Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:37 AM GMT

PDB ID	:	3PIB
Title	:	Crystal structure of red fluorescent protein eqFP578 crystallized at pH 5.5
Authors	:	Pletnev, S.; Pletneva, N.V.; Pletnev, V.Z.
Deposited on	:	2010-11-05
Resolution	:	1.15 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:

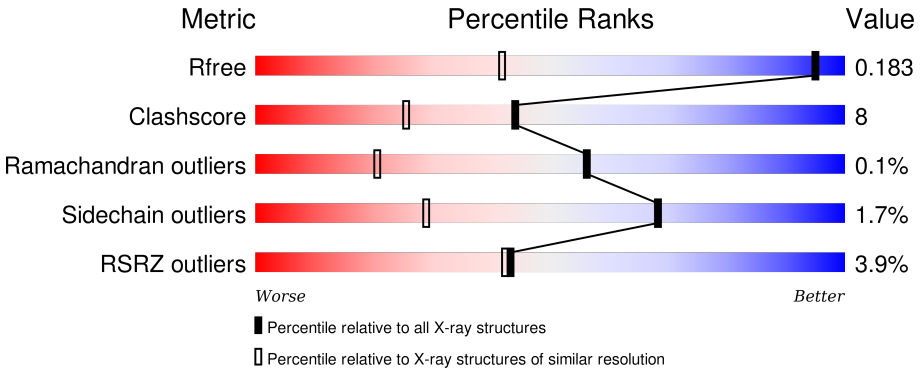
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.15 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	1036 (1.20-1.12)
Clashscore	102246	1109 (1.20-1.12)
Ramachandran outliers	100387	1058 (1.20-1.12)
Sidechain outliers	100360	1058 (1.20-1.12)
RSRZ outliers	91569	1038 (1.20-1.12)

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	236	6% 87% 8%
1	B	236	5% 89% 11%
1	C	236	2% 86% 8%
1	D	236	3% 89% 6%

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
2	GOL	A	250	-	-	X	X
2	GOL	B	250	-	-	X	X
2	GOL	C	250	-	-	X	X
2	GOL	D	250	-	-	X	X

2 Entry composition

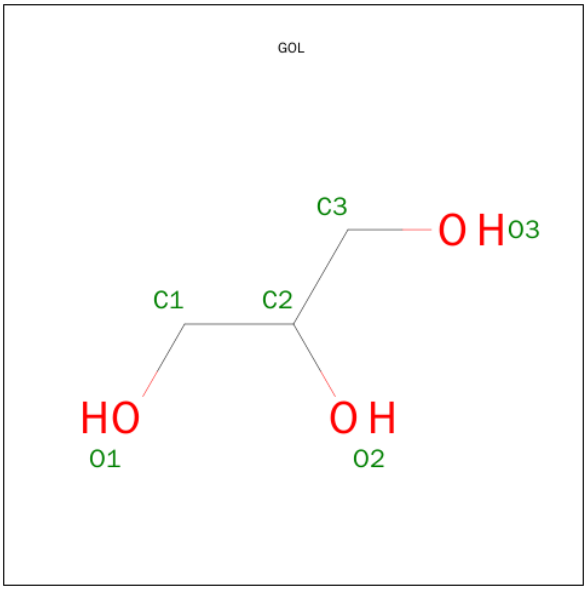
There are 3 unique types of molecules in this entry. The entry contains 15517 atoms, of which 7046 are hydrogens and 0 are deuteriums.

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 eqFP578 fluorescent protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	227	Total	C	H	N	O	S	0	14	0
			3612	1201	1737	309	348	17			
1	B	236	Total	C	H	N	O	S	0	21	0
			3796	1276	1797	339	367	17			
1	C	226	Total	C	H	N	O	S	0	20	0
			3631	1219	1729	313	353	17			
1	D	228	Total	C	H	N	O	S	0	28	0
			3701	1244	1751	322	368	16			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			14	3	8	3		
2	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is water.

