:B:13:LEU:HG	1:B:14:TYR:H	1.73	0.53
1:E:91:GLU:HG2	1:H:124:VAL:HG12	1.91	0.52
1:A:105:THR:HG23	1:C:122:ARG:HD3	1.91	0.52
1:E:39:GLN:CG	1:E:63:NRQ:CE	2.80	0.52
1:H:41:MET:HB2	1:H:63:NRQ:HE2A	1.91	0.52
1:E:164:LEU:HD12	2:E:257:HOH:O	2.09	0.52
1:D:39:GLN:HE22	1:D:66:SER:HB3	1.74	0.52
1:E:202:ILE:CG2	1:E:202:ILE:O	2.57	0.52
1:D:73:THR:HA	2:D:272:HOH:O	2.09	0.52
1:F:214:HIS:HD2	2:F:266:HOH:O	1.91	0.52
1:F:22:HIS:CD2	1:F:52:PRO:CG	2.93	0.52
1:D:185:LYS:HD2	2:D:264:HOH:O	2.09	0.52
2:E:260:HOH:O	1:H:125:ASN:HB2	2.10	0.52
1:B:197:ARG:HG3	1:B:197:ARG:NH1	2.24	0.51
1:D:207:LYS:O	1:D:208:GLU:HB2	2.10	0.51
1:F:106:GLN:CG	1:F:119:VAL:HG22	2.40	0.51
1:H:106:GLN:HG2	1:H:119:VAL:HG22	1.92	0.51
1:A:122:ARG:HD3	1:C:105:THR:CG2	2.40	0.51
1:D:224:LEU:HG	2:D:237:HOH:O	2.11	0.51
1:B:189:MET:HE2	2:B:246:HOH:O	2.09	0.51
1:F:122:ARG:HH12	1:G:120:LYS:CB	2.09	0.51
1:C:22:HIS:CD2	1:C:52:PRO:CG	2.94	0.51
1:G:63:NRQ:HE1	1:G:160:MET:SD	2.51	0.51
1:A:106:GLN:HG2	1:A:119:VAL:HG22	1.93	0.51
1:E:120:LYS:HB3	1:H:122:ARG:NH1	2.26	0.50
1:G:13:LEU:HD23	1:G:14:TYR:N	2.26	0.50
1:A:13:LEU:HG	1:A:14:TYR:H	1.76	0.50
1:D:152:GLY:O	1:D:189:MET:HE2	2.11	0.50
1:A:122:ARG:HD3	1:C:105:THR:HG23	1.94	0.50
1:C:207:LYS:O	1:C:208:GLU:HB2	2.10	0.50
1:A:22:HIS:CD2	1:A:52:PRO:CG	2.94	0.50
1:A:105:THR:CG2	1:C:122:ARG:HD3	2.42	0.50
1:H:22:HIS:CE1	2:H:262:HOH:O	2.64	0.50
1:C:25:LYS:HB2	1:C:47:GLU:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:63:NRQ:CD1	1:E:197:ARG:HH21	2.25	0.50
1:H:207:LYS:O	1:H:208:GLU:HB2	2.11	0.50
1:D:185:LYS:CG	2:D:264:HOH:O	2.59	0.50
1:F:91:GLU:HG2	1:G:124:VAL:HG12	1.94	0.50
1:B:203:LYS:HB2	1:B:212:GLU:HB3	1.94	0.50
1:H:63:NRQ:CD1	1:H:197:ARG:NH2	2.75	0.49
1:B:39:GLN:HG3	1:B:63:NRQ:CE	2.42	0.49
1:F:41:MET:CB	1:F:63:NRQ:HE3	2.40	0.49
1:C:134:GLN:OE1	1:H:138:LEU:HD23	2.12	0.49
1:G:63:NRQ:HG12	1:G:213:GLN:NE2	2.27	0.49
1:E:122:ARG:HD3	1:H:105:THR:HG23	1.93	0.49
1:F:89:THR:HB	1:G:21:ASN:HD21	1.76	0.49
1:G:173:ASN:ND2	2:G:244:HOH:O	2.44	0.49
1:H:63:NRQ:HA31	1:H:63:NRQ:N1	2.28	0.49
1:F:21:ASN:HD21	1:G:89:THR:HB	1.78	0.49
1:B:124:VAL:HG12	1:D:91:GLU:HG2	1.95	0.49
1:B:100:GLY:N	2:B:254:HOH:O	2.44	0.49
1:E:106:GLN:CG	1:E:119:VAL:HG22	2.43	0.49
1:E:203:LYS:HB2	1:E:212:GLU:HB3	1.94	0.49
1:D:13:LEU:HD23	1:D:14:TYR:N	2.28	0.49
1:C:13:LEU:HG	1:C:14:TYR:H	1.78	0.48
1:C:53:PHE:HD1	1:C:54:ALA:O	1.96	0.48
1:F:203:LYS:HB2	1:F:212:GLU:HB3	1.94	0.48
1:G:25:LYS:HB2	1:G:47:GLU:HB2	1.95	0.48
1:A:63:NRQ:CG2	1:A:197:ARG:HE	2.27	0.48
1:G:208:GLU:HB2	2:G:255:HOH:O	2.14	0.48
