



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:15 PM UTC

PDB ID : 4XVP / pdb_00004xvp
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

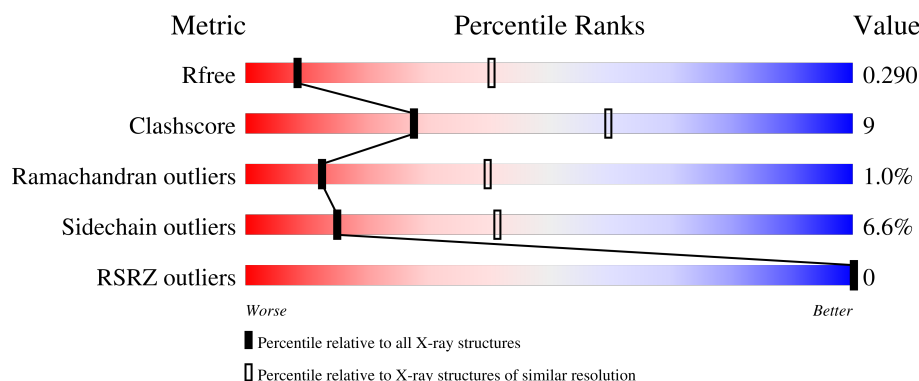
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. 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	
1	B	272	
1	C	272	
2	D	170	
2	E	170	

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Mol	Chain	Length	Quality of chain
2	F	170	70% 21% • 7%

2 Entry composition

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	C	N	O	S	0	0	0
			1824	1161	307	350	6			
1	B	228	Total	C	N	O	S	0	0	0
			1824	1161	307	350	6			
1	C	228	Total	C	N	O	S	0	0	0
			1824	1161	307	350	6			

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

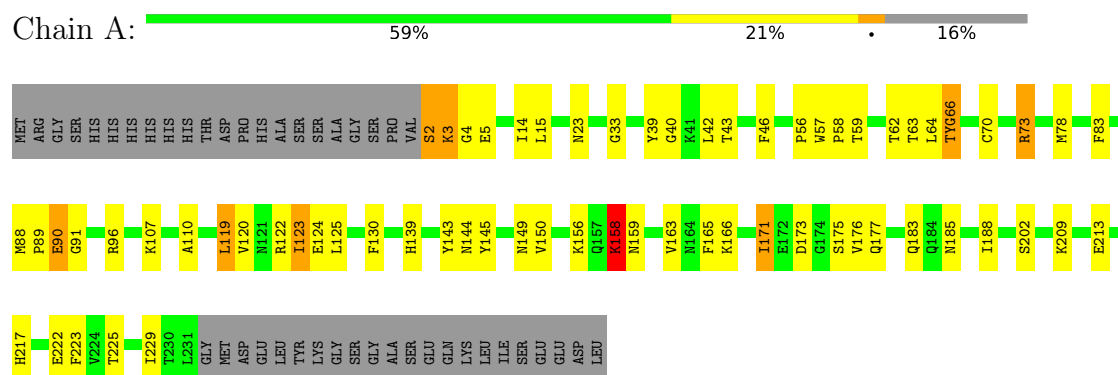
- Molecule 2 is a protein called BGFP-C.

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

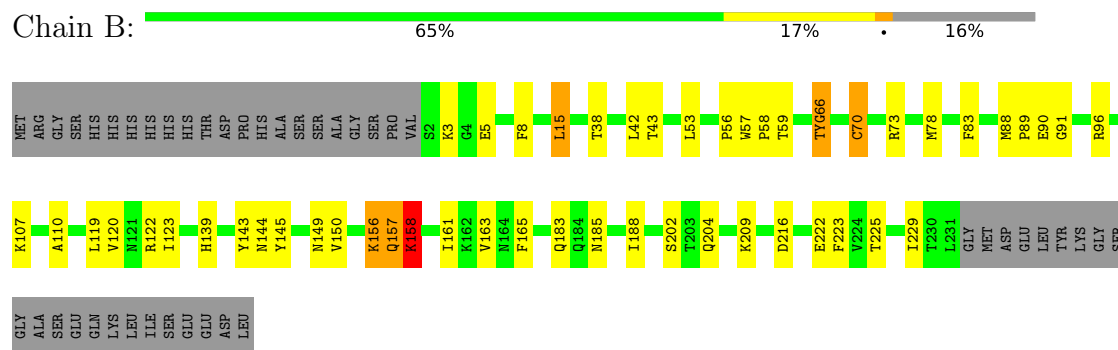
3 Residue-property plots [i](#)

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.

