



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:56 PM UTC

PDB ID : 1B9C / pdb_00001b9c
Title : Green Fluorescent Protein Mutant F99S, M153T and V163A
Authors : Battistutta, R.; Negro, A.; Zanotti, G.
Deposited on : 1999-02-09
Resolution : 2.40 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

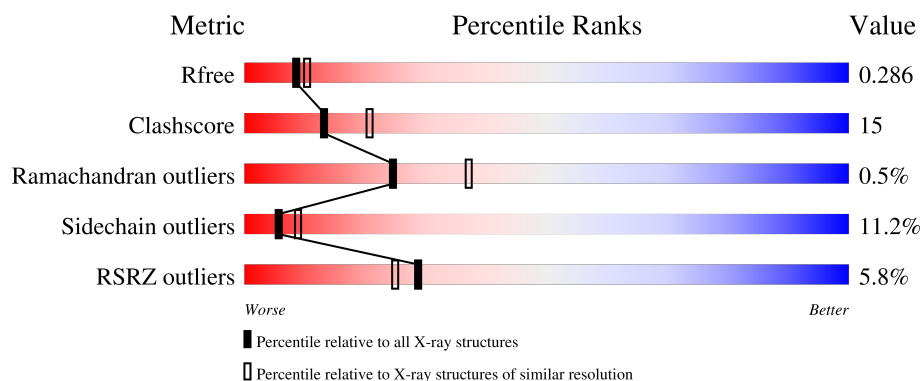
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	
1	B	236	
1	C	236	
1	D	236	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7466 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 PROTEIN (GREEN FLUORESCENT PROTEIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1795	1139	303	348	5			
1	B	225	Total	C	N	O	S	0	0	0
			1795	1139	303	348	5			
1	C	225	Total	C	N	O	S	0	0	0
			1795	1139	303	348	5			
1	D	225	Total	C	N	O	S	0	0	0
			1795	1139	303	348	5			

There are 28 discrepancies between the modelled and reference sequences:

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	1	ALA	MET	engineered mutation	UNP P42212
A	99	SER	PHE	engineered mutation	UNP P42212
A	153	THR	MET	engineered mutation	UNP P42212
A	163	ALA	VAL	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	1	ALA	MET	engineered mutation	UNP P42212
B	99	SER	PHE	engineered mutation	UNP P42212
B	153	THR	MET	engineered mutation	UNP P42212
B	163	ALA	VAL	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	1	ALA	MET	engineered mutation	UNP P42212
C	99	SER	PHE	engineered mutation	UNP P42212
C	153	THR	MET	engineered mutation	UNP P42212
C	163	ALA	VAL	engineered mutation	UNP P42212

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Chain	Residue	Modelled	Actual	Comment	Reference
D	66	CRO	SER	chromophore	UNP P42212
D	66	CRO	TYR	chromophore	UNP P42212
D	66	CRO	GLY	chromophore	UNP P42212
D	1	ALA	MET	engineered mutation	UNP P42212
D	99	SER	PHE	engineered mutation	UNP P42212
D	153	THR	MET	engineered mutation	UNP P42212
D	163	ALA	VAL	engineered mutation	UNP P42212

