



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2017 – 09:33 AM EST

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 : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

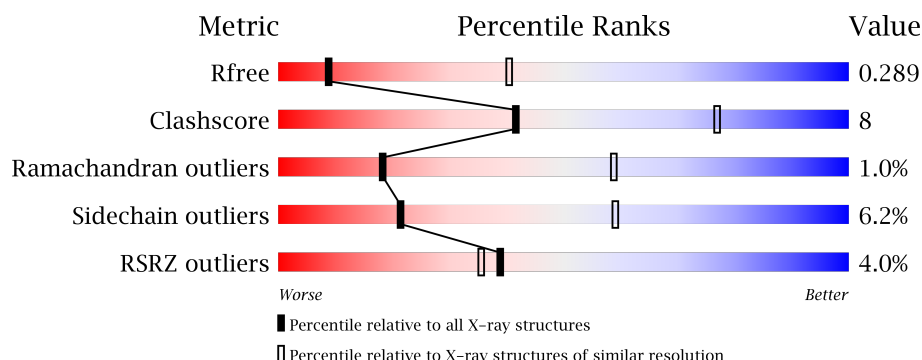
1 Overall quality at a glance

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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (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. 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	<div> <div>3%</div> <div>60% 22% 16%</div> </div>
1	B	272	<div> <div>8%</div> <div>65% 17% 16%</div> </div>
1	C	272	<div> <div>66% 17% 16%</div> </div>
2	D	170	<div> <div>4%</div> <div>72% 20% 7%</div> </div>
2	E	170	<div> <div>6%</div> <div>73% 19% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	170	<div><div><div>%</div><div><div></div></div><div>72%</div><div>20%</div><div>• 7%</div></div></div>

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

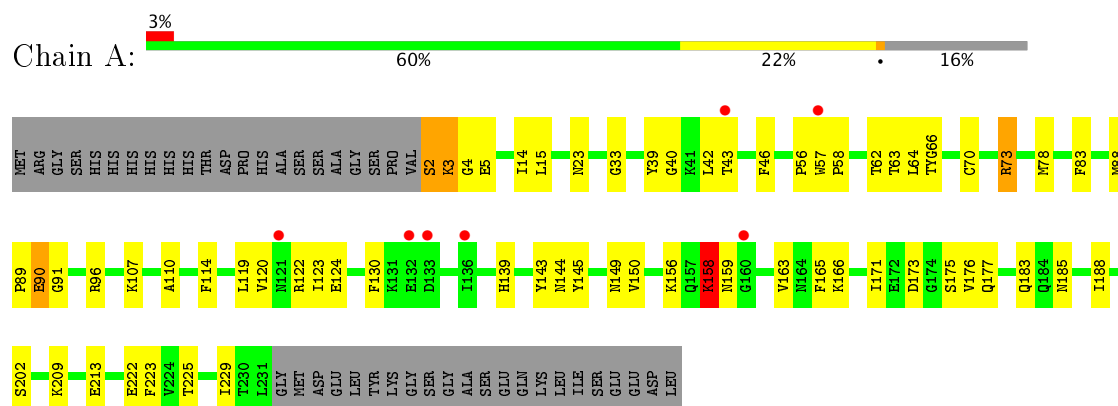
- Molecule 2 is a protein called BGFP-C.

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			

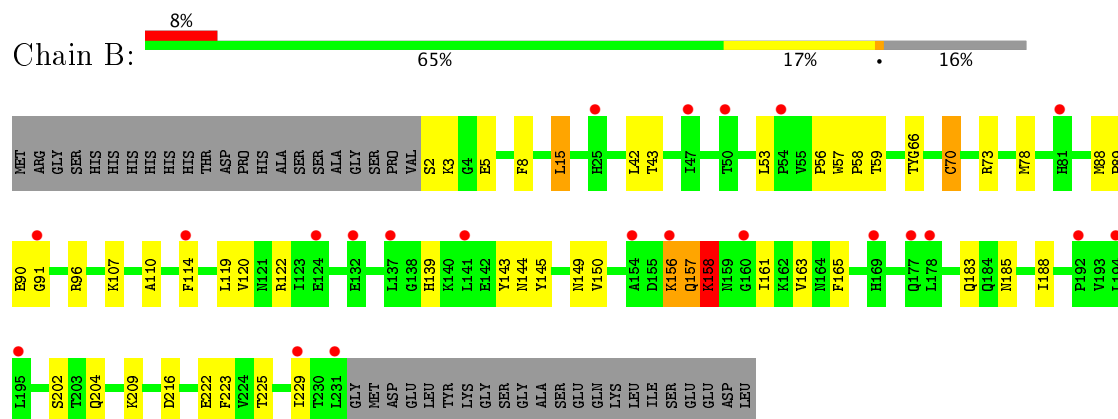
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