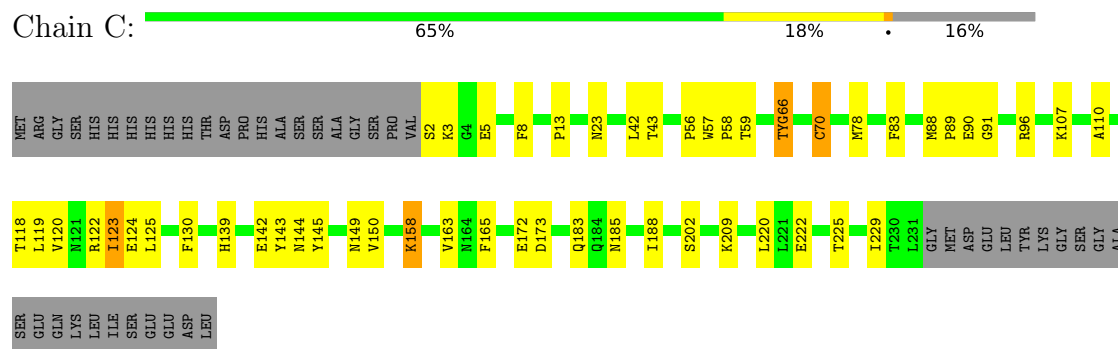
• Molecule 1: Green fluorescent protein



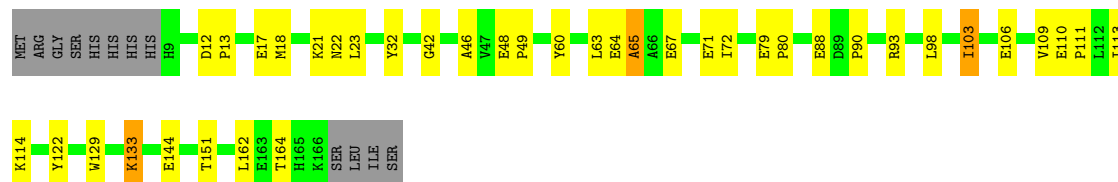
• Molecule 1: Green fluorescent protein



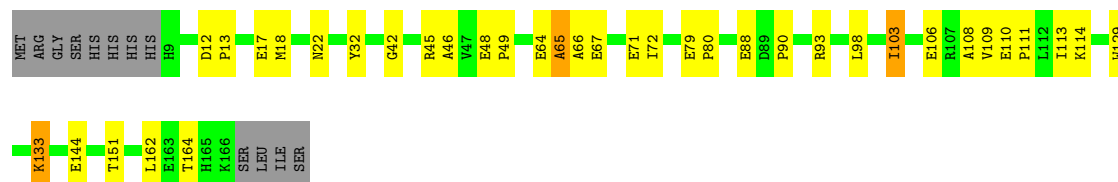
• Molecule 1: Green fluorescent protein



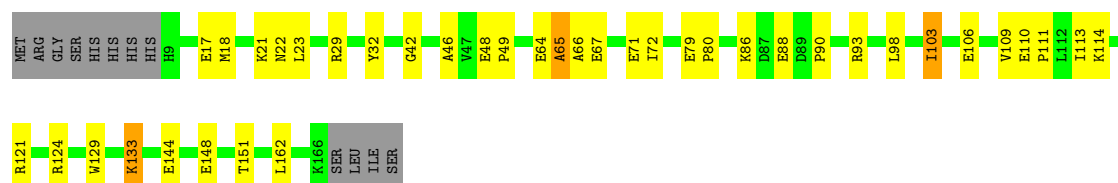
• Molecule 2: BGFP-C

Chain D:  70% 21% 7%

• Molecule 2: BGFP-C

Chain E:  71% 20% 7%

• Molecule 2: BGFP-C

Chain F:  70% 21% 7%

4 Data and refinement statistics

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 46.70 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.70-3.40) 96.7 (46.70-3.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.292 0.213 , 0.290	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 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.75	0/1842	0.89	1/2489 (0.0%)
1	B	0.65	0/1842	0.83	0/2489
1	C	0.82	0/1842	0.90	0/2489
2	D	0.74	0/1239	0.92	2/1666 (0.1%)
2	E	0.66	0/1239	0.88	1/1666 (0.1%)
2	F	0.83	0/1239	0.92	2/1666 (0.1%)
All	All	0.74	0/9243	0.89	6/12465 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	103	ILE	CB-CA-C	-6.25	102.47	112.16
2	E	103	ILE	CB-CA-C	-5.68	103.36	112.16
2	D	67	GLU	N-CA-C	-5.59	105.34	111.82
2	F	67	GLU	N-CA-C	-5.35	105.61	111.82
1	A	217	HIS	N-CA-C	5.27	115.25	108.34
2	D	103	ILE	CB-CA-C	-5.13	104.20	112.16

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	50	0
1	B	1824	0	1775	27	0
1	C	1824	0	1774	31	1
2	D	1224	0	1238	24	0
2	E	1224	0	1238	24	0
2	F	1224	0	1238	22	1
All	All	9144	0	9038	164	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 9.

