



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:33 PM UTC

PDB ID : 4W7X / pdb_00004w7x
Title : Crystal Structure of Full-Length Split GFP Mutant E115C Disulfide Dimer,
P 1 21 1 Space Group
Authors : Leibly, D.J.; Waldo, G.S.; Yeates, T.O.
Deposited on : 2014-08-22
Resolution : 2.80 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

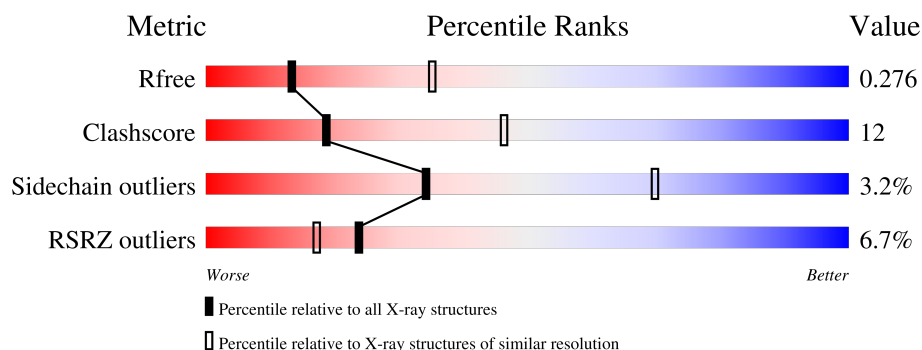
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	229	7% 73% 20% . .
1	B	229	7% 76% 18% . .
1	C	229	6% 72% 24% . .
1	D	229	6% 75% 18% . 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CRO	C	66	-	-	X	-

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7089 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.

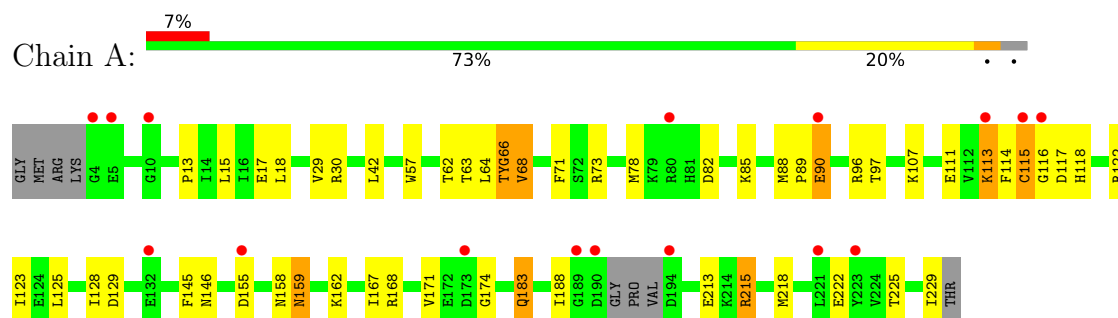
- Molecule 1 is a protein called fluorescent protein E115C/T118H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1781	1134	303	340	4			
1	B	221	Total	C	N	O	S	0	0	0
			1770	1129	299	338	4			
1	C	224	Total	C	N	O	S	0	0	0
			1793	1141	307	341	4			
1	D	216	Total	C	N	O	S	0	0	0
			1745	1112	298	331	4			

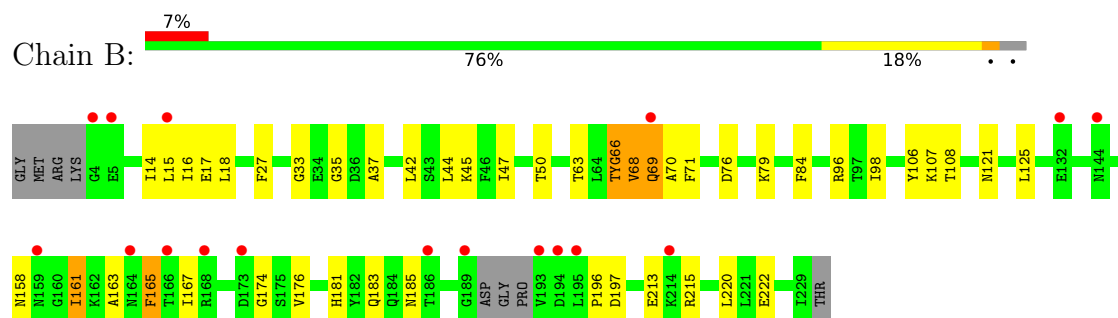
3 Residue-property plots [i](#)

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.