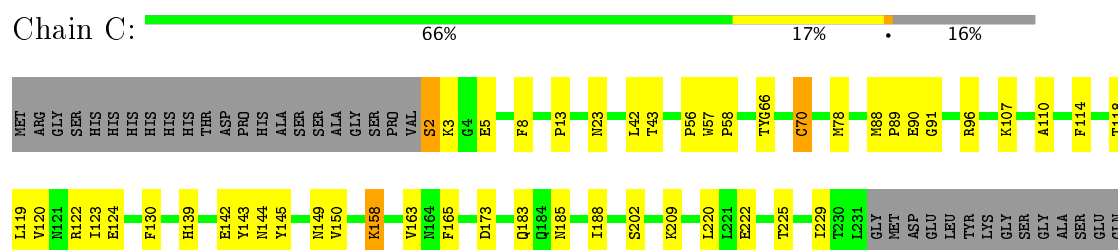
• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein



• Molecule 1: Green fluorescent protein

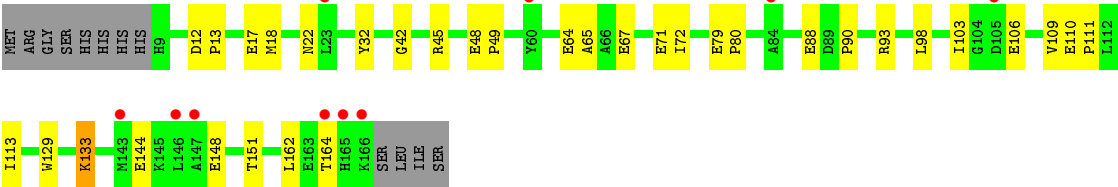


LYS
LEU
ILE
SER
SER
GLU
GLU
ASP
LEU

• Molecule 2: BGFP-C



• Molecule 2: BGFP-C



• Molecule 2: BGFP-C



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 46.72 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.209 , 0.292 0.212 , 0.289	Depositor DCC
R_{free} test set	887 reflections (5.27%)	DCC
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	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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	0.57	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(°)	Ideal(°)
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.

All (145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:171:ILE:HD13	1:A:175:SER:C	2.30	0.51
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
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
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
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: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
1:A:40:GLY:HA3	1:A:73:ARG:HB2	1.97	0.47
2:E:79:GLU:HB2	2:E:80:PRO:HD3	1.97	0.47
1:A:158:LYS:HG3	1:A:159:ASN:H	1.79	0.47
1:C:57:TRP:HB2	1:C:58:PRO:HD3	1.96	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:17:GLU:O	2:F:18:MET:C	2.55	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
1:A:14:ILE:N	1:A:33:GLY:O	2.47	0.45
1:A:3:LYS:HD2	1:A:4:GLY:N	2.32	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
1:C:88:MET:SD	1:C:91:GLY:HA2	2.57	0.44
2:D:32:TYR:C	2:D:32:TYR:CD1	2.91	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:91:GLY:HA3	1:B:188:ILE:HD12	1.99	0.44
1:B:57:TRP:HB2	1:B:58:PRO:HD3	2.00	0.44
2:E:144:GLU:HA	2:E:162:LEU:HD11	1.99	0.44
2:F:46:ALA:C	2:F:49:PRO:HD2	2.38	0.44
1:B:58:PRO:O	1:B:59:THR:C	2.55	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
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: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
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
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:D:46:ALA:C	2:D:49:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:83:PHE:C	1:A:83:PHE:CD2	2.94	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: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
1:A:123:ILE:HG22	1:A:124:GLU:N	2.36	0.41
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:CD1	1:A:171:ILE:N	2.81	0.41
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:E:17:GLU:O	2:E:18:MET:C	2.59	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

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

5.3.1 Protein backbone

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%)	38	75
1	B	223/272 (82%)	206 (92%)	16 (7%)	1 (0%)	38	75
1	C	223/272 (82%)	202 (91%)	20 (9%)	1 (0%)	38	75
2	D	156/170 (92%)	146 (94%)	7 (4%)	3 (2%)	9	45
2	E	156/170 (92%)	147 (94%)	6 (4%)	3 (2%)	9	45
2	F	156/170 (92%)	145 (93%)	9 (6%)	2 (1%)	14	53
All	All	1137/1326 (86%)	1047 (92%)	79 (7%)	11 (1%)	18	59

