Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:36 PM GMT

PDB ID	:	3U8A
Title	:	Crystal structure of monomeric reversibly photoswitchable red fluorescent protein rsTagRFP in the OFF state
Authors	:	Pletnev, S.
Deposited on	:	2011-10-16
Resolution	:	1.78 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

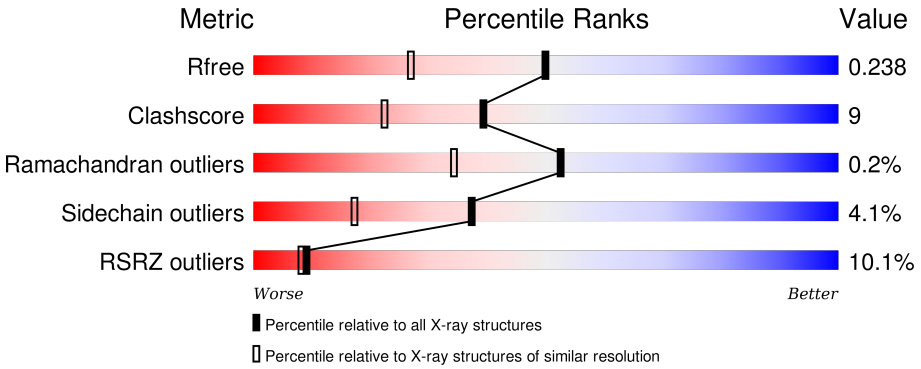
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.78 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}	91344	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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	7% 74% 18% • 8%
1	B	243	10% 75% 17% 8%
1	C	243	8% 74% 14% • 8%
1	D	243	12% 77% 14% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7676 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 Fluorescent protein rsTagRFP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1786	1135	304	334	13			
1	B	224	Total	C	N	O	S	0	0	0
			1786	1135	304	334	13			
1	C	224	Total	C	N	O	S	0	0	0
			1786	1135	304	334	13			
1	D	224	Total	C	N	O	S	0	0	0
			1786	1135	304	334	13			

- Molecule 2 is water.

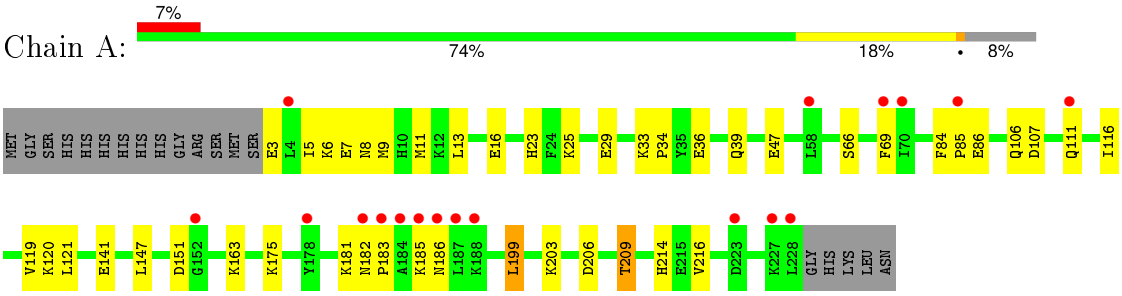
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	128	Total	O	0	0
			128	128		
2	C	146	Total	O	0	0
			146	146		
2	D	116	Total	O	0	0
			116	116		

3 Residue-property plots (i)

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

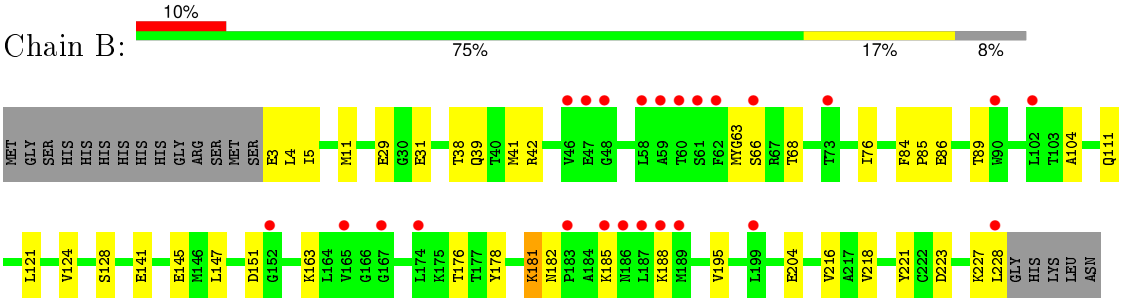
- Molecule 1: Fluorescent protein rsTagRFP

