Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 11:30 am GMT

PDB ID	:	5MSE
Title	:	GFP nuclear transport receptor mimic 3B8
Authors	:	Huyton, T.; Gorlich, D.
Deposited on	:	2017-01-04
Resolution	:	1.66 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:

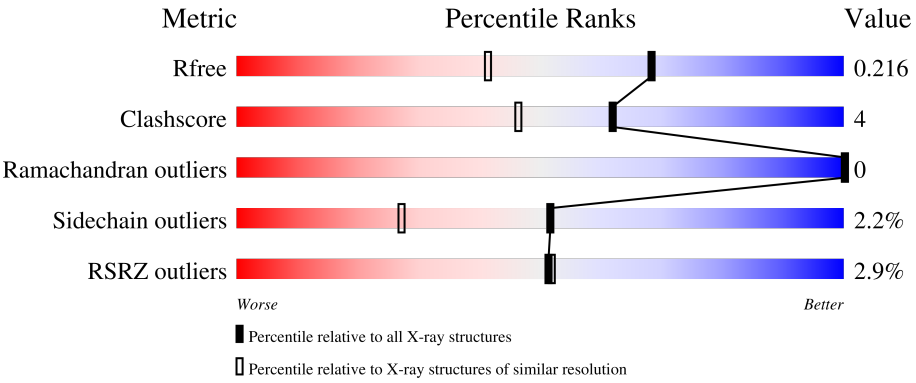
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.66 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	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	238	3% 77% 13% • 6%
1	B	238	3% 79% 13% • 6%
1	C	238	3% 79% 14% • 5%
1	D	238	3% 79% 13% • 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8179 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 Green fluorescent protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	1	0
			1837	1155	328	341	13			
1	C	227	Total	C	N	O	S	0	1	0
			1852	1164	331	344	13			
1	D	224	Total	C	N	O	S	0	1	0
			1837	1155	328	341	13			
1	B	224	Total	C	N	O	S	0	1	0
			1837	1155	328	341	13			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP P42212
A	0	GLY	-	expression tag	UNP P42212
A	1	THR	-	expression tag	UNP P42212
A	3	ARG	LYS	engineered mutation	UNP P42212
A	26	ARG	LYS	engineered mutation	UNP P42212
A	30	ARG	SER	engineered mutation	UNP P42212
A	41	MET	LYS	engineered mutation	UNP P42212
A	45	ARG	LYS	engineered mutation	UNP P42212
A	52	ARG	LYS	engineered mutation	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	72	ALA	SER	engineered mutation	UNP P42212
A	79	ARG	LYS	engineered mutation	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	87	THR	ALA	engineered mutation	UNP P42212
A	97	MET	THR	engineered mutation	UNP P42212
A	99	TYR	PHE	engineered mutation	UNP P42212
A	101	GLU	LYS	engineered mutation	UNP P42212
A	105	ALA	ASN	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	ARG	LYS	engineered mutation	UNP P42212
A	111	VAL	GLU	engineered mutation	UNP P42212
A	113	ARG	LYS	engineered mutation	UNP P42212
A	126	ARG	LYS	engineered mutation	UNP P42212
A	128	THR	ILE	engineered mutation	UNP P42212
A	131	ARG	LYS	engineered mutation	UNP P42212
A	140	ARG	LYS	engineered mutation	UNP P42212
A	145	PHE	TYR	engineered mutation	UNP P42212
A	149	MET	ASN	engineered mutation	UNP P42212
A	156	ARG	LYS	engineered mutation	UNP P42212
A	158	ARG	LYS	engineered mutation	UNP P42212
A	162	ARG	LYS	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	164	MET	ASN	engineered mutation	UNP P42212
A	166	ASN	LYS	engineered mutation	UNP P42212
A	167	THR	ILE	engineered mutation	UNP P42212
A	171	VAL	ILE	engineered mutation	UNP P42212
A	176	GLU	VAL	engineered mutation	UNP P42212
A	178	VAL	LEU	engineered mutation	UNP P42212
A	180	MET	ASP	engineered mutation	UNP P42212
A	198	ASP	ASN	engineered mutation	UNP P42212
A	202	TYR	SER	engineered mutation	UNP P42212
A	204	MET	GLN	engineered mutation	UNP P42212
A	206	LEU	ALA	engineered mutation	UNP P42212
A	209	VAL	LYS	engineered mutation	UNP P42212
A	214	ARG	LYS	engineered mutation	UNP P42212
A	221	ARG	LEU	engineered mutation	UNP P42212
A	225	MET	THR	engineered mutation	UNP P42212
A	231	LEU	HIS	engineered mutation	UNP P42212
A	238	ARG	LYS	engineered mutation	UNP P42212
C	-1	ALA	-	expression tag	UNP P42212
C	0	GLY	-	expression tag	UNP P42212
C	1	THR	-	expression tag	UNP P42212
C	3	ARG	LYS	engineered mutation	UNP P42212
C	26	ARG	LYS	engineered mutation	UNP P42212
C	30	ARG	SER	engineered mutation	UNP P42212
C	41	MET	LYS	engineered mutation	UNP P42212
C	45	ARG	LYS	engineered mutation	UNP P42212
C	52	ARG	LYS	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	66	CRO	GLY	chromophore	UNP P42212
C	72	ALA	SER	engineered mutation	UNP P42212
C	79	ARG	LYS	engineered mutation	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	87	THR	ALA	engineered mutation	UNP P42212
C	97	MET	THR	engineered mutation	UNP P42212
C	99	TYR	PHE	engineered mutation	UNP P42212
C	101	GLU	LYS	engineered mutation	UNP P42212
C	105	ALA	ASN	engineered mutation	UNP P42212
C	107	ARG	LYS	engineered mutation	UNP P42212
C	111	VAL	GLU	engineered mutation	UNP P42212
C	113	ARG	LYS	engineered mutation	UNP P42212
C	126	ARG	LYS	engineered mutation	UNP P42212
C	128	THR	ILE	engineered mutation	UNP P42212
C	131	ARG	LYS	engineered mutation	UNP P42212
C	140	ARG	LYS	engineered mutation	UNP P42212
C	145	PHE	TYR	engineered mutation	UNP P42212
C	149	MET	ASN	engineered mutation	UNP P42212
C	156	ARG	LYS	engineered mutation	UNP P42212
C	158	ARG	LYS	engineered mutation	UNP P42212