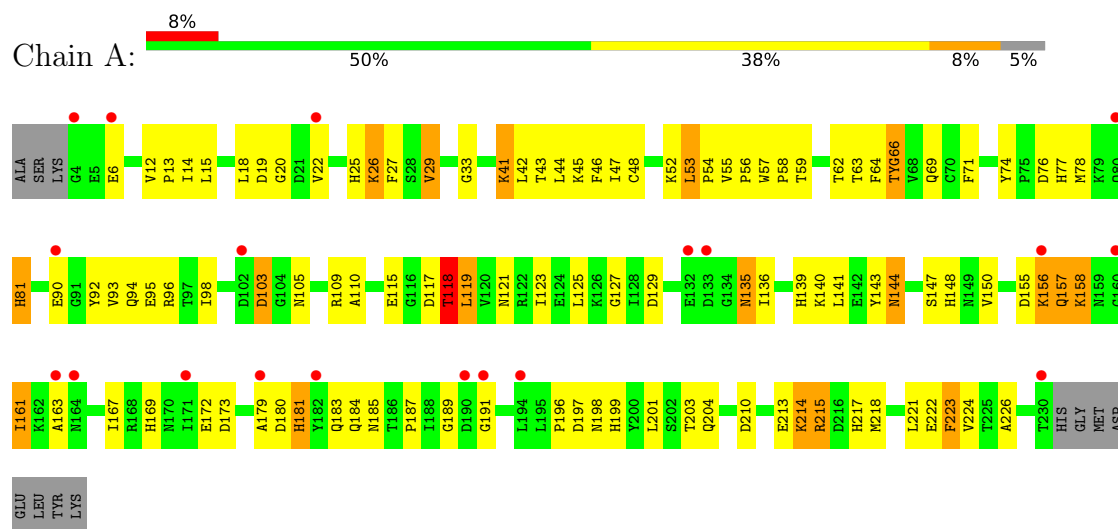
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	39	Total O 39 39	0	0
2	B	41	Total O 41 41	0	0
2	C	110	Total O 110 110	0	0
2	D	96	Total O 96 96	0	0

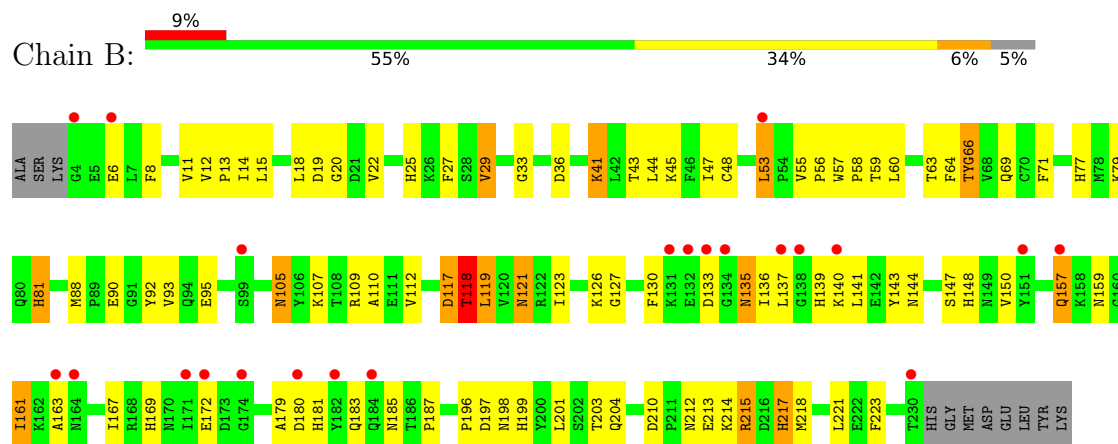
3 Residue-property plots [i](#)

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.

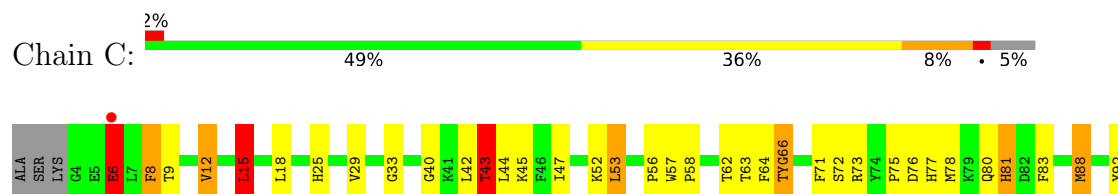
• Molecule 1: PROTEIN (GREEN FLUORESCENT PROTEIN)

