Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:59 PM BST

PDB ID	:	6XWY
Title	:	Highly pH-resistant long stokes-shift, red fluorescent protein mCRISPRed
Authors	:	Erdogan, M.; Fabritius, A.; Basquin, J.; Griesbeck, O.
Deposited on	:	2020-01-24
Resolution	:	1.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

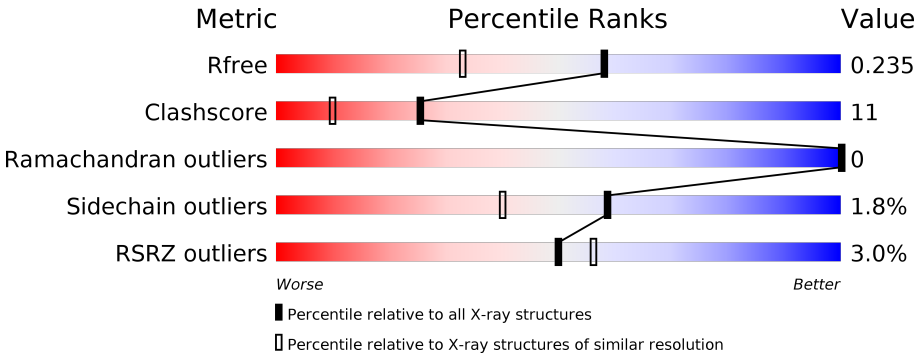
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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	219	3% 84% 14%
1	B	219	3% 80% 16%
1	C	219	2% 84% 15%
1	D	219	5% 78% 20%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7583 atoms, of which 24 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 Red fluorescent protein eqFP611.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1738	1100	299	328	11			
1	B	216	Total	C	N	O	S	0	0	0
			1717	1086	295	325	11			
1	C	218	Total	C	N	O	S	0	0	0
			1734	1097	298	328	11			
1	D	217	Total	C	N	O	S	0	0	0
			1731	1095	298	327	11			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8ISF8
A	2	PRO	-	expression tag	UNP Q8ISF8
A	11	LYS	MET	conflict	UNP Q8ISF8
A	21	HIS	TYR	conflict	UNP Q8ISF8
A	30	GLU	ASP	conflict	UNP Q8ISF8
A	32	ARG	ASN	conflict	UNP Q8ISF8
A	35	GLU	MET	conflict	UNP Q8ISF8
A	37	VAL	THR	conflict	UNP Q8ISF8
A	45	ILE	VAL	conflict	UNP Q8ISF8
A	63	NRQ	MET	chromophore	UNP Q8ISF8
A	63	NRQ	TYR	chromophore	UNP Q8ISF8
A	63	NRQ	GLY	chromophore	UNP Q8ISF8
A	66	ARG	LYS	conflict	UNP Q8ISF8
A	71	TYR	HIS	conflict	UNP Q8ISF8
A	72	PRO	THR	conflict	UNP Q8ISF8
A	73	ALA	LYS	conflict	UNP Q8ISF8
A	74	ASP	GLY	conflict	UNP Q8ISF8
A	101	VAL	PHE	conflict	UNP Q8ISF8
A	104	THR	MET	conflict	UNP Q8ISF8
A	113	GLU	CYS	conflict	UNP Q8ISF8
A	117	ASN	HIS	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	118	VAL	ALA	conflict	UNP Q8ISF8
A	121	ARG	THR	conflict	UNP Q8ISF8
A	130	PRO	ALA	conflict	UNP Q8ISF8
A	141	ALA	PRO	conflict	UNP Q8ISF8
A	142	ASP	ASN	conflict	UNP Q8ISF8
A	146	MET	LEU	conflict	UNP Q8ISF8
A	157	LEU	SER	conflict	UNP Q8ISF8
A	158	ASP	GLN	conflict	UNP Q8ISF8
A	159	ARG	MET	conflict	UNP Q8ISF8
A	162	LYS	ASN	conflict	UNP Q8ISF8
A	168	HIS	TYR	conflict	UNP Q8ISF8
A	170	HIS	SER	conflict	UNP Q8ISF8
A	172	ASN	SER	conflict	UNP Q8ISF8
A	174	VAL	GLU	conflict	UNP Q8ISF8
A	184	GLY	GLU	conflict	UNP Q8ISF8
A	185	ASP	ASN	conflict	UNP Q8ISF8
A	186	ILE	PHE	conflict	UNP Q8ISF8
A	191	VAL	PHE	conflict	UNP Q8ISF8
A	193	ALA	PHE	conflict	UNP Q8ISF8
A	201	ILE	LEU	conflict	UNP Q8ISF8
A	206	ASN	LYS	conflict	UNP Q8ISF8
A	208	THR	MET	conflict	UNP Q8ISF8
A	209	TYR	PHE	conflict	UNP Q8ISF8
A	213	ARG	HIS	conflict	UNP Q8ISF8
A	215	VAL	HIS	conflict	UNP Q8ISF8
A	220	TYR	PHE	conflict	UNP Q8ISF8
A	221	SER	CYS	conflict	UNP Q8ISF8
B	1	GLY	-	expression tag	UNP Q8ISF8
B	2	PRO	-	expression tag	UNP Q8ISF8
B	11	LYS	MET	conflict	UNP Q8ISF8
B	21	HIS	TYR	conflict	UNP Q8ISF8
B	30	GLU	ASP	conflict	UNP Q8ISF8
B	32	ARG	ASN	conflict	UNP Q8ISF8
B	35	GLU	MET	conflict	UNP Q8ISF8
B	37	VAL	THR	conflict	UNP Q8ISF8
B	45	ILE	VAL	conflict	UNP Q8ISF8
B	63	NRQ	MET	chromophore	UNP Q8ISF8
B	63	NRQ	TYR	chromophore	UNP Q8ISF8
B	63	NRQ	GLY	chromophore	UNP Q8ISF8
B	66	ARG	LYS	conflict	UNP Q8ISF8
B	71	TYR	HIS	conflict	UNP Q8ISF8
B	72	PRO	THR	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	73	ALA	LYS	conflict	UNP Q8ISF8
B	74	ASP	GLY	conflict	UNP Q8ISF8
B	101	VAL	PHE	conflict	UNP Q8ISF8
B	104	THR	MET	conflict	UNP Q8ISF8
B	113	GLU	CYS	conflict	UNP Q8ISF8
B	117	ASN	HIS	conflict	UNP Q8ISF8
B	118	VAL	ALA	conflict	UNP Q8ISF8
B	121	ARG	THR	conflict	UNP Q8ISF8
B	130	PRO	ALA	conflict	UNP Q8ISF8
B	141	ALA	PRO	conflict	UNP Q8ISF8
B	142	ASP	ASN	conflict	UNP Q8ISF8
B	146	MET	LEU	conflict	UNP Q8ISF8
B	157	LEU	SER	conflict	UNP Q8ISF8
B	158	ASP	GLN	conflict	UNP Q8ISF8
B	159	ARG	MET	conflict	UNP Q8ISF8
B	162	LYS	ASN	conflict	UNP Q8ISF8
B	168	HIS	TYR	conflict	UNP Q8ISF8
B	170	HIS	SER	conflict	UNP Q8ISF8