C	162	ARG	LYS	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	164	MET	ASN	engineered mutation	UNP P42212
C	166	ASN	LYS	engineered mutation	UNP P42212
C	167	THR	ILE	engineered mutation	UNP P42212
C	171	VAL	ILE	engineered mutation	UNP P42212
C	176	GLU	VAL	engineered mutation	UNP P42212
C	178	VAL	LEU	engineered mutation	UNP P42212
C	180	MET	ASP	engineered mutation	UNP P42212
C	198	ASP	ASN	engineered mutation	UNP P42212
C	202	TYR	SER	engineered mutation	UNP P42212
C	204	MET	GLN	engineered mutation	UNP P42212
C	206	LEU	ALA	engineered mutation	UNP P42212
C	209	VAL	LYS	engineered mutation	UNP P42212
C	214	ARG	LYS	engineered mutation	UNP P42212
C	221	ARG	LEU	engineered mutation	UNP P42212
C	225	MET	THR	engineered mutation	UNP P42212
C	231	LEU	HIS	engineered mutation	UNP P42212
C	238	ARG	LYS	engineered mutation	UNP P42212
D	-1	ALA	-	expression tag	UNP P42212
D	0	GLY	-	expression tag	UNP P42212
D	1	THR	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	ARG	LYS	engineered mutation	UNP P42212
D	26	ARG	LYS	engineered mutation	UNP P42212
D	30	ARG	SER	engineered mutation	UNP P42212
D	41	MET	LYS	engineered mutation	UNP P42212
D	45	ARG	LYS	engineered mutation	UNP P42212
D	52	ARG	LYS	engineered mutation	UNP P42212
D	64	LEU	PHE	engineered mutation	UNP P42212
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	72	ALA	SER	engineered mutation	UNP P42212
D	79	ARG	LYS	engineered mutation	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212
D	87	THR	ALA	engineered mutation	UNP P42212
D	97	MET	THR	engineered mutation	UNP P42212
D	99	TYR	PHE	engineered mutation	UNP P42212
D	101	GLU	LYS	engineered mutation	UNP P42212
D	105	ALA	ASN	engineered mutation	UNP P42212
D	107	ARG	LYS	engineered mutation	UNP P42212
D	111	VAL	GLU	engineered mutation	UNP P42212
D	113	ARG	LYS	engineered mutation	UNP P42212
D	126	ARG	LYS	engineered mutation	UNP P42212
D	128	THR	ILE	engineered mutation	UNP P42212
D	131	ARG	LYS	engineered mutation	UNP P42212
D	140	ARG	LYS	engineered mutation	UNP P42212
D	145	PHE	TYR	engineered mutation	UNP P42212
D	149	MET	ASN	engineered mutation	UNP P42212
D	156	ARG	LYS	engineered mutation	UNP P42212
D	158	ARG	LYS	engineered mutation	UNP P42212
D	162	ARG	LYS	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	164	MET	ASN	engineered mutation	UNP P42212
D	166	ASN	LYS	engineered mutation	UNP P42212
D	167	THR	ILE	engineered mutation	UNP P42212
D	171	VAL	ILE	engineered mutation	UNP P42212
D	176	GLU	VAL	engineered mutation	UNP P42212
D	178	VAL	LEU	engineered mutation	UNP P42212
D	180	MET	ASP	engineered mutation	UNP P42212
D	198	ASP	ASN	engineered mutation	UNP P42212
D	202	TYR	SER	engineered mutation	UNP P42212
D	204	MET	GLN	engineered mutation	UNP P42212
D	206	LEU	ALA	engineered mutation	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	209	VAL	LYS	engineered mutation	UNP P42212
D	214	ARG	LYS	engineered mutation	UNP P42212
D	221	ARG	LEU	engineered mutation	UNP P42212
D	225	MET	THR	engineered mutation	UNP P42212
D	231	LEU	HIS	engineered mutation	UNP P42212
D	238	ARG	LYS	engineered mutation	UNP P42212
B	-1	ALA	-	expression tag	UNP P42212
B	0	GLY	-	expression tag	UNP P42212
B	1	THR	-	expression tag	UNP P42212
B	3	ARG	LYS	engineered mutation	UNP P42212
B	26	ARG	LYS	engineered mutation	UNP P42212
B	30	ARG	SER	engineered mutation	UNP P42212
B	41	MET	LYS	engineered mutation	UNP P42212
B	45	ARG	LYS	engineered mutation	UNP P42212
B	52	ARG	LYS	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	72	ALA	SER	engineered mutation	UNP P42212
B	79	ARG	LYS	engineered mutation	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	87	THR	ALA	engineered mutation	UNP P42212
B	97	MET	THR	engineered mutation	UNP P42212
B	99	TYR	PHE	engineered mutation	UNP P42212
B	101	GLU	LYS	engineered mutation	UNP P42212
B	105	ALA	ASN	engineered mutation	UNP P42212
B	107	ARG	LYS	engineered mutation	UNP P42212
B	111	VAL	GLU	engineered mutation	UNP P42212
B	113	ARG	LYS	engineered mutation	UNP P42212
B	126	ARG	LYS	engineered mutation	UNP P42212
B	128	THR	ILE	engineered mutation	UNP P42212
B	131	ARG	LYS	engineered mutation	UNP P42212
B	140	ARG	LYS	engineered mutation	UNP P42212
B	145	PHE	TYR	engineered mutation	UNP P42212
B	149	MET	ASN	engineered mutation	UNP P42212
B	156	ARG	LYS	engineered mutation	UNP P42212
B	158	ARG	LYS	engineered mutation	UNP P42212
B	162	ARG	LYS	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	164	MET	ASN	engineered mutation	UNP P42212
B	166	ASN	LYS	engineered mutation	UNP P42212