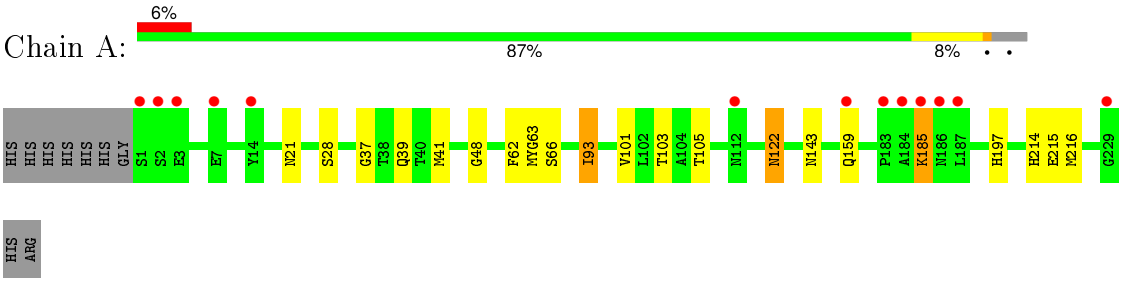
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	184	Total	O	0	0
			184	184		
3	C	175	Total	O	0	0
			175	175		
3	D	184	Total	O	0	0
			184	184		

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.

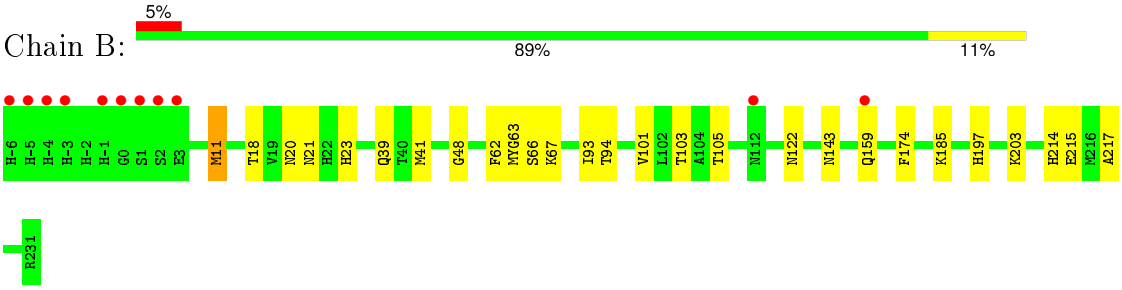
- Molecule 1: eqFP578 fluorescent protein

Chain A:



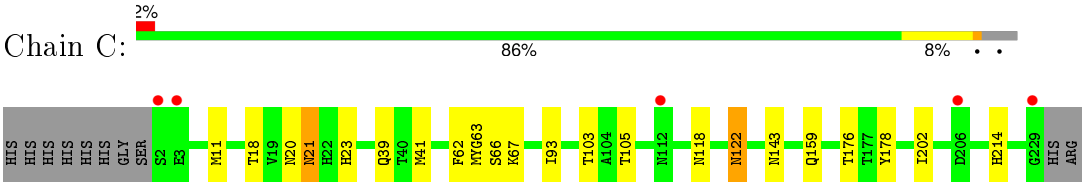
- Molecule 1: eqFP578 fluorescent protein

Chain B:



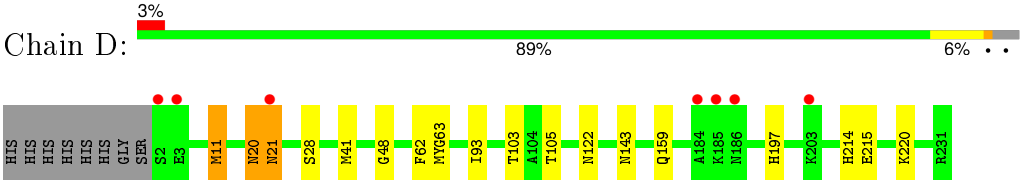
- Molecule 1: eqFP578 fluorescent protein

Chain C:



- Molecule 1: eqFP578 fluorescent protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	161.25Å 161.25Å 75.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.91 – 1.15 35.91 – 1.15	Depositor EDS
% Data completeness (in resolution range)	92.8 (35.91-1.15) 92.8 (35.91-1.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.15Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.155 , 0.176 0.162 , 0.183	Depositor DCC
R_{free} test set	3201 reflections (1.03%)	DCC
Wilson B-factor (Å^2)	11.1	Xtriage
Anisotropy	0.740	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 47.9	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 314505 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15517	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: GOL, 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	0.50	0/1935	0.70	0/2604
1	B	0.49	0/2078	0.69	1/2795 (0.0%)
1	C	0.48	0/1972	0.65	0/2655
1	D	0.51	0/2027	0.72	0/2726
All	All	0.50	0/8012	0.69	1/10780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	20	ASN	CB-CA-C	5.35	121.10	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	1737	1859	34	0
1	B	1999	1797	1957	41	0
1	C	1902	1729	1874	38	0
1	D	1950	1751	1883	41	0
2	A	6	8	7	7	0
2	B	6	8	8	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	8	8	6	0
2	D	6	8	7	7	0
3	A	178	0	0	1	1
3	B	184	0	0	1	0
3	C	175	0	0	1	0
3	D	184	0	0	1	1
All	All	8471	7046	7603	124	1

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 8.