B	172	ASN	SER	conflict	UNP Q8ISF8
B	174	VAL	GLU	conflict	UNP Q8ISF8
B	184	GLY	GLU	conflict	UNP Q8ISF8
B	185	ASP	ASN	conflict	UNP Q8ISF8
B	186	ILE	PHE	conflict	UNP Q8ISF8
B	191	VAL	PHE	conflict	UNP Q8ISF8
B	193	ALA	PHE	conflict	UNP Q8ISF8
B	201	ILE	LEU	conflict	UNP Q8ISF8
B	206	ASN	LYS	conflict	UNP Q8ISF8
B	208	THR	MET	conflict	UNP Q8ISF8
B	209	TYR	PHE	conflict	UNP Q8ISF8
B	213	ARG	HIS	conflict	UNP Q8ISF8
B	215	VAL	HIS	conflict	UNP Q8ISF8
B	220	TYR	PHE	conflict	UNP Q8ISF8
B	221	SER	CYS	conflict	UNP Q8ISF8
C	1	GLY	-	expression tag	UNP Q8ISF8
C	2	PRO	-	expression tag	UNP Q8ISF8
C	11	LYS	MET	conflict	UNP Q8ISF8
C	21	HIS	TYR	conflict	UNP Q8ISF8
C	30	GLU	ASP	conflict	UNP Q8ISF8
C	32	ARG	ASN	conflict	UNP Q8ISF8
C	35	GLU	MET	conflict	UNP Q8ISF8
C	37	VAL	THR	conflict	UNP Q8ISF8
C	45	ILE	VAL	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	63	NRQ	MET	chromophore	UNP Q8ISF8
C	63	NRQ	TYR	chromophore	UNP Q8ISF8
C	63	NRQ	GLY	chromophore	UNP Q8ISF8
C	66	ARG	LYS	conflict	UNP Q8ISF8
C	71	TYR	HIS	conflict	UNP Q8ISF8
C	72	PRO	THR	conflict	UNP Q8ISF8
C	73	ALA	LYS	conflict	UNP Q8ISF8
C	74	ASP	GLY	conflict	UNP Q8ISF8
C	101	VAL	PHE	conflict	UNP Q8ISF8
C	104	THR	MET	conflict	UNP Q8ISF8
C	113	GLU	CYS	conflict	UNP Q8ISF8
C	117	ASN	HIS	conflict	UNP Q8ISF8
C	118	VAL	ALA	conflict	UNP Q8ISF8
C	121	ARG	THR	conflict	UNP Q8ISF8
C	130	PRO	ALA	conflict	UNP Q8ISF8
C	141	ALA	PRO	conflict	UNP Q8ISF8
C	142	ASP	ASN	conflict	UNP Q8ISF8
C	146	MET	LEU	conflict	UNP Q8ISF8
C	157	LEU	SER	conflict	UNP Q8ISF8
C	158	ASP	GLN	conflict	UNP Q8ISF8
C	159	ARG	MET	conflict	UNP Q8ISF8
C	162	LYS	ASN	conflict	UNP Q8ISF8
C	168	HIS	TYR	conflict	UNP Q8ISF8
C	170	HIS	SER	conflict	UNP Q8ISF8
C	172	ASN	SER	conflict	UNP Q8ISF8
C	174	VAL	GLU	conflict	UNP Q8ISF8
C	184	GLY	GLU	conflict	UNP Q8ISF8
C	185	ASP	ASN	conflict	UNP Q8ISF8
C	186	ILE	PHE	conflict	UNP Q8ISF8
C	191	VAL	PHE	conflict	UNP Q8ISF8
C	193	ALA	PHE	conflict	UNP Q8ISF8
C	201	ILE	LEU	conflict	UNP Q8ISF8
C	206	ASN	LYS	conflict	UNP Q8ISF8
C	208	THR	MET	conflict	UNP Q8ISF8
C	209	TYR	PHE	conflict	UNP Q8ISF8
C	213	ARG	HIS	conflict	UNP Q8ISF8
C	215	VAL	HIS	conflict	UNP Q8ISF8
C	220	TYR	PHE	conflict	UNP Q8ISF8
C	221	SER	CYS	conflict	UNP Q8ISF8
D	1	GLY	-	expression tag	UNP Q8ISF8
D	2	PRO	-	expression tag	UNP Q8ISF8
D	11	LYS	MET	conflict	UNP Q8ISF8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	HIS	TYR	conflict	UNP Q8ISF8
D	30	GLU	ASP	conflict	UNP Q8ISF8
D	32	ARG	ASN	conflict	UNP Q8ISF8
D	35	GLU	MET	conflict	UNP Q8ISF8
D	37	VAL	THR	conflict	UNP Q8ISF8
D	45	ILE	VAL	conflict	UNP Q8ISF8
D	63	NRQ	MET	chromophore	UNP Q8ISF8
D	63	NRQ	TYR	chromophore	UNP Q8ISF8
D	63	NRQ	GLY	chromophore	UNP Q8ISF8
D	66	ARG	LYS	conflict	UNP Q8ISF8
D	71	TYR	HIS	conflict	UNP Q8ISF8
D	72	PRO	THR	conflict	UNP Q8ISF8
D	73	ALA	LYS	conflict	UNP Q8ISF8
D	74	ASP	GLY	conflict	UNP Q8ISF8
D	101	VAL	PHE	conflict	UNP Q8ISF8
D	104	THR	MET	conflict	UNP Q8ISF8
D	113	GLU	CYS	conflict	UNP Q8ISF8
D	117	ASN	HIS	conflict	UNP Q8ISF8
D	118	VAL	ALA	conflict	UNP Q8ISF8
D	121	ARG	THR	conflict	UNP Q8ISF8
D	130	PRO	ALA	conflict	UNP Q8ISF8
D	141	ALA	PRO	conflict	UNP Q8ISF8
D	142	ASP	ASN	conflict	UNP Q8ISF8
D	146	MET	LEU	conflict	UNP Q8ISF8
D	157	LEU	SER	conflict	UNP Q8ISF8
D	158	ASP	GLN	conflict	UNP Q8ISF8
D	159	ARG	MET	conflict	UNP Q8ISF8
D	162	LYS	ASN	conflict	UNP Q8ISF8
D	168	HIS	TYR	conflict	UNP Q8ISF8
D	170	HIS	SER	conflict	UNP Q8ISF8
D	172	ASN	SER	conflict	UNP Q8ISF8
D	174	VAL	GLU	conflict	UNP Q8ISF8
D	184	GLY	GLU	conflict	UNP Q8ISF8
D	185	ASP	ASN	conflict	UNP Q8ISF8
D	186	ILE	PHE	conflict	UNP Q8ISF8
D	191	VAL	PHE	conflict	UNP Q8ISF8
D	193	ALA	PHE	conflict	UNP Q8ISF8
D	201	ILE	LEU	conflict	UNP Q8ISF8
D	206	ASN	LYS	conflict	UNP Q8ISF8
D	208	THR	MET	conflict	UNP Q8ISF8
D	209	TYR	PHE	conflict	UNP Q8ISF8
D	213	ARG	HIS	conflict	UNP Q8ISF8