Continued on next page...

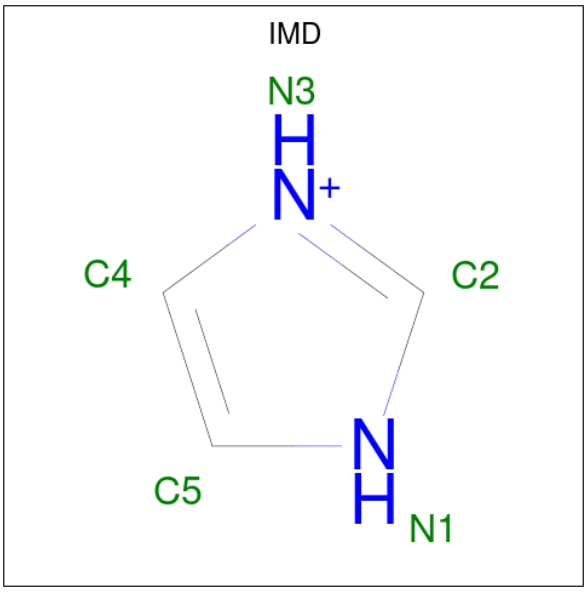
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	167	THR	ILE	engineered mutation	UNP P42212
B	171	VAL	ILE	engineered mutation	UNP P42212
B	176	GLU	VAL	engineered mutation	UNP P42212
B	178	VAL	LEU	engineered mutation	UNP P42212
B	180	MET	ASP	engineered mutation	UNP P42212
B	198	ASP	ASN	engineered mutation	UNP P42212
B	202	TYR	SER	engineered mutation	UNP P42212
B	204	MET	GLN	engineered mutation	UNP P42212
B	206	LEU	ALA	engineered mutation	UNP P42212
B	209	VAL	LYS	engineered mutation	UNP P42212
B	214	ARG	LYS	engineered mutation	UNP P42212
B	221	ARG	LEU	engineered mutation	UNP P42212
B	225	MET	THR	engineered mutation	UNP P42212
B	231	LEU	HIS	engineered mutation	UNP P42212
B	238	ARG	LYS	engineered mutation	UNP P42212

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	C	2	Total Na 2 2	0	0
2	D	2	Total Na 2 2	0	0
2	B	2	Total Na 2 2	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N 5 3 2	0	0
3	A	1	Total C N 5 3 2	0	0
3	C	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

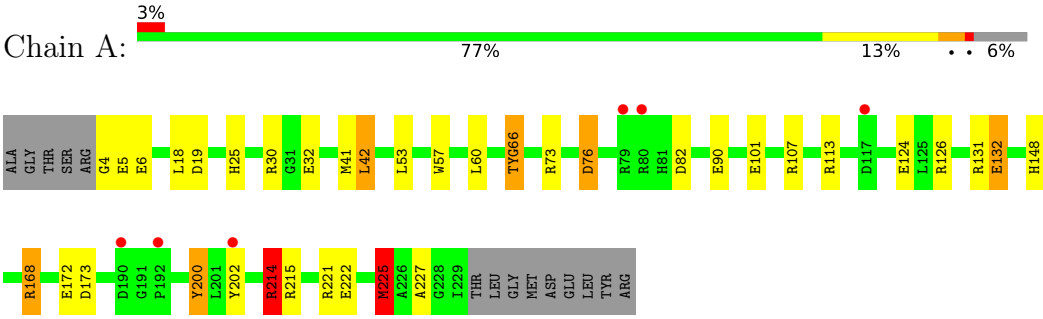
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	187	Total O 187 187	0	0
4	C	213	Total O 213 213	0	0
4	D	192	Total O 192 192	0	0
4	B	196	Total O 196 196	0	0

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.