Chain A:



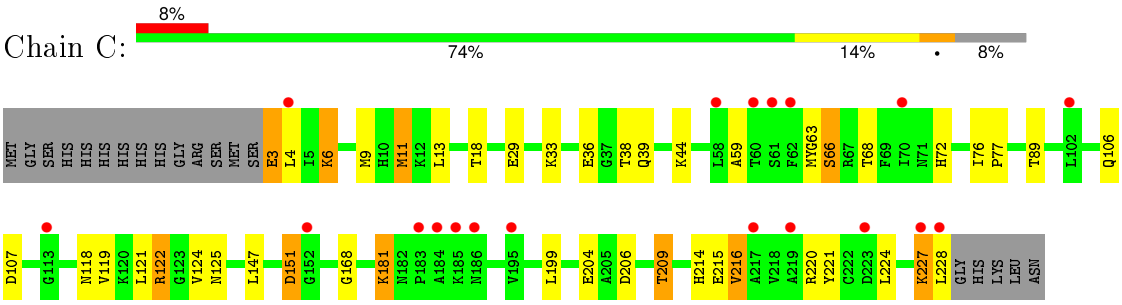
- Molecule 1: Fluorescent protein rsTagRFP

Chain B:



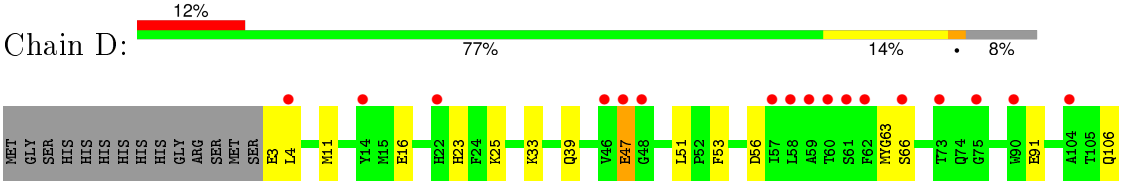
- Molecule 1: Fluorescent protein rsTagRFP

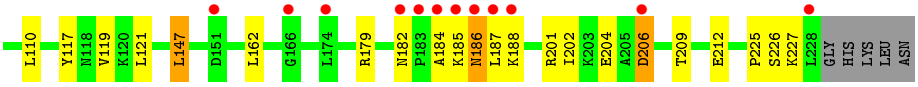
Chain C:



- Molecule 1: Fluorescent protein rsTagRFP

Chain D:




L110
Y117
N118
V119
K120
L121
L147
D151
L162
G166
L174
R179
N182
P183
A184
K185
N186
L187
K188
R201
I202
K203
E204
A205
D206
T209
E212
P225
S226
K227
L228
GLY
HIS
LYS
LEU
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.75Å 69.64Å 73.95Å 78.61° 83.77° 72.16°	Depositor
Resolution (Å)	26.65 – 1.78 29.56 – 1.78	Depositor EDS
% Data completeness (in resolution range)	93.9 (26.65-1.78) 89.5 (29.56-1.78)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.182 , 0.235 0.186 , 0.238	Depositor DCC
R_{free} test set	1650 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 82793 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7676	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	0/1804	0.81	2/2435 (0.1%)
1	B	0.77	3/1804 (0.2%)	0.74	0/2435
1	C	0.84	1/1804 (0.1%)	0.81	2/2435 (0.1%)
1	D	0.73	0/1804	0.77	1/2435 (0.0%)
All	All	0.79	4/7216 (0.1%)	0.78	5/9740 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	124	VAL	CB-CG1	-6.57	1.39	1.52
1	B	104	ALA	CA-CB	-5.33	1.41	1.52
1	B	145	GLU	CG-CD	5.19	1.59	1.51
1	C	66	SER	N-CA	-5.01	1.36	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	147	LEU	CA-CB-CG	-6.76	99.75	115.30
1	A	199	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	147	LEU	CA-CB-CG	-5.48	102.69	115.30
1	C	72	HIS	CB-CA-C	5.28	120.95	110.40
1	A	147	LEU	CA-CB-CG	-5.13	103.50	115.30

