Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 05:12 PM EDT

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 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 (i) 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 (i)) were used in the production of this report:

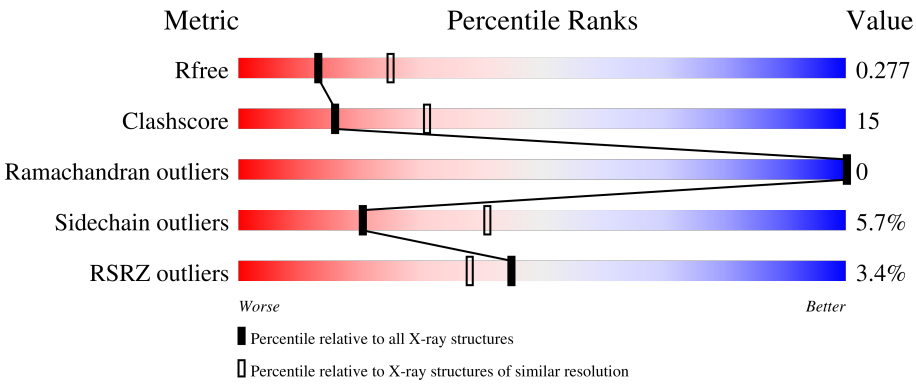
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	2%, 70%, 19%, •, 10%
1	B	243	2%, 66%, 22%, •, 10%
1	C	243	2%, 63%, 25%, •, 10%
1	D	243	2%, 67%, 22%, •, 9%
1	E	243	3%, 67%, 21%, •, 10%

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Mol	Chain	Length	Quality of chain
1	F	243	2% 63% 26% • 10%
1	G	243	6% 66% 21% • 10%
1	H	243	5% 64% 24% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	NRQ	E	63	-	-	X	-
1	NRQ	F	63	-	-	X	-
1	NRQ	H	63	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14324 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
			Total	C	N	O	S			
1	A	219	1745	1108	295	329	13	0	0	0
1	B	219	1745	1108	295	329	13	0	0	0
1	C	219	1745	1108	295	329	13	0	0	0
1	D	222	1768	1123	299	333	13	0	0	0
1	E	219	1745	1108	295	329	13	0	0	0
1	F	219	1745	1108	295	329	13	0	0	0
1	G	219	1745	1108	295	329	13	0	0	0
1	H	219	1745	1108	295	329	13	0	0	0

- Molecule 2 is water.

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

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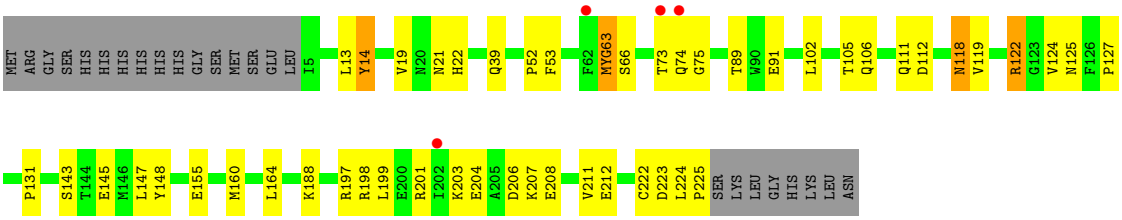
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	G	28	28	28	0	0
			Total	O		
2	H	35	35	35	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

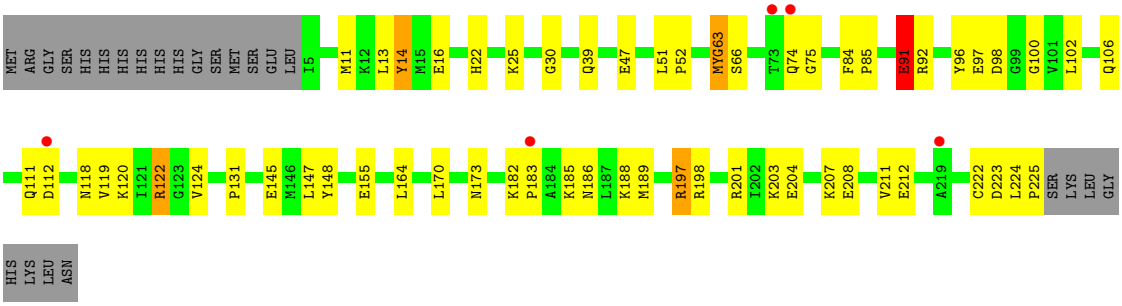
• Molecule 1: Far-red fluorescent protein mKate

Chain A:



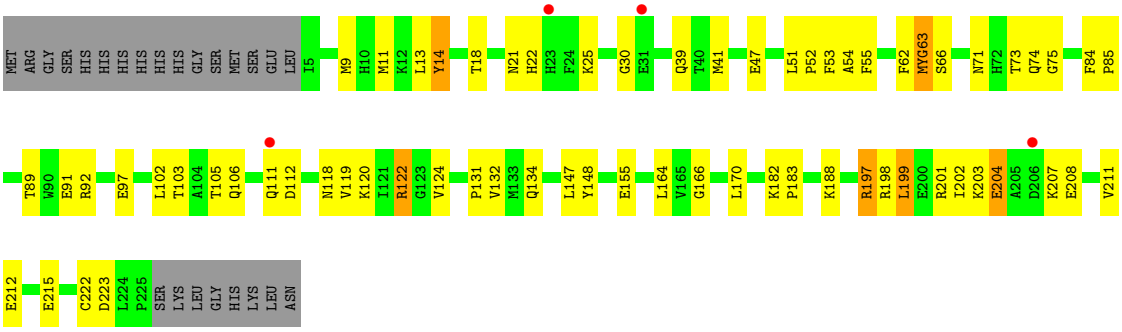
• Molecule 1: Far-red fluorescent protein mKate

Chain B:



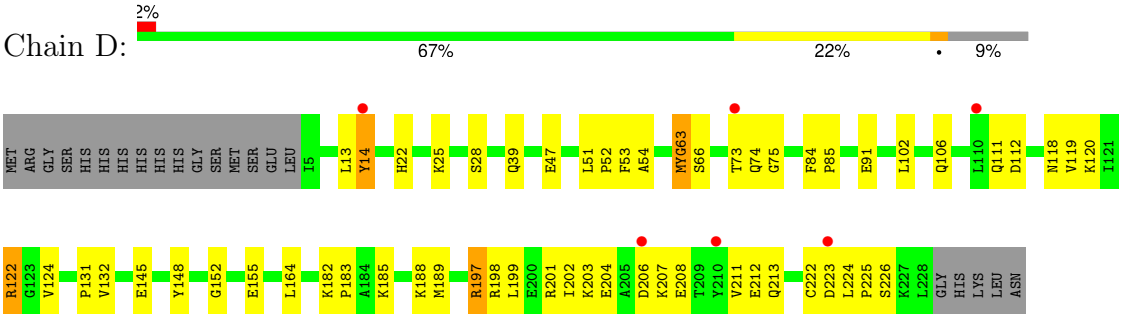
• Molecule 1: Far-red fluorescent protein mKate

Chain C:



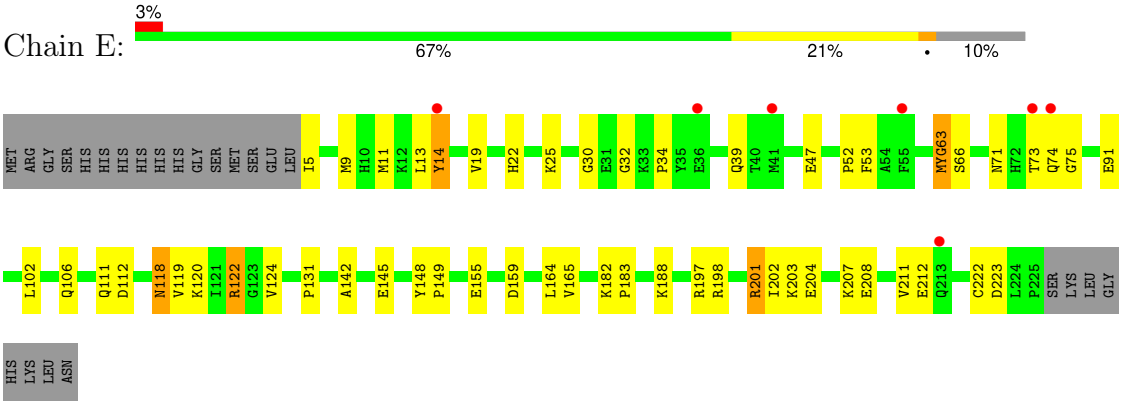
• Molecule 1: Far-red fluorescent protein mKate

Chain D:



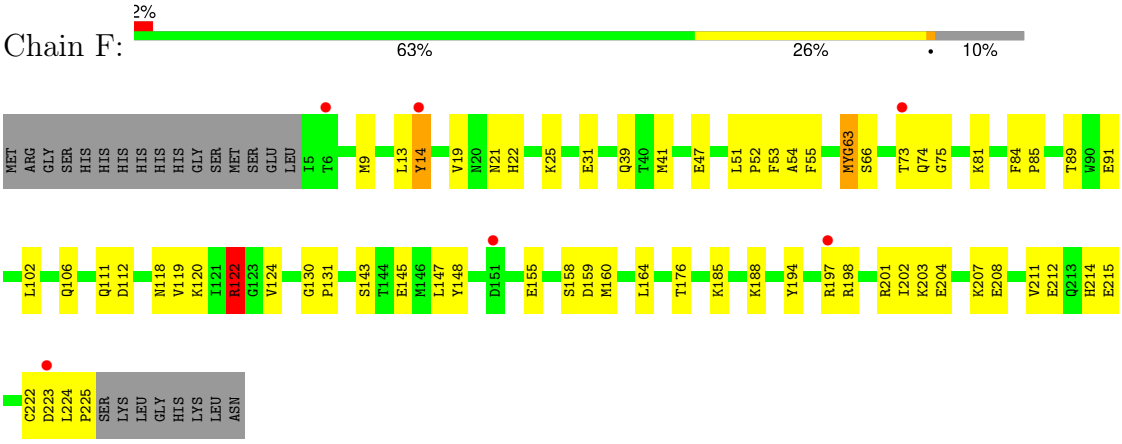
• Molecule 1: Far-red fluorescent protein mKate