1:H:203:LYS:HB2	1:H:212:GLU:HB3	1.95	0.48
1:B:182:LYS:HG2	1:B:183:PRO:HD2	1.94	0.48
1:F:53:PHE:HD1	1:F:54:ALA:O	1.97	0.48
1:C:132:VAL:HB	2:C:239:HOH:O	2.14	0.48
1:A:63:NRQ:N2	1:A:63:NRQ:HD2	2.29	0.48
1:G:13:LEU:HG	1:G:14:TYR:H	1.79	0.48
1:D:13:LEU:HG	1:D:14:TYR:H	1.79	0.48
1:A:131:PRO:HB3	1:A:164:LEU:HD22	1.96	0.48
1:D:63:NRQ:CG1	1:D:199:LEU:CD1	2.92	0.48
1:H:198:ARG:NE	2:H:290:HOH:O	2.37	0.48
1:H:25:LYS:HB2	1:H:47:GLU:HB2	1.95	0.48
1:G:207:LYS:O	1:G:208:GLU:HB2	2.14	0.48
1:F:207:LYS:O	1:F:208:GLU:HB2	2.14	0.48
1:E:39:GLN:OE1	1:E:63:NRQ:HE3	2.14	0.47
1:G:22:HIS:CD2	1:G:52:PRO:CG	2.96	0.47
1:G:203:LYS:HB2	1:G:212:GLU:HB3	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:39:GLN:HE22	1:E:66:SER:HB3	1.78	0.47
1:D:63:NRQ:CD2	1:D:197:ARG:HD2	2.44	0.47
1:E:39:GLN:CD	1:E:63:NRQ:CE	2.82	0.47
1:B:131:PRO:HB3	1:B:164:LEU:HD22	1.95	0.47
1:B:207:LYS:O	1:B:208:GLU:HB2	2.15	0.47
1:D:63:NRQ:SD	1:D:213:GLN:NE2	2.87	0.47
1:C:204:GLU:CB	2:C:252:HOH:O	2.63	0.47
1:A:145:GLU:HB2	1:A:197:ARG:HH12	1.80	0.47
1:H:53:PHE:HD1	1:H:54:ALA:O	1.97	0.47
1:A:160:MET:HA	2:A:235:HOH:O	2.14	0.47
1:D:63:NRQ:SD	1:D:199:LEU:HD11	2.55	0.47
1:B:22:HIS:CD2	1:B:52:PRO:CG	2.96	0.47
1:A:13:LEU:HD23	1:A:14:TYR:N	2.29	0.47
1:C:170:LEU:CD1	2:C:242:HOH:O	2.43	0.46
1:G:224:LEU:HA	1:G:225:PRO:HD3	1.69	0.46
1:E:22:HIS:CD2	1:E:52:PRO:CG	2.98	0.46
1:G:11:MET:HG2	1:G:30:GLY:O	2.14	0.46
1:H:22:HIS:CD2	1:H:52:PRO:CG	2.97	0.46
1:E:131:PRO:HB3	1:E:164:LEU:HD22	1.97	0.46
1:D:51:LEU:HA	1:D:52:PRO:HD3	1.75	0.46
1:H:134:GLN:HG2	2:H:283:HOH:O	2.15	0.46
1:D:183:PRO:CB	2:D:264:HOH:O	2.63	0.46
1:H:106:GLN:CG	1:H:119:VAL:HG22	2.46	0.46
1:D:106:GLN:HG2	1:D:119:VAL:HG22	1.98	0.46
1:H:41:MET:CB	1:H:63:NRQ:HE3	2.46	0.46
1:F:81:LYS:NZ	2:F:250:HOH:O	2.49	0.46
1:C:13:LEU:HD23	1:C:14:TYR:N	2.31	0.46
1:D:206:ASP:O	1:D:207:LYS:HB2	2.16	0.46
1:E:13:LEU:HD23	1:E:14:TYR:N	2.30	0.46
1:H:19:VAL:HB	1:H:53:PHE:CE2	2.51	0.46
1:H:84:PHE:HB3	1:H:85:PRO:HA	1.98	0.46
1:D:224:LEU:HA	1:D:225:PRO:HD3	1.74	0.46
1:F:224:LEU:HA	1:F:225:PRO:HD3	1.75	0.46
1:A:63:NRQ:CD1	1:A:197:ARG:NE	2.76	0.46
1:F:13:LEU:HD23	1:F:14:TYR:N	2.31	0.46
1:A:148:TYR:CZ	1:A:155:GLU:HB2	2.51	0.46
1:B:13:LEU:HD23	1:B:14:TYR:N	2.31	0.45
1:D:148:TYR:CZ	1:D:155:GLU:HB2	2.51	0.45
1:B:106:GLN:HG2	1:B:119:VAL:HG22	1.97	0.45
1:C:204:GLU:HB2	2:C:252:HOH:O	2.15	0.45
1:G:222:CYS:HB3	1:H:198:ARG:HH22	1.82	0.45
1:H:63:NRQ:CD1	1:H:197:ARG:NE	2.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:ARG:NH2	2:A:276:HOH:O	2.50	0.45