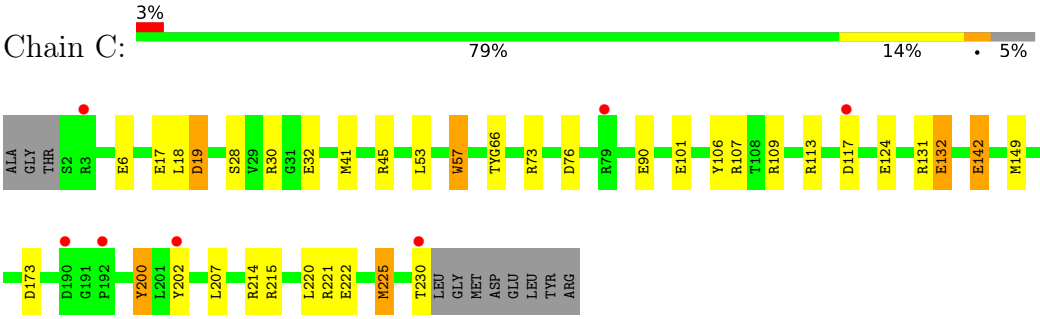
• Molecule 1: Green fluorescent protein

Chain A:



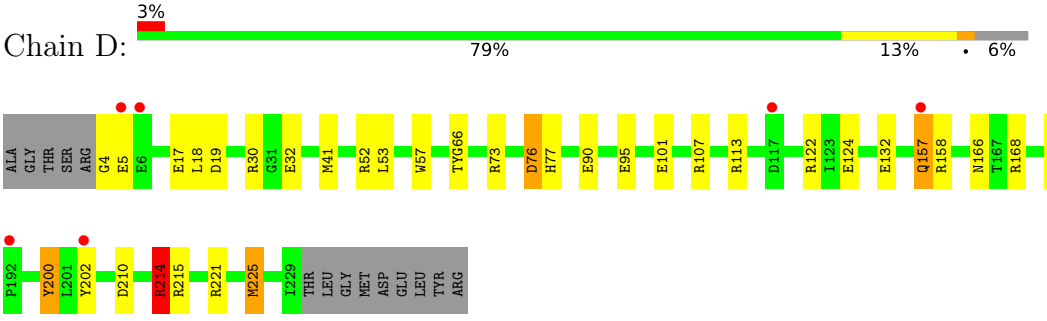
• Molecule 1: Green fluorescent protein

Chain C:



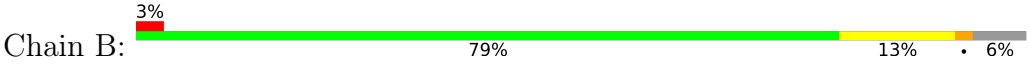
• Molecule 1: Green fluorescent protein

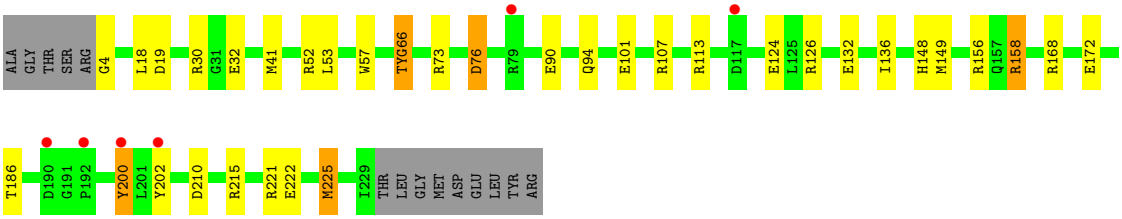
Chain D:



• Molecule 1: Green fluorescent protein

Chain B:




ALA GLY THR SER ARG G4 L18 D19 R30 G31 E32 M41 R52 L53 W57 TYG66 R73 D76 R79 E90 Q94 E101 R107 R113 D117 E124 L125 R126 E132 I136 H148 M149 R156 Q157 R158 R168 E172
T186 D190 G191 P192 Y200 L201 Y202 D210 R215 R221 E222 M225 I229 THR LEU GLY MET ASP GLU LEU TYR ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.40Å 73.40Å 93.93Å 90.00° 93.73° 90.00°	Depositor
Resolution (Å)	46.86 – 1.66 46.86 – 1.66	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.86-1.66) 98.4 (46.86-1.66)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.66Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.206 0.186 , 0.216	Depositor DCC
R_{free} test set	5744 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8179	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: CRO, NA, IMD