Chain E:



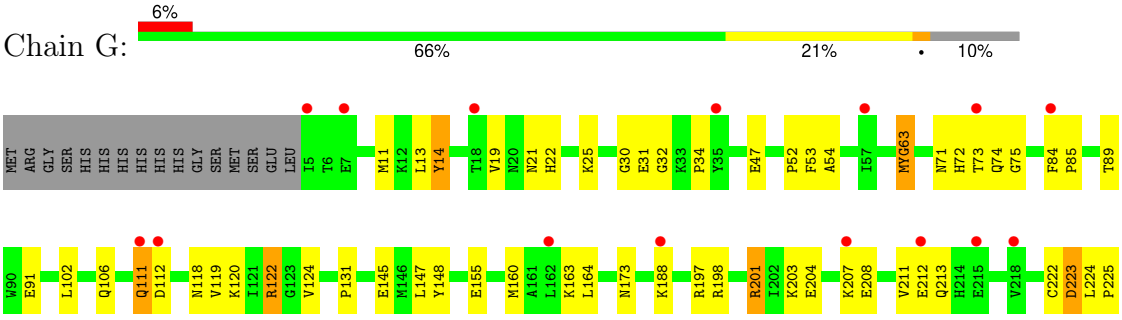
• Molecule 1: Far-red fluorescent protein mKate

Chain F:



• Molecule 1: Far-red fluorescent protein mKate

Chain G:



SER LYS LEU GLY HIS LYS LEU ASN

- Molecule 1: Far-red fluorescent protein mKate

Chain H:

MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY SER MET SER GLU LEU I5 T6 E7 N8 M9 L13 Y14 T18 V19 N20 N21 H22 K25 K33 P34 Y35 Q39 T40 M41 R42 E47 L51 P52 F53 A54 MYG63 S66 K67 T68 F69 T73 Q74 G75 F79

F84 P85 E91 R92 L102 T105 Q106 Q111 D112 N118 V119 R122 G123 V124 N125 P131 V132 M133 Q134 L138 E145 M146 L147 Y148 E155 M160 K163 L164 G168 K182 P183 A184 K185 K188 R197 R198 L199 E200 R201 I202 K203 E204

K207 E208 V211 E212 V218 C222 D223 L224 P225 SER LYS LEU GLY HIS LYS LEU ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.58 (at 2.61Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.235 , 0.282 0.232 , 0.277	Depositor DCC
R_{free} test set	2508 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	53.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.094 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14324	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NRQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 15.

