



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 11:46 AM UTC

PDB ID : 8JKC / pdb_00008jkc
Title : Crystal structure of the Green fluorescent protein SE_A277 variant at pH 4.5
Authors : Shin, S.C.
Deposited on : 2023-06-01
Resolution : 1.95 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

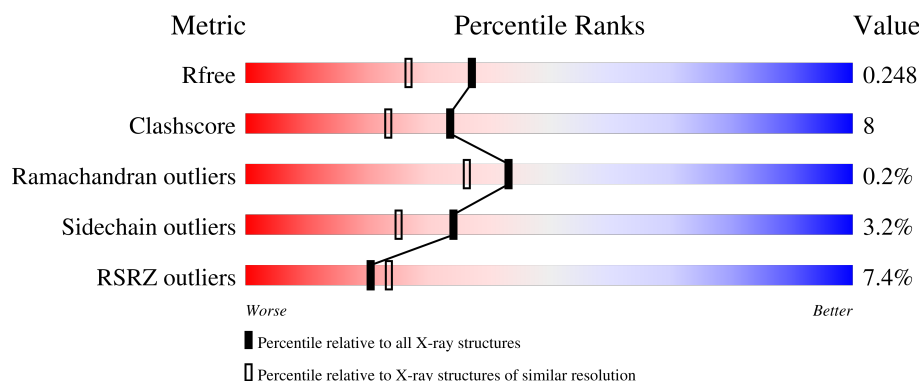
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	236	7% 77% 15% • 5%
1	B	236	6% 85% 8% • 5%
1	C	236	7% 81% 12% • 5%
1	D	236	8% 81% 13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7796 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	225	Total	C	N	O	S	0	0	0
			1807	1153	304	344	6			
1	B	225	Total	C	N	O	S	0	0	0
			1807	1153	304	344	6			
1	C	225	Total	C	N	O	S	0	0	0
			1807	1153	304	344	6			
1	D	225	Total	C	N	O	S	0	0	0
			1807	1153	304	344	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LEU	PHE	engineered mutation	UNP P42212
A	66	CRO	SER	chromophore	UNP P42212
A	66	CRO	TYR	chromophore	UNP P42212
A	66	CRO	GLY	chromophore	UNP P42212
A	80	ARG	GLN	engineered mutation	UNP P42212
A	147	ASP	SER	engineered mutation	UNP P42212
A	149	GLN	ASN	engineered mutation	UNP P42212
A	163	ALA	VAL	engineered mutation	UNP P42212
A	175	GLY	SER	engineered mutation	UNP P42212
A	202	PHE	SER	engineered mutation	UNP P42212
A	204	THR	GLN	engineered mutation	UNP P42212
A	206	THR	ALA	engineered mutation	UNP P42212
B	64	LEU	PHE	engineered mutation	UNP P42212
B	66	CRO	SER	chromophore	UNP P42212
B	66	CRO	TYR	chromophore	UNP P42212
B	66	CRO	GLY	chromophore	UNP P42212
B	80	ARG	GLN	engineered mutation	UNP P42212
B	147	ASP	SER	engineered mutation	UNP P42212
B	149	GLN	ASN	engineered mutation	UNP P42212
B	163	ALA	VAL	engineered mutation	UNP P42212
B	175	GLY	SER	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
B	202	PHE	SER	engineered mutation	UNP P42212
B	204	THR	GLN	engineered mutation	UNP P42212
B	206	THR	ALA	engineered mutation	UNP P42212
C	64	LEU	PHE	engineered mutation	UNP P42212
C	66	CRO	SER	chromophore	UNP P42212
C	66	CRO	TYR	chromophore	UNP P42212
C	66	CRO	GLY	chromophore	UNP P42212
C	80	ARG	GLN	engineered mutation	UNP P42212
C	147	ASP	SER	engineered mutation	UNP P42212
C	149	GLN	ASN	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212
C	175	GLY	SER	engineered mutation	UNP P42212
C	202	PHE	SER	engineered mutation	UNP P42212
C	204	THR	GLN	engineered mutation	UNP P42212
C	206	THR	ALA	engineered mutation	UNP P42212
D	64	LEU	PHE	engineered mutation	UNP P42212
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	80	ARG	GLN	engineered mutation	UNP P42212
D	147	ASP	SER	engineered mutation	UNP P42212
D	149	GLN	ASN	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212
D	175	GLY	SER	engineered mutation	UNP P42212
D	202	PHE	SER	engineered mutation	UNP P42212
D	204	THR	GLN	engineered mutation	UNP P42212
D	206	THR	ALA	engineered mutation	UNP P42212