1:F:145:GLU:HB2	1:F:197:ARG:HH12	1.82	0.45
1:E:19:VAL:HB	1:E:53:PHE:CE2	2.52	0.45
1:H:33:LYS:HB3	2:H:282:HOH:O	2.17	0.45
1:F:160:MET:HA	2:F:247:HOH:O	2.17	0.45
1:H:51:LEU:HD23	2:H:262:HOH:O	2.16	0.45
1:A:122:ARG:NH1	1:C:120:LYS:HB3	2.31	0.45
1:D:84:PHE:HB3	1:D:85:PRO:HA	1.99	0.45
1:G:198:ARG:NH2	1:H:222:CYS:HB3	2.31	0.45
1:C:199:LEU:C	1:C:199:LEU:CD2	2.80	0.45
1:B:74:GLN:O	1:B:75:GLY:C	2.54	0.45
1:C:203:LYS:HB2	1:C:212:GLU:HB3	1.99	0.45
1:F:13:LEU:HG	1:F:14:TYR:H	1.82	0.44
1:E:63:NRQ:HD1	1:E:197:ARG:HH21	1.82	0.44
1:C:63:NRQ:N1	1:C:63:NRQ:CA3	2.76	0.44
1:D:63:NRQ:CB1	1:D:199:LEU:CD1	2.95	0.44
1:G:106:GLN:CG	1:G:119:VAL:HG22	2.47	0.44
1:A:147:LEU:HA	1:A:155:GLU:O	2.17	0.44
1:C:11:MET:HG2	1:C:30:GLY:O	2.18	0.44
1:H:39:GLN:HE22	1:H:66:SER:HB3	1.82	0.44
1:F:51:LEU:HA	1:F:52:PRO:HD3	1.72	0.44
1:C:147:LEU:HA	1:C:155:GLU:O	2.17	0.44
1:H:131:PRO:HB3	1:H:164:LEU:HD22	2.00	0.44
1:E:74:GLN:O	1:E:75:GLY:C	2.55	0.44
1:H:182:LYS:HG2	1:H:183:PRO:HD2	2.00	0.44
1:F:66:SER:N	2:F:246:HOH:O	2.50	0.44
1:H:148:TYR:CZ	1:H:155:GLU:HB2	2.53	0.44
1:A:63:NRQ:HE1	1:A:143:SER:OG	2.17	0.44
1:E:13:LEU:HG	1:E:14:TYR:N	2.32	0.44
1:E:159:ASP:OD2	1:F:159:ASP:OD2	2.36	0.44
1:A:203:LYS:HB2	1:A:212:GLU:HB3	2.00	0.44
1:D:182:LYS:HG2	1:D:183:PRO:HD2	2.00	0.43
1:B:13:LEU:HG	1:B:14:TYR:N	2.33	0.43
1:B:39:GLN:HG3	1:B:63:NRQ:HE2A	2.00	0.43
1:E:207:LYS:O	1:E:208:GLU:HB2	2.17	0.43
1:C:131:PRO:HB3	1:C:164:LEU:HD22	2.00	0.43
1:B:186:ASN:ND2	2:B:291:HOH:O	2.50	0.43
1:A:19:VAL:HB	1:A:53:PHE:CE2	2.53	0.43
1:F:84:PHE:HB3	1:F:85:PRO:HA	2.00	0.43
1:G:131:PRO:HB3	1:G:164:LEU:HD22	2.00	0.43
1:C:39:GLN:NE2	1:C:215:GLU:OE1	2.51	0.43
1:H:41:MET:CB	1:H:63:NRQ:CE	2.96	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:158:SER:CB	2:F:282:HOH:O	2.66	0.43
1:A:21:ASN:HD21	1:C:89:THR:CB	2.30	0.43
1:D:106:GLN:CG	1:D:119:VAL:HG22	2.49	0.43
1:C:106:GLN:HG2	1:C:119:VAL:HG22	2.01	0.43
1:B:25:LYS:HB2	1:B:47:GLU:HB2	2.01	0.43
1:F:131:PRO:HB3	1:F:164:LEU:HD22	2.00	0.43
1:B:84:PHE:HB3	1:B:85:PRO:HA	2.01	0.43
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.30	0.43
1:F:39:GLN:NE2	1:F:215:GLU:OE1	2.52	0.43
1:C:74:GLN:O	1:C:75:GLY:C	2.57	0.43
1:F:74:GLN:O	1:F:75:GLY:C	2.57	0.43
1:C:84:PHE:HB3	1:C:85:PRO:HA	2.01	0.43
1:D:63:NRQ:CG1	1:D:199:LEU:HD12	2.45	0.43
1:C:197:ARG:CG	1:C:197:ARG:HH11	2.29	0.43
1:G:74:GLN:O	1:G:75:GLY:C	2.56	0.42
1:C:71:ASN:OD1	1:C:73:THR:HG23	2.19	0.42
1:E:13:LEU:CG	1:E:14:TYR:N	2.82	0.42
1:G:53:PHE:HD1	1:G:54:ALA:O	2.02	0.42
1:H:13:LEU:HD23	1:H:14:TYR:N	2.35	0.42