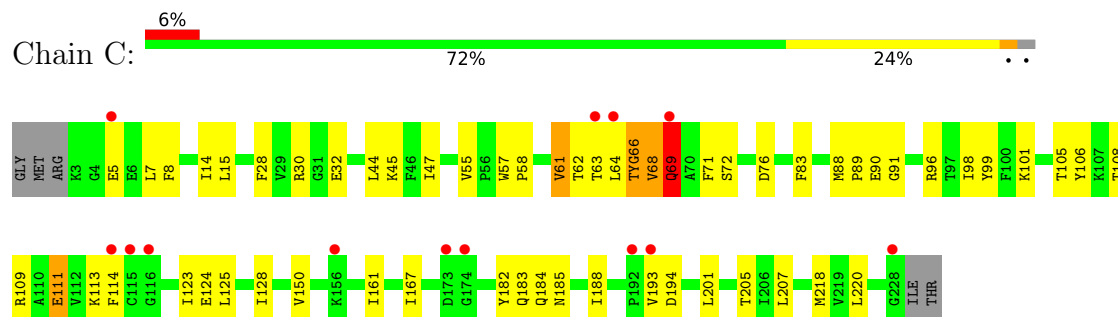
• Molecule 1: fluorescent protein E115C/T118H



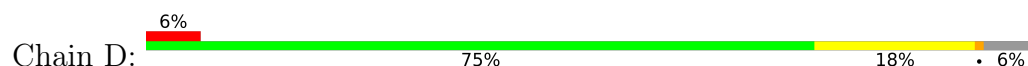
• Molecule 1: fluorescent protein E115C/T118H

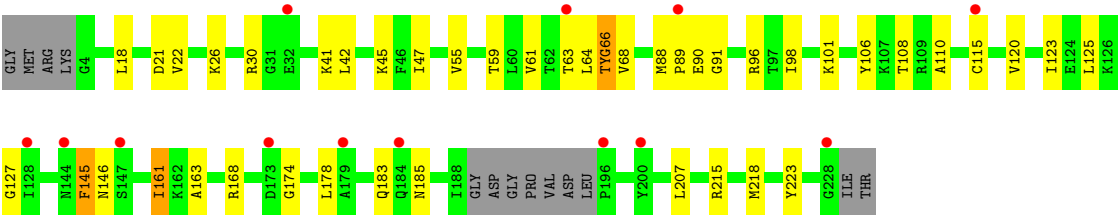


• Molecule 1: fluorescent protein E115C/T118H



• Molecule 1: fluorescent protein E115C/T118H





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.84Å 70.47Å 116.78Å 90.00° 92.56° 90.00°	Depositor
Resolution (Å)	66.77 – 2.80 66.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (66.77-2.80) 99.7 (66.77-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1555)	Depositor
R, R_{free}	0.217 , 0.269 (Not available) , 0.276	Depositor DCC
R_{free} test set	2689 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7089	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.06% 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

5.1 Standard geometry

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	0.38	1/1797 (0.1%)	0.77	6/2427 (0.2%)
1	B	0.37	0/1786	0.76	4/2415 (0.2%)
1	C	0.37	1/1811 (0.1%)	0.73	1/2448 (0.0%)
1	D	0.32	0/1761	0.71	1/2377 (0.0%)
All	All	0.36	2/7155 (0.0%)	0.75	12/9667 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	VAL	N-CA	-7.43	1.32	1.46
1	C	68	VAL	N-CA	-7.42	1.32	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	68	VAL	N-CA-CB	9.24	127.20	111.50
1	B	197	ASP	N-CA-C	-6.85	101.70	110.53
1	B	69	GLN	N-CA-C	-6.02	104.51	112.34
1	B	165	PHE	N-CA-C	5.67	117.47	108.79
1	B	174	GLY	N-CA-C	-5.63	106.89	115.00
1	D	174	GLY	N-CA-C	-5.59	107.65	114.92
1	A	116	GLY	N-CA-C	5.49	119.31	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	CYS	CA-C-N	5.33	125.90	119.98
1	A	115	CYS	C-N-CA	5.33	125.90	119.98
1	A	159	ASN	CB-CA-C	5.17	119.23	111.89
1	C	69	GLN	N-CA-C	-5.05	105.90	111.71
1	A	174	GLY	N-CA-C	-5.00	107.80	115.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	CYS	Peptide