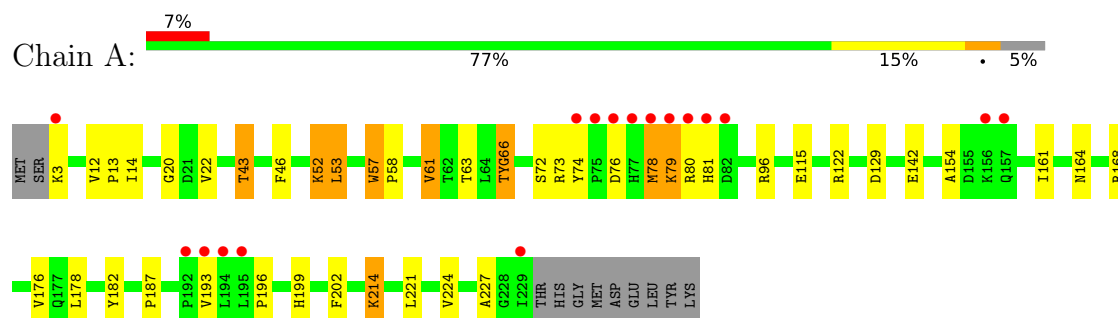
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	127	Total O 127 127	0	0
2	B	149	Total O 149 149	0	0
2	C	162	Total O 162 162	0	0
2	D	130	Total O 130 130	0	0

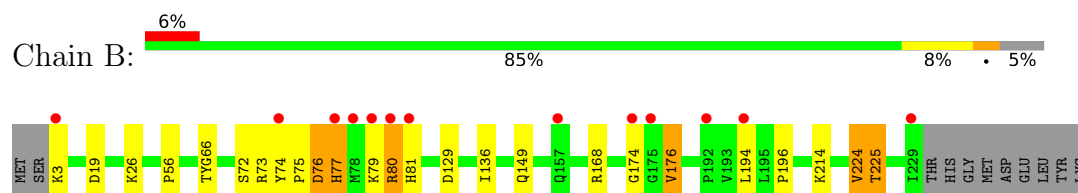
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

