wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 09:46 pm BST

PDB ID	:	4XVP
Title	:	X-ray structure of bGFP-C / EGFP complex
Authors	:	Chevrel, A.; Urvoas, A.; Li de la Sierra-Gallay, I.; Van Tilbeurgh, H.; Minard, P.; Valerio-Lepiniec, M.
Deposited on	:	2015-01-27
Resolution	:	3.40 Å(reported)

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

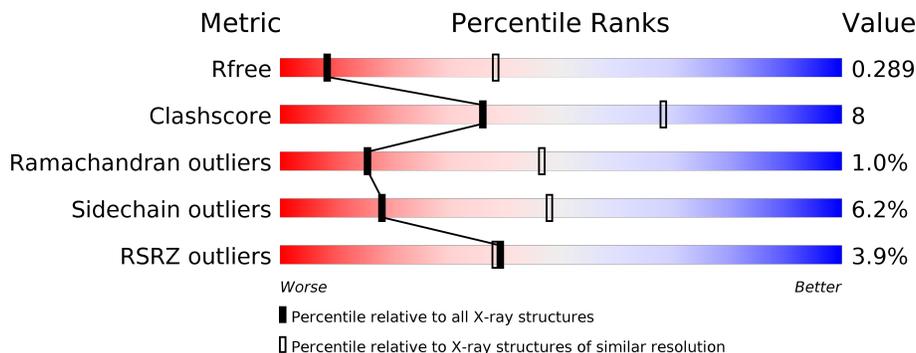|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	Percentile Ranks	Value
Rfree		0.289
Clashscore		8
Ramachandran outliers		1.0%
Sidechain outliers		6.2%
RSRZ outliers		3.9%