All (124) 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:93[B]:ILE:HD11	1:B:101:VAL:HG13	1.40	1.02
1:B:93[B]:ILE:HD11	1:B:101:VAL:CG1	2.04	0.87
1:D:215:GLU:OE1	2:D:250:GOL:H12	1.80	0.81
1:B:215:GLU:OE2	2:B:250:GOL:H2	1.82	0.80
1:A:63:NRQ:C2	2:A:250:GOL:H11	2.11	0.80
1:C:21[A]:ASN:C	1:C:21[A]:ASN:HD22	1.84	0.79
1:B:18[B]:THR:CG2	1:B:23:HIS:ND1	2.47	0.77
1:C:18[B]:THR:HG22	1:C:23:HIS:ND1	2.00	0.77
1:A:122:ASN:HD21	1:B:105[A]:THR:HG23	1.51	0.76
1:C:20[A]:ASN:O	1:C:21[A]:ASN:CG	2.25	0.76
1:B:159[A]:GLN:CD	1:C:159[A]:GLN:HG3	2.06	0.76
1:D:28[B]:SER:OG	1:D:41[B]:MET:CG	2.36	0.74
1:A:101:VAL:HG11	1:B:93[A]:ILE:HD12	1.70	0.73
1:D:63:NRQ:C2	2:D:250:GOL:H11	2.18	0.73
1:D:20[A]:ASN:O	1:D:21[A]:ASN:ND2	2.21	0.73
1:B:18[B]:THR:HG22	1:B:23:HIS:ND1	2.04	0.73
1:C:66:SER:C	2:C:250:GOL:H11	2.10	0.71
1:C:20[A]:ASN:O	1:C:21[A]:ASN:ND2	2.24	0.70
1:A:159[A]:GLN:HG3	1:D:159[A]:GLN:CD	2.11	0.70
1:C:122[A]:ASN:HD21	1:D:105[A]:THR:HG23	1.55	0.70
1:D:93:ILE:HD13	1:D:103[A]:THR:HG22	1.73	0.70
1:D:93:ILE:CD1	1:D:103[A]:THR:HG22	2.22	0.69
1:B:159[A]:GLN:HG3	1:C:159[A]:GLN:CD	2.14	0.68
1:C:21[A]:ASN:C	1:C:21[A]:ASN:ND2	2.48	0.66
1:B:93[B]:ILE:CD1	1:B:101:VAL:HG13	2.20	0.65
1:C:63:NRQ:HE2	1:C:143:ASN:HD21	1.62	0.65
1:A:28[B]:SER:OG	1:A:41[B]:MET:CE	2.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:NRQ:HE2	1:A:143:ASN:HD21	1.64	0.62
1:D:28[B]:SER:OG	1:D:41[B]:MET:HG2	1.99	0.62
1:A:28[B]:SER:OG	1:A:41[B]:MET:HE2	2.00	0.62
1:B:63:NRQ:HE2	1:B:143:ASN:HD21	1.65	0.62
1:C:18[B]:THR:CG2	1:C:23:HIS:ND1	2.62	0.62
1:C:103[B]:THR:HG21	1:D:103[B]:THR:OG1	2.00	0.61
1:C:20[A]:ASN:O	1:C:21[A]:ASN:CB	2.47	0.61
1:D:63:NRQ:CA2	2:D:250:GOL:H11	2.30	0.61
1:A:159[A]:GLN:CD	1:D:159[A]:GLN:HG3	2.20	0.61
1:A:103[B]:THR:HG21	1:B:103[B]:THR:HG1	1.66	0.60
1:C:67:LYS:HD2	2:C:250:GOL:C1	2.31	0.60
1:A:93:ILE:HD12	1:B:101:VAL:HG11	1.83	0.60
1:A:63:NRQ:CA2	2:A:250:GOL:C1	2.81	0.59
1:B:215:GLU:CD	2:B:250:GOL:H2	2.25	0.58
1:B:18[B]:THR:HG21	1:B:23:HIS:ND1	2.20	0.57
1:D:41[B]:MET:SD	1:D:62:PHE:HB3	2.44	0.57
1:A:159[A]:GLN:HG3	1:D:159[A]:GLN:OE1	2.05	0.56
1:D:93:ILE:HD13	1:D:103[A]:THR:CG2	2.34	0.56
1:B:159[A]:GLN:NE2	1:C:159[A]:GLN:HG3	2.20	0.56
1:A:21[B]:ASN:ND2	1:B:105[B]:THR:HG23	2.21	0.56
1:A:105[A]:THR:HG23	1:B:122[A]:ASN:OD1	2.06	0.56
1:B:41[C]:MET:SD	1:B:62:PHE:HB3	2.46	0.55
1:B:18[B]:THR:HG21	1:B:23:HIS:CE1	2.42	0.55
1:D:63:NRQ:HE2	1:D:143:ASN:HD21	1.72	0.54
1:C:214:HIS:HD2	3:C:275:HOH:O	1.89	0.54
1:A:63:NRQ:CA2	2:A:250:GOL:H11	2.38	0.54
1:C:21[B]:ASN:ND2	1:D:105[B]:THR:HG23	2.24	0.53
1:D:11[A]:MET:HG3	1:D:41[A]:MET:SD	2.49	0.53