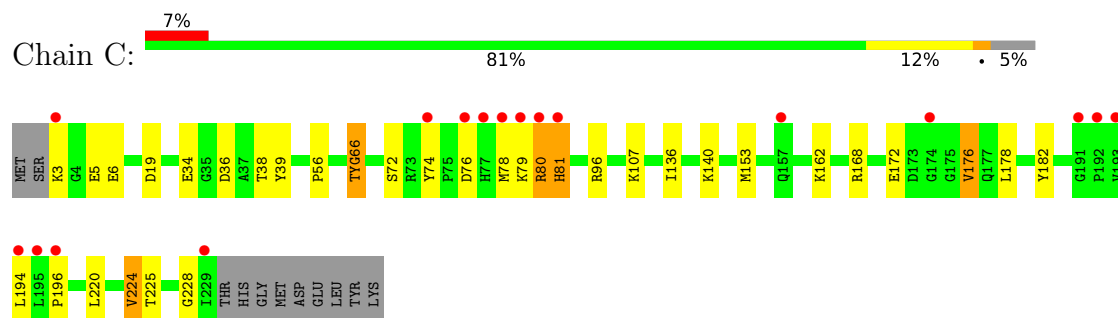
- Molecule 1: Green fluorescent protein



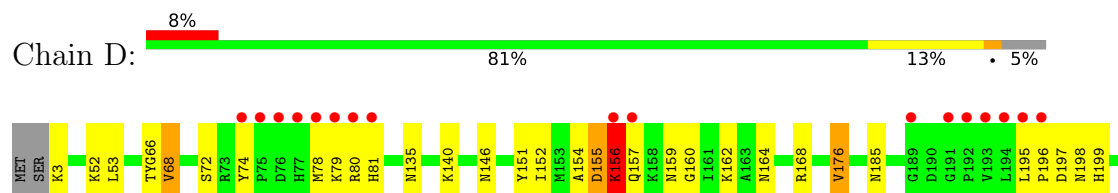
- Molecule 1: Green fluorescent protein

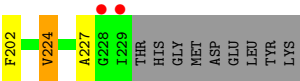


- Molecule 1: Green fluorescent protein



- Molecule 1: Green fluorescent protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.79Å 80.63Å 179.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 1.95 48.02 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.02-1.95) 99.1 (48.02-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.201 , 0.246 0.203 , 0.248	Depositor DCC
R_{free} test set	2002 reflections (2.46%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7796	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	1.06	12/1826 (0.7%)	0.70	1/2467 (0.0%)
1	B	0.38	0/1826	0.73	3/2467 (0.1%)
1	C	0.38	0/1826	0.58	0/2467
1	D	0.35	0/1826	0.59	1/2467 (0.0%)
All	All	0.62	12/7304 (0.2%)	0.65	5/9868 (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	C	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	TRP	C-O	-8.98	1.15	1.24
1	A	52	LYS	C-O	-6.66	1.16	1.24
1	A	12	VAL	C-O	-6.61	1.16	1.23
1	A	43	THR	C-O	-6.01	1.17	1.24
1	A	61	VAL	C-O	-5.83	1.17	1.24
1	A	58	PRO	C-O	-5.63	1.16	1.24
1	A	53	LEU	C-O	-5.46	1.17	1.24
1	A	22	VAL	C-O	-5.39	1.18	1.24
1	A	14	ILE	C-O	-5.27	1.18	1.24
1	A	63	THR	C-O	-5.26	1.18	1.24
1	A	46	PHE	C-O	-5.07	1.17	1.24
1	A	13	PRO	C-O	-5.05	1.17	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	GLY	N-CA-C	17.52	139.17	114.64
1	B	174	GLY	CA-C-N	-7.52	115.74	122.43
1	B	174	GLY	C-N-CA	-7.52	115.74	122.43
1	D	155	ASP	N-CA-C	-6.65	102.46	110.44
1	A	20	GLY	N-CA-C	5.27	121.09	111.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	81	HIS	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	1807	0	1746	33	0
1	B	1807	0	1746	22	0
1	C	1807	0	1745	27	0
1	D	1807	0	1746	31	0
2	A	127	0	0	1	0
2	B	149	0	0	1	0
2	C	162	0	0	3	0
2	D	130	0	0	4	0
All	All	7796	0	6983	109	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 8.