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	1786	0	1744	35	0
1	B	1786	0	1744	30	0
1	C	1786	0	1743	37	0
1	D	1786	0	1744	27	0
2	A	142	0	0	5	0
2	B	128	0	0	5	0
2	C	146	0	0	7	0
2	D	116	0	0	2	0
All	All	7676	0	6975	125	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 (125) 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:120:LYS:HE2	2:A:317:HOH:O	1.69	0.93
1:B:185:LYS:HD3	2:B:256:HOH:O	1.69	0.91
1:C:6:LYS:HA	1:C:6:LYS:HE2	1.56	0.88
1:C:68:THR:HG23	2:C:256:HOH:O	1.75	0.87
1:B:3:GLU:HA	2:B:389:HOH:O	1.76	0.85
1:A:206:ASP:HB2	1:A:209:THR:HG22	1.59	0.81
1:D:182:ASN:ND2	1:D:185:LYS:HB2	1.97	0.80
1:C:151:ASP:OD2	1:C:151:ASP:O	2.01	0.77
1:D:39:GLN:HE22	1:D:66:SER:HB3	1.50	0.76
1:A:119:VAL:O	1:A:120:LYS:HD3	1.88	0.74
1:B:121:LEU:C	1:B:121:LEU:HD12	2.10	0.72
1:A:111:GLN:HG2	1:A:116:ILE:HG13	1.71	0.71
1:A:119:VAL:C	1:A:120:LYS:HD3	2.12	0.70
1:D:182:ASN:CG	1:D:185:LYS:HB2	2.12	0.69
1:A:5:ILE:HA	1:A:9:MET:CE	2.23	0.69
1:C:9:MET:HG2	2:C:310:HOH:O	1.93	0.69
1:A:5:ILE:HA	1:A:9:MET:HE2	1.76	0.68
1:A:39:GLN:HE22	1:A:66:SER:HB3	1.59	0.68
1:A:214:HIS:HD2	2:A:311:HOH:O	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:OD1	2:C:367:HOH:O	2.12	0.66
1:D:206:ASP:HB2	1:D:209:THR:OG1	1.95	0.66
1:C:121:LEU:C	1:C:121:LEU:HD12	2.16	0.66
1:C:106:GLN:HG3	1:C:119:VAL:HG22	1.79	0.65
1:C:227:LYS:N	1:C:227:LYS:HD2	2.11	0.64
1:D:25:LYS:HB2	1:D:47:GLU:HG3	1.78	0.64
1:B:41:MET:HB2	1:B:63:NRQ:CE	2.27	0.63
1:A:6:LYS:H	1:A:9:MET:CE	2.12	0.63
1:D:202:ILE:HB	1:D:212:GLU:HG2	1.80	0.63
1:D:4:LEU:HD22	1:D:110:LEU:HD23	1.79	0.63
1:C:18:THR:HG21	1:C:122:ARG:NH1	2.15	0.62
1:A:182:ASN:HD22	1:A:185:LYS:HD2	1.66	0.61
1:C:204:GLU:HG3	2:C:526:HOH:O	2.00	0.61
1:C:89:THR:HG23	1:C:181:LYS:HD2	1.83	0.60
1:D:66:SER:HG	1:D:117:TYR:HH	1.49	0.60
1:A:106:GLN:NE2	2:A:316:HOH:O	2.35	0.60
1:C:6:LYS:CE	1:C:6:LYS:HA	2.31	0.59
1:D:121:LEU:C	1:D:121:LEU:HD12	2.23	0.59
1:C:39:GLN:HE22	1:C:66:SER:CB	2.16	0.58
1:C:33:LYS:HD2	1:C:36:GLU:OE1	2.03	0.58
2:B:302:HOH:O	1:C:168:GLY:HA2	2.04	0.56