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	1781	0	1725	36	0
1	B	1770	0	1708	41	0
1	C	1793	0	1735	65	0
1	D	1745	0	1694	33	0
All	All	7089	0	6862	166	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (166) 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:C:64:LEU:O	1:C:66:CRO:CA3	1.73	1.34
1:C:64:LEU:O	1:C:66:CRO:HA31	0.93	1.10
1:C:64:LEU:C	1:C:66:CRO:HA31	1.82	1.03
1:C:7:LEU:HD11	1:C:89:PRO:HG3	1.46	0.94
1:D:115:CYS:SG	1:D:120:VAL:CG2	2.56	0.93
1:D:61:VAL:HB	1:D:145:PHE:CZ	2.04	0.92
1:D:115:CYS:SG	1:D:120:VAL:HG23	2.09	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:CRO:HD1	1:C:66:CRO:N2	1.87	0.88
1:B:66:CRO:N2	1:B:66:CRO:HD1	1.87	0.88
1:A:66:CRO:HD1	1:A:66:CRO:N2	1.88	0.87
1:D:61:VAL:HG11	1:D:145:PHE:CE2	2.11	0.86
1:C:66:CRO:N2	1:C:66:CRO:OG1	2.12	0.82
1:C:66:CRO:HG11	1:C:220:LEU:HD21	1.61	0.81
1:D:61:VAL:CG1	1:D:145:PHE:CE2	2.66	0.79
1:C:193:VAL:HG12	1:C:194:ASP:N	1.99	0.77
1:D:115:CYS:SG	1:D:120:VAL:HG21	2.25	0.77
1:A:111:GLU:HB3	1:A:113:LYS:HD3	1.68	0.76
1:B:42:LEU:HD11	1:B:68:VAL:HG23	1.70	0.72
1:C:64:LEU:O	1:C:66:CRO:HA32	1.88	0.70
1:C:58:PRO:O	1:C:61:VAL:HG23	1.92	0.70
1:A:57:TRP:HB3	1:A:218:MET:HE3	1.72	0.69
1:A:17:GLU:OE2	1:A:30:ARG:NH1	2.23	0.69
1:C:69:GLN:O	1:C:71:PHE:N	2.27	0.68
1:A:15:LEU:HD23	1:B:15:LEU:HD11	1.74	0.68
1:C:83:PHE:CD1	1:C:193:VAL:HG11	2.29	0.67
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.76	0.67
1:B:163:ALA:HB3	1:B:183:GLN:HG2	1.78	0.66
1:D:163:ALA:HB3	1:D:183:GLN:HB3	1.78	0.66
1:C:66:CRO:CG1	1:C:220:LEU:HD21	2.26	0.65
1:C:61:VAL:O	1:C:66:CRO:OG1	2.13	0.65
1:A:66:CRO:HE1	1:A:222:GLU:OE2	1.96	0.64
1:A:15:LEU:CD2	1:B:15:LEU:HD11	2.27	0.64
1:C:7:LEU:HD11	1:C:89:PRO:CG	2.26	0.64
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.80	0.64
1:B:27:PHE:HB2	1:B:50:THR:HG21	1.79	0.63
1:D:22:VAL:HG12	1:D:127:GLY:HA3	1.80	0.63
1:B:68:VAL:O	1:B:70:ALA:N	2.32	0.63