All (109) 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:80:ARG:O	1:C:194:LEU:HD13	1.46	1.15
1:B:81:HIS:HB3	1:B:196:PRO:HA	1.48	0.96
1:A:214:LYS:HD3	1:A:214:LYS:H	1.34	0.93
1:B:80:ARG:HG2	1:B:80:ARG:HH11	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:HIS:HE1	1:D:197:ASP:HB2	1.44	0.83
1:A:76:ASP:HA	1:A:79:LYS:HG3	1.59	0.81
1:B:76:ASP:HA	1:B:79:LYS:HB2	1.62	0.81
1:A:78:MET:HE1	1:A:227:ALA:CA	2.13	0.78
1:A:168:ARG:HH11	1:A:178:LEU:HD21	1.49	0.78
1:D:156:LYS:HA	1:D:195:LEU:HD22	1.68	0.76
1:A:78:MET:HE1	1:A:227:ALA:HA	1.72	0.72
1:A:168:ARG:HG3	1:A:176:VAL:HG11	1.71	0.71
1:A:115:GLU:HG2	1:B:26:LYS:HB2	1.74	0.69
1:A:43:THR:HG22	1:A:221:LEU:HD13	1.75	0.68
1:D:168:ARG:HG3	1:D:176:VAL:HG11	1.75	0.67
1:D:146:ASN:OD1	2:D:301:HOH:O	2.13	0.67
1:D:81:HIS:CE1	1:D:197:ASP:HB2	2.28	0.66
1:C:80:ARG:O	1:C:194:LEU:CD1	2.35	0.65
1:B:72:SER:HB2	1:B:224:VAL:HG22	1.78	0.65
1:C:3:LYS:HB2	1:C:6:GLU:OE1	1.96	0.65
1:A:168:ARG:NH1	1:A:178:LEU:HD21	2.13	0.63
1:B:76:ASP:HA	1:B:79:LYS:HD3	1.82	0.62
1:B:80:ARG:HG2	1:B:80:ARG:NH1	2.12	0.60
1:A:78:MET:HE1	1:A:227:ALA:C	2.27	0.59
1:A:115:GLU:HG2	1:B:26:LYS:CB	2.33	0.59
1:C:81:HIS:HB3	1:C:196:PRO:HB3	1.85	0.59
1:A:78:MET:C	1:A:80:ARG:H	2.10	0.58
1:A:168:ARG:HG3	1:A:176:VAL:CG1	2.33	0.58
1:D:168:ARG:HG3	1:D:176:VAL:CG1	2.34	0.57
1:B:3:LYS:N	2:B:305:HOH:O	2.38	0.57
1:B:72:SER:HA	1:B:224:VAL:HG13	1.86	0.57
1:D:52:LYS:HD3	1:D:53:LEU:N	2.20	0.56
1:C:79:LYS:O	1:C:80:ARG:C	2.45	0.56
1:D:3:LYS:N	2:D:304:HOH:O	2.38	0.55
1:D:155:ASP:HB2	1:D:162:LYS:HG2	1.87	0.55
1:C:80:ARG:C	1:C:194:LEU:HD13	2.30	0.54
1:D:68:VAL:N	2:D:306:HOH:O	2.41	0.54
1:D:199:HIS:HB2	1:D:227:ALA:O	2.08	0.54
1:A:74:TYR:OH	1:A:199:HIS:HE1	1.91	0.53
1:B:214:LYS:HD3	1:B:214:LYS:H	1.73	0.52
1:D:154:ALA:HB2	1:D:196:PRO:O	2.10	0.52
1:A:43:THR:HG22	1:A:221:LEU:CD1	2.38	0.52
1:D:81:HIS:CE1	1:D:197:ASP:H	2.28	0.52
1:C:78:MET:HA	1:C:81:HIS:CD2	2.45	0.52
1:C:78:MET:HE1	1:C:228:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ALA:HB2	1:A:196:PRO:O	2.10	0.51
1:D:74:TYR:HD2	1:D:78:MET:HG2	1.76	0.50
1:B:80:ARG:O	1:B:194:LEU:HD13	2.11	0.50
1:B:81:HIS:HB3	1:B:196:PRO:CA	2.33	0.50
1:C:66:CRO:HG11	1:C:220:LEU:HD21	1.94	0.50
1:A:122:ARG:CZ	1:B:19:ASP:HB2	2.42	0.49
1:C:78:MET:HA	1:C:81:HIS:HD2	1.76	0.49
1:B:77:HIS:ND1	1:B:77:HIS:N	2.52	0.48