1:B:76:ILE:HG12	1:B:221:TYR:CZ	2.40	0.56
1:A:175:LYS:HE3	2:A:442:HOH:O	2.06	0.56
1:A:120:LYS:N	1:A:120:LYS:HD3	2.21	0.55
1:C:76:ILE:HG12	1:C:221:TYR:CZ	2.40	0.55
1:D:182:ASN:HD22	1:D:185:LYS:HD2	1.71	0.55
1:A:66:SER:N	2:A:300:HOH:O	2.39	0.54
1:A:111:GLN:HG2	1:A:116:ILE:CG1	2.36	0.54
1:A:107:ASP:OD1	1:A:181:LYS:HE2	2.07	0.54
1:C:77:PRO:HA	2:C:239:HOH:O	2.08	0.54
1:A:214:HIS:CG	1:D:227:LYS:HE2	2.44	0.53
1:A:86:GLU:HG2	1:A:182:ASN:HB2	1.90	0.53
1:D:51:LEU:HD13	1:D:53:PHE:CZ	2.44	0.53
1:A:121:LEU:C	1:A:121:LEU:HD12	2.29	0.53
1:B:11:MET:HE3	1:B:31:GLU:HA	1.91	0.52
1:C:220:ARG:HG3	1:C:221:TYR:O	2.10	0.52
1:A:33:LYS:HB2	1:A:36:GLU:HB2	1.91	0.52
1:A:6:LYS:O	1:A:8:ASN:N	2.42	0.52
1:C:59:ALA:HB1	1:C:199:LEU:HD21	1.92	0.51
1:C:63:NRQ:HB12	1:C:215:GLU:OE1	2.10	0.51
1:A:16:GLU:OE2	1:A:23:HIS:NE2	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:NRQ:HD2	1:C:63:NRQ:O2	2.11	0.51
1:A:86:GLU:H	1:A:86:GLU:CD	2.13	0.51
1:B:111:GLN:NE2	2:B:396:HOH:O	2.38	0.51
1:B:41:MET:HB2	1:B:63:NRQ:HE3	1.92	0.51
1:A:33:LYS:HD2	1:A:36:GLU:HG3	1.92	0.51
1:D:39:GLN:NE2	1:D:66:SER:HB3	2.24	0.50
1:B:68:THR:HG23	2:B:245:HOH:O	2.11	0.50
1:B:41:MET:CB	1:B:63:NRQ:CE	2.88	0.50
1:B:141:GLU:CD	1:B:163:LYS:HE2	2.32	0.50
1:D:106:GLN:HG3	1:D:119:VAL:HG22	1.93	0.50
1:B:147:LEU:HD12	1:B:195:VAL:HG23	1.94	0.49
1:B:86:GLU:HG2	1:B:182:ASN:HB2	1.94	0.49
1:C:11:MET:HE1	1:C:39:GLN:HB2	1.94	0.49
1:B:41:MET:CB	1:B:63:NRQ:HE3	2.42	0.49
1:D:186:ASN:HD22	1:D:187:LEU:N	2.10	0.49
1:C:38:THR:HG22	1:C:216:VAL:HG13	1.94	0.48
1:B:89:THR:HG23	1:B:181:LYS:HD2	1.94	0.48
1:A:6:LYS:H	1:A:9:MET:HE1	1.79	0.47
1:C:18:THR:CG2	1:C:122:ARG:NH1	2.77	0.47
1:B:121:LEU:O	1:B:121:LEU:HD12	2.14	0.47
1:B:218:VAL:HG23	1:C:224:LEU:HD21	1.96	0.47
1:C:206:ASP:O	1:C:209:THR:HB	2.14	0.47
1:B:84:PHE:HB3	1:B:85:PRO:HA	1.97	0.47
1:B:3:GLU:HG3	1:B:5:ILE:H	1.80	0.47
1:C:63:NRQ:O3	1:C:106:GLN:NE2	2.40	0.46
1:A:141:GLU:OE2	1:A:163:LYS:HD3	2.15	0.46
1:C:44:LYS:HE2	2:C:333:HOH:O	2.14	0.46