1:B:42:LEU:HD11	1:B:68:VAL:CG2	2.30	0.61
1:C:63:THR:CG2	1:C:108:THR:HG21	2.30	0.61
1:B:68:VAL:O	1:B:69:GLN:C	2.43	0.61
1:C:193:VAL:CG1	1:C:194:ASP:N	2.63	0.61
1:D:108:THR:HG22	1:D:125:LEU:HG	1.81	0.60
1:D:88:MET:HA	1:D:89:PRO:C	2.27	0.59
1:C:68:VAL:HG23	1:C:68:VAL:O	2.01	0.59
1:C:193:VAL:HG12	1:C:194:ASP:H	1.66	0.59
1:A:62:THR:HG21	1:A:167:ILE:HG13	1.85	0.58
1:A:66:CRO:N2	1:A:66:CRO:CD1	2.63	0.58
1:C:63:THR:HG22	1:C:108:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:C	1:C:66:CRO:CA3	2.58	0.57
1:C:66:CRO:N2	1:C:66:CRO:CD1	2.62	0.57
1:C:69:GLN:O	1:C:72:SER:N	2.35	0.57
1:C:83:PHE:CE1	1:C:193:VAL:HG11	2.39	0.57
1:A:15:LEU:HD23	1:B:15:LEU:CD1	2.35	0.57
1:D:18:LEU:HD11	1:D:125:LEU:HB2	1.86	0.56
1:D:146:ASN:ND2	1:D:168:ARG:O	2.39	0.56
1:C:193:VAL:CG1	1:C:194:ASP:H	2.18	0.56
1:B:167:ILE:HG13	1:B:181:HIS:CE1	2.41	0.56
1:D:101:LYS:HG3	1:D:178:LEU:HB2	1.88	0.56
1:A:78:MET:HE3	1:A:229:ILE:HD12	1.88	0.55
1:C:89:PRO:O	1:C:91:GLY:N	2.40	0.55
1:D:41:LYS:NZ	1:D:223:TYR:OH	2.34	0.54
1:B:161:ILE:HG21	1:B:196:PRO:HG3	1.90	0.54
1:C:69:GLN:C	1:C:71:PHE:H	2.15	0.53
1:D:61:VAL:HB	1:D:145:PHE:CE2	2.43	0.53
1:A:97:THR:HG22	1:A:107:LYS:HG2	1.90	0.53
1:D:61:VAL:HG11	1:D:145:PHE:CD2	2.44	0.53
1:C:66:CRO:CG1	1:C:220:LEU:CD2	2.86	0.53
1:A:155:ASP:OD2	1:A:162:LYS:HG3	2.09	0.53
1:C:5:GLU:C	1:C:7:LEU:H	2.15	0.52
1:A:42:LEU:HB2	1:A:222:GLU:HB2	1.91	0.52
1:A:68:VAL:HB	1:A:71:PHE:HD2	1.74	0.52
1:A:73:ARG:HB3	1:A:225:THR:HG22	1.90	0.52
1:C:69:GLN:C	1:C:71:PHE:N	2.66	0.52
1:D:61:VAL:CB	1:D:145:PHE:CZ	2.86	0.52
1:B:98:ILE:HB	1:B:106:TYR:HB2	1.92	0.51
1:C:66:CRO:O2	1:C:96:ARG:NH2	2.42	0.51
1:C:161:ILE:HG13	1:C:185:ASN:HB2	1.92	0.51
1:C:111:GLU:HG2	1:C:188:ILE:HD11	1.93	0.51
1:A:17:GLU:OE1	1:A:122:ARG:NH1	2.43	0.51
1:B:165:PHE:HE2	1:B:167:ILE:HD11	1.75	0.51
1:C:58:PRO:C	1:C:61:VAL:HG23	2.36	0.50
1:A:13:PRO:HB2	1:A:118:HIS:CD2	2.46	0.50