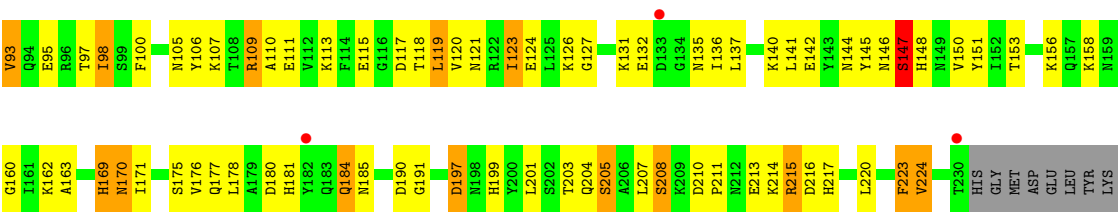


• Molecule 1: PROTEIN (GREEN FLUORESCENT PROTEIN)

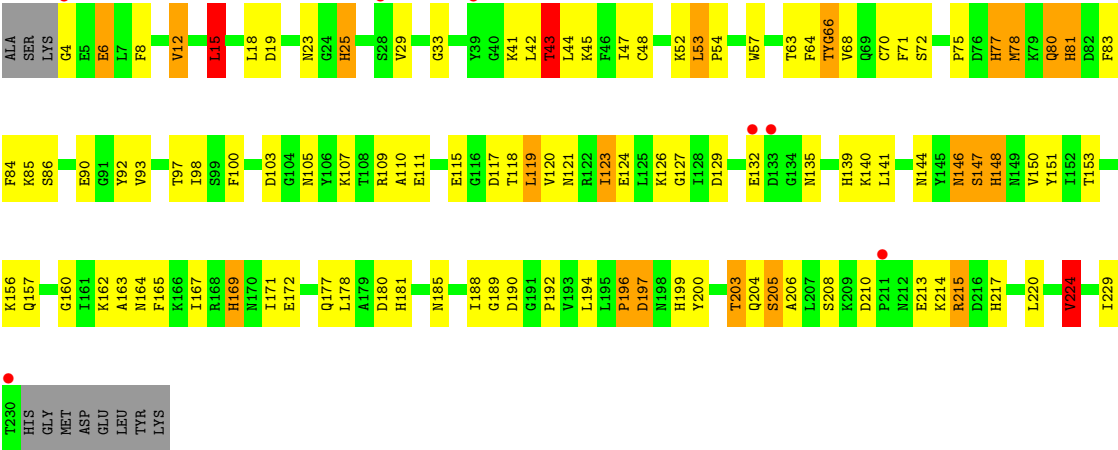


• Molecule 1: PROTEIN (GREEN FLUORESCENT PROTEIN)





● Molecule 1: PROTEIN (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	83.48Å 85.37Å 140.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	89.9 (30.00-2.40) 94.6 (30.00-2.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.35 (at 2.44Å)	Xtriage
Refinement program	X-PLOR 3.8.5	Depositor
R, R_{free}	0.204 , 0.280 0.219 , 0.286	Depositor DCC
R_{free} test set	3663 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7466	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.31% 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	1.03	15/1814 (0.8%)	1.72	34/2453 (1.4%)
1	B	1.09	15/1814 (0.8%)	1.74	28/2453 (1.1%)
1	C	1.30	15/1814 (0.8%)	2.00	50/2453 (2.0%)
1	D	1.28	12/1814 (0.7%)	1.95	54/2453 (2.2%)
All	All	1.18	57/7256 (0.8%)	1.86	166/9812 (1.7%)