1:D:13:LEU:HB3	1:D:28:SER:OG	2.19	0.42
1:A:127:PRO:HD2	2:A:254:HOH:O	2.17	0.42
1:F:148:TYR:CZ	1:F:155:GLU:HB2	2.54	0.42
1:A:224:LEU:HA	1:A:225:PRO:HD3	1.72	0.42
1:B:224:LEU:HA	1:B:225:PRO:HD3	1.77	0.42
1:B:51:LEU:HD23	2:B:268:HOH:O	2.19	0.42
1:E:25:LYS:HB2	1:E:47:GLU:HB2	2.02	0.42
1:A:21:ASN:HD21	1:C:89:THR:HB	1.84	0.42
1:E:63:NRQ:N1	1:E:63:NRQ:CA3	2.83	0.42
1:C:148:TYR:CZ	1:C:155:GLU:HB2	2.55	0.42
1:A:207:LYS:O	1:A:208:GLU:HB2	2.18	0.42
1:G:148:TYR:CZ	1:G:155:GLU:HB2	2.54	0.42
1:A:74:GLN:O	1:A:75:GLY:C	2.58	0.42
1:B:91:GLU:CG	1:D:124:VAL:HG12	2.44	0.42
1:A:13:LEU:C	1:A:13:LEU:HD23	2.40	0.42
1:F:130:GLY:N	2:F:242:HOH:O	2.53	0.42
1:G:72:HIS:HB2	2:G:251:HOH:O	2.19	0.42
1:E:32:GLY:O	1:E:34:PRO:HD3	2.20	0.42
1:E:182:LYS:HG2	1:E:183:PRO:HD2	2.02	0.42
1:D:53:PHE:HD1	1:D:54:ALA:O	2.02	0.41
1:E:142:ALA:HB3	1:F:194:TYR:OH	2.19	0.41
1:C:39:GLN:HE22	1:C:66:SER:HB3	1.85	0.41
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:55:PHE:CD2	1:C:55:PHE:O	2.73	0.41
1:E:124:VAL:HG12	1:H:91:GLU:CG	2.46	0.41
1:F:19:VAL:HB	1:F:53:PHE:CE2	2.56	0.41
1:C:199:LEU:O	1:C:199:LEU:CD2	2.68	0.41
1:G:19:VAL:HB	1:G:53:PHE:CE2	2.55	0.41
1:B:148:TYR:CZ	1:B:155:GLU:HB2	2.55	0.41
1:B:96:TYR:CB	2:B:254:HOH:O	2.63	0.41
1:H:13:LEU:HG	1:H:14:TYR:N	2.35	0.41
1:E:122:ARG:HD3	1:H:105:THR:CG2	2.51	0.41
1:E:71:ASN:OD1	1:E:73:THR:HG23	2.20	0.41
1:A:89:THR:OG1	1:C:21:ASN:ND2	2.52	0.41
1:C:92:ARG:O	1:C:103:THR:HA	2.20	0.41
1:H:160:MET:HA	2:H:266:HOH:O	2.19	0.41
1:D:131:PRO:HB3	1:D:164:LEU:HD22	2.03	0.41
1:B:66:SER:N	2:B:262:HOH:O	2.53	0.41
1:A:206:ASP:O	1:A:207:LYS:HB2	2.21	0.41
1:F:202:ILE:HG22	1:F:202:ILE:O	2.19	0.41
1:G:13:LEU:C	1:G:13:LEU:HD23	2.40	0.41
1:F:147:LEU:HA	1:F:155:GLU:O	2.21	0.41
1:D:203:LYS:HB2	1:D:212:GLU:HB3	2.02	0.41
1:C:39:GLN:OE1	1:C:63:NRQ:CE	2.69	0.41
1:F:63:NRQ:CZ	1:F:197:ARG:HG3	2.51	0.41
1:H:63:NRQ:HB12	1:H:199:LEU:CD1	2.49	0.41
1:C:13:LEU:C	1:C:13:LEU:HD23	2.41	0.41
1:B:11:MET:HG2	1:B:30:GLY:O	2.21	0.41
1:E:148:TYR:CZ	1:E:155:GLU:HB2	2.55	0.41
1:F:55:PHE:CD2	1:F:55:PHE:O	2.73	0.41
1:E:11:MET:HG2	1:E:30:GLY:O	2.20	0.41
1:F:124:VAL:HG12	1:G:91:GLU:HG2	2.03	0.41
1:D:202:ILE:O	1:D:202:ILE:HG22	2.21	0.41
1:C:51:LEU:HA	1:C:52:PRO:HD3	1.73	0.41
1:G:147:LEU:HA	1:G:155:GLU:O	2.21	0.41
1:H:92:ARG:HD2	1:H:92:ARG:HH11	1.76	0.41
1:B:122:ARG:NH1	1:D:120:LYS:CB	2.83	0.40
1:A:13:LEU:HG	1:A:14:TYR:N	2.36	0.40
1:H:74:GLN:O	1:H:75:GLY:C	2.60	0.40
1:D:74:GLN:O	1:D:75:GLY:C	2.59	0.40
1:F:39:GLN:HE22	1:F:66:SER:HB3	1.87	0.40
1:E:148:TYR:HA	1:E:149:PRO:HD3	1.97	0.40