1:A:113:LYS:HG2	1:A:188:ILE:CD1	2.42	0.50
1:B:161:ILE:CG2	1:B:196:PRO:HG3	2.41	0.50
1:A:89:PRO:O	1:A:90:GLU:C	2.55	0.50
1:B:76:ASP:HA	1:B:79:LYS:HE2	1.93	0.50
1:C:58:PRO:HA	1:C:61:VAL:CG2	2.41	0.50
1:B:45:LYS:HE2	1:B:47:ILE:HD11	1.94	0.49
1:A:88:MET:HA	1:A:89:PRO:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:VAL:C	1:B:70:ALA:N	2.66	0.49
1:C:96:ARG:HG2	1:C:183:GLN:HB3	1.94	0.49
1:A:18:LEU:HB3	1:A:29:VAL:HB	1.94	0.49
1:B:14:ILE:HD11	1:B:35:GLY:HA3	1.95	0.49
1:B:63:THR:HG21	1:B:125:LEU:HD12	1.94	0.49
1:D:98:ILE:HB	1:D:106:TYR:HB2	1.94	0.49
1:D:61:VAL:CB	1:D:145:PHE:CE2	2.96	0.49
1:A:63:THR:HG21	1:A:125:LEU:HD12	1.94	0.49
1:B:96:ARG:HB2	1:B:108:THR:OG1	2.13	0.49
1:C:62:THR:HG21	1:C:167:ILE:HG13	1.94	0.48
1:C:89:PRO:O	1:C:90:GLU:C	2.56	0.48
1:C:150:VAL:HB	1:C:201:LEU:HB2	1.95	0.48
1:B:42:LEU:HB2	1:B:222:GLU:HB2	1.95	0.48
1:C:109:ARG:NH1	1:C:124:GLU:OE1	2.46	0.48
1:B:69:GLN:C	1:B:71:PHE:N	2.71	0.47
1:D:161:ILE:HG13	1:D:185:ASN:HB2	1.96	0.47
1:C:5:GLU:C	1:C:7:LEU:N	2.69	0.47
1:C:45:LYS:HE2	1:C:47:ILE:HD11	1.98	0.46
1:D:89:PRO:O	1:D:90:GLU:C	2.57	0.46
1:B:161:ILE:HG13	1:B:185:ASN:HB2	1.96	0.46
1:A:117:ASP:HB2	1:B:17:GLU:CD	2.41	0.46
1:A:213:GLU:OE2	1:A:215:ARG:HD3	2.16	0.46
1:B:69:GLN:OE1	1:B:84:PHE:CE1	2.69	0.46
1:C:66:CRO:HD1	1:C:66:CRO:OG1	2.16	0.46
1:A:158:ASN:O	1:A:159:ASN:OD1	2.34	0.46
1:C:111:GLU:HB3	1:C:113:LYS:CE	2.45	0.46
1:C:32:GLU:OE2	1:D:215:ARG:NH1	2.44	0.46
1:C:76:ASP:N	1:C:76:ASP:OD1	2.49	0.46
1:D:42:LEU:HD11	1:D:68:VAL:HG23	1.98	0.45
1:B:69:GLN:C	1:B:71:PHE:H	2.24	0.45
1:C:88:MET:HA	1:C:89:PRO:C	2.41	0.45
1:B:220:LEU:HD21	1:B:222:GLU:HG3	1.98	0.45
1:C:28:PHE:HE1	1:C:30:ARG:HG3	1.82	0.45
1:A:66:CRO:CE1	1:A:222:GLU:OE2	2.64	0.45
1:C:99:TYR:HA	1:C:105:THR:HG22	1.99	0.45
1:C:8:PHE:CZ	1:C:88:MET:HG3	2.52	0.45
1:C:83:PHE:CD1	1:C:193:VAL:CG1	2.98	0.45
1:A:117:ASP:HB2	1:B:17:GLU:OE1	2.17	0.44