1:A:214:HIS:HD2	3:A:653:HOH:O	1.90	0.53
1:C:105[A]:THR:HG23	1:D:122[A]:ASN:OD1	2.09	0.53
1:C:103[A]:THR:OG1	1:D:103[A]:THR:HG21	2.09	0.53
1:A:197:HIS:HE1	2:A:250:GOL:O2	1.92	0.52
1:B:11[A]:MET:HG3	1:B:41[A]:MET:HE1	1.90	0.52
1:A:41[A]:MET:SD	1:A:62:PHE:HB3	2.50	0.52
1:B:214:HIS:HD2	3:B:260:HOH:O	1.93	0.52
1:B:159[A]:GLN:OE1	1:C:159[A]:GLN:HG3	2.10	0.51
1:D:214:HIS:HD2	3:D:279:HOH:O	1.94	0.51
1:B:217:ALA:CB	2:B:250:GOL:H12	2.41	0.51
1:A:159[A]:GLN:OE1	1:D:159[A]:GLN:HG3	2.11	0.51
1:D:215:GLU:CD	2:D:250:GOL:H12	2.31	0.51
1:A:63:NRQ:CA2	2:A:250:GOL:H12	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LYS:HD2	1:A:185:LYS:H	1.76	0.49
1:D:215:GLU:OE1	2:D:250:GOL:C1	2.55	0.49
1:D:28[B]:SER:OG	1:D:41[B]:MET:HG3	2.11	0.49
1:C:67:LYS:HD2	2:C:250:GOL:H12	1.94	0.49
1:A:103[A]:THR:OG1	1:B:103[A]:THR:HG21	2.12	0.49
1:A:103[B]:THR:HG21	1:B:103[B]:THR:OG1	2.13	0.49
1:B:197:HIS:HE1	2:B:250:GOL:O2	1.96	0.48
1:A:103[B]:THR:CG2	1:B:103[B]:THR:HG1	2.25	0.48
1:A:197:HIS:CE1	2:A:250:GOL:O2	2.66	0.48
1:D:20[A]:ASN:O	1:D:21[A]:ASN:CB	2.60	0.48
1:B:203[B]:LYS:HB3	1:B:203[B]:LYS:HE2	1.64	0.48
1:A:185:LYS:CD	1:A:185:LYS:H	2.26	0.48
1:B:67:LYS:HD2	2:B:250:GOL:H31	1.96	0.47
1:C:41[C]:MET:HE3	1:C:41[C]:MET:HB3	1.45	0.47
1:D:21[A]:ASN:ND2	1:D:21[A]:ASN:C	2.69	0.46
1:D:21[A]:ASN:HD22	1:D:21[A]:ASN:C	2.19	0.46
1:A:93:ILE:HG13	1:A:103[B]:THR:HG22	1.98	0.46
1:B:159[A]:GLN:HG3	1:C:159[A]:GLN:NE2	2.31	0.46
1:D:20[A]:ASN:O	1:D:21[A]:ASN:CG	2.54	0.45
1:A:39:GLN:HE22	1:A:66:SER:CB	2.29	0.45
1:A:215:GLU:OE1	2:A:250:GOL:H12	2.17	0.45
1:C:63:NRQ:C2	2:C:250:GOL:H12	2.47	0.45
1:B:39:GLN:HE22	1:B:66:SER:CB	2.31	0.44
1:B:159[A]:GLN:CD	1:C:159[A]:GLN:CG	2.83	0.44
1:D:63:NRQ:CA2	2:D:250:GOL:C1	2.95	0.44
1:C:41[C]:MET:CE	1:C:62:PHE:HB3	2.47	0.44
1:C:39:GLN:HE22	1:C:66:SER:CB	2.31	0.43
1:B:66:SER:C	2:B:250:GOL:H32	2.39	0.43
1:B:217:ALA:HB2	2:B:250:GOL:H12	2.00	0.42
1:C:67:LYS:HD2	2:C:250:GOL:H11	2.00	0.42
1:B:159[A]:GLN:CG	1:C:159[A]:GLN:CD	2.85	0.42
1:C:21[B]:ASN:HD21	1:D:105[B]:THR:HG23	1.84	0.42
1:C:41[C]:MET:HE1	1:C:62:PHE:HB3	2.02	0.41
1:A:122:ASN:ND2	1:B:105[A]:THR:HG23	2.28	0.41
1:B:94:THR:HA	1:B:174:PHE:HB3	2.03	0.41
1:D:197:HIS:HE1	2:D:250:GOL:O2	2.03	0.41
1:A:21[B]:ASN:HD21	1:B:105[B]:THR:HG23	1.85	0.41
1:C:122[A]:ASN:HD21	1:D:105[A]:THR:CG2	2.29	0.41
1:D:93:ILE:HD12	1:D:103[A]:THR:HG22	1.99	0.41
1:A:37:GLY:O	1:A:216:MET:HA	2.21	0.41
1:C:176:THR:HG21	1:C:178:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159[A]:GLN:HG3	1:D:159[A]:GLN:NE2	2.36	0.40
1:C:66:SER:N	2:C:250:GOL:C1	2.85	0.40