Worse　　　　　　　　　　　　　　　　　　　Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	272	2% — 60% 22% • 16%
1	B	272	8% — 65% 17% • 16%
1	C	272	66% 17% • 16%
2	D	170	4% — 72% 20% • 7%
2	E	170	6% — 73% 19% • 7%
2	F	170	% — 72% 20% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9144 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	228	Total 1824	C 1161	N 307	O 350	S 6	0	0	0
1	B	228	Total 1824	C 1161	N 307	O 350	S 6	0	0	0
1	C	228	Total 1824	C 1161	N 307	O 350	S 6	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP P42212
A	-19	ARG	-	expression tag	UNP P42212
A	-18	GLY	-	expression tag	UNP P42212
A	-17	SER	-	expression tag	UNP P42212
A	-16	HIS	-	expression tag	UNP P42212
A	-15	HIS	-	expression tag	UNP P42212
A	-14	HIS	-	expression tag	UNP P42212
A	-13	HIS	-	expression tag	UNP P42212
A	-12	HIS	-	expression tag	UNP P42212
A	-11	HIS	-	expression tag	UNP P42212
A	-10	THR	-	expression tag	UNP P42212
A	-9	ASP	-	expression tag	UNP P42212
A	-8	PRO	-	expression tag	UNP P42212
A	-7	HIS	-	expression tag	UNP P42212
A	-6	ALA	-	expression tag	UNP P42212
A	-5	SER	-	expression tag	UNP P42212
A	-4	SER	-	expression tag	UNP P42212
A	-3	ALA	-	expression tag	UNP P42212
A	-2	GLY	-	expression tag	UNP P42212
A	-1	SER	-	expression tag	UNP P42212
A	0	PRO	-	expression tag	UNP P42212
A	1	VAL	-	expression tag	UNP P42212
A	64	LEU	PHE	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	231	LEU	HIS	engineered mutation	UNP P42212
A	239	GLY	-	expression tag	UNP P42212
A	240	SER	-	expression tag	UNP P42212
A	241	GLY	-	expression tag	UNP P42212
A	242	ALA	-	expression tag	UNP P42212
A	243	SER	-	expression tag	UNP P42212
A	244	GLU	-	expression tag	UNP P42212
A	245	GLN	-	expression tag	UNP P42212
A	246	LYS	-	expression tag	UNP P42212
A	247	LEU	-	expression tag	UNP P42212
A	248	ILE	-	expression tag	UNP P42212
A	249	SER	-	expression tag	UNP P42212
A	250	GLU	-	expression tag	UNP P42212
A	251	GLU	-	expression tag	UNP P42212
A	252	ASP	-	expression tag	UNP P42212
A	253	LEU	-	expression tag	UNP P42212
B	-20	MET	-	initiating methionine	UNP P42212
B	-19	ARG	-	expression tag	UNP P42212
B	-18	GLY	-	expression tag	UNP P42212
B	-17	SER	-	expression tag	UNP P42212
B	-16	HIS	-	expression tag	UNP P42212
B	-15	HIS	-	expression tag	UNP P42212
B	-14	HIS	-	expression tag	UNP P42212
B	-13	HIS	-	expression tag	UNP P42212
B	-12	HIS	-	expression tag	UNP P42212
B	-11	HIS	-	expression tag	UNP P42212
B	-10	THR	-	expression tag	UNP P42212
B	-9	ASP	-	expression tag	UNP P42212
B	-8	PRO	-	expression tag	UNP P42212
B	-7	HIS	-	expression tag	UNP P42212
B	-6	ALA	-	expression tag	UNP P42212
B	-5	SER	-	expression tag	UNP P42212
B	-4	SER	-	expression tag	UNP P42212
B	-3	ALA	-	expression tag	UNP P42212
B	-2	GLY	-	expression tag	UNP P42212
B	-1	SER	-	expression tag	UNP P42212
B	0	PRO	-	expression tag	UNP P42212
B	1	VAL	-	expression tag	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	231	LEU	HIS	engineered mutation	UNP P42212
B	239	GLY	-	expression tag	UNP P42212
B	240	SER	-	expression tag	UNP P42212
B	241	GLY	-	expression tag	UNP P42212
B	242	ALA	-	expression tag	UNP P42212
B	243	SER	-	expression tag	UNP P42212
B	244	GLU	-	expression tag	UNP P42212
B	245	GLN	-	expression tag	UNP P42212
B	246	LYS	-	expression tag	UNP P42212
B	247	LEU	-	expression tag	UNP P42212
B	248	ILE	-	expression tag	UNP P42212
B	249	SER	-	expression tag	UNP P42212
B	250	GLU	-	expression tag	UNP P42212
B	251	GLU	-	expression tag	UNP P42212
B	252	ASP	-	expression tag	UNP P42212
B	253	LEU	-	expression tag	UNP P42212
C	-20	MET	-	initiating methionine	UNP P42212
C	-19	ARG	-	expression tag	UNP P42212
C	-18	GLY	-	expression tag	UNP P42212
C	-17	SER	-	expression tag	UNP P42212
C	-16	HIS	-	expression tag	UNP P42212
C	-15	HIS	-	expression tag	UNP P42212
C	-14	HIS	-	expression tag	UNP P42212
C	-13	HIS	-	expression tag	UNP P42212
C	-12	HIS	-	expression tag	UNP P42212
C	-11	HIS	-	expression tag	UNP P42212
C	-10	THR	-	expression tag	UNP P42212
C	-9	ASP	-	expression tag	UNP P42212
C	-8	PRO	-	expression tag	UNP P42212
C	-7	HIS	-	expression tag	UNP P42212
C	-6	ALA	-	expression tag	UNP P42212
C	-5	SER	-	expression tag	UNP P42212
C	-4	SER	-	expression tag	UNP P42212
C	-3	ALA	-	expression tag	UNP P42212
C	-2	GLY	-	expression tag	UNP P42212
C	-1	SER	-	expression tag	UNP P42212
C	0	PRO	-	expression tag	UNP P42212
C	1	VAL	-	expression tag	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	231	LEU	HIS	engineered mutation	UNP P42212
C	239	GLY	-	expression tag	UNP P42212
C	240	SER	-	expression tag	UNP P42212
C	241	GLY	-	expression tag	UNP P42212
C	242	ALA	-	expression tag	UNP P42212
C	243	SER	-	expression tag	UNP P42212
C	244	GLU	-	expression tag	UNP P42212
C	245	GLN	-	expression tag	UNP P42212
C	246	LYS	-	expression tag	UNP P42212
C	247	LEU	-	expression tag	UNP P42212
C	248	ILE	-	expression tag	UNP P42212
C	249	SER	-	expression tag	UNP P42212
C	250	GLU	-	expression tag	UNP P42212
C	251	GLU	-	expression tag	UNP P42212
C	252	ASP	-	expression tag	UNP P42212
C	253	LEU	-	expression tag	UNP P42212