1:D:64:LEU:C	1:D:66:CRO:HA31	2.42	0.44
1:B:165:PHE:CE2	1:B:167:ILE:HD11	2.50	0.44
1:C:63:THR:HG21	1:C:125:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:GLU:HG2	1:C:113:LYS:HE2	1.98	0.44
1:A:64:LEU:O	1:A:66:CRO:HA31	2.17	0.44
1:B:66:CRO:HE1	1:B:222:GLU:OE2	2.17	0.44
1:C:205:THR:HG23	1:C:220:LEU:HD11	1.99	0.44
1:B:68:VAL:HB	1:B:71:PHE:HD2	1.83	0.44
1:D:110:ALA:HB2	1:D:123:ILE:HG23	2.00	0.43
1:C:32:GLU:CD	1:D:30:ARG:HH22	2.27	0.43
1:C:63:THR:HG21	1:C:108:THR:HG21	1.99	0.43
1:A:82:ASP:OD2	1:A:85:LYS:HD2	2.18	0.43
1:B:18:LEU:HD11	1:B:125:LEU:HB2	2.00	0.43
1:C:89:PRO:HB3	1:C:114:PHE:HB2	2.01	0.43
1:C:98:ILE:HD12	1:C:106:TYR:HD2	1.83	0.43
1:B:158:ASN:HA	1:C:184:GLN:HE22	1.84	0.43
1:A:66:CRO:OH	1:A:145:PHE:HE2	2.02	0.43
1:A:68:VAL:HB	1:A:71:PHE:CD2	2.54	0.43
1:B:16:ILE:HG12	1:B:121:ASN:HB3	1.99	0.42
1:B:37:ALA:HB2	1:B:71:PHE:HA	2.01	0.42
1:A:146:ASN:ND2	1:A:168:ARG:O	2.51	0.42
1:C:14:ILE:HD12	1:C:44:LEU:HD11	2.01	0.42
1:C:57:TRP:CE3	1:C:218:MET:HG2	2.55	0.42
1:A:42:LEU:HD11	1:A:68:VAL:HG23	2.00	0.42
1:D:89:PRO:O	1:D:91:GLY:N	2.52	0.42
1:B:42:LEU:CD1	1:B:68:VAL:CG2	2.97	0.42
1:C:207:LEU:HG	1:C:218:MET:HE1	2.01	0.42
1:D:96:ARG:HB2	1:D:108:THR:OG1	2.19	0.41
1:D:207:LEU:HD22	1:D:218:MET:HE1	2.03	0.41
1:B:69:GLN:O	1:B:71:PHE:N	2.53	0.41
1:B:33:GLY:HA3	1:B:44:LEU:HD23	2.03	0.41
1:C:5:GLU:O	1:C:7:LEU:N	2.53	0.41
1:D:21:ASP:OD2	1:D:26:LYS:HE2	2.21	0.41
1:D:63:THR:CG2	1:D:108:THR:HG21	2.51	0.41
1:D:63:THR:HG22	1:D:108:THR:HG21	2.03	0.41
1:B:66:CRO:N2	1:B:66:CRO:CD1	2.62	0.41
1:C:89:PRO:C	1:C:91:GLY:N	2.79	0.41
1:A:128:ILE:HD12	1:A:129:ASP:OD2	2.22	0.40
1:B:107:LYS:NZ	1:C:182:TYR:OH	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	191/197 (97%)	184 (96%)	7 (4%)	30	65
1	B	189/197 (96%)	184 (97%)	5 (3%)	40	75
1	C	191/197 (97%)	183 (96%)	8 (4%)	26	61
1	D	187/197 (95%)	183 (98%)	4 (2%)	47	79
All	All	758/788 (96%)	734 (97%)	24 (3%)	34	70