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 (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	77	HIS	CD2-NE2	-8.01	1.29	1.37
1	D	77	HIS	CD2-NE2	-7.49	1.29	1.37
1	D	181	HIS	CD2-NE2	-7.48	1.29	1.37
1	C	81	HIS	CD2-NE2	-7.45	1.29	1.37
1	A	169	HIS	CD2-NE2	-7.28	1.29	1.37
1	C	77	HIS	CD2-NE2	-7.16	1.29	1.37
1	B	181	HIS	CD2-NE2	-7.09	1.30	1.37
1	C	208	SER	CA-CB	-7.05	1.43	1.53
1	B	148	HIS	CD2-NE2	-7.05	1.30	1.37
1	C	199	HIS	CD2-NE2	-7.04	1.30	1.37
1	B	139	HIS	CD2-NE2	-6.99	1.30	1.37
1	A	81	HIS	CD2-NE2	-6.91	1.30	1.37
1	D	217	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	217	HIS	CD2-NE2	-6.73	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	HIS	CD2-NE2	-6.71	1.30	1.37
1	C	169	HIS	CD2-NE2	-6.66	1.30	1.37
1	B	217	HIS	CD2-NE2	-6.64	1.30	1.37
1	B	81	HIS	CD2-NE2	-6.60	1.30	1.37
1	A	25	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	139	HIS	CG-ND1	-6.54	1.31	1.38
1	C	181	HIS	CD2-NE2	-6.47	1.30	1.37
1	D	199	HIS	CD2-NE2	-6.45	1.30	1.37
1	C	217	HIS	CD2-NE2	-6.41	1.30	1.37
1	B	169	HIS	CD2-NE2	-6.38	1.30	1.37
1	D	181	HIS	CA-CB	-6.33	1.44	1.53
1	B	199	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	77	HIS	CD2-NE2	-6.28	1.30	1.37
1	D	81	HIS	CD2-NE2	-6.25	1.30	1.37
1	A	139	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	25	HIS	CD2-NE2	-6.21	1.31	1.37
1	D	192	PRO	CA-CB	-6.14	1.46	1.53
1	A	148	HIS	CD2-NE2	-6.05	1.31	1.37
1	C	25	HIS	CD2-NE2	-5.91	1.31	1.37
1	A	199	HIS	CD2-NE2	-5.85	1.31	1.37
1	C	100	PHE	CA-CB	-5.83	1.45	1.53
1	C	148	HIS	CD2-NE2	-5.79	1.31	1.37
1	D	169	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	139	HIS	CG-ND1	-5.53	1.32	1.38
1	D	148	HIS	CD2-NE2	-5.52	1.31	1.37
1	D	25	HIS	CD2-NE2	-5.51	1.31	1.37
1	B	118	THR	CA-CB	5.48	1.61	1.53
1	C	93	VAL	N-CA	-5.48	1.38	1.46
1	C	81	HIS	CG-ND1	-5.46	1.32	1.38
1	D	139	HIS	CD2-NE2	-5.45	1.31	1.37
1	A	118	THR	CA-CB	5.43	1.63	1.53
1	B	181	HIS	CG-ND1	-5.37	1.32	1.38
1	A	199	HIS	CG-ND1	-5.31	1.32	1.38
1	A	169	HIS	CG-ND1	-5.29	1.32	1.38
1	C	109	ARG	CA-C	-5.27	1.46	1.52
1	A	77	HIS	CG-ND1	-5.26	1.32	1.38
1	A	81	HIS	CG-ND1	-5.25	1.32	1.38
1	B	217	HIS	CG-ND1	-5.25	1.32	1.38
1	B	148	HIS	CG-ND1	-5.23	1.32	1.38
1	D	199	HIS	CG-ND1	-5.20	1.32	1.38
1	B	25	HIS	CG-ND1	-5.15	1.32	1.38
1	C	77	HIS	CG-ND1	-5.12	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	HIS	CG-ND1	-5.07	1.32	1.38