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%)	185 (93%)	14 (7%)	18	55
1	B	199/235 (85%)	181 (91%)	18 (9%)	11	41
1	C	199/235 (85%)	188 (94%)	11 (6%)	25	63
2	D	122/133 (92%)	117 (96%)	5 (4%)	35	71
2	E	122/133 (92%)	116 (95%)	6 (5%)	29	66
2	F	122/133 (92%)	116 (95%)	6 (5%)	29	66
All	All	963/1104 (87%)	903 (94%)	60 (6%)	21	59

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
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	114	PHE
1	A	144	ASN
1	A	145	TYR
1	A	158	LYS
1	A	173	ASP
1	A	202	SER
1	A	225	THR
1	B	2	SER
1	B	3	LYS
1	B	5	GLU
1	B	15	LEU
1	B	43	THR
1	B	70	CYS
1	B	73	ARG
1	B	90	GLU
1	B	107	LYS
1	B	114	PHE
1	B	144	ASN
1	B	145	TYR
1	B	156	LYS
1	B	157	GLN
1	B	158	LYS
1	B	161	ILE

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Mol	Chain	Res	Type
1	B	202	SER
1	B	225	THR
1	C	2	SER
1	C	3	LYS
1	C	43	THR
1	C	70	CYS
1	C	90	GLU
1	C	107	LYS
1	C	114	PHE
1	C	144	ASN
1	C	145	TYR
1	C	202	SER
1	C	225	THR
2	D	98	LEU
2	D	103	ILE
2	D	113	ILE
2	D	133	LYS
2	D	151	THR
2	E	98	LEU
2	E	103	ILE
2	E	113	ILE
2	E	133	LYS
2	E	148	GLU
2	E	151	THR
2	F	98	LEU
2	F	103	ILE
2	F	113	ILE
2	F	133	LYS
2	F	148	GLU
2	F	151	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	144	ASN
1	A	146	ASN
1	A	177	GLN
1	A	184	GLN
1	A	185	ASN
1	B	94	GLN
1	B	144	ASN

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Mol	Chain	Res	Type
1	B	159	ASN
1	B	170	ASN
1	B	177	GLN
1	B	184	GLN
1	B	185	ASN
1	B	204	GLN
1	C	94	GLN
1	C	144	ASN
1	C	146	ASN
1	C	177	GLN
1	C	184	GLN
1	C	185	ASN
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	23,23,24	3.68	7 (30%)	27,32,34	3.90	7 (25%)
1	CRO	B	66	1	23,23,24	3.58	5 (21%)	27,32,34	4.02	11 (40%)
1	CRO	C	66	1	23,23,24	3.92	7 (30%)	27,32,34	4.08	9 (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	-	0/12/31/32	0/2/2/2
1	CRO	C	66	1	-	0/12/31/32	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	CA1-C1	-4.93	1.44	1.51
1	A	66	CRO	C2-N3	-3.88	1.30	1.39
1	B	66	CRO	C2-N3	-3.72	1.30	1.39
1	A	66	CRO	CA2-C2	-3.30	1.45	1.48
1	C	66	CRO	C2-N3	-3.19	1.32	1.39
1	A	66	CRO	CA1-C1	-3.06	1.46	1.51
1	B	66	CRO	CA1-C1	-2.72	1.47	1.51
1	C	66	CRO	C1-N3	-2.50	1.32	1.37
1	C	66	CRO	CA2-C2	-2.27	1.46	1.48
1	A	66	CRO	CA2-N2	-2.02	1.34	1.38
1	A	66	CRO	O2-C2	2.21	1.28	1.23
1	B	66	CRO	O2-C2	2.43	1.28	1.23
1	A	66	CRO	C1-N2	2.78	1.36	1.32
1	C	66	CRO	C1-N2	2.95	1.36	1.32
1	C	66	CRO	O2-C2	3.23	1.30	1.23
1	B	66	CRO	C1-N2	3.87	1.38	1.32
1	B	66	CRO	CB2-CA2	15.28	1.48	1.35
1	A	66	CRO	CB2-CA2	15.90	1.49	1.35
1	C	66	CRO	CB2-CA2	16.60	1.49	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-14.48	123.16	130.97
1	A	66	CRO	O2-C2-CA2	-8.87	126.19	130.97
1	B	66	CRO	O2-C2-CA2	-6.55	127.44	130.97
1	A	66	CRO	C2-CA2-N2	-5.10	105.20	108.93
1	B	66	CRO	C2-CA2-N2	-4.65	105.53	108.93
1	C	66	CRO	CG2-CB2-CA2	-4.08	125.45	130.19
1	B	66	CRO	CG2-CB2-CA2	-3.72	125.86	130.19
1	A	66	CRO	CG2-CB2-CA2	-3.61	126.00	130.19
1	A	66	CRO	O3-C3-CA3	-3.37	115.23	126.38
1	C	66	CRO	C2-CA2-N2	-3.12	106.65	108.93
1	C	66	CRO	CA1-C1-N3	-3.06	121.07	124.75
1	B	66	CRO	O3-C3-CA3	-2.91	116.78	126.38
1	C	66	CRO	O3-C3-CA3	-2.32	118.69	126.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	CB2-CA2-N2	-2.31	125.28	128.79
1	B	66	CRO	CE2-CZ-CE1	-2.09	115.99	119.74
1	C	66	CRO	CD1-CE1-CZ	2.13	122.29	119.88
1	B	66	CRO	CD1-CE1-CZ	2.44	122.64	119.88
1	B	66	CRO	N3-C1-N2	2.54	113.21	111.45
1	C	66	CRO	CB2-CA2-C2	2.83	125.88	122.32
1	A	66	CRO	CA3-N3-C1	3.33	131.09	127.20
1	B	66	CRO	CA3-N3-C1	3.64	131.46	127.20
1	A	66	CRO	CB2-CA2-C2	4.65	128.16	122.32
1	C	66	CRO	N3-C1-N2	4.68	114.69	111.45
1	B	66	CRO	CB2-CA2-C2	5.45	129.18	122.32
1	C	66	CRO	CA2-C2-N3	12.10	108.70	103.30
1	A	66	CRO	CA2-C2-N3	15.21	110.08	103.30
1	B	66	CRO	CA2-C2-N3	16.37	110.60	103.30