All (1) 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)
3:A:655:HOH:O	3:D:659:HOH:O[4_554]	1.98	0.22

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	236/236 (100%)	231 (98%)	5 (2%)	0	100 100
1	B	251/236 (106%)	248 (99%)	3 (1%)	0	100 100
1	C	240/236 (102%)	237 (99%)	3 (1%)	0	100 100
1	D	246/236 (104%)	240 (98%)	4 (2%)	2 (1%)	24 3
All	All	973/944 (103%)	956 (98%)	15 (2%)	2 (0%)	56 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	20[A]	ASN
1	D	20[B]	ASN

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	208/202 (103%)	205 (99%)	3 (1%)	74 37
1	B	222/202 (110%)	217 (98%)	5 (2%)	58 17
1	C	212/202 (105%)	205 (97%)	7 (3%)	45 7
1	D	217/202 (107%)	212 (98%)	5 (2%)	58 17
All	All	859/808 (106%)	839 (98%)	20 (2%)	68 17

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ILE
1	A	122	ASN
1	A	185	LYS
1	B	11[A]	MET
1	B	11[B]	MET
1	B	21[A]	ASN
1	B	21[B]	ASN
1	B	185	LYS
1	C	11[A]	MET
1	C	11[B]	MET
1	C	21[A]	ASN
1	C	21[B]	ASN
1	C	118	ASN
1	C	122[A]	ASN
1	C	122[B]	ASN
1	D	11[A]	MET
1	D	11[B]	MET
1	D	21[A]	ASN
1	D	21[B]	ASN
1	D	220	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22[A]	HIS
1	A	39	GLN
1	A	112	ASN
1	A	118	ASN
1	A	122	ASN

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Mol	Chain	Res	Type
1	A	143	ASN
1	A	214	HIS
1	B	-1	HIS
1	B	22[A]	HIS
1	B	39	GLN
1	B	125	ASN
1	B	134	GLN
1	B	143	ASN
1	B	186	ASN
1	B	214	HIS
1	C	39	GLN
1	C	125	ASN
1	C	134	GLN
1	C	143	ASN
1	C	186	ASN
1	C	214	HIS
1	D	22[A]	HIS
1	D	39	GLN
1	D	125	ASN
1	D	143	ASN
1	D	214	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	2.97	13 (56%)	23,32,34	4.11	12 (52%)
1	NRQ	B	63	1	23,24,25	2.79	6 (26%)	23,32,34	3.44	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	NRQ	C	63	1	23,24,25	3.28	13 (56%)	23,32,34	3.32	8 (34%)
1	NRQ	D	63	1	23,24,25	2.02	8 (34%)	23,32,34	3.58	9 (39%)