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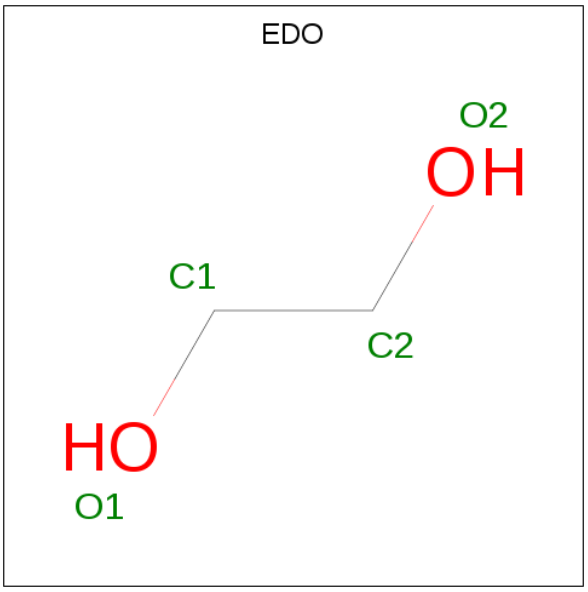
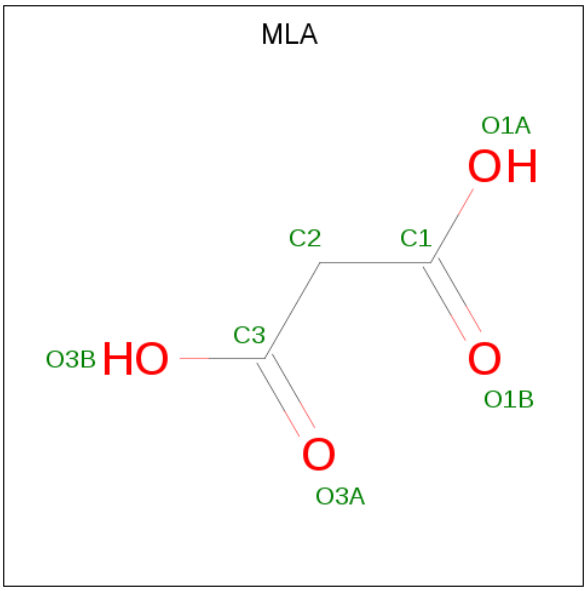
Chain	Residue	Modelled	Actual	Comment	Reference
D	215	VAL	HIS	conflict	UNP Q8ISF8
D	220	TYR	PHE	conflict	UNP Q8ISF8
D	221	SER	CYS	conflict	UNP Q8ISF8

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 9 3 2 4	0	0
3	A	1	Total C H O 9 3 2 4	0	0
3	B	1	Total C H O 9 3 2 4	0	0

- Molecule 4 is water.