1:A:13:LEU:HD23	1:A:13:LEU:C	2.35	0.46
1:D:184:ALA:HB3	2:D:525:HOH:O	2.16	0.46
1:D:206:ASP:OD1	1:D:206:ASP:N	2.48	0.46
1:A:25:LYS:HD2	1:A:47:GLU:OE1	2.15	0.46
1:C:151:ASP:CG	1:C:151:ASP:O	2.53	0.46
1:C:11:MET:CE	1:C:39:GLN:HB2	2.46	0.46
1:B:63:NRQ:HD2	1:B:63:NRQ:O2	2.16	0.46
1:A:206:ASP:O	1:A:209:THR:HB	2.16	0.45
1:C:124:VAL:O	1:C:125:ASN:HB2	2.16	0.45
1:B:147:LEU:CD1	1:B:195:VAL:HG23	2.46	0.45
1:C:121:LEU:O	1:C:121:LEU:HD12	2.17	0.45
1:B:39:GLN:HE22	1:B:66:SER:HB3	1.82	0.44
1:B:4:LEU:CD1	1:B:85:PRO:HB3	2.48	0.44
1:C:3:GLU:HG2	1:C:4:LEU:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:ASN:ND2	1:D:185:LYS:HD2	2.32	0.44
1:D:91:GLU:CD	1:D:179:ARG:HH12	2.21	0.44
1:A:84:PHE:HB3	1:A:85:PRO:HA	1.99	0.44
1:D:201:ARG:HD2	1:D:204:GLU:OE1	2.17	0.43
1:D:16:GLU:OE2	1:D:23:HIS:NE2	2.46	0.43
1:C:107:ASP:OD1	1:C:181:LYS:HE3	2.19	0.43
1:B:38:THR:HG22	1:B:216:VAL:HG13	2.01	0.43
1:B:29:GLU:OE2	1:B:42:ARG:NH2	2.52	0.43
1:A:6:LYS:H	1:A:9:MET:HE2	1.82	0.43
1:B:4:LEU:HD11	1:B:85:PRO:HB3	2.01	0.43
1:B:228:LEU:HD12	2:C:370:HOH:O	2.17	0.43
1:D:56:ASP:HB3	1:D:162:LEU:HD11	2.00	0.42
1:B:227:LYS:HD3	1:C:214:HIS:CG	2.55	0.42
1:A:216:VAL:HG11	1:D:225:PRO:HD2	2.01	0.42
1:C:13:LEU:HD23	1:C:13:LEU:C	2.40	0.42
1:D:63:NRQ:HD2	1:D:63:NRQ:O2	2.20	0.42
1:D:33:LYS:HB3	2:D:277:HOH:O	2.19	0.42
1:D:188:LYS:HD3	1:D:188:LYS:HA	1.83	0.42
1:B:176:THR:HG21	1:B:178:TYR:CZ	2.55	0.41
1:A:34:PRO:HA	1:A:69:PHE:HA	2.02	0.41
1:B:141:GLU:OE1	1:B:163:LYS:HE2	2.21	0.41
1:C:121:LEU:C	1:C:121:LEU:CD1	2.87	0.41
1:A:181:LYS:O	1:A:183:PRO:HD3	2.21	0.41
1:D:206:ASP:HB2	1:D:209:THR:HG1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	219/243 (90%)	209 (95%)	9 (4%)	1 (0%)	34 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	219/243 (90%)	215 (98%)	3 (1%)	1 (0%)	34 16
1	C	219/243 (90%)	214 (98%)	5 (2%)	0	100 100
1	D	219/243 (90%)	211 (96%)	8 (4%)	0	100 100
All	All	876/972 (90%)	849 (97%)	25 (3%)	2 (0%)	52 34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	B	151	ASP