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	ASP	CA-CB-CG	15.56	128.16	112.60
1	C	215	ARG	CD-NE-CZ	12.60	142.04	124.40
1	D	215	ARG	CD-NE-CZ	11.36	140.30	124.40
1	C	43	THR	CA-CB-OG1	-10.54	93.78	109.60
1	D	181	HIS	CB-CG-CD2	-9.72	118.56	131.20
1	C	64	PHE	CA-CB-CG	9.23	123.03	113.80
1	C	215	ARG	NE-CZ-NH2	-9.11	111.00	119.20
1	C	181	HIS	CB-CG-CD2	-9.01	119.48	131.20
1	C	215	ARG	NE-CZ-NH1	8.88	130.38	121.50
1	C	107	LYS	N-CA-C	-8.58	93.51	108.69
1	C	170	ASN	CA-CB-CG	8.49	121.09	112.60
1	C	109	ARG	N-CA-C	-8.38	94.58	108.32
1	A	117	ASP	CA-CB-CG	8.26	120.86	112.60
1	D	43	THR	CA-CB-OG1	-8.24	97.25	109.60
1	D	215	ARG	NE-CZ-NH2	-8.10	111.91	119.20
1	D	117	ASP	CA-CB-CG	8.06	120.66	112.60
1	D	109	ARG	N-CA-C	-8.01	94.07	108.48
1	A	184	GLN	CA-CB-CG	7.92	129.93	114.10
1	B	196	PRO	N-CA-C	7.71	123.30	111.57
1	C	43	THR	CA-CB-CG2	7.69	123.58	110.50
1	B	117	ASP	CA-CB-CG	7.56	120.16	112.60
1	D	107	LYS	N-CA-C	-7.51	95.40	108.69
1	D	215	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	C	199	HIS	CB-CG-CD2	-7.30	121.71	131.20
1	D	57	TRP	CA-C-N	7.18	127.02	119.05
1	D	57	TRP	C-N-CA	7.18	127.02	119.05
1	A	129	ASP	CA-CB-CG	7.09	119.69	112.60
1	D	44	LEU	N-CA-C	7.09	120.96	109.40
1	D	64	PHE	CA-CB-CG	7.09	120.89	113.80
1	B	77	HIS	CB-CG-CD2	-7.06	122.03	131.20
1	C	57	TRP	CA-C-N	7.03	127.01	119.28
1	C	57	TRP	C-N-CA	7.03	127.01	119.28
1	C	44	LEU	N-CA-C	6.98	120.78	109.40
1	C	124	GLU	N-CA-C	-6.90	97.33	109.06
1	C	197	ASP	CA-CB-CG	6.90	119.50	112.60
1	D	77	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	D	199	HIS	CB-CG-CD2	-6.76	122.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	SER	N-CA-CB	-6.72	100.61	111.22
1	A	173	ASP	CA-CB-CG	6.57	119.17	112.60
1	C	210	ASP	CA-CB-CG	6.55	119.15	112.60
1	A	196	PRO	N-CA-C	6.51	122.65	111.77
1	B	79	LYS	CA-C-N	6.51	131.74	120.68
1	B	79	LYS	C-N-CA	6.51	131.74	120.68
1	A	41	LYS	CA-C-O	6.39	127.60	120.70
1	D	129	ASP	N-CA-C	6.37	120.63	112.86
1	C	15	LEU	N-CA-C	-6.36	97.19	108.13
1	D	100	PHE	CA-CB-CG	-6.35	107.45	113.80
1	A	41	LYS	N-CA-C	6.32	119.70	109.40
1	D	146	ASN	CA-CB-CG	-6.23	106.37	112.60
1	D	43	THR	CA-CB-CG2	6.21	121.05	110.50
1	C	76	ASP	CA-CB-CG	6.20	118.80	112.60
1	D	210	ASP	CA-CB-CG	6.19	118.79	112.60
1	C	147	SER	CA-CB-OG	-6.12	98.86	111.10
1	D	217	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	B	19	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	216	ASP	N-CA-C	-6.08	100.85	109.96
1	D	15	LEU	N-CA-C	-6.05	97.72	108.13
1	A	19	ASP	CA-CB-CG	6.05	118.65	112.60
1	A	77	HIS	CA-CB-CG	5.98	119.78	113.80
1	C	190	ASP	CA-CB-CG	5.97	118.57	112.60
1	C	57	TRP	CE2-CD2-CG	-5.94	100.07	107.20
1	D	97	THR	CA-CB-OG1	-5.94	100.69	109.60
1	D	19	ASP	N-CA-C	-5.92	98.75	108.76
1	A	184	GLN	CB-CG-CD	-5.88	102.61	112.60