All (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:GLN:HG3	1:E:63:NRQ:CE	2.07	0.84
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:A:118:ASN:HB2	2:A:258:HOH:O	1.80	0.79
1:H:163:LYS:HB3	2:H:267:HOH:O	1.82	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:C:199:LEU:C	1:C:199:LEU:HD23	2.09	0.72
1:F:197:ARG:NH2	2:F:282:HOH:O	2.22	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:C:22:HIS:CD2	1:C:52:PRO:HG2	2.27	0.69
1:E:124:VAL:HG12	1:H:91:GLU:HG3	1.74	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:B:91:GLU:HG3	1:D:124:VAL:HG12	1.75	0.68
1:H:63:NRQ:HD1	1:H:197:ARG:HH21	1.58	0.68
1:C:201:ARG:HD3	1:C:211:VAL:HG13	1.74	0.68
1:F:63:NRQ:CG2	1:F:197:ARG:HE	2.06	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:A:222:CYS:HB3	1:B:198:ARG:NH2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ARG:HD3	1:E:211:VAL:HG13	1.77	0.67
1:G:208:GLU:OE1	2:G:257:HOH:O	2.10	0.67
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:C:166:GLY:O	1:H:203:LYS:HE2	1.96	0.66
1:H:22:HIS:CD2	1:H:52:PRO:HG2	2.30	0.66
1:A:222:CYS:HB3	1:B:198:ARG:HH22	1.61	0.66
1:G:145:GLU:HB3	1:G:197:ARG:HH12	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:HG2	1:C:197:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:145:GLU:HB3	1:A:197:ARG:HH12	1.65	0.60
1:B:197:ARG:HG2	1:B:197:ARG:NH1	1.97	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:63:NRQ:CD1	1:F:197:ARG:HE	2.17	0.58
1:F:120:LYS:CB	1:G:122:ARG:NH1	2.61	0.58
1:A:21:ASN:ND2	1:C:89:THR:OG1	2.37	0.57
1:D:197:ARG:HG3	1:D:197:ARG:HH11	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:A:73:THR:HA	2:A:238:HOH:O	2.04	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:F:41:MET:HB2	1:F:63:NRQ:CE	2.34	0.57
1:E:106:GLN:HG2	1:E:119:VAL:HG22	1.87	0.56
1:F:63:NRQ:HD1	1:F:197:ARG:HH21	1.70	0.56
1:B:122:ARG:HH12	1:D:120:LYS:HB3	1.70	0.55
1:E:202:ILE:HG22	1:E:202:ILE:O	2.06	0.55
1:F:63:NRQ:CD1	1:F:197:ARG:HH21	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:NRQ:CD1	1:E:197:ARG:HE	2.19	0.54
1:E:63:NRQ:N1	1:E:63:NRQ:HA31	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
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:G:106:GLN:HG2	1:G:119:VAL:HG22	1.91	0.53
1:H:13:LEU:HG	1:H:14:TYR:H	1.73	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:B:13:LEU:HG	1:B:14:TYR:H	1.73	0.53
1:F:63:NRQ:HE1	1:F:143:SER:OG	2.08	0.53
1:A:105:THR:HG23	1:C:122:ARG:HD3	1.91	0.52
1:E:91:GLU:HG2	1:H:124:VAL:HG12	1.91	0.52
1:D:39:GLN:HE22	1:D:66:SER:HB3	1.74	0.52
1:E:39:GLN:CG	1:E:63:NRQ:CE	2.80	0.52
1:E:164:LEU:HD12	2:E:257:HOH:O	2.09	0.52
1:H:41:MET:HB2	1:H:63:NRQ:HE2A	1.91	0.52
1:D:73:THR:HA	2:D:272:HOH:O	2.09	0.52
1:E:202:ILE:O	1:E:202:ILE:CG2	2.57	0.52
1:F:214:HIS:HD2	2:F:266:HOH:O	1.91	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:F:22:HIS:CD2	1:F:52:PRO:CG	2.93	0.52
1:B:197:ARG:NH1	1:B:197:ARG:HG3	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:B:189:MET:HE2	2:B:246:HOH:O	2.09	0.51
1:D:224:LEU:HG	2:D:237:HOH:O	2.11	0.51
1:C:22:HIS:CD2	1:C:52:PRO:CG	2.94	0.51
1:F:122:ARG:HH12	1:G:120:LYS:CB	2.09	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:A:122:ARG:HD3	1:C:105:THR:HG23	1.94	0.50
1:D:152:GLY:O	1:D:189:MET:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:25:LYS:HB2	1:C:47:GLU:HB2	1.93	0.50
1:H:22:HIS:CE1	2:H:262:HOH:O	2.64	0.50
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:B:203:LYS:HB2	1:B:212:GLU:HB3	1.94	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:39:GLN:HG3	1:B:63:NRQ:CE	2.42	0.49
1:H:63:NRQ:CD1	1:H:197:ARG:NH2	2.75	0.49
1:C:134:GLN:OE1	1:H:138:LEU:HD23	2.12	0.49
1:F:41:MET:CB	1:F:63:NRQ:HE3	2.40	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:63:NRQ:HG12	1:G:213:GLN:NE2	2.27	0.49