- Molecule 2 is a protein called BGFP-C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	158	Total 1224	C 763	N 219	O 238	S 4	0	0	0
2	E	158	Total 1224	C 763	N 219	O 238	S 4	0	0	0
2	F	158	Total 1224	C 763	N 219	O 238	S 4	0	0	0

# 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 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.
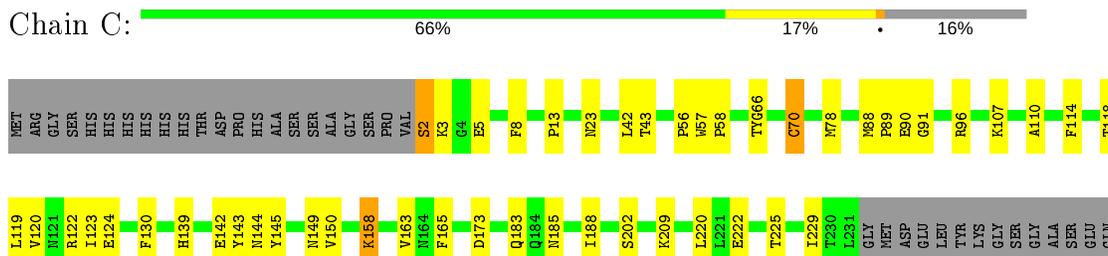
- Molecule 1: Green fluorescent protein
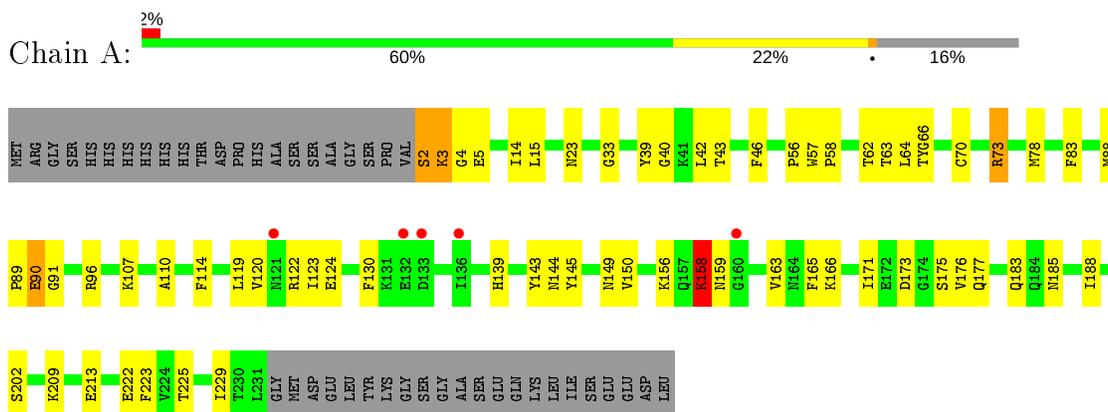
- Molecule 1: Green fluorescent protein
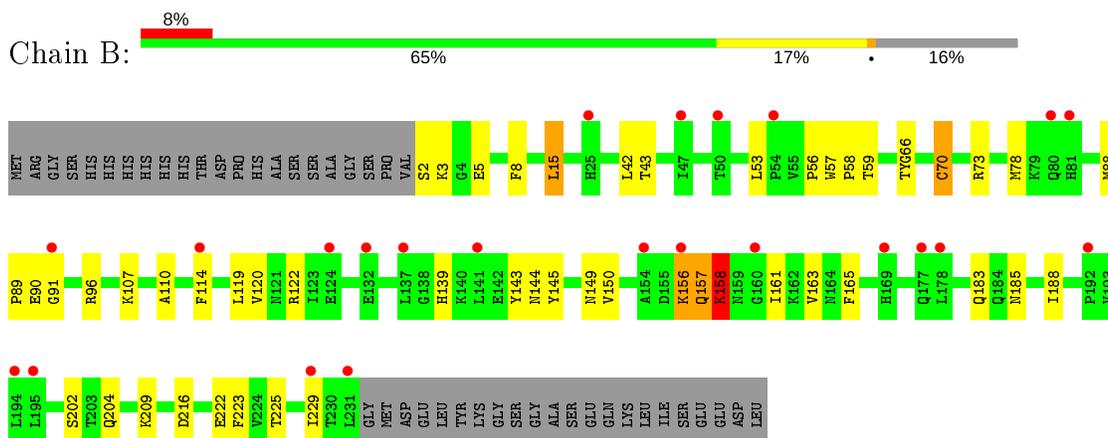
- Molecule 1: Green fluorescent protein