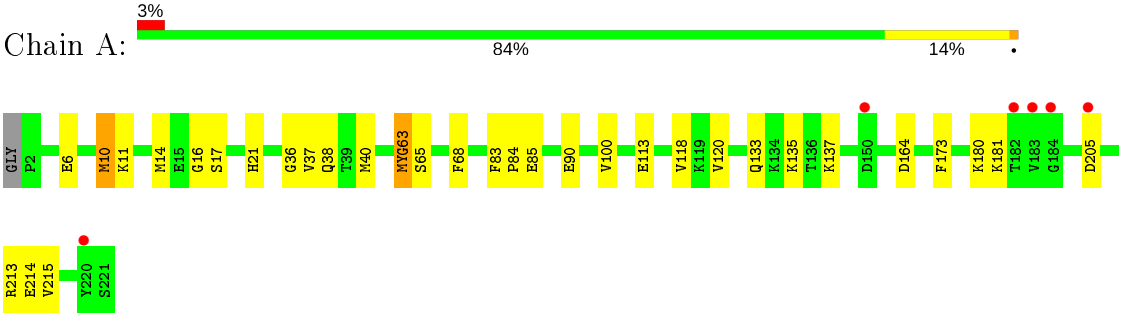
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	155	Total O 155 155	0	0
4	B	156	Total O 156 156	0	0
4	C	145	Total O 145 145	0	0
4	D	150	Total O 150 150	0	0

3 Residue-property plots

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.

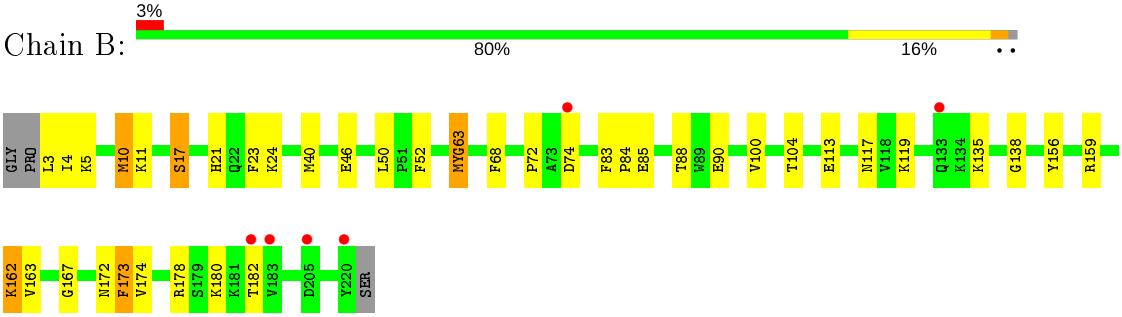
- Molecule 1: Red fluorescent protein eqFP611

Chain A:



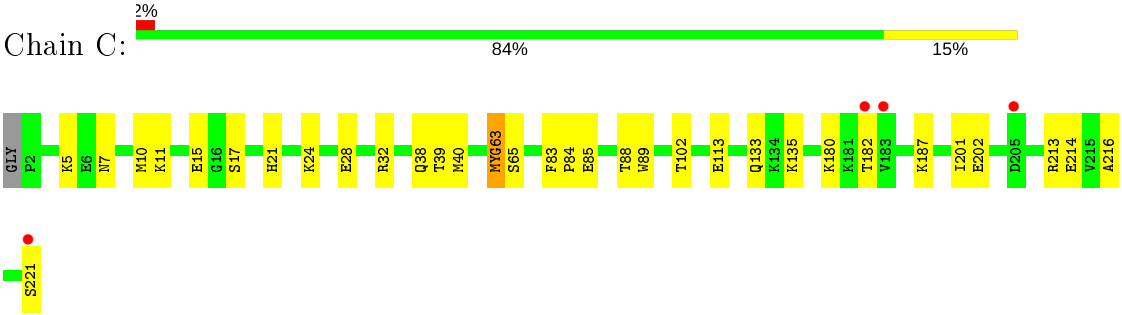
- Molecule 1: Red fluorescent protein eqFP611

Chain B:



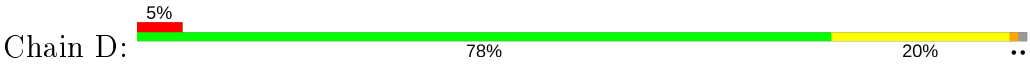
- Molecule 1: Red fluorescent protein eqFP611

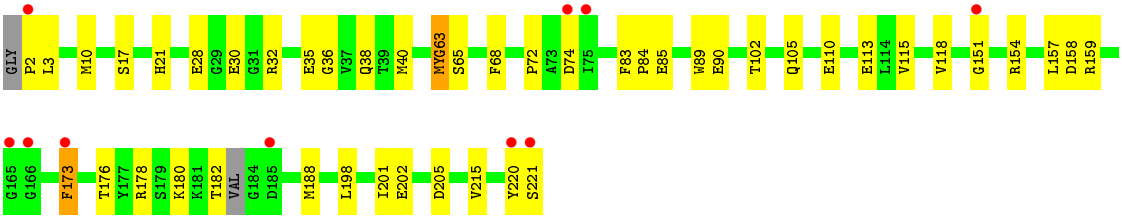
Chain C:



- Molecule 1: Red fluorescent protein eqFP611

Chain D:




GLY
P2
L3
M10
S17
H21
E28
G29
E30
G31
R32
E35
G36
V37
Q38
T39
M40
MYG63
S65
F68
P72
A73
D74
I75
F83
P84
E85
W89
E90
T102
Q105
E110
E113
L114
V115
V118
G151
R154
L157
D158
R159
G165
G166
F173
T176
Y177
R178
S179
K180
K181
T182
VAL
G184
D185
M188
L198
I201
E202
D205
V215
Y220
S221

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	92.02Å 96.86Å 232.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 1.75 48.43 – 1.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.43-1.75) 99.9 (48.43-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.75Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.203 , 0.232 0.210 , 0.235	Depositor DCC
R_{free} test set	5237 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	26.8	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.065 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7583	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