1:A:53:LEU:HD22	1:A:57:TRP:CE2	2.48	0.48
1:C:78:MET:O	1:C:81:HIS:HB2	2.13	0.48
1:C:19:ASP:OD1	2:C:301:HOH:O	2.20	0.48
1:A:78:MET:C	1:A:80:ARG:N	2.71	0.48
1:D:160:GLY:HA3	1:D:185:ASN:O	2.13	0.48
1:C:36:ASP:OD1	1:C:38:THR:HG22	2.14	0.47
1:D:155:ASP:O	1:D:157:GLN:N	2.48	0.47
1:D:74:TYR:CD2	1:D:78:MET:HG2	2.50	0.47
1:B:75:PRO:HB2	1:B:77:HIS:CE1	2.50	0.46
1:D:151:TYR:CZ	1:D:198:ASN:HB3	2.50	0.46
1:D:80:ARG:HD2	1:D:81:HIS:HD2	1.80	0.46
1:A:78:MET:O	1:A:80:ARG:N	2.49	0.46
1:D:72:SER:HA	1:D:224:VAL:HG13	1.97	0.46
1:A:187:PRO:HG3	1:A:193:VAL:HG11	1.97	0.46
1:A:72:SER:HA	1:A:224:VAL:HG13	1.98	0.46
1:A:72:SER:HB2	1:A:224:VAL:HG22	1.98	0.45
1:A:142:GLU:OE2	2:A:301:HOH:O	2.21	0.45
1:C:78:MET:HE1	1:C:228:GLY:CA	2.46	0.45
1:D:79:LYS:HE3	1:D:79:LYS:HB2	1.78	0.45
1:C:153:MET:HB2	1:C:162:LYS:HG2	1.98	0.45
1:C:72:SER:HB2	1:C:224:VAL:HG22	1.99	0.45
1:A:61:VAL:O	1:A:66:CRO:N1	2.50	0.45
1:B:73:ARG:HB3	1:B:225:THR:HB	1.99	0.45
1:C:107:LYS:HG3	2:C:360:HOH:O	2.16	0.44
1:B:168:ARG:HG2	1:B:176:VAL:HG11	1.98	0.44
1:C:72:SER:OG	1:C:74:TYR:CE1	2.70	0.44
1:C:56:PRO:HD3	1:C:136:ILE:O	2.17	0.43
1:C:72:SER:HA	1:C:224:VAL:HG13	1.98	0.43
1:A:202:PHE:HE1	1:A:227:ALA:HB3	1.84	0.43
1:B:56:PRO:HD3	1:B:136:ILE:O	2.17	0.43
1:D:146:ASN:ND2	2:D:313:HOH:O	2.52	0.43
1:B:149:GLN:H	1:B:149:GLN:HG2	1.58	0.43
1:C:168:ARG:HD3	2:C:429:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:HIS:O	1:D:196:PRO:HB3	2.19	0.43
1:C:5:GLU:OE2	1:C:79:LYS:O	2.37	0.43
1:D:135:ASN:HA	1:D:140:LYS:HB2	2.01	0.42
1:B:80:ARG:HH11	1:B:80:ARG:CG	2.21	0.42
1:D:78:MET:HE3	1:D:78:MET:HB2	1.62	0.42
1:D:72:SER:CB	1:D:224:VAL:HG22	2.49	0.42
1:C:168:ARG:HD2	1:C:176:VAL:HG11	2.02	0.42
1:A:81:HIS:O	1:A:196:PRO:HB3	2.19	0.42
1:D:155:ASP:CG	1:D:162:LYS:HE3	2.44	0.42
1:C:96:ARG:HA	1:C:182:TYR:O	2.20	0.41
1:D:202:PHE:O	1:D:224:VAL:HA	2.20	0.41
1:A:161:ILE:C	1:A:161:ILE:HD12	2.45	0.41
1:C:72:SER:CB	1:C:224:VAL:HG22	2.50	0.41
1:A:96:ARG:HA	1:A:182:TYR:O	2.20	0.41
1:A:227:ALA:HB2	1:C:39:TYR:CE1	2.56	0.41
1:A:78:MET:CE	1:A:227:ALA:C	2.93	0.41
1:A:73:ARG:HD2	1:A:73:ARG:C	2.46	0.40
1:D:72:SER:OG	1:D:74:TYR:CE1	2.74	0.40
1:B:72:SER:OG	1:B:74:TYR:CE1	2.75	0.40
1:D:152:ILE:O	1:D:198:ASN:HA	2.22	0.40
1:D:157:GLN:C	1:D:159:ASN:H	2.30	0.40
1:A:202:PHE:CE1	1:A:227:ALA:HB3	2.56	0.40
1:C:140:LYS:C	1:C:172:GLU:HG3	2.47	0.40