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	1.37	11/1860 (0.6%)	1.28	24/2516 (1.0%)
1	B	1.37	10/1860 (0.5%)	1.28	17/2516 (0.7%)
1	C	1.34	11/1875 (0.6%)	1.23	17/2537 (0.7%)
1	D	1.34	9/1860 (0.5%)	1.25	18/2516 (0.7%)
All	All	1.36	41/7455 (0.5%)	1.26	76/10085 (0.8%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLY	N-CA	9.87	1.60	1.46
1	D	4	GLY	N-CA	9.46	1.60	1.46
1	B	4	GLY	N-CA	7.98	1.58	1.46
1	A	172	GLU	CD-OE1	7.45	1.33	1.25
1	A	132	GLU	CD-OE1	7.41	1.33	1.25
1	B	200	TYR	CB-CG	-7.25	1.40	1.51
1	B	222	GLU	CG-CD	7.25	1.62	1.51
1	B	52	ARG	CZ-NH1	7.05	1.42	1.33
1	D	132	GLU	CG-CD	6.99	1.62	1.51
1	B	90	GLU	CD-OE1	6.94	1.33	1.25
1	A	90	GLU	CD-OE1	6.82	1.33	1.25
1	A	132	GLU	CD-OE2	6.76	1.33	1.25
1	A	222	GLU	CG-CD	6.73	1.62	1.51
1	D	90	GLU	CD-OE1	6.73	1.33	1.25
1	C	132	GLU	CG-CD	6.72	1.62	1.51
1	A	200	TYR	CB-CG	-6.70	1.41	1.51
1	C	200	TYR	CB-CG	-6.50	1.42	1.51
1	C	101	GLU	CD-OE2	6.43	1.32	1.25
1	B	124	GLU	CD-OE1	6.42	1.32	1.25
1	D	124	GLU	CD-OE1	6.32	1.32	1.25
1	A	132	GLU	CG-CD	6.27	1.61	1.51
1	C	90	GLU	CD-OE1	6.23	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	132	GLU	CD-OE1	6.19	1.32	1.25
1	C	124	GLU	CD-OE1	5.92	1.32	1.25
1	B	132	GLU	CG-CD	5.92	1.60	1.51
1	C	17	GLU	CD-OE2	5.89	1.32	1.25
1	C	106	TYR	CE1-CZ	5.84	1.46	1.38
1	D	101	GLU	CD-OE1	5.80	1.32	1.25
1	D	200	TYR	CB-CG	-5.78	1.43	1.51
1	B	132	GLU	CD-OE1	5.68	1.31	1.25
1	C	28	SER	CA-CB	5.63	1.61	1.52
1	D	90	GLU	CD-OE2	5.52	1.31	1.25
1	A	124	GLU	CD-OE1	5.42	1.31	1.25
1	C	132	GLU	CD-OE1	5.31	1.31	1.25
1	A	6	GLU	CD-OE2	5.29	1.31	1.25
1	B	19	ASP	CG-OD1	5.21	1.37	1.25
1	C	57	TRP	CG-CD1	-5.19	1.29	1.36
1	B	101	GLU	CD-OE1	5.16	1.31	1.25
1	C	222	GLU	CG-CD	5.12	1.59	1.51
1	D	52	ARG	CZ-NH2	5.09	1.39	1.33
1	A	172	GLU	CG-CD	5.03	1.59	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	52	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	D	107	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	A	73	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	107	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	221	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	221	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	D	221	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	41	MET	CG-SD-CE	8.40	113.63	100.20
1	B	113	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	B	19	ASP	CB-CG-OD1	8.09	125.58	118.30
1	A	19	ASP	CB-CG-OD1	8.08	125.57	118.30
1	C	107	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	B	19	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	D	113	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	73	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	225	MET	CG-SD-CE	-7.28	88.55	100.20
1	C	45	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	B	107	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	C	168	ARG	NE-CZ-NH2	-7.11	116.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	221	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	73	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	113	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	41	MET	CG-SD-CE	6.87	111.19	100.20
1	A	42	LEU	CB-CG-CD2	6.68	122.36	111.00
1	A	168	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	C	41	MET	CG-SD-CE	6.61	110.77	100.20
1	A	19	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	D	225	MET	CG-SD-CE	-6.52	89.76	100.20
1	C	225	MET	CG-SD-CE	-6.47	89.85	100.20
1	D	73	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	210	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	D	73	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	D	215	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	107	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	73	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	113	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	214	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	113	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	107	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	73	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	B	215	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	41	MET	CG-SD-CE	6.08	109.94	100.20
1	A	225	MET	CG-SD-CE	6.08	109.93	100.20
1	B	76	ASP	CB-CG-OD1	-6.03	112.87	118.30
1	D	168	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	76	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	C	214	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	210	ASP	CB-CG-OD2	-5.62	113.25	118.30
1	B	215	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	19	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	126	ARG	NE-CZ-NH1	5.57	123.09	120.30
1	A	156	ARG	CG-CD-NE	-5.57	100.11	111.80
1	D	19	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	19	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	D	107	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	B	126	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	C	215	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	76	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	B	136	ILE	CA-CB-CG1	-5.43	100.68	111.00
1	A	215	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	172	GLU	OE1-CD-OE2	5.39	129.77	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	124	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	A	156	ARG	CB-CG-CD	5.32	125.42	111.60
1	D	95	GLU	OE1-CD-OE2	5.28	129.63	123.30
1	A	42	LEU	CB-CG-CD1	-5.25	102.07	111.00
1	C	109	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	5	GLU	CB-CA-C	-5.20	100.01	110.40
1	C	142	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	A	82	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	173	ASP	CB-CG-OD1	5.09	122.89	118.30
1	D	5	GLU	CB-CA-C	-5.09	100.23	110.40
1	C	107	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	131	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	214	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	173	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	131	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	1837	0	1750	20	0
1	B	1837	0	1750	16	0
1	C	1852	0	1756	15	0
1	D	1837	0	1750	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	10	0	10	2	0
3	B	5	0	5	0	0
3	C	5	0	5	0	0
4	A	187	0	0	3	1
4	B	196	0	0	3	2
4	C	213	0	0	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	192	0	0	3	0
All	All	8179	0	7026	64	2

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 4.