5.1 Standard geometry

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

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	0.46	0/1753	0.62	0/2363
1	B	0.45	0/1731	0.64	0/2336
1	C	0.40	0/1749	0.65	2/2359 (0.1%)
1	D	0.39	0/1745	0.61	0/2350
All	All	0.43	0/6978	0.63	2/9408 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	187	LYS	CA-CB-CG	5.11	124.64	113.40
1	C	187	LYS	CD-CE-NZ	-5.01	100.18	111.70

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	1738	0	1691	30	0
1	B	1717	0	1656	47	0
1	C	1734	0	1680	29	0
1	D	1731	0	1681	46	0
2	A	4	6	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	6	6	0	0
2	D	4	6	6	2	0
3	A	14	4	4	1	0
3	B	7	2	2	1	0
4	A	155	0	0	1	0
4	B	156	0	0	6	0
4	C	145	0	0	2	0
4	D	150	0	0	6	0
All	All	7559	24	6732	145	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 11.

All (145) 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:D:157:LEU:CD2	1:D:159:ARG:HG2	1.74	1.16
1:D:157:LEU:HD22	1:D:159:ARG:CG	1.75	1.15
1:B:24:LYS:HD3	1:B:46:GLU:HB2	1.30	1.12
1:D:157:LEU:HD22	1:D:159:ARG:HG2	1.07	1.06
1:A:10:MET:CE	1:A:68:PHE:CE1	2.44	0.99
1:B:117:ASN:HB3	4:B:519:HOH:O	1.64	0.96
1:A:10:MET:CE	1:A:68:PHE:CZ	2.48	0.95
1:B:72:PRO:HB2	1:B:74:ASP:OD2	1.70	0.92
1:A:10:MET:HE3	1:A:68:PHE:CZ	2.06	0.90
1:B:24:LYS:HD3	1:B:46:GLU:CB	2.06	0.84
1:C:201:ILE:HG13	1:C:213:ARG:HG3	1.62	0.82
1:D:63:NRQ:HE2	1:D:157:LEU:HD11	1.61	0.82
1:A:10:MET:HE1	1:A:68:PHE:CZ	2.16	0.81
1:B:24:LYS:CD	1:B:46:GLU:HB2	2.09	0.80
1:D:151:GLY:HA2	1:D:188:MET:HE3	1.65	0.78
1:A:11:LYS:HG3	1:A:113:GLU:OE2	1.86	0.75
1:A:10:MET:HE1	1:A:68:PHE:CE1	2.24	0.69
1:A:100:VAL:HG21	1:C:102:THR:HG21	1.74	0.69
1:B:138:GLY:O	1:B:162:LYS:HB2	1.92	0.69
1:B:3:LEU:HD12	1:B:5:LYS:HD3	1.75	0.68
1:B:163:VAL:HG22	1:B:167:GLY:C	2.14	0.68
1:C:133:GLN:CB	1:C:135:LYS:HD2	2.23	0.67
1:B:24:LYS:N	1:B:24:LYS:HD2	2.10	0.67
2:A:301:EDO:H21	4:A:491:HOH:O	1.95	0.66
1:D:205:ASP:N	4:D:403:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:SER:N	4:D:402:HOH:O	2.26	0.64
1:B:88:THR:HG23	1:B:180:LYS:HD2	1.80	0.63
3:B:302:MLA:HC22	4:B:401:HOH:O	1.99	0.63
1:D:40:MET:HB2	1:D:63:NRQ:CE	2.28	0.63
1:C:133:GLN:HB2	1:C:135:LYS:HD2	1.81	0.62
1:D:10:MET:HE1	1:D:68:PHE:CZ	2.35	0.62
1:D:105:GLN:HG2	1:D:118:VAL:HG22	1.81	0.62
1:B:163:VAL:HG22	1:B:167:GLY:O	2.00	0.62
1:B:119:LYS:HB3	1:B:119:LYS:NZ	2.15	0.62
1:C:11:LYS:HG3	1:C:113:GLU:OE2	2.00	0.62
1:D:154:ARG:NH1	1:D:176:THR:HG23	2.15	0.62
1:D:105:GLN:CG	1:D:118:VAL:HG22	2.31	0.61
1:A:83:PHE:HB3	1:A:84:PRO:HA	1.81	0.61
1:C:15:GLU:HG2	1:C:24:LYS:HE2	1.84	0.60
1:B:11:LYS:HG3	1:B:113:GLU:OE1	2.01	0.60
1:A:90:GLU:HG2	4:C:390:HOH:O	2.01	0.60
1:B:23:PHE:C	1:B:24:LYS:HD2	2.22	0.60
1:C:201:ILE:CG1	1:C:213:ARG:HG3	2.30	0.59
1:D:83:PHE:HB3	1:D:84:PRO:HA	1.83	0.59
1:C:83:PHE:HB3	1:C:84:PRO:HA	1.85	0.59
1:B:3:LEU:HD12	1:B:5:LYS:CD	2.32	0.58
1:D:110:GLU:O	1:D:113:GLU:HB2	2.03	0.58
1:A:10:MET:HE2	1:A:68:PHE:CE1	2.36	0.58
1:B:3:LEU:CD1	1:B:5:LYS:HD3	2.33	0.58
1:C:133:GLN:HB3	1:C:135:LYS:HD2	1.86	0.57
1:A:100:VAL:HG21	1:C:102:THR:CG2	2.34	0.57
1:B:85:GLU:HG2	1:C:180:LYS:HE3	1.87	0.57
1:B:40:MET:HB2	1:B:63:NRQ:CE	2.36	0.55
1:C:40:MET:HB2	1:C:63:NRQ:CE	2.37	0.55
1:D:63:NRQ:HE2	1:D:157:LEU:CD1	2.35	0.55
1:B:180:LYS:HE2	1:C:85:GLU:HG2	1.88	0.54
1:B:83:PHE:HB3	1:B:84:PRO:HA	1.88	0.54
1:D:38:GLN:HE22	1:D:65:SER:CB	2.20	0.54
1:A:213:ARG:NE	3:A:302:MLA:O3B	2.34	0.53
1:A:133:GLN:O	1:A:135:LYS:HD2	2.08	0.53
1:D:176:THR:HG21	1:D:178:ARG:CZ	2.39	0.53
1:B:100:VAL:HG21	1:D:102:THR:HG21	1.91	0.52
1:B:24:LYS:HD3	1:B:46:GLU:OE1	2.09	0.52
1:D:17:SER:HA	1:D:21:HIS:O	2.09	0.52
1:D:157:LEU:HD23	1:D:158:ASP:N	2.25	0.52
1:D:90:GLU:HG3	4:D:429:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:LEU:HD21	1:D:159:ARG:HG2	1.81	0.51
1:C:214:GLU:OE1	1:C:216:ALA:HB2	2.11	0.51