1	D	25	HIS	CB-CG-CD2	-5.88	123.56	131.20
1	C	77	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	156	LYS	CA-C-N	5.87	128.07	120.44
1	A	156	LYS	C-N-CA	5.87	128.07	120.44
1	D	103	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	169	HIS	CB-CG-CD2	-5.83	123.61	131.20
1	C	156	LYS	N-CA-C	-5.83	104.62	110.97
1	A	121	ASN	OD1-CG-ND2	-5.83	116.77	122.60
1	C	81	HIS	CB-CG-CD2	-5.79	123.67	131.20
1	D	81	HIS	CB-CG-CD2	-5.77	123.70	131.20
1	D	197	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	217	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	C	8	PHE	N-CA-C	5.72	119.34	112.93
1	B	210	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	98	ILE	N-CA-C	-5.70	99.67	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	GLU	N-CA-C	-5.67	99.77	109.24
1	B	41	LYS	N-CA-C	5.67	118.64	109.40
1	D	169	HIS	ND1-CE1-NE2	5.65	114.05	108.40
1	C	88	MET	N-CA-C	5.64	117.73	110.39
1	D	78	MET	CA-CB-CG	5.64	125.39	114.10
1	D	188	ILE	N-CA-C	-5.59	105.65	110.74
1	B	57	TRP	CG-CD2-CE3	5.59	139.49	133.90
1	A	210	ASP	CA-C-N	5.58	125.26	119.56
1	A	210	ASP	C-N-CA	5.58	125.26	119.56
1	A	135	ASN	N-CA-C	5.58	119.59	112.34
1	B	36	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	224	VAL	CB-CA-C	-5.54	102.25	110.33
1	B	135	ASN	CA-CB-CG	5.53	118.13	112.60
1	C	25	HIS	CB-CG-CD2	-5.53	124.00	131.20
1	A	199	HIS	CB-CG-CD2	-5.52	124.03	131.20
1	A	148	HIS	CB-CG-CD2	-5.51	124.03	131.20
1	B	20	GLY	O-C-N	5.51	128.08	123.29
1	B	57	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	A	189	GLY	O-C-N	5.50	129.85	122.70
1	D	57	TRP	CE2-CD2-CG	-5.48	100.62	107.20
1	C	137	LEU	CD1-CG-CD2	-5.48	98.75	110.80
1	C	217	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	A	121	ASN	CA-CB-CG	5.45	118.05	112.60
1	B	19	ASP	N-CA-C	-5.44	98.33	108.02
1	C	115	GLU	N-CA-C	-5.44	96.93	107.44
1	D	139	HIS	CB-CG-CD2	-5.44	124.13	131.20
1	A	217	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	D	90	GLU	CB-CG-CD	5.41	121.80	112.60
1	B	159	ASN	CA-CB-CG	5.41	118.00	112.60
1	B	169	HIS	CB-CG-CD2	-5.41	124.17	131.20
1	B	148	HIS	CB-CG-CD2	-5.40	124.18	131.20
1	A	57	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	B	81	HIS	CB-CG-CD2	-5.38	124.21	131.20
1	B	187	PRO	N-CA-C	5.37	119.67	111.34
1	B	105	ASN	N-CA-C	5.36	117.40	108.99
1	D	164	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	D	8	PHE	N-CA-C	5.33	118.89	112.93
1	C	12	VAL	CA-C-N	5.32	125.58	119.83
1	C	12	VAL	C-N-CA	5.32	125.58	119.83
1	D	115	GLU	N-CA-C	-5.32	97.17	107.44
1	A	77	HIS	CB-CG-CD2	-5.31	124.29	131.20
1	B	135	ASN	N-CA-C	5.31	118.86	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	LYS	CA-CB-CG	5.30	124.71	114.10
1	B	199	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	D	6	GLU	N-CA-C	5.27	119.46	113.19