1:G:32:GLY:O	1:G:34:PRO:HD3	2.21	0.40
1:G:163:LYS:HB3	2:G:236:HOH:O	2.20	0.40
1:D:132:VAL:HB	2:D:269:HOH:O	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:84:PHE:HB3	1:G:85:PRO:HA	2.03	0.40
1:C:182:LYS:HG2	1:C:183:PRO:HD2	2.03	0.40
1:H:147:LEU:HA	1:H:155:GLU:O	2.21	0.40
1:B:147:LEU:HA	1:B:155:GLU:O	2.22	0.40
1:G:71:ASN:OD1	1:G:73:THR:HG23	2.21	0.40
1:C:202:ILE:HG22	1:C:202:ILE:O	2.21	0.40
1:F:63:NRQ:CD1	1:F:197:ARG:NE	2.85	0.40
1:B:13:LEU:CG	1:B:14:TYR:N	2.84	0.40
1:H:39:GLN:NE2	1:H:69:PHE:HB2	2.36	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:202:ILE:O	1:G:111:GLN:OE1[2_656]	1.76	0.44
1:D:206:ASP:OD1	1:E:118:ASN:ND2[2_545]	2.02	0.18
1:B:185:LYS:NZ	1:H:42:ARG:NE[2_545]	2.06	0.14
1:F:31:GLU:OE1	1:H:185:LYS:NZ[2_646]	2.10	0.10
1:E:202:ILE:O	1:G:111:GLN:CD[2_656]	2.19	0.01

## 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	214/243 (88%)	205 (96%)	9 (4%)	0	100	100
1	B	214/243 (88%)	200 (94%)	14 (6%)	0	100	100
1	C	214/243 (88%)	203 (95%)	11 (5%)	0	100	100
1	D	217/243 (89%)	200 (92%)	17 (8%)	0	100	100
1	E	214/243 (88%)	201 (94%)	13 (6%)	0	100	100
1	F	214/243 (88%)	202 (94%)	12 (6%)	0	100	100
1	G	214/243 (88%)	203 (95%)	11 (5%)	0	100	100
1	H	214/243 (88%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1715/1944 (88%)	1619 (94%)	96 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	187/208 (90%)	178 (95%)	9 (5%)	35	64
1	B	187/208 (90%)	176 (94%)	11 (6%)	28	52
1	C	187/208 (90%)	175 (94%)	12 (6%)	25	47
1	D	190/208 (91%)	179 (94%)	11 (6%)	28	53
1	E	187/208 (90%)	176 (94%)	11 (6%)	28	52
1	F	187/208 (90%)	176 (94%)	11 (6%)	28	52
1	G	187/208 (90%)	177 (95%)	10 (5%)	32	58
1	H	187/208 (90%)	176 (94%)	11 (6%)	28	52
All	All	1499/1664 (90%)	1413 (94%)	86 (6%)	29	54

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	TYR
1	A	102	LEU
1	A	111	GLN
1	A	112	ASP
1	A	118	ASN
1	A	122	ARG
1	A	188	LYS
1	A	204	GLU
1	A	223	ASP
1	B	14	TYR
1	B	91	GLU
1	B	102	LEU
1	B	111	GLN

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Mol	Chain	Res	Type
1	B	112	ASP
1	B	118	ASN
1	B	122	ARG
1	B	188	LYS
1	B	197	ARG
1	B	204	GLU
1	B	223	ASP
1	C	9	MET
1	C	14	TYR
1	C	102	LEU
1	C	111	GLN
1	C	112	ASP
1	C	118	ASN
1	C	122	ARG
1	C	188	LYS
1	C	197	ARG
1	C	199	LEU
1	C	204	GLU
1	C	223	ASP
1	D	14	TYR
1	D	102	LEU
1	D	111	GLN
1	D	112	ASP
1	D	118	ASN
1	D	122	ARG
1	D	188	LYS
1	D	197	ARG
1	D	204	GLU
1	D	223	ASP
1	D	226	SER
1	E	9	MET
1	E	14	TYR
1	E	102	LEU
1	E	111	GLN
1	E	112	ASP
1	E	118	ASN
1	E	122	ARG
1	E	188	LYS
1	E	201	ARG