1:A:10:MET:HE3	1:A:68:PHE:CE1	2.31	0.50
1:B:88:THR:HG21	1:C:182:THR:CG2	2.42	0.50
1:B:182:THR:HA	4:B:410:HOH:O	2.11	0.50
1:D:72:PRO:HB2	1:D:74:ASP:OD1	2.11	0.50
1:A:17:SER:HA	1:A:21:HIS:O	2.12	0.49
1:D:151:GLY:CA	1:D:188:MET:HE3	2.38	0.49
1:C:63:NRQ:N1	1:C:63:NRQ:HA31	2.28	0.49
1:D:40:MET:HB2	1:D:63:NRQ:HE2A	1.94	0.49
1:D:157:LEU:HD22	1:D:159:ARG:HG3	1.82	0.48
1:B:17:SER:HA	1:B:21:HIS:O	2.14	0.48
1:B:50:LEU:HD13	1:B:52:PHE:CZ	2.48	0.48
1:B:90:GLU:HB2	1:B:104:THR:HG22	1.95	0.48
1:C:39:THR:OG1	1:C:213:ARG:NE	2.46	0.48
1:C:5:LYS:NZ	4:C:304:HOH:O	2.40	0.48
1:D:176:THR:HG21	1:D:178:ARG:NH2	2.29	0.48
1:B:100:VAL:HG21	1:D:102:THR:CG2	2.45	0.47
1:D:36:GLY:O	1:D:215:VAL:HA	2.14	0.47
1:B:178:ARG:NH2	4:D:408:HOH:O	2.47	0.47
1:C:17:SER:HA	1:C:21:HIS:O	2.15	0.47
1:D:74:ASP:OD2	1:D:220:TYR:HE2	1.98	0.46
1:B:119:LYS:HB3	1:B:119:LYS:HZ3	1.80	0.46
1:D:63:NRQ:N1	1:D:63:NRQ:HA31	2.31	0.46
1:B:159:ARG:HD2	1:B:173:PHE:CE1	2.51	0.46
1:B:85:GLU:HG2	1:C:180:LYS:CE	2.46	0.46
1:D:3:LEU:HD22	1:D:84:PRO:HB3	1.97	0.45
1:A:83:PHE:C	1:A:181:LYS:HZ1	2.19	0.45
1:C:24:LYS:HB2	1:C:24:LYS:HE3	1.46	0.45
1:D:32:ARG:NH2	1:D:35:GLU:OE1	2.42	0.45
1:D:182:THR:O	1:D:182:THR:OG1	2.27	0.45
1:B:24:LYS:HE3	4:B:497:HOH:O	2.16	0.45
1:B:3:LEU:HD12	1:B:5:LYS:HZ2	1.81	0.45
1:B:180:LYS:CE	1:C:85:GLU:HG2	2.47	0.45
1:B:74:ASP:N	1:B:74:ASP:OD2	2.48	0.45
1:D:85:GLU:O	1:D:180:LYS:HE2	2.17	0.45
1:B:172:ASN:OD1	2:D:301:EDO:H11	2.17	0.45
1:A:85:GLU:O	1:A:180:LYS:HE2	2.16	0.45
1:A:38:GLN:HE22	1:A:65:SER:HB3	1.83	0.44
1:A:6:GLU:HG2	2:A:301:EDO:H11	1.99	0.44
1:A:11:LYS:HB3	1:A:11:LYS:HE2	1.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLY:HA2	1:A:120:VAL:O	2.18	0.44
1:A:14:MET:HB2	1:A:118:VAL:CG1	2.48	0.43
1:D:3:LEU:CD2	1:D:84:PRO:HB3	2.48	0.43
1:D:105:GLN:HG3	1:D:118:VAL:HG22	2.00	0.43
1:C:88:THR:HG23	1:C:180:LYS:HD2	2.00	0.43
1:B:63:NRQ:N2	1:B:63:NRQ:HD1	2.34	0.43
1:A:100:VAL:CG2	1:C:102:THR:HG21	2.45	0.43
1:C:63:NRQ:HA32	1:C:89:TRP:CZ2	2.54	0.43
1:D:10:MET:HE2	1:D:30:GLU:HA	2.01	0.43
1:A:37:VAL:HG22	1:A:215:VAL:HG22	2.01	0.43
1:B:3:LEU:HD13	1:B:4:ILE:C	2.39	0.43
1:B:3:LEU:HD22	4:B:515:HOH:O	2.17	0.42
1:B:135:LYS:HE3	1:B:135:LYS:HB2	1.85	0.42
1:C:38:GLN:HE22	1:C:65:SER:HB3	1.84	0.42
1:A:36:GLY:O	1:A:215:VAL:HA	2.19	0.42
1:D:198:LEU:HD23	1:D:198:LEU:C	2.40	0.42
1:A:40:MET:HB2	1:A:63:NRQ:CE	2.50	0.42
1:D:110:GLU:HG3	1:D:115:VAL:HG21	2.00	0.42
1:B:10:MET:CE	1:B:68:PHE:CZ	3.03	0.42
1:B:156:TYR:CE1	1:B:174:VAL:HG13	2.54	0.42
1:B:3:LEU:HD13	1:B:3:LEU:C	2.40	0.42
1:C:63:NRQ:HD1	1:C:63:NRQ:N2	2.35	0.42
1:D:159:ARG:HD2	1:D:173:PHE:CE1	2.55	0.41
1:D:201:ILE:O	1:D:202:GLU:HG3	2.20	0.41
1:A:10:MET:HE3	1:A:68:PHE:HZ	1.71	0.41
1:A:63:NRQ:HD1	1:A:214:GLU:OE1	2.20	0.41
1:B:11:LYS:NZ	1:B:11:LYS:HB2	2.36	0.41
1:A:137:LYS:HD2	1:A:164:ASP:OD2	2.21	0.41
1:A:63:NRQ:N2	1:A:63:NRQ:HD1	2.36	0.41
1:B:72:PRO:HB3	4:B:467:HOH:O	2.20	0.41
1:C:11:LYS:CG	1:C:113:GLU:OE2	2.68	0.41
1:D:151:GLY:O	1:D:188:MET:HE1	2.20	0.41
1:B:63:NRQ:HA31	1:B:63:NRQ:N1	2.35	0.40
2:D:301:EDO:H21	4:D:404:HOH:O	2.21	0.40
1:D:40:MET:CB	1:D:63:NRQ:HE2A	2.51	0.40
1:D:63:NRQ:HA32	1:D:89:TRP:CZ2	2.57	0.40
1:C:7:ASN:CG	1:C:32:ARG:HH11	2.23	0.40
1:D:2:PRO:N	4:D:414:HOH:O	2.55	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	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
1	B	211/219 (96%)	207 (98%)	4 (2%)	0	100	100
1	C	213/219 (97%)	208 (98%)	5 (2%)	0	100	100
1	D	210/219 (96%)	206 (98%)	4 (2%)	0	100	100
All	All	847/876 (97%)	829 (98%)	18 (2%)	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	185/185 (100%)	182 (98%)	3 (2%)	62	45
1	B	181/185 (98%)	177 (98%)	4 (2%)	52	29
1	C	184/185 (100%)	180 (98%)	4 (2%)	52	29
1	D	184/185 (100%)	182 (99%)	2 (1%)	73	60
All	All	734/740 (99%)	721 (98%)	13 (2%)	59	40