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLU
1	A	113	LYS
1	A	114	PHE
1	A	123	ILE
1	A	171	VAL
1	A	183	GLN
1	A	215	ARG
1	B	68	VAL
1	B	161	ILE
1	B	176	VAL
1	B	213	GLU
1	B	215	ARG
1	C	15	LEU
1	C	55	VAL
1	C	61	VAL
1	C	69	GLN
1	C	101	LYS
1	C	111	GLU

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Mol	Chain	Res	Type
1	C	123	ILE
1	C	128	ILE
1	D	55	VAL
1	D	59	THR
1	D	145	PHE
1	D	161	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	HIS
1	B	158	ASN
1	C	158	ASN
1	C	184	GLN
1	D	139	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CRO	D	66	1	22,23,24	3.38	6 (27%)	30,32,34	3.06	9 (30%)
1	CRO	A	66	1	22,23,24	3.51	5 (22%)	30,32,34	3.19	7 (23%)
1	CRO	B	66	1	22,23,24	3.33	4 (18%)	30,32,34	3.19	7 (23%)
1	CRO	C	66	1	22,23,24	3.73	7 (31%)	30,32,34	3.42	8 (26%)

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	D	66	1	-	1/12/31/32	0/2/2/2
1	CRO	A	66	1	-	1/12/31/32	0/2/2/2
1	CRO	B	66	1	-	1/12/31/32	0/2/2/2
1	CRO	C	66	1	-	7/12/31/32	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	CRO	CB2-CA2	14.18	1.48	1.35
1	A	66	CRO	CB2-CA2	14.16	1.48	1.35
1	C	66	CRO	CB2-CA2	14.14	1.48	1.35
1	D	66	CRO	CB2-CA2	12.09	1.46	1.35
1	C	66	CRO	OG1-CB1	5.71	1.58	1.43
1	A	66	CRO	CA1-N1	-5.38	1.32	1.47
1	D	66	CRO	CA2-C2	-5.10	1.43	1.48
1	D	66	CRO	C2-N3	-4.93	1.28	1.40
1	C	66	CRO	CA1-N1	-4.92	1.33	1.47
1	D	66	CRO	CA1-N1	-4.41	1.35	1.47
1	A	66	CRO	C1-N2	3.93	1.38	1.32
1	B	66	CRO	C1-N2	3.89	1.37	1.32
1	C	66	CRO	C1-N2	3.88	1.37	1.32
1	C	66	CRO	C2-N3	-3.01	1.33	1.40
1	A	66	CRO	C2-N3	-2.99	1.33	1.40
1	B	66	CRO	C2-N3	-2.99	1.33	1.40
1	C	66	CRO	O2-C2	2.93	1.29	1.23
1	D	66	CRO	C1-N2	2.87	1.36	1.32
1	B	66	CRO	O2-C2	2.86	1.28	1.23
1	A	66	CRO	O2-C2	2.85	1.28	1.23
1	C	66	CRO	CG1-CB1	-2.82	1.43	1.51
1	D	66	CRO	CA2-N2	-2.81	1.32	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-8.64	125.50	131.02
1	A	66	CRO	O2-C2-CA2	-8.56	125.56	131.02
1	B	66	CRO	O2-C2-CA2	-8.55	125.56	131.02
1	D	66	CRO	CA2-C2-N3	8.40	110.55	103.50
1	D	66	CRO	O2-C2-CA2	-8.35	125.69	131.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	CG2-CB2-CA2	-8.33	119.97	129.87
1	C	66	CRO	CG2-CB2-CA2	-8.32	119.98	129.87
1	A	66	CRO	CG2-CB2-CA2	-8.31	119.99	129.87
1	C	66	CRO	CB2-CA2-C2	7.42	131.35	122.36
1	A	66	CRO	CB2-CA2-C2	7.38	131.30	122.36
1	B	66	CRO	CB2-CA2-C2	7.36	131.27	122.36
1	C	66	CRO	CA2-C2-N3	6.46	108.92	103.50
1	B	66	CRO	CA2-C2-N3	6.40	108.88	103.50
1	A	66	CRO	CA2-C2-N3	6.39	108.86	103.50
1	D	66	CRO	C1-CA1-N1	6.09	120.67	109.78
1	C	66	CRO	CG1-CB1-CA1	5.98	125.85	112.18
1	D	66	CRO	C2-N3-C1	-5.29	105.62	108.07
1	A	66	CRO	CB2-CA2-N2	-4.76	122.31	128.76
1	C	66	CRO	CB2-CA2-N2	-4.73	122.34	128.76
1	B	66	CRO	CB2-CA2-N2	-4.69	122.39	128.76
1	D	66	CRO	C2-CA2-N2	-4.55	105.69	108.95
1	C	66	CRO	C2-N3-C1	-4.35	106.05	108.07
1	B	66	CRO	C2-N3-C1	-4.31	106.07	108.07
1	A	66	CRO	C2-N3-C1	-4.27	106.09	108.07
1	D	66	CRO	O3-C3-CA3	-3.82	108.26	125.47
1	C	66	CRO	C2-CA2-N2	-3.68	106.31	108.95
1	B	66	CRO	C2-CA2-N2	-3.65	106.33	108.95
1	A	66	CRO	C2-CA2-N2	-3.57	106.40	108.95
1	D	66	CRO	CB2-CA2-C2	3.48	126.57	122.36
1	D	66	CRO	CA1-C1-N3	-2.39	121.86	124.69
1	D	66	CRO	C3-CA3-N3	2.06	117.11	112.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	N1-CA1-CB1-CG1
1	C	66	CRO	C1-CA1-CB1-OG1
1	C	66	CRO	N2-C1-CA1-CB1
1	C	66	CRO	N3-C1-CA1-CB1
1	D	66	CRO	N1-CA1-CB1-CG1
1	B	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	C3-CA3-N3-C2
1	C	66	CRO	C1-CA1-CB1-CG1
1	C	66	CRO	N1-CA1-CB1-OG1