1	E	204	GLU
1	E	223	ASP
1	F	14	TYR

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Mol	Chain	Res	Type
1	F	73	THR
1	F	102	LEU
1	F	111	GLN
1	F	112	ASP
1	F	118	ASN
1	F	122	ARG
1	F	176	THR
1	F	188	LYS
1	F	204	GLU
1	F	223	ASP
1	G	14	TYR
1	G	102	LEU
1	G	111	GLN
1	G	112	ASP
1	G	118	ASN
1	G	122	ARG
1	G	188	LYS
1	G	201	ARG
1	G	204	GLU
1	G	223	ASP
1	H	14	TYR
1	H	68	THR
1	H	91	GLU
1	H	102	LEU
1	H	111	GLN
1	H	112	ASP
1	H	118	ASN
1	H	122	ARG
1	H	188	LYS
1	H	204	GLU
1	H	223	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	111	GLN
1	A	118	ASN
1	B	21	ASN
1	B	111	GLN
1	B	118	ASN
1	C	21	ASN

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Mol	Chain	Res	Type
1	C	111	GLN
1	C	118	ASN
1	D	21	ASN
1	D	111	GLN
1	D	118	ASN
1	E	21	ASN
1	E	111	GLN
1	E	118	ASN
1	F	21	ASN
1	F	111	GLN
1	F	118	ASN
1	G	21	ASN
1	G	111	GLN
1	G	118	ASN
1	G	213	GLN
1	H	21	ASN
1	H	111	GLN
1	H	118	ASN

### 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	63	1	24,24,25	3.52	2 (8%)	30,32,34	2.34	6 (20%)
1	NRQ	B	63	1	24,24,25	4.38	3 (12%)	30,32,34	2.07	8 (26%)
1	NRQ	C	63	1	24,24,25	3.57	3 (12%)	30,32,34	1.71	6 (20%)
1	NRQ	D	63	1	24,24,25	3.58	3 (12%)	30,32,34	1.90	6 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	NRQ	E	63	1	24,24,25	3.71	4 (16%)	30,32,34	2.09	10 (33%)
1	NRQ	F	63	1	24,24,25	3.97	6 (25%)	30,32,34	2.72	11 (36%)
1	NRQ	G	63	1	24,24,25	3.96	3 (12%)	30,32,34	1.63	5 (16%)
1	NRQ	H	63	1	24,24,25	3.55	3 (12%)	30,32,34	1.67	5 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	A	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	B	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	E	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	F	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	G	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	H	63	1	-	0/9/31/32	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	NRQ	O3-C3	20.47	1.25	1.11
1	G	63	NRQ	O3-C3	16.79	1.22	1.11
1	E	63	NRQ	O3-C3	16.43	1.22	1.11
1	A	63	NRQ	O3-C3	16.40	1.22	1.11
1	H	63	NRQ	O3-C3	16.23	1.22	1.11
1	D	63	NRQ	O3-C3	15.07	1.21	1.11
1	C	63	NRQ	O3-C3	14.51	1.21	1.11
1	F	63	NRQ	O3-C3	14.48	1.21	1.11
1	G	63	NRQ	OH-CZ	8.75	1.59	1.37
1	F	63	NRQ	OH-CZ	8.69	1.59	1.37
1	D	63	NRQ	OH-CZ	7.15	1.55	1.37
1	C	63	NRQ	C1-CA1	-7.10	1.38	1.48
1	E	63	NRQ	C1-CA1	-6.30	1.39	1.48
1	C	63	NRQ	OH-CZ	5.50	1.51	1.37
1	F	63	NRQ	CB2-CA2	5.36	1.38	1.35
1	F	63	NRQ	C1-CA1	-5.28	1.41	1.48
1	F	63	NRQ	CA2-C2	4.19	1.53	1.48
1	D	63	NRQ	CA2-C2	4.09	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	63	NRQ	OH-CZ	4.07	1.47	1.37