All (164) 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
1:A:46:PHE:CD1	1:A:64:LEU:HD21	2.26	0.70
1:A:156:LYS:CG	2:D:164:THR:HG22	2.23	0.69
1:A:171:ILE:HD13	1:A:176:VAL:N	2.08	0.69
2:D:90:PRO:HA	2:D:93:ARG:HG2	1.79	0.64
1:B:156:LYS:HG2	1:B:157:GLN:N	2.13	0.64
1:A:223:PHE:CD1	2:E:13:PRO:HB2	2.34	0.63
2:E:90:PRO:HA	2:E:93:ARG:HG2	1.81	0.63
1:B:143:TYR:CZ	1:B:209:LYS:HE2	2.35	0.62
1:C:143:TYR:CZ	1:C:209:LYS:HE2	2.35	0.62
2:F:90:PRO:HA	2:F:93:ARG:HG2	1.82	0.61
1:A:171:ILE:HD12	1:A:171:ILE:N	2.15	0.61
1:A:3:LYS:NZ	1:A:90:GLU:OE2	2.34	0.60
1:A:39:TYR:CE1	2:E:17:GLU:HA	2.39	0.57
1:A:62:THR:O	1:A:66:CRO:C2	2.52	0.57
1:A:143:TYR:CZ	1:A:209:LYS:HE2	2.39	0.57
1:A:213:GLU:OE2	1:C:158:LYS:NZ	2.38	0.57
1:A:171:ILE:HD13	1:A:175:SER:C	2.30	0.56
1:C:42:LEU:HB2	1:C:222:GLU:HB3	1.87	0.56
1:C:23:ASN:HD21	1:C:130:PHE:N	2.04	0.56
1:C:149:ASN:ND2	2:F:71:GLU:OE2	2.36	0.55
1:C:66:CRO:HD1	1:C:66:CRO:N2	2.23	0.54
2:D:129:TRP:CH2	2:D:133:LYS:HG3	2.43	0.54
2:F:48:GLU:HB2	2:F:49:PRO:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:VAL:HB	1:C:183:GLN:HB3	1.90	0.53
1:C:66:CRO:HG11	1:C:220:LEU:HD21	1.91	0.53
1:A:63:THR:HA	1:A:96:ARG:NH1	2.24	0.53
1:B:66:CRO:O2	1:B:96:ARG:NH2	2.37	0.53
2:E:48:GLU:HB2	2:E:49:PRO:HD3	1.90	0.52
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.58	0.52
2:D:48:GLU:HB2	2:D:49:PRO:HD3	1.90	0.52
1:C:183:GLN:HE21	1:C:185:ASN:HD21	1.58	0.52
1:C:56:PRO:HG3	1:C:139:HIS:HA	1.93	0.51
1:A:163:VAL:HB	1:A:183:GLN:HB3	1.91	0.51
2:D:32:TYR:CE2	2:D:64:GLU:CG	2.94	0.51
1:C:110:ALA:HA	1:C:122:ARG:O	2.12	0.50
2:D:32:TYR:CE2	2:D:64:GLU:HG2	2.47	0.50
2:F:32:TYR:CE2	2:F:64:GLU:CG	2.94	0.50
2:F:17:GLU:O	2:F:18:MET:C	2.55	0.50
1:A:42:LEU:HB2	1:A:222:GLU:HB3	1.94	0.50
2:F:32:TYR:CE2	2:F:64:GLU:HG2	2.47	0.49