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	66	CRO	1	0
1	A	66	CRO	6	0
1	B	66	CRO	3	0
1	C	66	CRO	14	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 [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, 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	220/229 (96%)	0.47	16 (7%) 21 15	25, 44, 81, 119	0
1	B	220/229 (96%)	0.41	17 (7%) 19 14	27, 40, 69, 159	0
1	C	223/229 (97%)	0.54	13 (5%) 29 22	32, 51, 79, 109	0
1	D	215/229 (93%)	0.62	13 (6%) 27 21	36, 56, 86, 129	0
All	All	878/916 (95%)	0.51	59 (6%) 24 17	25, 48, 81, 159	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	115	CYS	6.4
1	B	193	VAL	6.3
1	A	116	GLY	5.0
1	B	195	LEU	4.9
1	A	189	GLY	4.6
1	B	194	ASP	4.5
1	A	190	ASP	4.1
1	B	166	THR	4.1
1	A	115	CYS	3.8
1	A	4	GLY	3.8
1	B	4	GLY	3.8
1	D	144	ASN	3.7
1	D	196	PRO	3.6
1	B	132	GLU	3.3
1	C	115	CYS	3.3
1	D	228	GLY	3.2
1	A	223	TYR	3.2
1	B	173	ASP	3.2
1	C	173	ASP	3.1
1	D	32	GLU	3.1
1	A	155	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	63	THR	2.9
1	C	116	GLY	2.9
1	A	5	GLU	2.8
1	B	214	LYS	2.8
1	A	80	ARG	2.8
1	D	89	PRO	2.7
1	C	69	GLN	2.7
1	A	132	GLU	2.6
1	C	114	PHE	2.6
1	B	168	ARG	2.5
1	C	64	LEU	2.5
1	B	15	LEU	2.5
1	D	147	SER	2.5
1	A	10	GLY	2.4
1	A	90	GLU	2.4
1	A	221	LEU	2.4
1	A	113	LYS	2.4
1	B	164	ASN	2.4
1	B	144	ASN	2.3
1	D	179	ALA	2.3
1	B	186	THR	2.3
1	C	156	LYS	2.3
1	A	173	ASP	2.2
1	D	63	THR	2.2
1	B	189	GLY	2.2
1	C	174	GLY	2.2
1	D	200	TYR	2.2
1	B	5	GLU	2.2
1	D	184	GLN	2.2
1	C	228	GLY	2.1
1	A	194	ASP	2.1
1	B	69	GLN	2.1
1	D	128	ILE	2.1
1	C	192	PRO	2.0
1	B	159	ASN	2.0
1	C	5	GLU	2.0
1	D	173	ASP	2.0
1	C	193	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
1	CRO	A	66	22/23	0.83	0.15	40,41,43,44	0
1	CRO	C	66	22/23	0.84	0.15	51,51,52,52	0
1	CRO	B	66	22/23	0.89	0.12	37,37,38,39	0
1	CRO	D	66	22/23	0.91	0.10	40,41,42,44	0

6.3 Carbohydrates [i](#)

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.