1:G:173:ASN:ND2	2:G:244:HOH:O	2.44	0.49
1:F:21:ASN:HD21	1:G:89:THR:HB	1.78	0.49
1:H:63:NRQ:N1	1:H:63:NRQ:HA31	2.28	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:D:13:LEU:HD23	1:D:14:TYR:N	2.28	0.49
1:E:203:LYS:HB2	1:E:212:GLU:HB3	1.94	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:B:182:LYS:HG2	1:B:183:PRO:HD2	1.94	0.48
1:H:203:LYS:HB2	1:H:212:GLU:HB3	1.95	0.48
1:C:132:VAL:HB	2:C:239:HOH:O	2.14	0.48
1:F:53:PHE:HD1	1:F:54:ALA:O	1.97	0.48
1:A:63:NRQ:HD2	1:A:63:NRQ:N2	2.29	0.48
1:A:131:PRO:HB3	1:A:164:LEU:HD22	1.96	0.48
1:D:13:LEU:HG	1:D:14:TYR:H	1.79	0.48
1:G:13:LEU:HG	1:G:14:TYR:H	1.79	0.48
1:D:63:NRQ:CG1	1:D:199:LEU:CD1	2.92	0.48
1:H:25:LYS:HB2	1:H:47:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:198:ARG:NE	2:H:290:HOH:O	2.37	0.48
1:F:207:LYS:O	1:F:208:GLU:HB2	2.14	0.48
1:G:207:LYS:O	1:G: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
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:B:131:PRO:HB3	1:B:164:LEU:HD22	1.95	0.47
1:E:39:GLN:CD	1:E:63:NRQ:CE	2.82	0.47
1:B:207:LYS:O	1:B:208:GLU:HB2	2.15	0.47
1:C:204:GLU:CB	2:C:252:HOH:O	2.63	0.47
1:D:63:NRQ:SD	1:D:213:GLN:NE2	2.87	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:A:13:LEU:HD23	1:A:14:TYR:N	2.29	0.47
1:B:22:HIS:CD2	1:B:52:PRO:CG	2.96	0.47
1:D:63:NRQ:SD	1:D:199:LEU:HD11	2.55	0.47
1:C:170:LEU:CD1	2:C:242:HOH:O	2.43	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:G:224:LEU:HA	1:G:225:PRO:HD3	1.69	0.46
1:E:131:PRO:HB3	1:E:164:LEU:HD22	1.97	0.46
1:H:22:HIS:CD2	1:H:52:PRO:CG	2.97	0.46
1:D:51:LEU:HA	1:D:52:PRO:HD3	1.75	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:H:134:GLN:HG2	2:H:283:HOH:O	2.15	0.46
1:D:106:GLN:HG2	1:D:119:VAL:HG22	1.98	0.46
1:F:81:LYS:NZ	2:F:250:HOH:O	2.49	0.46
1:H:41:MET:CB	1:H:63:NRQ:HE3	2.46	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:A:148:TYR:CZ	1:A:155:GLU:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:HD23	1:F:14:TYR:N	2.31	0.46
1:B:13:LEU:HD23	1:B:14:TYR:N	2.31	0.45
1:B:106:GLN:HG2	1:B:119:VAL:HG22	1.97	0.45
1:D:148:TYR:CZ	1:D:155:GLU:HB2	2.51	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
1:A:197:ARG:NH2	2:A:276:HOH:O	2.50	0.45
1:E:19:VAL:HB	1:E:53:PHE:CE2	2.52	0.45
1:F:145:GLU:HB2	1:F:197:ARG:HH12	1.82	0.45
1:F:160:MET:HA	2:F:247:HOH:O	2.17	0.45
1:H:33:LYS:HB3	2:H:282:HOH:O	2.17	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:H:51:LEU:HD23	2:H:262:HOH:O	2.16	0.45
1:B:74:GLN:O	1:B:75:GLY:C	2.54	0.45
1:C:199:LEU:C	1:C:199:LEU:CD2	2.80	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:A:147:LEU:HA	1:A:155:GLU:O	2.17	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: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:C:147:LEU:HA	1:C:155:GLU:O	2.17	0.44
1:F:51:LEU:HA	1:F:52:PRO:HD3	1.72	0.44
1:E:74:GLN:O	1:E:75:GLY:C	2.55	0.44
1:F:66:SER:N	2:F:246:HOH:O	2.50	0.44
1:H:131:PRO:HB3	1:H:164:LEU:HD22	2.00	0.44
1:H:148:TYR:CZ	1:H:155:GLU:HB2	2.53	0.44
1:H:182:LYS:HG2	1:H:183:PRO:HD2	2.00	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: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:D:182:LYS:HG2	1:D:183:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:207:LYS:O	1:E:208:GLU:HB2	2.17	0.43
1:A:19:VAL:HB	1:A:53:PHE:CE2	2.53	0.43
1:B:186:ASN:ND2	2:B:291:HOH:O	2.50	0.43
1:C:131:PRO:HB3	1:C:164:LEU:HD22	2.00	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
1:A:21:ASN:HD21	1:C:89:THR:CB	2.30	0.43
1:C:106:GLN:HG2	1:C:119:VAL:HG22	2.01	0.43
1:D:106:GLN:CG	1:D:119:VAL:HG22	2.49	0.43
1:F:158:SER:CB	2:F:282:HOH:O	2.66	0.43
1:B:25:LYS:HB2	1:B:47:GLU:HB2	2.01	0.43
1:B:84:PHE:HB3	1:B:85:PRO:HA	2.01	0.43
1:F:131:PRO:HB3	1:F:164:LEU:HD22	2.00	0.43
1:D:197:ARG:HH11	1:D:197:ARG:CG	2.30	0.43