All (64) 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:200:TYR:HE2	1:A:202[B]:TYR:CE2	1.90	0.90
1:C:200:TYR:HE2	1:C:202[B]:TYR:CE2	1.94	0.84
1:B:200:TYR:HE2	1:B:202[B]:TYR:CE2	1.98	0.82
1:D:172:GLU:OE1	4:D:401:HOH:O	2.00	0.78
1:D:17:GLU:OE1	1:D:122:ARG:NH1	2.21	0.71
1:C:200:TYR:CE2	1:C:202[B]:TYR:CE2	2.80	0.69
1:A:200:TYR:CE2	1:A:202[B]:TYR:CZ	2.81	0.69
1:A:200:TYR:CE2	1:A:202[B]:TYR:CE2	2.78	0.67
1:B:186:THR:HG23	4:B:450:HOH:O	1.95	0.66
1:D:214:ARG:HA	1:D:214:ARG:HE	1.62	0.64
1:B:148:HIS:CE1	1:B:168:ARG:H	2.16	0.63
1:A:25:HIS:NE2	4:A:401:HOH:O	2.19	0.62
1:C:19:ASP:OD1	4:C:401:HOH:O	2.16	0.62
1:B:200:TYR:CE2	1:B:202[B]:TYR:CE2	2.85	0.60
1:B:148:HIS:HE1	1:B:168:ARG:H	1.50	0.59
1:A:148:HIS:CE1	1:A:168:ARG:H	2.20	0.59
1:B:200:TYR:CE2	1:B:202[B]:TYR:CZ	2.91	0.58
1:A:30:ARG:HH12	1:A:32:GLU:CD	2.07	0.57
1:B:158:ARG:HG3	1:B:186:THR:HG22	1.87	0.57
1:B:30:ARG:HH12	1:B:32:GLU:CD	2.08	0.56
3:A:304:IMD:H2	4:C:528:HOH:O	2.05	0.55
1:D:30:ARG:HH12	1:D:32:GLU:CD	2.10	0.55
1:A:148:HIS:HE1	1:A:168:ARG:H	1.55	0.55
1:D:53:LEU:HD22	1:D:57:TRP:CE2	2.42	0.55
1:B:158:ARG:HH11	1:B:186:THR:CG2	2.20	0.55
1:B:53:LEU:HD22	1:B:57:TRP:CE2	2.42	0.55
1:C:230:THR:HA	4:C:581:HOH:O	2.06	0.54
1:D:200:TYR:HE2	1:D:202[B]:TYR:CE2	2.25	0.54
1:C:53:LEU:HD22	1:C:57:TRP:CE2	2.43	0.54
1:B:66:CRO:OH	1:B:148:HIS:HD2	1.89	0.54
1:A:53:LEU:HD22	1:A:57:TRP:CE2	2.43	0.54
1:A:60:LEU:C	4:A:420:HOH:O	2.47	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ARG:HH12	1:C:32:GLU:CD	2.10	0.53
1:C:142:GLU:OE1	4:C:402:HOH:O	2.19	0.53
1:A:200:TYR:HE2	1:A:202[B]:TYR:CZ	2.19	0.53
1:B:158:ARG:HH11	1:B:186:THR:HG22	1.72	0.53
1:A:157:GLN:NE2	1:A:157:GLN:H	2.05	0.53
1:A:66:CRO:OH	1:A:148:HIS:HD2	1.90	0.52
1:C:200:TYR:CE2	1:C:202[B]:TYR:CZ	2.97	0.52
1:D:157:GLN:NE2	1:D:157:GLN:H	2.07	0.51
1:A:214:ARG:HE	1:A:214:ARG:HA	1.76	0.51
1:D:166:ASN:HD22	1:D:180:MET:HA	1.76	0.49
1:A:42:LEU:HD12	1:A:42:LEU:C	2.33	0.49
1:B:156:ARG:NH2	4:B:408:HOH:O	2.47	0.48
1:C:19:ASP:HB2	4:C:416:HOH:O	2.14	0.47
1:C:149:MET:CG	1:C:202[B]:TYR:CE1	2.98	0.46
1:C:132:GLU:OE1	4:C:403:HOH:O	2.20	0.45
1:D:77:HIS:HD2	4:D:539:HOH:O	1.99	0.45
1:B:94:GLN:NE2	4:B:409:HOH:O	2.48	0.45
1:A:132:GLU:HG3	4:A:565:HOH:O	2.17	0.45
1:A:101:GLU:OE1	3:A:304:IMD:H5	2.17	0.44
1:C:18:LEU:C	1:C:18:LEU:HD23	2.38	0.44
1:B:149:MET:CG	1:B:202[B]:TYR:CE1	3.01	0.43
1:D:214:ARG:HE	1:D:214:ARG:CA	2.31	0.43
1:A:18:LEU:C	1:A:18:LEU:HD23	2.38	0.43
1:A:214:ARG:HE	1:A:214:ARG:CA	2.32	0.42
1:A:66:CRO:HD1	1:A:66:CRO:N2	2.35	0.42
1:C:117:ASP:HB3	4:C:576:HOH:O	2.19	0.41
1:D:18:LEU:C	1:D:18:LEU:HD23	2.40	0.41
1:D:214:ARG:NH1	4:D:410:HOH:O	2.51	0.41
1:A:225:MET:CE	1:A:227:ALA:HB2	2.51	0.41
1:B:18:LEU:C	1:B:18:LEU:HD23	2.41	0.41
1:C:149:MET:HG2	1:C:202[B]:TYR:CE1	2.56	0.41
1:C:207:LEU:CD2	1:C:220:LEU:HD13	2.52	0.40

All (2) 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)
4:C:564:HOH:O	4:B:497:HOH:O[2_345]	2.10	0.10
4:A:418:HOH:O	4:B:547:HOH:O[2_445]	2.12	0.08