LYS LEU ILE SER GLU ASP LEU

● Molecule 2: BGFP-C

Chain D:

MET ARG GLY SER HIS HIS HIS HIS H9 D12 P13 K21 N22 L23 Y32 G42 A46 V47 E48 P49 Y60 L63 E64 A65 E71 I72 E79 P80 E88 D89 P90 R93 L98 I103 E106 V109 E110 P111 L112 I113 L116 Y122

W129 K133 E144 K145 L146 T151 A154 A158 L162 E163 T164 H165 K166 SER LEU ILE SER

● Molecule 2: BGFP-C

Chain E:

MET ARG GLY SER HIS HIS HIS HIS H9 D12 P13 E17 M18 N22 L23 Y32 G42 R45 E48 P49 Y60 E64 A65 A66 E67 E71 I72 E79 P80 A84 E88 D89 P90 R93 L98 I103 G104 D105 E106 V109 E110 P111 L112

I113 W129 K133 M143 E144 K145 L146 A147 E148 T151 L162 E163 T164 H165 K166 SER LEU ILE SER

● Molecule 2: BGFP-C

Chain F:

MET ARG GLY SER HIS HIS HIS HIS H9 E17 M18 K21 N22 L23 R29 Y32 G42 A46 V47 E48 P49 E64 A65 E71 I72 E79 P80 K86 D87 E88 D89 P90 R93 L98 I103 E106 V109 E110 P111 L112 I113 R121 R124

W129 K133 M143 E144 E148 T151 L162 K166 SER LEU ILE SER

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.52Å 71.55Å 179.20Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	46.70 – 3.40 46.72 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.70-3.40) 96.5 (46.72-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.292 0.212 , 0.289	Depositor DCC
R_{free} test set	888 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.6	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.7	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9144	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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

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	0.57	0/1842	0.70	0/2489
1	B	0.48	0/1842	0.65	0/2489
1	C	0.62	0/1842	0.73	0/2489
2	D	0.53	0/1239	0.72	0/1666
2	E	0.45	0/1239	0.68	0/1666
2	F	0.59	0/1239	0.72	1/1666 (0.1%)
All	All	0.55	0/9243	0.70	1/12465 (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	F	124	ARG	NE-CZ-NH1	5.32	122.96	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	1824	0	1775	46	0
1	B	1824	0	1775	26	0
1	C	1824	0	1774	28	1
2	D	1224	0	1238	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1224	0	1238	19	0
2	F	1224	0	1238	18	1
All	All	9144	0	9038	145	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.

The worst 5 of 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:A:156:LYS:HG3	2:D:164:THR:HG22	1.52	0.90
1:A:46:PHE:CE1	1:A:64:LEU:HD21	2.08	0.89
1:A:23:ASN:OD1	1:A:130:PHE:HB2	1.84	0.78
1:C:66:CRO:HG11	1:C:220:LEU:CD2	2.13	0.77
1:A:46:PHE:CE1	1:A:64:LEU:CD2	2.72	0.73

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)
1:C:173:ASP:OD1	2:F:86:LYS:NZ[4_749]	1.89	0.31