There are no symmetry-related clashes.

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	220/236 (93%)	216 (98%)	3 (1%)	1 (0%)	24	16
1	B	220/236 (93%)	217 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	220/236 (93%)	213 (97%)	7 (3%)	0	100	100
1	D	220/236 (93%)	214 (97%)	5 (2%)	1 (0%)	24	16
All	All	880/944 (93%)	860 (98%)	18 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	LYS
1	D	156	LYS

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	193/205 (94%)	187 (97%)	6 (3%)	35	26
1	B	193/205 (94%)	186 (96%)	7 (4%)	31	21
1	C	193/205 (94%)	186 (96%)	7 (4%)	31	21
1	D	193/205 (94%)	188 (97%)	5 (3%)	40	33
All	All	772/820 (94%)	747 (97%)	25 (3%)	34	25

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	52	LYS
1	A	78	MET
1	A	129	ASP
1	A	164	ASN
1	A	214	LYS
1	B	76	ASP
1	B	77	HIS
1	B	80	ARG
1	B	129	ASP

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	224	VAL
1	B	225	THR
1	C	34	GLU
1	C	76	ASP
1	C	80	ARG
1	C	176	VAL
1	C	178	LEU
1	C	224	VAL
1	C	225	THR
1	D	68	VAL
1	D	156	LYS
1	D	164	ASN
1	D	176	VAL
1	D	224	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	199	HIS
1	B	81	HIS
1	B	164	ASN
1	C	164	ASN
1	C	184	GLN
1	D	81	HIS
1	D	105	ASN
1	D	146	ASN
1	D	149	GLN
1	D	184	GLN