There are no chirality outliers.

There are no torsion outliers.

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 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 ⓘ

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%)	0.29	7 (3%) 49 46	68, 113, 146, 171	0
1	B	227/272 (83%)	0.71	22 (9%) 8 9	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%) 41 37	64, 101, 155, 178	0
2	E	158/170 (92%)	0.38	10 (6%) 21 20	89, 141, 179, 193	0
2	F	158/170 (92%)	-0.20	1 (0%) 89 86	52, 89, 151, 174	0
All	All	1155/1326 (87%)	0.21	46 (3%) 39 35	52, 114, 174, 222	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	LEU	5.3
1	B	231	LEU	5.0
2	D	166	LYS	4.5
2	E	166	LYS	4.1
1	B	194	LEU	4.0
1	B	229	ILE	3.8
1	B	132	GLU	3.5
1	B	169	HIS	3.4
1	B	160	GLY	3.3
1	B	177	GLN	3.3
2	E	23	LEU	3.1
2	F	143	MET	3.0
2	E	164	THR	3.0
2	D	158	ALA	3.0
1	B	91	GLY	2.9
2	E	60	TYR	2.8
1	B	124	GLU	2.8
2	E	105	ASP	2.8
1	B	192	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	114	PHE	2.6
2	E	165	HIS	2.6
1	B	141	LEU	2.6
1	A	160	GLY	2.6
2	D	154	ALA	2.5
1	B	156	LYS	2.5
2	E	146	LEU	2.5
1	B	81	HIS	2.4
2	E	84	ALA	2.4
1	A	133	ASP	2.4
2	E	143	MET	2.4
1	B	25	HIS	2.3
1	B	54	PRO	2.3
2	D	144	GLU	2.3
1	A	136	ILE	2.3
1	A	132	GLU	2.3
2	D	116	LEU	2.2
1	B	178	LEU	2.2
1	B	50	THR	2.2
1	B	47	ILE	2.1
2	E	147	ALA	2.1
1	A	121	ASN	2.1
1	B	154	ALA	2.1
1	B	137	LEU	2.1
2	D	146	LEU	2.0
1	A	57	TRP	2.0
1	A	43	THR	2.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CRO	B	66	22/23	0.92	0.26	-	97,131,145,150	0
1	CRO	A	66	22/23	0.98	0.20	-	78,93,102,104	0
1	CRO	C	66	22/23	0.97	0.24	-	55,73,82,100	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.