1:C:74:GLN:O	1:C:75:GLY:C	2.57	0.43
1:F:39:GLN:NE2	1:F:215:GLU:OE1	2.52	0.43
1:C:84:PHE:HB3	1:C:85:PRO:HA	2.01	0.43
1:F:74:GLN:O	1:F:75:GLY:C	2.57	0.43
1:C:197:ARG:HH11	1:C:197:ARG:CG	2.29	0.43
1:D:63:NRQ:CG1	1:D:199:LEU:HD12	2.45	0.43
1:C:71:ASN:OD1	1:C:73:THR:HG23	2.19	0.42
1:G:74:GLN:O	1:G:75:GLY:C	2.56	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:A:127:PRO:HD2	2:A:254:HOH:O	2.17	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:D:13:LEU:HB3	1:D:28:SER:OG	2.19	0.42
1:F:148:TYR:CZ	1:F:155:GLU:HB2	2.54	0.42
1:H:13:LEU:HD23	1:H:14:TYR:N	2.35	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:A:74:GLN:O	1:A:75:GLY:C	2.58	0.42
1:A:207:LYS:O	1:A:208:GLU:HB2	2.18	0.42
1:C:148:TYR:CZ	1:C:155:GLU:HB2	2.55	0.42
1:E:63:NRQ:N1	1:E:63:NRQ:CA3	2.83	0.42
1:G:148:TYR:CZ	1:G:155:GLU:HB2	2.54	0.42
1:A:13:LEU:HD23	1:A:13:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:CG	1:D:124:VAL:HG12	2.44	0.42
1:E:32:GLY:O	1:E:34:PRO:HD3	2.20	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: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:B:39:GLN:HE22	1:B:66:SER:HB3	1.84	0.41
1:C:39:GLN:HE22	1:C:66:SER:HB3	1.85	0.41
1:C:55:PHE:O	1:C:55:PHE:CD2	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:B:148:TYR:CZ	1:B:155:GLU:HB2	2.55	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:A:89:THR:OG1	1:C:21:ASN:ND2	2.52	0.41
1:B:96:TYR:CB	2:B:254:HOH:O	2.63	0.41
1:C:92:ARG:O	1:C:103:THR:HA	2.20	0.41
1:E:71:ASN:OD1	1:E:73:THR:HG23	2.20	0.41
1:E:122:ARG:HD3	1:H:105:THR:CG2	2.51	0.41
1:H:13:LEU:HG	1:H:14:TYR:N	2.35	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:A:206:ASP:O	1:A:207:LYS:HB2	2.21	0.41
1:B:66:SER:N	2:B:262:HOH:O	2.53	0.41
1:F:202:ILE:O	1:F:202:ILE:HG22	2.19	0.41
1:D:203:LYS:HB2	1:D:212:GLU:HB3	2.02	0.41
1:F:147:LEU:HA	1:F:155:GLU:O	2.21	0.41
1:G:13:LEU:HD23	1:G:13:LEU:C	2.40	0.41
1:B:11:MET:HG2	1:B:30:GLY:O	2.21	0.41
1:C:13:LEU:HD23	1:C:13:LEU:C	2.41	0.41
1:C:39:GLN:OE1	1:C:63:NRQ:CE	2.69	0.41
1:D:202:ILE:O	1:D:202:ILE:HG22	2.21	0.41
1:E:11:MET:HG2	1:E:30:GLY:O	2.20	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:F:63:NRQ:CZ	1:F:197:ARG:HG3	2.51	0.41
1:F:124:VAL:HG12	1:G:91:GLU:HG2	2.03	0.41
1:H:63:NRQ:HB12	1:H:199:LEU:CD1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:ARG:HH11	1:H:92:ARG:HD2	1.76	0.41
1:A:13:LEU:HG	1:A:14:TYR:N	2.36	0.40
1:B:122:ARG:NH1	1:D:120:LYS:CB	2.83	0.40
1:D:74:GLN:O	1:D:75:GLY:C	2.59	0.40
1:H:74:GLN:O	1:H:75:GLY:C	2.60	0.40
1:E:148:TYR:HA	1:E:149:PRO:HD3	1.97	0.40
1:F:39:GLN:HE22	1:F:66:SER:HB3	1.87	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:C:182:LYS:HG2	1:C:183:PRO:HD2	2.03	0.40
1:D:132:VAL:HB	2:D:269:HOH:O	2.21	0.40
1:G:84:PHE:HB3	1:G:85:PRO:HA	2.03	0.40
1:B:147:LEU:HA	1:B:155:GLU:O	2.22	0.40
1:C:202:ILE:O	1:C:202:ILE:HG22	2.21	0.40
1:G:71:ASN:OD1	1:G:73:THR:HG23	2.21	0.40
1:H:147:LEU:HA	1:H:155:GLU:O	2.21	0.40
1:B:13:LEU:CG	1:B:14:TYR:N	2.84	0.40
1:F:63:NRQ:CD1	1:F:197:ARG:NE	2.85	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	Interatomic distance (Å)	Clash overlap (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 (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	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
All	All	1715/1944 (88%)	1619 (94%)	96 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	187/208 (90%)	178 (95%)	9 (5%)	25	49
1	B	187/208 (90%)	176 (94%)	11 (6%)	19	39
1	C	187/208 (90%)	175 (94%)	12 (6%)	17	35
1	D	190/208 (91%)	179 (94%)	11 (6%)	20	40
1	E	187/208 (90%)	176 (94%)	11 (6%)	19	39
1	F	187/208 (90%)	176 (94%)	11 (6%)	19	39
1	G	187/208 (90%)	177 (95%)	10 (5%)	22	45
1	H	187/208 (90%)	176 (94%)	11 (6%)	19	39
All	All	1499/1664 (90%)	1413 (94%)	86 (6%)	20	41