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	190/206 (92%)	182 (96%)	8 (4%)	36 16
1	B	190/206 (92%)	185 (97%)	5 (3%)	54 35
1	C	190/206 (92%)	179 (94%)	11 (6%)	25 8
1	D	190/206 (92%)	183 (96%)	7 (4%)	41 21
All	All	760/824 (92%)	729 (96%)	31 (4%)	37 17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	11	MET
1	A	29	GLU
1	A	151	ASP
1	A	186	ASN
1	A	199	LEU
1	A	203	LYS
1	A	209	THR
1	B	128	SER

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Mol	Chain	Res	Type
1	B	181	LYS
1	B	188	LYS
1	B	204	GLU
1	B	223	ASP
1	C	3	GLU
1	C	6	LYS
1	C	11	MET
1	C	29	GLU
1	C	122	ARG
1	C	151	ASP
1	C	181	LYS
1	C	209	THR
1	C	216	VAL
1	C	227	LYS
1	C	228	LEU
1	D	3	GLU
1	D	11	MET
1	D	47	GLU
1	D	147	LEU
1	D	186	ASN
1	D	206	ASP
1	D	226	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	213	GLN
1	B	8	ASN
1	B	10	HIS
1	C	23	HIS
1	C	39	GLN
1	D	8	ASN
1	D	10	HIS
1	D	82	GLN
1	D	186	ASN
1	D	213	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	23,24,25	1.62	5 (21%)	23,32,34	3.70	10 (43%)
1	NRQ	B	63	1	23,24,25	1.47	4 (17%)	23,32,34	4.42	10 (43%)
1	NRQ	C	63	1	23,24,25	1.52	5 (21%)	23,32,34	2.60	7 (30%)
1	NRQ	D	63	1	23,24,25	1.37	4 (17%)	23,32,34	2.48	7 (30%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	CG2-CB2	-4.39	1.38	1.46
1	D	63	NRQ	CG2-CB2	-2.73	1.41	1.46
1	B	63	NRQ	CG2-CB2	-2.60	1.41	1.46
1	C	63	NRQ	CG2-CB2	-2.30	1.42	1.46
1	D	63	NRQ	O2-C2	-2.01	1.18	1.23
1	C	63	NRQ	CD1-CG2	2.17	1.43	1.39
1	C	63	NRQ	CB2-CA2	2.28	1.37	1.35
1	B	63	NRQ	CA2-C2	2.29	1.51	1.48
1	A	63	NRQ	CB2-CA2	2.32	1.37	1.35
1	D	63	NRQ	CB2-CA2	2.35	1.37	1.35
1	A	63	NRQ	CA1-N1	2.55	1.36	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	CD1-CG2	2.85	1.44	1.39
1	A	63	NRQ	CA2-C2	3.02	1.51	1.48
1	C	63	NRQ	CA1-N1	3.34	1.38	1.28
1	B	63	NRQ	CA1-N1	3.37	1.38	1.28
1	B	63	NRQ	CB2-CA2	3.57	1.38	1.35
1	C	63	NRQ	CA2-C2	3.77	1.52	1.48
1	D	63	NRQ	CA1-N1	3.85	1.40	1.28