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 (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	NRQ	CG2-CB2	-5.90	1.34	1.46
1	C	63	NRQ	CE2-CD2	-4.77	1.30	1.38
1	A	63	NRQ	OH-CZ	-4.30	1.26	1.37
1	B	63	NRQ	CG2-CB2	-4.10	1.38	1.46
1	D	63	NRQ	CE-SD	-4.03	1.54	1.78
1	C	63	NRQ	OH-CZ	-3.96	1.27	1.37
1	B	63	NRQ	OH-CZ	-3.94	1.27	1.37
1	A	63	NRQ	CA2-C2	-3.69	1.44	1.48
1	A	63	NRQ	CG1-CB1	-3.21	1.41	1.51
1	B	63	NRQ	CA2-C2	-2.97	1.45	1.48
1	A	63	NRQ	C2-N3	-2.88	1.33	1.39
1	C	63	NRQ	CE-SD	-2.88	1.61	1.78
1	A	63	NRQ	CE-SD	-2.86	1.61	1.78
1	A	63	NRQ	C1-N2	-2.63	1.27	1.33
1	C	63	NRQ	C1-N2	-2.35	1.28	1.33
1	C	63	NRQ	C2-N3	-2.32	1.34	1.39
1	C	63	NRQ	CG1-CB1	-2.22	1.44	1.51
1	D	63	NRQ	CB2-CA2	-2.20	1.33	1.35
1	A	63	NRQ	CG2-CB2	-2.20	1.42	1.46
1	D	63	NRQ	C2-N3	-2.19	1.35	1.39
1	D	63	NRQ	CG1-CB1	-2.18	1.44	1.51
1	C	63	NRQ	C1-N3	2.12	1.43	1.38
1	D	63	NRQ	CE1-CD1	2.19	1.42	1.38
1	A	63	NRQ	CG1-SD	2.28	1.93	1.81
1	C	63	NRQ	CA3-N3	2.32	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	NRQ	C1-N3	2.49	1.43	1.38
1	B	63	NRQ	CD1-CG2	2.74	1.44	1.39
1	D	63	NRQ	CA2-C2	3.03	1.51	1.48
1	A	63	NRQ	CD1-CG2	3.04	1.45	1.39
1	A	63	NRQ	CE1-CD1	3.37	1.44	1.38
1	C	63	NRQ	CB1-CA1	3.48	1.62	1.51
1	D	63	NRQ	CD1-CG2	3.52	1.46	1.39
1	D	63	NRQ	CA3-N3	4.09	1.54	1.47
1	C	63	NRQ	CD1-CG2	4.45	1.47	1.39
1	C	63	NRQ	CE2-CZ	4.63	1.48	1.38
1	B	63	NRQ	CE2-CZ	4.77	1.48	1.38
1	A	63	NRQ	CB2-CA2	5.83	1.40	1.35
1	A	63	NRQ	CE2-CZ	6.97	1.53	1.38
1	C	63	NRQ	CB2-CA2	9.14	1.43	1.35
1	B	63	NRQ	CB2-CA2	9.46	1.43	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	NRQ	CA2-C2-N3	-8.49	99.14	103.40
1	A	63	NRQ	CB1-CA1-N1	-7.85	110.51	124.94
1	D	63	NRQ	CB2-CA2-N2	-7.18	115.83	128.67
1	B	63	NRQ	CB1-CA1-N1	-7.14	111.81	124.94
1	A	63	NRQ	CB2-CA2-N2	-7.10	115.97	128.67
1	A	63	NRQ	CE1-CD1-CG2	-6.83	112.75	121.29
1	C	63	NRQ	CB1-CA1-N1	-5.86	114.17	124.94
1	B	63	NRQ	CB2-CA2-N2	-5.16	119.45	128.67
1	D	63	NRQ	CB1-CA1-N1	-5.00	115.74	124.94
1	B	63	NRQ	CE1-CZ-CE2	-4.22	113.78	119.79
1	B	63	NRQ	CE1-CD1-CG2	-3.98	116.32	121.29
1	D	63	NRQ	N3-C1-N2	-3.77	108.98	113.26
1	A	63	NRQ	O2-C2-CA2	-3.56	129.02	130.95
1	A	63	NRQ	CE1-CZ-CE2	-3.34	115.03	119.79
1	C	63	NRQ	CE1-CD1-CG2	-3.24	117.24	121.29
1	C	63	NRQ	CB2-CA2-N2	-3.20	122.94	128.67
1	C	63	NRQ	CB1-CG1-SD	-2.92	105.71	112.88
1	A	63	NRQ	CB1-CG1-SD	-2.59	106.53	112.88
1	A	63	NRQ	N3-C1-N2	-2.49	110.44	113.26
1	D	63	NRQ	CA3-N3-C2	-2.46	119.99	123.99
1	D	63	NRQ	CE1-CD1-CG2	-2.23	118.50	121.29
1	B	63	NRQ	O2-C2-CA2	-2.09	129.82	130.95
1	C	63	NRQ	CD1-CE1-CZ	2.33	122.57	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	NRQ	O2-C2-CA2	2.79	132.45	130.95
1	B	63	NRQ	CA2-C2-N3	3.29	105.05	103.40
1	C	63	NRQ	CB2-CA2-C2	3.33	127.24	122.36
1	A	63	NRQ	CD1-CG2-CD2	3.81	123.47	117.64
1	A	63	NRQ	CA2-C2-N3	4.22	105.51	103.40
1	A	63	NRQ	CG2-CB2-CA2	4.48	136.03	130.22
1	D	63	NRQ	O2-C2-CA2	4.56	133.41	130.95
1	D	63	NRQ	CG2-CB2-CA2	4.78	136.42	130.22
1	B	63	NRQ	CD1-CE1-CZ	6.02	126.83	119.87
1	B	63	NRQ	CG2-CB2-CA2	6.18	138.25	130.22
1	A	63	NRQ	CD1-CE1-CZ	6.37	127.23	119.87
1	B	63	NRQ	CB2-CA2-C2	7.21	132.92	122.36
1	D	63	NRQ	CB2-CA2-C2	7.78	133.75	122.36
1	A	63	NRQ	CB2-CA2-C2	9.49	136.26	122.36
1	C	63	NRQ	CG2-CB2-CA2	12.32	146.21	130.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	63	NRQ	5	0
1	B	63	NRQ	1	0
1	C	63	NRQ	2	0
1	D	63	NRQ	4	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands 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	$\#\|Z\| > 2$
2	GOL	A	250	-	5,5,5	1.13	0	5,5,5	0.52	0
2	GOL	B	250	-	5,5,5	1.04	0	5,5,5	1.28	1 (20%)
2	GOL	C	250	-	5,5,5	0.87	0	5,5,5	0.66	0
2	GOL	D	250	-	5,5,5	1.23	0	5,5,5	0.54	0