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	C	66	1	22,23,24	4.87	9 (40%)	30,32,34	3.29	12 (40%)
1	CRO	D	66	1	22,23,24	5.47	9 (40%)	30,32,34	2.62	9 (30%)
1	CRO	B	66	1	22,23,24	5.74	10 (45%)	30,32,34	2.72	10 (33%)
1	CRO	A	66	1	22,23,24	5.74	10 (45%)	30,32,34	2.72	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	C	66	1	-	5/12/31/32	0/2/2/2
1	CRO	D	66	1	-	2/12/31/32	0/2/2/2
1	CRO	B	66	1	-	2/12/31/32	0/2/2/2
1	CRO	A	66	1	-	2/12/31/32	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CB2-CA2	18.01	1.52	1.35
1	B	66	CRO	CB2-CA2	18.00	1.52	1.35
1	C	66	CRO	CB2-CA2	17.90	1.52	1.35
1	D	66	CRO	CB2-CA2	17.29	1.51	1.35
1	B	66	CRO	CA2-C2	-11.62	1.36	1.48
1	A	66	CRO	CA2-C2	-11.60	1.36	1.48
1	A	66	CRO	OG1-CB1	-11.10	1.13	1.43
1	B	66	CRO	OG1-CB1	-11.10	1.13	1.43
1	D	66	CRO	CA2-C2	-10.31	1.37	1.48
1	D	66	CRO	OG1-CB1	-10.25	1.16	1.43
1	C	66	CRO	CA2-C2	-8.63	1.39	1.48
1	C	66	CRO	O2-C2	7.75	1.38	1.23
1	B	66	CRO	O2-C2	6.55	1.36	1.23
1	A	66	CRO	O2-C2	6.54	1.36	1.23
1	D	66	CRO	C2-N3	-6.12	1.25	1.40
1	D	66	CRO	O2-C2	5.64	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	CRO	C1-N3	-5.28	1.28	1.37
1	A	66	CRO	CA2-N2	-4.82	1.28	1.38
1	B	66	CRO	CA2-N2	-4.80	1.28	1.38
1	A	66	CRO	C2-N3	-4.76	1.29	1.40
1	B	66	CRO	C2-N3	-4.74	1.29	1.40
1	D	66	CRO	CA2-N2	-4.73	1.28	1.38
1	B	66	CRO	C1-N3	-4.64	1.29	1.37
1	A	66	CRO	C1-N3	-4.62	1.29	1.37
1	C	66	CRO	CG1-CB1	-4.26	1.39	1.51
1	D	66	CRO	CA3-N3	-3.45	1.40	1.47
1	C	66	CRO	C2-N3	-3.44	1.32	1.40
1	C	66	CRO	CG2-CB2	3.38	1.53	1.46
1	C	66	CRO	OG1-CB1	-2.99	1.35	1.43
1	A	66	CRO	CG2-CB2	2.65	1.51	1.46
1	B	66	CRO	CG2-CB2	2.65	1.51	1.46
1	D	66	CRO	CG2-CB2	2.58	1.51	1.46
1	C	66	CRO	CA2-N2	-2.51	1.33	1.38
1	B	66	CRO	CA3-N3	-2.51	1.42	1.47
1	A	66	CRO	CA3-N3	-2.50	1.42	1.47
1	B	66	CRO	C1-N2	-2.44	1.28	1.32
1	A	66	CRO	C1-N2	-2.39	1.28	1.32
1	C	66	CRO	C1-N3	-2.08	1.33	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	CRO	O2-C2-CA2	-9.92	124.69	131.02
1	C	66	CRO	CG1-CB1-CA1	9.35	133.55	112.18
1	D	66	CRO	O2-C2-CA2	-7.41	126.29	131.02
1	A	66	CRO	O2-C2-CA2	-6.80	126.68	131.02
1	B	66	CRO	O2-C2-CA2	-6.77	126.70	131.02
1	C	66	CRO	CG2-CB2-CA2	-6.43	122.22	129.87
1	D	66	CRO	CG2-CB2-CA2	-5.82	122.94	129.87
1	D	66	CRO	CA2-C2-N3	5.72	108.30	103.50
1	B	66	CRO	CG2-CB2-CA2	-5.58	123.24	129.87
1	A	66	CRO	CG2-CB2-CA2	-5.57	123.24	129.87
1	A	66	CRO	CA2-N2-C1	5.43	110.04	105.80
1	B	66	CRO	CA2-N2-C1	5.42	110.04	105.80
1	C	66	CRO	CA2-C2-N3	5.37	108.01	103.50
1	A	66	CRO	CA2-C2-N3	5.09	107.78	103.50
1	B	66	CRO	CA2-C2-N3	5.09	107.77	103.50
1	D	66	CRO	OG1-CB1-CA1	4.81	119.25	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CRO	C2-CA2-N2	-4.80	105.51	108.95
1	A	66	CRO	C2-CA2-N2	-4.79	105.52	108.95
1	D	66	CRO	C2-CA2-N2	-4.23	105.92	108.95
1	B	66	CRO	C1-CA1-N1	3.72	116.44	109.78
1	A	66	CRO	C1-CA1-N1	3.65	116.30	109.78
1	A	66	CRO	N3-C1-N2	-3.53	108.70	111.48
1	B	66	CRO	N3-C1-N2	-3.47	108.75	111.48
1	D	66	CRO	C1-CA1-N1	3.28	115.64	109.78
1	A	66	CRO	OG1-CB1-CA1	3.18	115.78	109.00
1	B	66	CRO	OG1-CB1-CA1	3.17	115.75	109.00
1	D	66	CRO	O3-C3-CA3	-3.04	111.77	125.47
1	C	66	CRO	C2-CA2-N2	-2.77	106.97	108.95
1	A	66	CRO	CA1-C1-N3	2.66	127.83	124.69
1	B	66	CRO	CA1-C1-N3	2.62	127.78	124.69
1	C	66	CRO	CA1-C1-N2	2.57	127.37	123.88
1	C	66	CRO	C1-CA1-N1	-2.50	105.31	109.78
1	D	66	CRO	CB2-CA2-N2	2.49	132.14	128.76
1	C	66	CRO	CA2-N2-C1	2.28	107.58	105.80
1	B	66	CRO	O3-C3-CA3	-2.27	115.24	125.47
1	A	66	CRO	O3-C3-CA3	-2.27	115.25	125.47
1	C	66	CRO	OG1-CB1-CA1	2.25	113.80	109.00
1	C	66	CRO	CB2-CA2-N2	2.22	131.77	128.76
1	D	66	CRO	CA2-N2-C1	2.15	107.48	105.80
1	C	66	CRO	CD2-CG2-CB2	-2.08	114.07	121.22
1	C	66	CRO	CD2-CG2-CD1	2.03	120.66	117.65