1:A:183:GLN:HE21	1:A:185:ASN:HD21	1.61	0.49
1:B:204:GLN:HE22	2:D:13:PRO:HD2	1.77	0.49
2:F:110:GLU:HB3	2:F:111:PRO:HD3	1.93	0.49
1:A:171:ILE:HD11	1:A:177:GLN:N	2.27	0.49
1:B:163:VAL:HB	1:B:183:GLN:HB3	1.95	0.49
1:A:149:ASN:ND2	2:D:71:GLU:OE2	2.44	0.49
2:D:32:TYR:C	2:D:32:TYR:CD1	2.91	0.49
1:C:23:ASN:HD21	1:C:130:PHE:H	1.59	0.49
1:B:15:LEU:O	1:B:120:VAL:HA	2.13	0.49
1:C:119:LEU:HD13	1:C:120:VAL:N	2.28	0.49
1:B:110:ALA:HA	1:B:122:ARG:O	2.13	0.48
2:F:46:ALA:C	2:F:49:PRO:HD2	2.38	0.48
1:A:110:ALA:HA	1:A:122:ARG:O	2.13	0.48
2:E:32:TYR:CE2	2:E:64:GLU:CG	2.96	0.48
1:B:58:PRO:O	1:B:59:THR:C	2.55	0.48
1:B:149:ASN:ND2	2:E:71:GLU:OE2	2.47	0.48
2:E:32:TYR:CE2	2:E:64:GLU:HG2	2.49	0.48
2:F:129:TRP:CH2	2:F:133:LYS:HG3	2.49	0.48
1:A:73:ARG:HG3	2:E:45:ARG:NH1	2.29	0.47
2:D:46:ALA:C	2:D:49:PRO:HD2	2.40	0.47
1:A:40:GLY:HA3	1:A:73:ARG:HB2	1.97	0.47
1:A:158:LYS:HG3	1:A:159:ASN:H	1.79	0.47
2:E:79:GLU:HB2	2:E:80:PRO:HD3	1.97	0.47
1:C:57:TRP:HB2	1:C:58:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:129:TRP:CH2	2:E:133:LYS:HG3	2.50	0.47
1:A:88:MET:SD	1:A:91:GLY:HA2	2.54	0.46
1:C:150:VAL:HG13	1:C:165:PHE:CD1	2.50	0.46
2:F:144:GLU:HA	2:F:162:LEU:HD11	1.98	0.46
1:A:83:PHE:CD2	1:A:83:PHE:C	2.94	0.46
1:C:13:PRO:HG2	1:C:118:THR:HA	1.98	0.46
1:C:88:MET:HB3	1:C:89:PRO:HA	1.98	0.46
1:B:150:VAL:HG13	1:B:165:PHE:CD1	2.50	0.46
2:D:79:GLU:HB2	2:D:80:PRO:HD3	1.98	0.46
2:F:79:GLU:HB2	2:F:80:PRO:HD3	1.98	0.46
1:C:8:PHE:CZ	1:C:70:CYS:HB2	2.50	0.45
1:C:91:GLY:HA3	1:C:188:ILE:HD12	1.99	0.45
1:A:96:ARG:NE	1:A:183:GLN:OE1	2.48	0.45
1:C:142:GLU:OE2	2:F:29:ARG:NH1	2.49	0.45
2:E:17:GLU:O	2:E:18:MET:C	2.59	0.45
1:A:150:VAL:HG13	1:A:165:PHE:CD1	2.51	0.45
1:C:96:ARG:NE	1:C:183:GLN:OE1	2.48	0.45
1:B:88:MET:SD	1:B:91:GLY:HA2	2.57	0.45