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
2	GOL	A	250	-	-	0/4/4/4	0/0/0/0
2	GOL	B	250	-	-	0/4/4/4	0/0/0/0
2	GOL	C	250	-	-	0/4/4/4	0/0/0/0
2	GOL	D	250	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	250	GOL	O3-C3-C2	-2.32	98.94	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	250	GOL	7	0
2	B	250	GOL	7	0
2	C	250	GOL	6	0
2	D	250	GOL	7	0

5.7 Other polymers (i)

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^{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	226/236 (95%)	0.14	13 (5%)	26	26	9, 13, 25, 39	1 (0%)
1	B	235/236 (99%)	0.13	11 (4%)	35	34	9, 13, 24, 33	6 (2%)
1	C	225/236 (95%)	0.04	5 (2%)	65	65	10, 14, 23, 37	0
1	D	227/236 (96%)	0.03	7 (3%)	52	52	10, 13, 23, 36	0
All	All	913/944 (96%)	0.09	36 (3%)	43	42	9, 13, 24, 39	7 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	GLY	7.9
1	B	1	SER	6.8
1	C	3	GLU	6.3
1	B	-5	HIS	5.4
1	A	2	SER	5.0
1	C	2	SER	4.9
1	B	-4	HIS	4.7
1	A	3	GLU	4.5
1	D	2[A]	SER	4.3
1	C	229	GLY	4.2
1	A	185	LYS	4.1
1	B	3	GLU	4.1
1	A	1	SER	4.0
1	B	-6	HIS	3.9
1	D	184	ALA	3.8
1	D	3[A]	GLU	3.8
1	D	185	LYS	3.6
1	A	229	GLY	3.5
1	B	-1	HIS	3.4
1	A	112	ASN	3.2
1	A	187	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	-3	HIS	3.2
1	C	112	ASN	3.2
1	A	184	ALA	3.1
1	A	186	ASN	3.1
1	C	206	ASP	2.9
1	A	183	PRO	2.5
1	D	203[A]	LYS	2.4
1	B	2	SER	2.4
1	B	159[A]	GLN	2.3
1	A	14	TYR	2.2
1	A	159[A]	GLN	2.1
1	D	186	ASN	2.1
1	B	112[A]	ASN	2.1
1	D	21[A]	ASN	2.1
1	A	7	GLU	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	D	63	23/24	0.98	0.08	-	10,11,19,21	0
1	NRQ	C	63	23/24	0.97	0.11	-	10,11,19,24	0
1	NRQ	B	63	23/24	0.98	0.09	-	10,11,18,20	0
1	NRQ	A	63	23/24	0.98	0.10	-	10,11,19,23	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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
2	GOL	C	250	6/6	0.91	0.22	9.82	17,28,35,37	14
2	GOL	D	250	6/6	0.86	0.23	8.02	21,27,33,36	14
2	GOL	A	250	6/6	0.88	0.21	7.07	17,27,36,36	14
2	GOL	B	250	6/6	0.93	0.17	6.33	17,29,35,35	14

6.5 Other polymers (i)

There are no such residues in this entry.