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	223/272 (82%)	201 (90%)	21 (9%)	1 (0%)	34	67
1	B	223/272 (82%)	206 (92%)	16 (7%)	1 (0%)	34	67
1	C	223/272 (82%)	202 (91%)	20 (9%)	1 (0%)	34	67
2	D	156/170 (92%)	146 (94%)	7 (4%)	3 (2%)	8	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	156/170 (92%)	147 (94%)	6 (4%)	3 (2%)	8	31
2	F	156/170 (92%)	145 (93%)	9 (6%)	2 (1%)	12	39
All	All	1137/1326 (86%)	1047 (92%)	79 (7%)	11 (1%)	15	46

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	158	LYS
1	A	158	LYS
1	B	158	LYS
2	D	22	ASN
2	E	22	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	199/235 (85%)	185 (93%)	14 (7%)	15	44
1	B	199/235 (85%)	181 (91%)	18 (9%)	9	32
1	C	199/235 (85%)	188 (94%)	11 (6%)	21	51
2	D	122/133 (92%)	117 (96%)	5 (4%)	30	59
2	E	122/133 (92%)	116 (95%)	6 (5%)	25	55
2	F	122/133 (92%)	116 (95%)	6 (5%)	25	55
All	All	963/1104 (87%)	903 (94%)	60 (6%)	18	48

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	157	GLN
1	C	3	LYS
2	F	103	ILE
1	B	202	SER
1	C	70	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	177	GLN
1	B	185	ASN
2	E	33	ASN
1	B	184	GLN
1	B	204	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 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	3.79	6 (26%)	30,32,34	3.87	12 (40%)
1	CRO	A	66	1	23,23,24	3.89	7 (30%)	30,32,34	3.73	9 (30%)
1	CRO	C	66	1	23,23,24	4.13	8 (34%)	30,32,34	3.86	11 (36%)

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	-	2/12/31/32	0/2/2/2
1	CRO	A	66	1	-	0/12/31/32	0/2/2/2
1	CRO	C	66	1	-	3/12/31/32	0/2/2/2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CB2-CA2	17.62	1.49	1.35
1	A	66	CRO	CB2-CA2	16.88	1.49	1.35
1	B	66	CRO	CB2-CA2	16.22	1.48	1.35
1	C	66	CRO	CA1-C1	-5.03	1.44	1.51
1	B	66	CRO	C1-N2	4.08	1.38	1.32

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	CA2-C2-N3	15.29	110.60	103.37
1	A	66	CRO	CA2-C2-N3	14.20	110.08	103.37
1	C	66	CRO	O2-C2-CA2	-13.88	123.16	130.96
1	C	66	CRO	CA2-C2-N3	11.27	108.70	103.37
1	A	66	CRO	O2-C2-CA2	-8.50	126.19	130.96

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	N2-C1-CA1-CB1
1	C	66	CRO	N3-C1-CA1-CB1
1	C	66	CRO	C3-CA3-N3-C2
1	B	66	CRO	N2-C1-CA1-CB1
1	B	66	CRO	N3-C1-CA1-CB1

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	66	CRO	1	0
1	A	66	CRO	3	0
1	C	66	CRO	5	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	227/272 (83%)	0.28	5 (2%)	62	60	68, 113, 146, 171	0
1	B	227/272 (83%)	0.71	23 (10%)	7	8	88, 154, 199, 222	0
1	C	227/272 (83%)	-0.15	0	100	100	57, 91, 121, 149	0
2	D	158/170 (92%)	0.16	6 (3%)	40	39	64, 101, 155, 178	0
2	E	158/170 (92%)	0.38	10 (6%)	20	21	89, 141, 179, 193	0
2	F	158/170 (92%)	-0.21	1 (0%)	89	89	52, 89, 151, 174	0
All	All	1155/1326 (87%)	0.21	45 (3%)	39	38	52, 114, 174, 222	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	5.3
1	B	231	LEU	5.1
2	D	166	LYS	4.5
2	E	166	LYS	4.2
1	B	194	LEU	4.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CRO	B	66	22/23	0.92	0.26	97,131,145,150	0
1	CRO	C	66	22/23	0.97	0.24	55,73,82,100	0
1	CRO	A	66	22/23	0.98	0.20	78,93,102,104	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.