1	B	63	NRQ	C1-CA1	-3.81	1.43	1.48
1	A	63	NRQ	C1-CA1	-3.15	1.43	1.48
1	H	63	NRQ	C1-CA1	-3.03	1.44	1.48
1	B	63	NRQ	CB2-CA2	-2.84	1.33	1.35
1	F	63	NRQ	CA3-C3	2.59	1.51	1.48
1	E	63	NRQ	CA3-N3	-2.26	1.45	1.47
1	G	63	NRQ	C1-CA1	-2.21	1.45	1.48
1	E	63	NRQ	C1-N2	-2.01	1.28	1.33

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	NRQ	C1-CA1-N1	8.95	132.44	121.83
1	F	63	NRQ	C1-CA1-N1	8.55	131.97	121.83
1	D	63	NRQ	CB1-CA1-C1	-7.08	99.52	118.06
1	F	63	NRQ	CB1-CA1-N1	-6.07	97.57	125.36
1	E	63	NRQ	C1-CA1-N1	5.77	128.67	121.83
1	B	63	NRQ	C1-CA1-N1	5.58	128.45	121.83
1	C	63	NRQ	C1-CA1-N1	5.40	128.23	121.83
1	G	63	NRQ	C1-CA1-N1	5.30	128.11	121.83
1	B	63	NRQ	CA3-N3-C1	4.89	131.38	124.10
1	F	63	NRQ	CB1-CA1-C1	4.67	130.29	118.06
1	H	63	NRQ	CB1-CA1-C1	4.63	130.19	118.06
1	E	63	NRQ	CA3-N3-C2	4.47	126.24	123.46
1	G	63	NRQ	CA3-N3-C1	4.27	130.46	124.10
1	A	63	NRQ	O2-C2-CA2	4.24	133.41	130.96
1	A	63	NRQ	CA3-N3-C1	4.00	130.05	124.10
1	E	63	NRQ	CG1-CB1-CA1	-3.93	104.97	112.76
1	E	63	NRQ	N3-C1-N2	3.93	116.31	113.24
1	H	63	NRQ	CB1-CA1-N1	-3.92	107.41	125.36
1	C	63	NRQ	CB1-CA1-N1	-3.71	108.39	125.36
1	B	63	NRQ	CE2-CD2-CG2	-3.52	116.86	121.30
1	A	63	NRQ	N3-C1-N2	3.48	115.95	113.24
1	D	63	NRQ	CA3-N3-C1	3.46	129.25	124.10
1	H	63	NRQ	CA3-N3-C1	3.38	129.13	124.10
1	F	63	NRQ	C2-CA2-N2	-3.33	106.41	108.91
1	F	63	NRQ	CG2-CB2-CA2	3.30	133.89	130.10
1	C	63	NRQ	CA1-C1-N3	-3.28	120.18	124.78
1	B	63	NRQ	CB1-CA1-C1	-3.26	109.52	118.06
1	F	63	NRQ	CA1-C1-N3	-3.17	120.34	124.78
1	H	63	NRQ	N3-C1-N2	3.13	115.68	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	NRQ	O2-C2-CA2	3.12	132.76	130.96
1	B	63	NRQ	CG2-CB2-CA2	3.09	133.65	130.10
1	C	63	NRQ	CA3-N3-C2	3.07	125.37	123.46
1	F	63	NRQ	CA3-N3-C2	2.93	125.28	123.46
1	A	63	NRQ	CA1-C1-N3	-2.91	120.69	124.78
1	G	63	NRQ	O2-C2-CA2	-2.82	129.32	130.96
1	F	63	NRQ	CA3-N3-C1	2.77	128.22	124.10
1	B	63	NRQ	N3-C1-N2	2.74	115.38	113.24
1	D	63	NRQ	CB1-CA1-N1	2.68	137.63	125.36
1	E	63	NRQ	CA2-C2-N3	-2.58	101.97	103.44
1	A	63	NRQ	CB1-CA1-N1	-2.54	113.71	125.36
1	H	63	NRQ	CG1-CB1-CA1	-2.53	107.76	112.76
1	D	63	NRQ	N3-C1-N2	2.51	115.20	113.24
1	E	63	NRQ	CB1-CA1-N1	-2.49	113.97	125.36
1	F	63	NRQ	N3-C1-N2	2.36	115.08	113.24
1	E	63	NRQ	CE2-CD2-CG2	-2.32	118.37	121.30
1	D	63	NRQ	CB2-CA2-C2	2.32	126.03	122.46
1	B	63	NRQ	CD1-CG2-CB2	-2.31	113.31	121.21
1	B	63	NRQ	CD1-CG2-CD2	2.21	121.09	117.66
1	G	63	NRQ	CB1-CA1-C1	-2.19	112.32	118.06
1	F	63	NRQ	CA2-C2-N3	2.19	104.69	103.44
1	D	63	NRQ	CG2-CB2-CA2	2.16	132.58	130.10