1:A:88:MET:HB3	1:A:89:PRO:HA	1.99	0.45
2:E:32:TYR:CD1	2:E:32:TYR:C	2.95	0.45
2:F:64:GLU:O	2:F:65:ALA:C	2.60	0.45
1:A:3:LYS:HD2	1:A:4:GLY:N	2.32	0.45
1:A:14:ILE:N	1:A:33:GLY:O	2.47	0.45
2:D:144:GLU:HA	2:D:162:LEU:HD11	1.98	0.45
2:E:42:GLY:HA2	2:E:72:ILE:HG12	1.98	0.44
2:E:46:ALA:C	2:E:49:PRO:HD2	2.41	0.44
1:A:64:LEU:C	1:A:64:LEU:HD23	2.43	0.44
1:C:88:MET:SD	1:C:91:GLY:HA2	2.57	0.44
2:D:17:GLU:O	2:D:18:MET:C	2.59	0.44
2:F:21:LYS:O	2:F:23:LEU:N	2.50	0.44
1:A:66:CRO:O2	1:A:96:ARG:NH2	2.31	0.44
1:B:42:LEU:HB2	1:B:222:GLU:HB3	1.99	0.44
1:B:57:TRP:HB2	1:B:58:PRO:HD3	2.00	0.44
1:B:91:GLY:HA3	1:B:188:ILE:HD12	1.99	0.44
2:E:144:GLU:HA	2:E:162:LEU:HD11	1.99	0.44
2:E:64:GLU:O	2:E:65:ALA:C	2.60	0.44
2:D:64:GLU:O	2:D:65:ALA:C	2.61	0.43
1:A:58:PRO:O	1:A:59:THR:C	2.59	0.43
1:A:91:GLY:HA3	1:A:188:ILE:HD12	2.01	0.43
1:B:156:LYS:HD2	2:E:164:THR:HG23	2.00	0.43
2:F:32:TYR:CE2	2:F:64:GLU:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:CRO:HG11	1:C:220:LEU:HD22	1.96	0.43
1:A:158:LYS:CG	1:A:159:ASN:H	2.32	0.43
1:B:83:PHE:CD2	1:B:83:PHE:C	2.97	0.43
1:B:96:ARG:NE	1:B:183:GLN:OE1	2.51	0.43
1:B:8:PHE:CZ	1:B:70:CYS:HB2	2.52	0.43
2:D:110:GLU:HB3	2:D:111:PRO:HD3	2.01	0.43
2:D:42:GLY:HA2	2:D:72:ILE:HG12	2.00	0.43
2:F:21:LYS:C	2:F:23:LEU:N	2.77	0.43
1:B:223:PHE:CD1	2:D:13:PRO:HB2	2.53	0.43
1:C:66:CRO:O2	1:C:96:ARG:NH2	2.41	0.43
2:F:32:TYR:CD1	2:F:32:TYR:C	2.97	0.43
1:A:125:LEU:C	1:A:125:LEU:HD23	2.44	0.43
1:A:15:LEU:O	1:A:120:VAL:HA	2.18	0.42
2:D:32:TYR:CE2	2:D:64:GLU:HG3	2.53	0.42
2:E:32:TYR:CE2	2:E:64:GLU:HG3	2.54	0.42
1:A:57:TRP:HB2	1:A:58:PRO:HD3	2.01	0.42
1:B:88:MET:HB3	1:B:89:PRO:HA	2.01	0.42
2:F:121:ARG:HG3	2:F:124:ARG:HH21	1.84	0.42
1:A:66:CRO:HD1	1:A:66:CRO:N2	2.34	0.42
1:B:158:LYS:N	1:B:158:LYS:HD2	2.34	0.42
2:E:64:GLU:C	2:E:66:ALA:N	2.77	0.42