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

Mol	Chain	Res	Type
1	A	14	TYR
1	A	102	LEU

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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
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 (i)

There are no RNA molecules in this entry.

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

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	H	63	1	24,24,25	1.34	2 (8%)	24,32,34	1.16	2 (8%)
1	NRQ	B	63	1	24,24,25	1.25	2 (8%)	24,32,34	1.60	7 (29%)
1	NRQ	C	63	1	24,24,25	1.98	2 (8%)	24,32,34	1.15	1 (4%)
1	NRQ	D	63	1	24,24,25	2.00	2 (8%)	24,32,34	1.35	5 (20%)
1	NRQ	A	63	1	24,24,25	1.05	1 (4%)	24,32,34	1.43	4 (16%)
1	NRQ	E	63	1	24,24,25	1.44	3 (12%)	24,32,34	1.48	5 (20%)
1	NRQ	G	63	1	24,24,25	2.21	1 (4%)	24,32,34	1.25	2 (8%)
1	NRQ	F	63	1	24,24,25	2.63	5 (20%)	24,32,34	1.71	8 (33%)

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	H	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	B	63	1	-	1/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	2/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	3/9/31/32	0/2/2/2
1	NRQ	A	63	1	-	2/9/31/32	0/2/2/2
1	NRQ	E	63	1	-	0/9/31/32	0/2/2/2
1	NRQ	G	63	1	-	2/9/31/32	0/2/2/2
1	NRQ	F	63	1	-	1/9/31/32	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	63	NRQ	OH-CZ	10.02	1.59	1.37
1	F	63	NRQ	OH-CZ	9.95	1.59	1.37
1	D	63	NRQ	OH-CZ	8.20	1.55	1.37
1	C	63	NRQ	C1-CA1	-6.42	1.38	1.48
1	C	63	NRQ	OH-CZ	6.32	1.51	1.37
1	E	63	NRQ	C1-CA1	-5.69	1.39	1.48
1	F	63	NRQ	C1-CA1	-4.75	1.41	1.48
1	H	63	NRQ	OH-CZ	4.69	1.47	1.37
1	F	63	NRQ	CA2-C2	4.18	1.53	1.48
1	D	63	NRQ	CA2-C2	4.07	1.52	1.48
1	F	63	NRQ	CB2-CA2	3.75	1.38	1.35
1	B	63	NRQ	C1-CA1	-3.40	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	C1-CA1	-2.80	1.43	1.48
1	H	63	NRQ	C1-CA1	-2.68	1.44	1.48
1	E	63	NRQ	C1-N2	-2.21	1.28	1.33
1	E	63	NRQ	OH-CZ	-2.17	1.32	1.37
1	B	63	NRQ	CB2-CA2	-2.15	1.33	1.35
1	F	63	NRQ	CD1-CE1	2.00	1.42	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	63	NRQ	C3-CA3-N3	3.85	121.20	112.43
1	A	63	NRQ	O2-C2-CA2	3.74	133.41	131.02
1	C	63	NRQ	C3-CA3-N3	3.74	120.94	112.43
1	F	63	NRQ	C2-CA2-N2	-3.55	106.41	108.95
1	F	63	NRQ	CG2-CB2-CA2	3.39	133.89	129.87
1	B	63	NRQ	CE2-CD2-CG2	-3.37	116.86	121.22
1	B	63	NRQ	CG2-CB2-CA2	3.19	133.65	129.87
1	A	63	NRQ	C3-CA3-N3	3.16	119.63	112.43
1	H	63	NRQ	C3-CA3-N3	3.14	119.58	112.43
1	E	63	NRQ	N3-C1-N2	3.11	116.31	112.62
1	D	63	NRQ	CB2-CA2-C2	3.03	126.03	122.36
1	F	63	NRQ	C3-CA3-N3	2.84	118.89	112.43
1	A	63	NRQ	N3-C1-N2	2.81	115.95	112.62
1	F	63	NRQ	O2-C2-CA2	2.73	132.76	131.02
1	D	63	NRQ	C3-CA3-N3	2.69	118.55	112.43
1	G	63	NRQ	O2-C2-CA2	-2.66	129.32	131.02
1	H	63	NRQ	N3-C1-N2	2.58	115.68	112.62
1	B	63	NRQ	C3-CA3-N3	2.44	117.98	112.43
1	E	63	NRQ	C3-CA3-N3	2.41	117.90	112.43
1	F	63	NRQ	CB2-CA2-C2	2.33	125.18	122.36
1	B	63	NRQ	N3-C1-N2	2.32	115.38	112.62