1	E	63	NRQ	CA1-C1-N3	-2.12	121.81	124.78
1	G	63	NRQ	N3-C1-N2	2.09	114.87	113.24
1	C	63	NRQ	N3-C1-N2	2.09	114.87	113.24
1	E	63	NRQ	CG2-CB2-CA2	2.05	132.46	130.10
1	E	63	NRQ	C2-CA2-N2	2.03	110.44	108.91
1	C	63	NRQ	CB1-CA1-C1	2.01	123.33	118.06

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	219/243 (90%)	0.23	5 (2%) 57 54	31, 54, 84, 102	0
1	B	219/243 (90%)	0.26	6 (2%) 52 49	36, 53, 85, 106	0
1	C	219/243 (90%)	0.30	7 (3%) 45 42	37, 55, 86, 102	0
1	D	222/243 (91%)	0.32	7 (3%) 45 42	37, 55, 86, 107	0
1	E	219/243 (90%)	0.22	8 (3%) 39 35	36, 54, 85, 102	0
1	F	219/243 (90%)	0.30	7 (3%) 45 42	35, 54, 85, 101	0
1	G	219/243 (90%)	0.58	18 (8%) 12 9	35, 57, 87, 105	0
1	H	219/243 (90%)	0.47	13 (5%) 22 18	38, 57, 85, 105	0
All	All	1755/1944 (90%)	0.34	71 (4%) 36 32	31, 55, 86, 107	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	THR	7.9
1	G	188	LYS	5.7
1	H	75	GLY	5.6
1	B	73	THR	4.6
1	D	206	ASP	4.5
1	B	74	GLN	3.8
1	G	7	GLU	3.7
1	D	210	TYR	3.5
1	H	73	THR	3.3
1	F	151	ASP	3.3
1	H	7	GLU	3.2
1	G	84	PHE	3.2
1	D	223	ASP	3.2
1	G	218	VAL	3.1
1	H	6	THR	3.1
1	C	111	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	74	GLN	3.0
1	H	74	GLN	2.9
1	F	14	TYR	2.9
1	G	162	LEU	2.8
1	G	212	GLU	2.8
1	H	218	VAL	2.8
1	H	5	ILE	2.8
1	B	219	ALA	2.7
1	G	111	GLN	2.7
1	C	23	HIS	2.6
1	G	5	ILE	2.6
1	C	206	ASP	2.5
1	G	112	ASP	2.5
1	H	223	ASP	2.5
1	G	57	ILE	2.5
1	A	202	ILE	2.5
1	H	79	PHE	2.5
1	D	14	TYR	2.4
1	B	112	ASP	2.4
1	G	215	GLU	2.4
1	F	73	THR	2.4
1	E	73	THR	2.4
1	E	14	TYR	2.4
1	H	168	GLY	2.3
1	C	31	GLU	2.3
1	E	55	PHE	2.3
1	G	35	TYR	2.3
1	F	223	ASP	2.3
1	B	183	PRO	2.3
1	A	74	GLN	2.2
1	D	110	LEU	2.2
1	G	34	PRO	2.2
1	E	36	GLU	2.2
1	E	213	GLN	2.2
1	H	111	GLN	2.2
1	G	73	THR	2.2
1	C	36	GLU	2.2
1	F	6	THR	2.2
1	G	9	MET	2.2
1	H	212	GLU	2.1
1	A	62	PHE	2.1
1	F	197	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	14	TYR	2.1
1	D	74	GLN	2.1
1	G	207	LYS	2.1
1	C	21	ASN	2.1
1	A	73	THR	2.0
1	G	40	THR	2.0
1	E	223	ASP	2.0
1	F	150	ALA	2.0
1	B	29	GLU	2.0
1	H	112	ASP	2.0
1	E	41	MET	2.0
1	A	223	ASP	2.0
1	G	18	THR	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
1	NRQ	D	63	23/24	0.25	1.21	32,52,77,79	0
1	NRQ	B	63	23/24	0.22	1.01	40,47,63,67	0
1	NRQ	H	63	23/24	0.22	0.53	38,61,84,91	0
1	NRQ	A	63	23/24	0.20	0.08	33,50,69,75	0
1	NRQ	F	63	23/24	0.17	-0.40	30,48,66,79	0
1	NRQ	G	63	23/24	0.18	-0.49	53,63,77,88	0
1	NRQ	E	63	23/24	0.13	-0.91	38,47,57,64	0
1	NRQ	C	63	23/24	0.14	-0.96	37,46,64,75	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.