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	173	PHE

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Mol	Chain	Res	Type
1	A	205	ASP
1	B	10	MET
1	B	17	SER
1	B	162	LYS
1	B	173	PHE
1	C	10	MET
1	C	28	GLU
1	C	202	GLU
1	C	221	SER
1	D	28	GLU
1	D	173	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN

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	B	63	1	23,24,25	2.26	7 (30%)	23,32,34	2.70	9 (39%)
1	NRQ	C	63	1	23,24,25	2.22	7 (30%)	23,32,34	3.23	7 (30%)
1	NRQ	A	63	1	23,24,25	2.26	8 (34%)	23,32,34	3.04	7 (30%)
1	NRQ	D	63	1	23,24,25	2.37	7 (30%)	23,32,34	2.32	5 (21%)

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	B	63	1	-	4/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	3/9/31/32	0/2/2/2
1	NRQ	A	63	1	-	3/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	4/9/31/32	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	NRQ	CA2-C2	5.67	1.54	1.48
1	B	63	NRQ	CA2-C2	5.32	1.53	1.48
1	D	63	NRQ	C1-N3	4.82	1.46	1.38
1	C	63	NRQ	CA2-C2	4.76	1.53	1.48
1	A	63	NRQ	C1-N3	4.74	1.46	1.38
1	B	63	NRQ	C1-N3	4.72	1.46	1.38
1	A	63	NRQ	CA2-C2	4.65	1.53	1.48
1	C	63	NRQ	CB2-CA2	-4.44	1.31	1.35
1	D	63	NRQ	C1-N2	4.27	1.42	1.33
1	C	63	NRQ	C1-N2	4.08	1.42	1.33
1	C	63	NRQ	C1-N3	3.96	1.44	1.38
1	A	63	NRQ	CB2-CA2	-3.94	1.31	1.35
1	D	63	NRQ	CB2-CA2	-3.94	1.31	1.35
1	A	63	NRQ	C1-N2	3.93	1.41	1.33
1	B	63	NRQ	CB2-CA2	-3.79	1.31	1.35
1	C	63	NRQ	C2-N3	3.58	1.48	1.39
1	B	63	NRQ	C1-N2	3.57	1.41	1.33
1	A	63	NRQ	C2-N3	3.46	1.48	1.39
1	B	63	NRQ	C2-N3	3.40	1.47	1.39
1	D	63	NRQ	C2-N3	3.35	1.47	1.39
1	B	63	NRQ	CG2-CB2	3.29	1.53	1.46
1	D	63	NRQ	CG2-CB2	3.18	1.53	1.46
1	C	63	NRQ	CG2-CB2	3.03	1.52	1.46
1	A	63	NRQ	CG2-CB2	2.91	1.52	1.46
1	D	63	NRQ	CA2-N2	2.73	1.44	1.38
1	C	63	NRQ	O2-C2	-2.51	1.17	1.23
1	A	63	NRQ	O2-C2	-2.38	1.18	1.23
1	A	63	NRQ	CA2-N2	2.26	1.43	1.38
1	B	63	NRQ	O2-C2	-2.00	1.18	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	NRQ	O2-C2-CA2	-10.68	124.97	130.96
1	A	63	NRQ	O2-C2-CA2	-9.39	125.69	130.96
1	A	63	NRQ	CA2-C2-N3	8.77	107.52	103.37
1	C	63	NRQ	CA2-C2-N3	8.58	107.43	103.37
1	B	63	NRQ	CA2-C2-N3	7.63	106.98	103.37
1	B	63	NRQ	O2-C2-CA2	-7.32	126.85	130.96
1	D	63	NRQ	O2-C2-CA2	-6.75	127.17	130.96
1	D	63	NRQ	CA2-C2-N3	6.61	106.50	103.37
1	C	63	NRQ	CD1-CG2-CD2	3.08	122.19	117.64
1	A	63	NRQ	CD1-CG2-CD2	2.90	121.94	117.64
1	C	63	NRQ	CE-SD-CG1	2.86	110.23	100.40
1	A	63	NRQ	CE-SD-CG1	2.82	110.07	100.40
1	B	63	NRQ	CG2-CB2-CA2	-2.80	126.51	129.94
1	B	63	NRQ	O3-C3-CA3	-2.74	118.10	126.39
1	C	63	NRQ	O3-C3-CA3	-2.73	118.14	126.39
1	B	63	NRQ	CD1-CG2-CD2	2.73	121.68	117.64
1	B	63	NRQ	C2-CA2-N2	-2.73	107.02	108.93
1	B	63	NRQ	CE-SD-CG1	2.69	109.64	100.40
1	A	63	NRQ	CE1-CD1-CG2	-2.55	117.93	121.25
1	A	63	NRQ	C2-CA2-N2	-2.53	107.16	108.93
1	D	63	NRQ	CD1-CG2-CD2	2.49	121.33	117.64
1	B	63	NRQ	CA2-N2-C1	2.31	108.56	104.33
1	D	63	NRQ	O3-C3-CA3	-2.31	119.41	126.39
1	C	63	NRQ	C2-CA2-N2	-2.23	107.37	108.93
1	C	63	NRQ	CE1-CD1-CG2	-2.20	118.38	121.25
1	D	63	NRQ	CE1-CD1-CG2	-2.16	118.43	121.25
1	B	63	NRQ	CE1-CD1-CG2	-2.14	118.46	121.25
1	A	63	NRQ	O3-C3-CA3	-2.11	120.02	126.39