1	B	63	NRQ	CD1-CG2-CD2	2.32	121.09	117.65
1	B	63	NRQ	CD1-CG2-CB2	-2.30	113.31	121.22
1	D	63	NRQ	CG2-CB2-CA2	2.28	132.58	129.87
1	D	63	NRQ	CB2-CA2-N2	-2.22	125.75	128.76
1	E	63	NRQ	CE2-CD2-CG2	-2.21	118.37	121.22
1	E	63	NRQ	CG2-CB2-CA2	2.18	132.46	129.87
1	D	63	NRQ	N3-C1-N2	2.17	115.20	112.62
1	F	63	NRQ	CD2-CE2-CZ	2.10	122.10	119.88
1	A	63	NRQ	CB2-CA2-C2	2.10	124.90	122.36
1	E	63	NRQ	C2-CA2-N2	2.08	110.44	108.95
1	F	63	NRQ	N3-C1-N2	2.07	115.08	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	NRQ	CD2-CE2-CZ	2.04	122.04	119.88
1	F	63	NRQ	O3-C3-CA3	-2.01	116.43	125.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	63	NRQ	13	0
1	B	63	NRQ	2	0
1	C	63	NRQ	5	0
1	D	63	NRQ	8	0
1	A	63	NRQ	8	0
1	E	63	NRQ	13	0
1	G	63	NRQ	3	0
1	F	63	NRQ	10	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	218/243 (89%)	0.17	4 (1%)	68	64	31, 54, 84, 102	0
1	B	218/243 (89%)	0.21	5 (2%)	60	54	36, 53, 85, 106	0
1	C	218/243 (89%)	0.24	4 (1%)	68	64	37, 55, 86, 102	0
1	D	221/243 (90%)	0.25	6 (2%)	54	48	37, 55, 86, 107	0
1	E	218/243 (89%)	0.17	7 (3%)	47	40	36, 54, 85, 102	0
1	F	218/243 (89%)	0.24	6 (2%)	53	46	35, 55, 85, 101	0
1	G	218/243 (89%)	0.52	15 (6%)	16	12	35, 57, 87, 105	0
1	H	218/243 (89%)	0.39	13 (5%)	21	16	38, 57, 85, 105	0
All	All	1747/1944 (89%)	0.27	60 (3%)	45	38	31, 55, 86, 107	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	73	THR	8.2
1	G	188	LYS	5.8
1	H	75	GLY	5.1
1	B	73	THR	4.7
1	D	206	ASP	4.3
1	B	74	GLN	3.9
1	G	7	GLU	3.8
1	D	210	TYR	3.4
1	F	151	ASP	3.2
1	H	73	THR	3.1
1	H	6	THR	3.0
1	G	84	PHE	3.0
1	G	212	GLU	3.0
1	D	223	ASP	3.0
1	G	218	VAL	3.0
1	E	74	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	74	GLN	2.9
1	H	7	GLU	2.9
1	C	111	GLN	2.8
1	H	218	VAL	2.8
1	F	14	TYR	2.8
1	G	5	ILE	2.7
1	B	219	ALA	2.7
1	G	162	LEU	2.7
1	H	5	ILE	2.7
1	H	79	PHE	2.6
1	C	23	HIS	2.5
1	G	111	GLN	2.5
1	B	183	PRO	2.5
1	H	223	ASP	2.5
1	H	168	GLY	2.5
1	D	14	TYR	2.5
1	G	215	GLU	2.4
1	C	206	ASP	2.4
1	F	73	THR	2.4
1	A	202	ILE	2.4
1	E	14	TYR	2.3
1	G	57	ILE	2.3
1	E	73	THR	2.3
1	F	223	ASP	2.2
1	A	74	GLN	2.2
1	H	111	GLN	2.2
1	D	110	LEU	2.2
1	G	112	ASP	2.2
1	E	55	PHE	2.2
1	B	112	ASP	2.2
1	F	6	THR	2.2
1	G	73	THR	2.2
1	C	31	GLU	2.1
1	E	36	GLU	2.1
1	F	197	ARG	2.1
1	A	62	PHE	2.1
1	A	73	THR	2.1
1	H	35	TYR	2.1
1	G	18	THR	2.1
1	H	112	ASP	2.1
1	G	35	TYR	2.0
1	G	207	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	213	GLN	2.0
1	E	41	MET	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	NRQ	D	63	23/24	0.85	0.26	32,52,77,79	0
1	NRQ	B	63	23/24	0.86	0.22	40,47,63,67	0
1	NRQ	G	63	23/24	0.90	0.18	53,63,77,88	0
1	NRQ	F	63	23/24	0.91	0.18	30,48,66,79	0
1	NRQ	H	63	23/24	0.91	0.21	38,61,84,91	0
1	NRQ	A	63	23/24	0.92	0.20	33,50,69,75	0
1	NRQ	C	63	23/24	0.94	0.15	37,46,64,75	0
1	NRQ	E	63	23/24	0.95	0.13	38,47,57,64	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.