2:F:88:GLU:O	2:F:93:ARG:NH1	2.52	0.42
1:A:2:SER:O	1:A:5:GLU:HG2	2.19	0.42
1:A:119:LEU:HD13	1:A:120:VAL:N	2.34	0.42
1:B:119:LEU:HD13	1:B:120:VAL:N	2.35	0.42
1:A:40:GLY:CA	1:A:73:ARG:HB2	2.50	0.41
2:E:88:GLU:O	2:E:93:ARG:NH1	2.53	0.41
1:C:58:PRO:O	1:C:59:THR:C	2.64	0.41
1:C:83:PHE:CD2	1:C:83:PHE:C	2.98	0.41
1:C:123:ILE:HG22	1:C:124:GLU:N	2.35	0.41
2:D:21:LYS:O	2:D:23:LEU:N	2.54	0.41
2:E:110:GLU:HB3	2:E:111:PRO:HD3	2.01	0.41
1:A:171:ILE:HD11	1:A:176:VAL:C	2.45	0.41
1:B:56:PRO:HG3	1:B:139:HIS:HA	2.02	0.41
2:D:106:GLU:O	2:D:109:VAL:HG23	2.19	0.41
2:F:106:GLU:O	2:F:109:VAL:HG23	2.20	0.41
1:A:78:MET:HG2	1:A:229:ILE:HB	2.03	0.41
1:C:2:SER:O	1:C:5:GLU:HG2	2.20	0.41
2:E:106:GLU:O	2:E:109:VAL:HG23	2.21	0.41
2:F:64:GLU:C	2:F:66:ALA:N	2.79	0.41
1:A:123:ILE:HG22	1:A:124:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HE2	2:D:122:TYR:CE2	2.56	0.41
1:B:53:LEU:N	1:B:216:ASP:OD2	2.50	0.41
1:B:78:MET:HG2	1:B:229:ILE:HB	2.03	0.41
1:A:171:ILE:N	1:A:171:ILE:CD1	2.81	0.41
1:C:125:LEU:C	1:C:125:LEU:HD23	2.46	0.40
2:D:88:GLU:O	2:D:93:ARG:NH1	2.54	0.40
2:E:64:GLU:O	2:E:67:GLU:N	2.55	0.40
1:B:156:LYS:HD3	1:B:156:LYS:H	1.86	0.40
2:D:60:TYR:O	2:D:63:LEU:HB3	2.21	0.40
2:F:42:GLY:HA2	2:F:72:ILE:HG12	2.03	0.40
1:A:56:PRO:HG3	1:A:139:HIS:HA	2.04	0.40
1:C:78:MET:HG2	1:C:229:ILE:HB	2.03	0.40
2:E:108:ALA:C	2:E:111:PRO:HD2	2.47	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	30	59
1	B	223/272 (82%)	206 (92%)	16 (7%)	1 (0%)	30	59
1	C	223/272 (82%)	202 (91%)	20 (9%)	1 (0%)	30	59
2	D	156/170 (92%)	146 (94%)	7 (4%)	3 (2%)	6	26
2	E	156/170 (92%)	147 (94%)	6 (4%)	3 (2%)	6	26
2	F	156/170 (92%)	145 (93%)	9 (6%)	2 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1137/1326 (86%)	1047 (92%)	79 (7%)	11 (1%)	12	40