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	63	NRQ	C2-CA2-CB2-CG2
1	C	63	NRQ	C2-CA2-CB2-CG2
1	A	63	NRQ	N2-CA2-CB2-CG2
1	A	63	NRQ	C2-CA2-CB2-CG2
1	D	63	NRQ	C2-CA2-CB2-CG2
1	B	63	NRQ	N2-CA2-CB2-CG2
1	C	63	NRQ	N2-CA2-CB2-CG2
1	D	63	NRQ	N2-CA2-CB2-CG2

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

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRQ	3	0
1	C	63	NRQ	4	0
1	A	63	NRQ	3	0
1	D	63	NRQ	7	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	EDO	A	301	-	3,3,3	0.44	0	2,2,2	0.54	0
3	MLA	B	302	-	0,6,6	0.00	-	0,7,7	0.00	-
3	MLA	A	303	-	0,6,6	0.00	-	0,7,7	0.00	-
2	EDO	D	301	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.33	0
3	MLA	A	302	-	0,6,6	0.00	-	0,7,7	0.00	-

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	EDO	A	301	-	-	1/1/1/1	-
3	MLA	B	302	-	-	0/0/4/4	-
3	MLA	A	303	-	-	0/0/4/4	-
2	EDO	D	301	-	-	1/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
3	MLA	A	302	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EDO	O1-C1-C2-O2
2	D	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EDO	2	0
3	B	302	MLA	1	0
2	D	301	EDO	2	0
3	A	302	MLA	1	0

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	217/219 (99%)	0.21	6 (2%) 53 58	20, 29, 53, 86	0
1	B	215/219 (98%)	0.20	6 (2%) 53 58	21, 33, 57, 78	0
1	C	217/219 (99%)	0.22	4 (1%) 68 76	20, 33, 58, 76	0
1	D	216/219 (98%)	0.32	10 (4%) 32 38	22, 34, 59, 75	0
All	All	865/876 (98%)	0.23	26 (3%) 50 56	20, 33, 57, 86	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	VAL	8.4
1	D	2	PRO	5.2
1	A	184	GLY	4.6
1	C	183	VAL	4.2
1	D	220	TYR	4.1
1	D	221	SER	3.6
1	D	74	ASP	3.2
1	A	150	ASP	3.0
1	B	183	VAL	2.8
1	A	182	THR	2.8
1	D	185	ASP	2.8
1	B	205	ASP	2.7
1	B	133	GLN	2.7
1	A	220	TYR	2.6
1	B	74	ASP	2.5
1	D	151	GLY	2.5
1	A	205	ASP	2.4
1	C	221	SER	2.2
1	B	220	TYR	2.2
1	B	182	THR	2.2
1	D	75	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	173	PHE	2.1
1	D	165	GLY	2.1
1	C	205	ASP	2.1
1	C	182	THR	2.1
1	D	166	GLY	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, 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	B-factors(Å^2)	Q<0.9
1	NRQ	A	63	23/24	0.94	0.11	23,28,36,40	0
1	NRQ	B	63	23/24	0.95	0.12	24,31,39,46	0
1	NRQ	D	63	23/24	0.95	0.10	28,34,39,46	0
1	NRQ	C	63	23/24	0.96	0.12	23,30,36,40	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	EDO	B	301	4/4	0.66	0.44	80,96,97,97	0
3	MLA	A	303	7/7	0.69	0.20	58,61,73,73	0
3	MLA	B	302	7/7	0.75	0.28	41,56,71,71	0
3	MLA	A	302	7/7	0.76	0.17	46,57,69,69	0
2	EDO	A	301	4/4	0.78	0.30	64,77,80,84	0
2	EDO	D	301	4/4	0.91	0.15	52,62,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.