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	66	CRO	N1-CA1-CB1-OG1
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	N2-CA2-CB2-CG2
1	C	66	CRO	C1-CA1-CB1-CG1
1	A	66	CRO	C1-CA1-CB1-CG1
1	B	66	CRO	C1-CA1-CB1-CG1
1	D	66	CRO	C1-CA1-CB1-CG1
1	A	66	CRO	N2-C1-CA1-CB1
1	B	66	CRO	N2-C1-CA1-CB1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	CRO	1	0
1	A	66	CRO	1	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	224/236 (94%)	0.27	17 (7%) 20 22	17, 27, 65, 83	0
1	B	224/236 (94%)	0.12	13 (5%) 29 33	15, 25, 55, 80	0
1	C	224/236 (94%)	0.21	17 (7%) 20 22	16, 25, 59, 76	0
1	D	224/236 (94%)	0.32	19 (8%) 16 19	17, 27, 65, 83	0
All	All	896/944 (94%)	0.23	66 (7%) 20 23	15, 26, 64, 83	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	ILE	7.1
1	C	194	LEU	6.3
1	B	229	ILE	6.3
1	B	174	GLY	5.7
1	C	81	HIS	5.7
1	D	194	LEU	5.3
1	A	194	LEU	4.9
1	A	229	ILE	4.7
1	D	77	HIS	4.7
1	D	229	ILE	4.7
1	D	193	VAL	4.5
1	A	193	VAL	4.4
1	A	77	HIS	4.4
1	B	80	ARG	4.3
1	A	79	LYS	4.1
1	C	77	HIS	4.0
1	B	79	LYS	3.9
1	D	192	PRO	3.9
1	C	195	LEU	3.9
1	D	156	LYS	3.9
1	B	77	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	81	HIS	3.7
1	C	193	VAL	3.7
1	C	192	PRO	3.7
1	C	3	LYS	3.7
1	A	74	TYR	3.6
1	D	78	MET	3.5
1	D	74	TYR	3.4
1	B	175	GLY	3.4
1	B	157	GLN	3.4
1	C	74	TYR	3.4
1	B	74	TYR	3.3
1	D	195	LEU	3.3
1	B	192	PRO	3.3
1	B	3	LYS	3.3
1	A	192	PRO	3.3
1	A	195	LEU	3.1
1	C	157	GLN	3.1
1	D	75	PRO	3.1
1	D	79	LYS	3.0
1	C	78	MET	3.0
1	C	79	LYS	2.9
1	B	194	LEU	2.9
1	D	81	HIS	2.9
1	D	196	PRO	2.8
1	A	157	GLN	2.8
1	C	80	ARG	2.7
1	A	81	HIS	2.7
1	C	174	GLY	2.6
1	A	76	ASP	2.6
1	D	191	GLY	2.6
1	B	78	MET	2.5
1	D	157	GLN	2.5
1	A	78	MET	2.4
1	A	156	LYS	2.4
1	A	80	ARG	2.3
1	C	76	ASP	2.3
1	D	76	ASP	2.2
1	C	191	GLY	2.2
1	A	75	PRO	2.2
1	A	82	ASP	2.1
1	D	228	GLY	2.1
1	D	80	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	3	LYS	2.1
1	C	196	PRO	2.0
1	D	189	GLY	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(Å ²)	Q<0.9
1	CRO	B	66	22/23	0.89	0.10	17,22,24,25	0
1	CRO	A	66	22/23	0.95	0.07	17,22,24,25	0
1	CRO	C	66	22/23	0.96	0.06	15,19,22,29	0
1	CRO	D	66	22/23	0.96	0.07	15,23,26,27	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.