All (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
2	F	22	ASN
2	D	65	ALA
2	E	65	ALA
2	D	12	ASP
2	F	65	ALA
2	E	12	ASP

5.3.2 Protein sidechains ⓘ

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%)	183 (92%)	16 (8%)	11	36
1	B	199/235 (85%)	181 (91%)	18 (9%)	9	30
1	C	199/235 (85%)	188 (94%)	11 (6%)	19	46
2	D	122/133 (92%)	116 (95%)	6 (5%)	22	49
2	E	122/133 (92%)	116 (95%)	6 (5%)	22	49
2	F	122/133 (92%)	115 (94%)	7 (6%)	18	45
All	All	963/1104 (87%)	899 (93%)	64 (7%)	15	41

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER

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Mol	Chain	Res	Type
1	A	3	LYS
1	A	43	THR
1	A	70	CYS
1	A	73	ARG
1	A	90	GLU
1	A	107	LYS
1	A	119	LEU
1	A	123	ILE
1	A	144	ASN
1	A	145	TYR
1	A	158	LYS
1	A	171	ILE
1	A	173	ASP
1	A	202	SER
1	A	225	THR
1	B	3	LYS
1	B	5	GLU
1	B	15	LEU
1	B	38	THR
1	B	43	THR
1	B	70	CYS
1	B	73	ARG
1	B	90	GLU
1	B	107	LYS
1	B	123	ILE
1	B	144	ASN
1	B	145	TYR
1	B	156	LYS
1	B	157	GLN
1	B	158	LYS
1	B	161	ILE
1	B	202	SER
1	B	225	THR
1	C	3	LYS
1	C	43	THR
1	C	70	CYS
1	C	90	GLU
1	C	107	LYS
1	C	123	ILE
1	C	144	ASN
1	C	145	TYR
1	C	172	GLU

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Mol	Chain	Res	Type
1	C	202	SER
1	C	225	THR
2	D	98	LEU
2	D	103	ILE
2	D	113	ILE
2	D	114	LYS
2	D	133	LYS
2	D	151	THR
2	E	98	LEU
2	E	103	ILE
2	E	113	ILE
2	E	114	LYS
2	E	133	LYS
2	E	151	THR
2	F	98	LEU
2	F	103	ILE
2	F	113	ILE
2	F	114	LYS
2	F	133	LYS
2	F	148	GLU
2	F	151	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	144	ASN
1	A	146	ASN
1	A	169	HIS
1	A	185	ASN
1	B	94	GLN
1	B	144	ASN
1	B	170	ASN
1	B	177	GLN
1	B	185	ASN
1	B	204	GLN
1	C	23	ASN
1	C	94	GLN
1	C	144	ASN
1	C	170	ASN
1	C	177	GLN
1	C	185	ASN

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Mol	Chain	Res	Type
2	D	33	ASN
2	E	33	ASN
2	F	33	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	A	66	1	22,23,24	3.48	6 (27%)	30,32,34	2.85	8 (26%)
1	CRO	B	66	1	22,23,24	3.43	6 (27%)	30,32,34	2.99	10 (33%)
1	CRO	C	66	1	22,23,24	3.64	7 (31%)	30,32,34	3.23	10 (33%)