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	NRQ	CB1-CA1-N1	-12.85	101.32	124.94
1	A	63	NRQ	CB1-CA1-N1	-10.96	104.80	124.94
1	A	63	NRQ	CB2-CA2-N2	-3.73	122.01	128.67
1	A	63	NRQ	C2-CA2-N2	-3.54	106.08	108.91
1	C	63	NRQ	CB2-CA2-N2	-3.37	122.65	128.67
1	D	63	NRQ	C2-CA2-N2	-3.33	106.25	108.91
1	B	63	NRQ	O2-C2-N3	-3.32	117.33	124.50
1	B	63	NRQ	C2-CA2-N2	-3.31	106.27	108.91
1	C	63	NRQ	C2-CA2-N2	-3.27	106.30	108.91
1	B	63	NRQ	CB2-CA2-N2	-3.10	123.12	128.67
1	D	63	NRQ	CB2-CA2-N2	-3.02	123.27	128.67
1	B	63	NRQ	CA3-N3-C2	-2.77	119.48	123.99
1	A	63	NRQ	CD1-CG2-CD2	-2.42	113.94	117.64
1	A	63	NRQ	CE-SD-CG1	-2.17	92.97	100.37
1	D	63	NRQ	C3-CA3-N3	3.28	120.17	113.00
1	B	63	NRQ	CA2-C2-N3	3.55	105.18	103.40
1	D	63	NRQ	CA2-C2-N3	3.88	105.35	103.40
1	C	63	NRQ	C3-CA3-N3	3.90	121.55	113.00
1	B	63	NRQ	C3-CA3-N3	4.03	121.82	113.00
1	A	63	NRQ	CA2-C2-N3	4.17	105.49	103.40
1	D	63	NRQ	O2-C2-CA2	4.35	133.30	130.95
1	C	63	NRQ	CA2-C2-N3	4.40	105.60	103.40
1	A	63	NRQ	C3-CA3-N3	4.87	123.66	113.00
1	A	63	NRQ	O2-C2-CA2	4.91	133.59	130.95
1	C	63	NRQ	O2-C2-CA2	5.04	133.66	130.95
1	C	63	NRQ	CG2-CB2-CA2	5.12	136.87	130.22
1	D	63	NRQ	CB2-CA2-C2	5.48	130.39	122.36
1	B	63	NRQ	CB2-CA2-C2	5.60	130.56	122.36
1	B	63	NRQ	CG2-CB2-CA2	5.74	137.66	130.22
1	C	63	NRQ	CB2-CA2-C2	5.91	131.02	122.36
1	A	63	NRQ	CG2-CB2-CA2	5.97	137.96	130.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	NRQ	CG2-CB2-CA2	6.34	138.45	130.22
1	A	63	NRQ	CB2-CA2-C2	6.48	131.85	122.36
1	B	63	NRQ	O2-C2-CA2	12.11	137.48	130.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRQ	5	0
1	C	63	NRQ	3	0
1	D	63	NRQ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	223/243 (91%)	0.43	18 (8%) 15 14	26, 46, 83, 138	0
1	B	223/243 (91%)	0.59	24 (10%) 8 7	25, 49, 79, 102	0
1	C	223/243 (91%)	0.43	19 (8%) 13 12	26, 47, 78, 123	0
1	D	223/243 (91%)	0.67	29 (13%) 5 4	28, 51, 80, 146	0
All	All	892/972 (91%)	0.53	90 (10%) 9 8	25, 48, 81, 146	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	184	ALA	9.8
1	D	187	LEU	7.1
1	D	184	ALA	7.1
1	D	186	ASN	6.5
1	B	187	LEU	6.2
1	D	183	PRO	6.0
1	C	228	LEU	5.8
1	A	228	LEU	5.3
1	C	152	GLY	5.1
1	A	183	PRO	4.7
1	B	188	LYS	4.6
1	D	185	LYS	4.6
1	C	183	PRO	4.5
1	B	189	MET	4.4
1	A	187	LEU	4.3
1	A	186	ASN	4.3
1	C	186	ASN	4.3
1	B	228	LEU	4.3
1	B	62	PHE	4.1
1	A	4	LEU	4.1
1	D	182	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	185	LYS	3.9
1	D	60	THR	3.9
1	B	66	SER	3.9
1	B	165	VAL	3.8
1	D	59	ALA	3.8
1	B	90	TRP	3.8
1	A	70	ILE	3.7
1	B	185	LYS	3.7
1	B	152	GLY	3.7
1	C	4	LEU	3.6
1	B	48	GLY	3.6
1	D	90	TRP	3.5
1	D	4	LEU	3.5
1	B	59	ALA	3.5
1	C	70	ILE	3.4
1	D	206	ASP	3.4
1	C	185	LYS	3.4
1	B	60	THR	3.3
1	D	62	PHE	3.2
1	B	46	VAL	3.2
1	D	73	THR	3.2
1	D	58	LEU	3.1
1	A	152	GLY	3.1
1	B	174	LEU	3.0
1	D	61	SER	3.0
1	C	184	ALA	3.0
1	D	228	LEU	3.0
1	D	151	ASP	2.9
1	D	166	GLY	2.8
1	B	199	LEU	2.8
1	C	58	LEU	2.8
1	C	62	PHE	2.8
1	A	182	ASN	2.7
1	B	183	PRO	2.7
1	B	73	THR	2.7
1	B	47	GLU	2.6
1	A	58	LEU	2.6
1	B	167	GLY	2.6
1	D	48	GLY	2.5
1	A	188	LYS	2.5
1	B	61	SER	2.4
1	B	58	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	102	LEU	2.4
1	C	61	SER	2.4
1	D	188	LYS	2.4
1	C	219	ALA	2.3
1	D	66	SER	2.3
1	A	227	LYS	2.3
1	C	227	LYS	2.3
1	C	195	VAL	2.3
1	D	75	GLY	2.3
1	C	223	ASP	2.3
1	D	174	LEU	2.3
1	B	186	ASN	2.3
1	A	111	GLN	2.2
1	D	14	TYR	2.2
1	A	223	ASP	2.2
1	D	22	HIS	2.2
1	D	46	VAL	2.2
1	C	217	ALA	2.1
1	D	57	ILE	2.1
1	C	113	GLY	2.1
1	A	69	PHE	2.1
1	C	102	LEU	2.1
1	A	85	PRO	2.1
1	D	47	GLU	2.1
1	D	104	ALA	2.0
1	A	178	TYR	2.0
1	C	60	THR	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. 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^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	NRQ	A	63	23/24	0.87	0.19	-	36,44,58,102	0
1	NRQ	C	63	23/24	0.91	0.15	-	41,50,58,59	0
1	NRQ	B	63	23/24	0.89	0.28	-	40,50,61,66	0
1	NRQ	D	63	23/24	0.91	0.26	-	45,52,70,79	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.