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	220/238 (92%)	216 (98%)	4 (2%)	0	100	100
1	B	220/238 (92%)	216 (98%)	4 (2%)	0	100	100
1	C	223/238 (94%)	219 (98%)	4 (2%)	0	100	100
1	D	220/238 (92%)	217 (99%)	3 (1%)	0	100	100
All	All	883/952 (93%)	868 (98%)	15 (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	195/205 (95%)	190 (97%)	5 (3%)	46	21
1	B	195/205 (95%)	192 (98%)	3 (2%)	65	44
1	C	195/205 (95%)	191 (98%)	4 (2%)	53	29
1	D	195/205 (95%)	190 (97%)	5 (3%)	46	21
All	All	780/820 (95%)	763 (98%)	17 (2%)	52	27

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ASP
1	A	157	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	158	ARG
1	A	214	ARG
1	A	225	MET
1	C	6	GLU
1	C	76	ASP
1	C	158	ARG
1	C	225	MET
1	D	76	ASP
1	D	157	GLN
1	D	158	ARG
1	D	214	ARG
1	D	225	MET
1	B	76	ASP
1	B	158	ARG
1	B	225	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	157	GLN
1	D	77	HIS
1	D	157	GLN
1	D	166	ASN
1	B	77	HIS
1	B	148	HIS

5.3.3 RNA (i)

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	CRO	B	66	1	23,23,24	3.00	9 (39%)	30,32,34	3.37	12 (40%)
1	CRO	D	66	1	23,23,24	2.88	6 (26%)	30,32,34	4.11	10 (33%)
1	CRO	C	66	1	23,23,24	3.05	7 (30%)	30,32,34	3.91	13 (43%)
1	CRO	A	66	1	23,23,24	3.02	6 (26%)	30,32,34	4.12	13 (43%)

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	CRO	B	66	1	-	0/12/31/32	0/2/2/2
1	CRO	D	66	1	-	0/12/31/32	0/2/2/2
1	CRO	C	66	1	-	0/12/31/32	0/2/2/2
1	CRO	A	66	1	-	0/12/31/32	0/2/2/2

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	11.49	1.44	1.35
1	C	66	CRO	CB2-CA2	11.19	1.44	1.35
1	B	66	CRO	CB2-CA2	10.30	1.43	1.35
1	D	66	CRO	CB2-CA2	10.11	1.43	1.35
1	B	66	CRO	CA1-C1	-5.38	1.43	1.51
1	D	66	CRO	CA1-C1	-5.24	1.44	1.51
1	C	66	CRO	CA1-C1	-5.23	1.44	1.51
1	A	66	CRO	CA1-C1	-4.60	1.44	1.51
1	B	66	CRO	C2-N3	-4.41	1.29	1.39
1	A	66	CRO	C2-N3	-4.39	1.29	1.39
1	D	66	CRO	C2-N3	-4.09	1.30	1.39
1	C	66	CRO	CA2-C2	-4.02	1.44	1.48
1	D	66	CRO	C1-N2	3.66	1.37	1.32
1	C	66	CRO	C1-N2	3.42	1.37	1.32
1	B	66	CRO	O2-C2	3.41	1.30	1.23
1	D	66	CRO	O2-C2	3.05	1.29	1.23
1	A	66	CRO	O2-C2	2.95	1.29	1.23
1	C	66	CRO	C2-N3	-2.91	1.33	1.39
1	C	66	CRO	O2-C2	2.88	1.29	1.23
1	B	66	CRO	C1-N2	2.84	1.36	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CA2-N2	-2.74	1.32	1.38
1	B	66	CRO	CE1-CD1	2.45	1.43	1.38
1	B	66	CRO	CE2-CD2	2.43	1.43	1.38
1	A	66	CRO	CA2-C2	-2.42	1.46	1.48
1	D	66	CRO	CA2-C2	-2.32	1.46	1.48
1	A	66	CRO	CE1-CD1	2.24	1.42	1.38
1	B	66	CRO	CA2-N2	-2.22	1.33	1.38
1	B	66	CRO	CA3-N3	-2.17	1.43	1.47