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	A	66	1	-	0/12/31/32	0/2/2/2
1	CRO	B	66	1	-	2/12/31/32	0/2/2/2
1	CRO	C	66	1	-	4/12/31/32	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CB2-CA2	15.27	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	14.62	1.49	1.35
1	B	66	CRO	CB2-CA2	14.05	1.48	1.35
1	A	66	CRO	C2-N3	-4.20	1.30	1.40
1	B	66	CRO	C1-N2	4.10	1.38	1.32
1	B	66	CRO	C2-N3	-4.03	1.30	1.40
1	C	66	CRO	O2-C2	3.49	1.30	1.23
1	C	66	CRO	C2-N3	-3.47	1.32	1.40
1	C	66	CRO	C1-N2	3.12	1.36	1.32
1	A	66	CRO	CA2-C2	-3.08	1.45	1.48
1	A	66	CRO	C1-N2	2.94	1.36	1.32
1	B	66	CRO	O2-C2	2.63	1.28	1.23
1	C	66	CRO	C1-N3	-2.59	1.32	1.37
1	A	66	CRO	O2-C2	2.40	1.28	1.23
1	A	66	CRO	CA2-N2	-2.15	1.34	1.38
1	C	66	CRO	CA2-C2	-2.12	1.46	1.48
1	C	66	CRO	CA2-N2	-2.10	1.34	1.38
1	B	66	CRO	CA2-N2	-2.08	1.34	1.38
1	B	66	CRO	CE1-CD1	2.03	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-12.31	123.16	131.02
1	B	66	CRO	CA2-C2-N3	8.46	110.60	103.50
1	A	66	CRO	CA2-C2-N3	7.84	110.08	103.50
1	A	66	CRO	O2-C2-CA2	-7.57	126.19	131.02
1	B	66	CRO	C2-N3-C1	-7.11	104.78	108.07
1	C	66	CRO	CA2-C2-N3	6.19	108.70	103.50
1	C	66	CRO	C2-N3-C1	-5.86	105.36	108.07
1	B	66	CRO	CB2-CA2-C2	5.63	129.18	122.36
1	B	66	CRO	O2-C2-CA2	-5.61	127.44	131.02
1	A	66	CRO	C2-CA2-N2	-5.24	105.20	108.95
1	A	66	CRO	C2-N3-C1	-4.81	105.84	108.07
1	A	66	CRO	CB2-CA2-C2	4.79	128.16	122.36
1	B	66	CRO	C2-CA2-N2	-4.77	105.53	108.95
1	C	66	CRO	N3-C1-N2	4.08	114.69	111.48
1	A	66	CRO	C1-CA1-N1	-3.75	103.08	109.78
1	C	66	CRO	CG2-CB2-CA2	-3.71	125.45	129.87
1	B	66	CRO	CG2-CB2-CA2	-3.37	125.86	129.87
1	A	66	CRO	CG2-CB2-CA2	-3.25	126.00	129.87
1	C	66	CRO	C2-CA2-N2	-3.22	106.65	108.95
1	C	66	CRO	CA1-C1-N3	-3.05	121.07	124.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	CB2-CA2-C2	2.91	125.88	122.36
1	B	66	CRO	CD1-CE1-CZ	2.61	122.64	119.88
1	B	66	CRO	CB2-CA2-N2	-2.56	125.28	128.76
1	B	66	CRO	CE2-CZ-CE1	-2.37	115.99	119.77
1	C	66	CRO	CD1-CE1-CZ	2.28	122.29	119.88
1	A	66	CRO	O3-C3-CA3	-2.28	115.23	125.47
1	B	66	CRO	N3-C1-N2	2.20	113.21	111.48
1	C	66	CRO	C1-CA1-N1	-2.05	106.11	109.78

There are no chirality outliers.

All (6) 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
1	C	66	CRO	N1-CA1-CB1-CG1

There are no ring outliers.

3 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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, 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%)	-0.46	0 100 100	68, 113, 146, 171	0
1	B	227/272 (83%)	-0.33	0 100 100	88, 154, 199, 222	0
1	C	227/272 (83%)	-0.63	0 100 100	57, 91, 121, 149	0
2	D	158/170 (92%)	-0.54	0 100 100	64, 101, 155, 178	0
2	E	158/170 (92%)	-0.45	0 100 100	89, 141, 179, 193	0
2	F	158/170 (92%)	-0.72	0 100 100	52, 89, 151, 174	0
All	All	1155/1326 (87%)	-0.51	0 100 100	52, 114, 174, 222	0

There are no RSRZ outliers to report.

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

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	0.95	0.09	97,131,145,150	0
1	CRO	A	66	22/23	0.96	0.07	78,93,102,104	0
1	CRO	C	66	22/23	0.97	0.06	55,73,82,100	0

6.3 Carbohydrates

There are no oligosaccharides 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.