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	66	CRO	O2-C2-CA2	-17.02	121.40	130.96
1	C	66	CRO	O2-C2-CA2	-14.17	123.01	130.96
1	A	66	CRO	O2-C2-CA2	-14.03	123.08	130.96
1	B	66	CRO	O2-C2-CA2	-13.03	123.64	130.96
1	D	66	CRO	CA2-C2-N3	10.34	108.26	103.37
1	C	66	CRO	CA2-C2-N3	10.33	108.25	103.37
1	A	66	CRO	CA2-C2-N3	10.23	108.21	103.37
1	A	66	CRO	C1-CA1-N1	-7.35	98.03	109.96
1	A	66	CRO	CA3-N3-C1	7.03	135.60	127.16
1	C	66	CRO	C1-CA1-N1	-6.48	99.45	109.96
1	B	66	CRO	C1-CA1-N1	-5.45	101.12	109.96
1	D	66	CRO	C1-CA1-N1	-5.35	101.27	109.96
1	B	66	CRO	CA2-C2-N3	4.54	105.52	103.37
1	B	66	CRO	CG2-CB2-CA2	-4.49	124.44	129.94
1	A	66	CRO	CG1-CB1-CA1	-4.41	101.77	112.16
1	A	66	CRO	N3-C1-N2	4.28	114.42	111.45
1	B	66	CRO	CG1-CB1-CA1	-4.13	102.41	112.16
1	D	66	CRO	CG2-CB2-CA2	-3.98	125.06	129.94
1	C	66	CRO	C2-N3-C1	-3.97	105.96	107.97
1	A	66	CRO	C2-CA2-N2	-3.84	106.25	108.93
1	B	66	CRO	CA2-N2-C1	-3.72	103.03	105.77
1	B	66	CRO	N3-C1-N2	3.66	113.99	111.45
1	C	66	CRO	CA3-N3-C1	3.66	131.55	127.16
1	C	66	CRO	CG1-CB1-CA1	-3.37	104.22	112.16
1	C	66	CRO	CD2-CG2-CD1	3.31	122.54	117.64
1	B	66	CRO	O2-C2-N3	3.26	130.83	124.35
1	D	66	CRO	CG1-CB1-CA1	-3.21	104.60	112.16
1	D	66	CRO	C2-CA2-N2	-3.09	106.77	108.93
1	D	66	CRO	O2-C2-N3	3.01	130.34	124.35
1	A	66	CRO	O3-C3-CA3	-2.94	117.51	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	66	CRO	O3-C3-CA3	-2.89	117.67	126.39
1	C	66	CRO	CB2-CA2-C2	2.86	125.69	122.28
1	A	66	CRO	C2-N3-C1	-2.82	106.54	107.97
1	B	66	CRO	CA1-C1-N3	-2.76	121.43	124.75
1	B	66	CRO	CA3-N3-C1	2.60	130.28	127.16
1	A	66	CRO	CA3-N3-C2	-2.59	117.86	123.80
1	C	66	CRO	CD1-CE1-CZ	-2.50	117.13	119.88
1	C	66	CRO	CE2-CZ-CE1	2.48	123.95	119.77
1	D	66	CRO	N3-C1-N2	2.45	113.15	111.45
1	C	66	CRO	CE1-CD1-CG2	-2.44	118.06	121.25
1	A	66	CRO	CD2-CG2-CD1	2.43	121.24	117.64
1	D	66	CRO	CA2-N2-C1	-2.42	103.99	105.77
1	D	66	CRO	CD2-CE2-CZ	-2.38	117.27	119.88
1	B	66	CRO	CD1-CE1-CZ	-2.19	117.48	119.88
1	A	66	CRO	O2-C2-N3	2.16	128.64	124.35
1	C	66	CRO	CD2-CG2-CB2	-2.11	114.02	121.22
1	A	66	CRO	CA1-C1-N2	-2.09	120.96	123.89
1	C	66	CRO	O2-C2-N3	2.02	128.35	124.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRO	1	0
1	A	66	CRO	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	IMD	A	303	-	3,5,5	0.42	0	4,5,5	0.59	0
3	IMD	C	303	-	3,5,5	0.46	0	4,5,5	0.59	0
3	IMD	A	304	-	3,5,5	0.38	0	4,5,5	0.46	0
3	IMD	B	303	-	3,5,5	0.39	0	4,5,5	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
3	IMD	A	303	-	-	-	0/1/1/1
3	IMD	C	303	-	-	-	0/1/1/1
3	IMD	A	304	-	-	-	0/1/1/1
3	IMD	B	303	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	IMD	2	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	223/238 (93%)	0.15	6 (2%)	54	55	14, 25, 45, 61	0
1	B	223/238 (93%)	0.08	6 (2%)	54	55	14, 24, 46, 60	0
1	C	226/238 (94%)	0.08	8 (3%)	44	45	14, 24, 49, 65	0
1	D	223/238 (93%)	0.14	6 (2%)	54	55	15, 25, 47, 61	0
All	All	895/952 (94%)	0.11	26 (2%)	51	52	14, 24, 48, 65	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202[A]	TYR	4.2
1	D	202[A]	TYR	4.1
1	A	202[A]	TYR	4.0
1	A	192	PRO	3.8
1	B	192	PRO	3.7
1	B	202[A]	TYR	3.7
1	A	190	ASP	3.6
1	A	117	ASP	3.3
1	D	117	ASP	3.3
1	A	79	ARG	3.0
1	B	117	ASP	3.0
1	B	79	ARG	2.9
1	C	230	THR	2.9
1	C	190	ASP	2.9
1	D	192	PRO	2.9
1	C	79	ARG	2.7
1	C	192	PRO	2.6
1	C	117	ASP	2.5
1	C	157	GLN	2.5
1	C	3	ARG	2.5
1	D	157	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	80	ARG	2.4
1	D	6	GLU	2.1
1	B	190	ASP	2.1
1	B	200	TYR	2.1
1	D	5	GLU	2.1

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	CRO	A	66	22/23	0.95	0.07	18,20,21,25	0
1	CRO	D	66	22/23	0.95	0.07	18,19,23,24	0
1	CRO	B	66	22/23	0.96	0.07	16,19,22,25	0
1	CRO	C	66	22/23	0.97	0.07	16,18,21,22	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
3	IMD	A	303	5/5	0.96	0.09	25,25,29,31	0
3	IMD	C	303	5/5	0.96	0.07	26,27,30,33	0
3	IMD	B	303	5/5	0.96	0.08	24,25,28,31	0
3	IMD	A	304	5/5	0.97	0.09	24,24,30,31	0
2	NA	C	302	1/1	0.98	0.06	22,22,22,22	0
2	NA	B	302	1/1	0.98	0.07	29,29,29,29	0
2	NA	B	301	1/1	0.99	0.07	21,21,21,21	0
2	NA	A	302	1/1	0.99	0.06	21,21,21,21	0
2	NA	C	301	1/1	0.99	0.08	28,28,28,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	301	1/1	0.99	0.07	27,27,27,27	0
2	NA	D	301	1/1	0.99	0.06	26,26,26,26	0
2	NA	D	302	1/1	0.99	0.09	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.