1	C	175	SER	CA-C-N	-5.26	115.80	123.06
1	C	175	SER	C-N-CA	-5.26	115.80	123.06
1	D	139	HIS	N-CA-C	5.25	118.44	111.30
1	D	4	GLY	CA-C-N	5.25	127.26	120.44
1	D	4	GLY	C-N-CA	5.25	127.26	120.44
1	A	181	HIS	CB-CG-CD2	-5.25	124.38	131.20
1	D	165	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	97	THR	CA-CB-OG1	-5.23	101.76	109.60
1	A	223	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	77	HIS	ND1-CG-CD2	5.21	111.31	106.10
1	C	6	GLU	N-CA-C	5.21	119.39	113.19
1	D	181	HIS	CB-CG-ND1	5.18	130.47	122.70
1	C	113	LYS	CB-CG-CD	5.17	123.19	111.30
1	A	81	HIS	CB-CG-CD2	-5.16	124.50	131.20
1	A	187	PRO	N-CA-C	5.15	119.41	111.21
1	C	146	ASN	CA-CB-CG	-5.15	107.45	112.60
1	D	23	ASN	CA-CB-CG	-5.15	107.45	112.60
1	D	121	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	C	223	PHE	N-CA-C	-5.14	99.73	108.26
1	C	57	TRP	CD1-CG-CD2	5.12	114.48	106.30
1	A	144	ASN	CA-CB-CG	5.11	117.71	112.60
1	D	80	GLN	N-CA-C	-5.11	107.00	113.18
1	A	172	GLU	N-CA-C	5.10	118.28	111.75
1	B	121	ASN	CA-CB-CG	5.09	117.69	112.60
1	D	215	ARG	CB-CG-CD	5.09	123.00	111.30
1	D	68	VAL	CA-CB-CG1	-5.08	101.76	110.40
1	D	12	VAL	CA-C-N	5.08	125.32	119.83
1	D	12	VAL	C-N-CA	5.08	125.32	119.83
1	B	126	LYS	CA-C-N	5.08	126.49	121.57
1	B	126	LYS	C-N-CA	5.08	126.49	121.57
1	A	20	GLY	O-C-N	5.08	127.71	123.29
1	D	169	HIS	CB-CG-CD2	-5.07	124.61	131.20
1	C	210	ASP	N-CA-C	-5.06	101.93	109.42
1	C	115	GLU	CB-CG-CD	5.05	121.19	112.60
1	D	41	LYS	N-CA-C	5.05	117.63	109.40
1	A	19	ASP	N-CA-C	-5.04	99.04	108.02
1	B	139	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	D	196	PRO	N-CA-C	5.04	122.85	112.47
1	A	103	ASP	CA-CB-CG	5.03	117.63	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	LEU	CA-C-O	5.02	123.03	119.32
1	C	121	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	C	131	LYS	N-CA-C	-5.01	102.45	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	GLY	Peptide

5.2 Too-close contacts ⓘ

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	1795	0	1730	61	0
1	B	1795	0	1730	49	0
1	C	1795	0	1730	60	0
1	D	1795	0	1730	52	0
2	A	39	0	0	3	0
2	B	41	0	0	0	0
2	C	110	0	0	8	0
2	D	96	0	0	6	0
All	All	7466	0	6920	210	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 15.

All (210) 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:203:THR:HG22	1:A:224:VAL:HG13	1.47	0.95
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.58	0.84
1:D:81:HIS:CD2	1:D:197:ASP:H	2.05	0.75
1:D:81:HIS:HD2	1:D:197:ASP:H	1.33	0.74
1:C:171:ILE:HD11	1:C:177:GLN:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:HIS:HD2	1:C:197:ASP:H	1.40	0.70
1:C:81:HIS:CD2	1:C:197:ASP:H	2.10	0.69
1:A:42:LEU:HD13	1:A:66:CRO:OG1	1.98	0.63
1:C:171:ILE:HD11	1:C:177:GLN:CB	2.29	0.63
1:C:93:VAL:HG22	1:C:111:GLU:HG2	1.81	0.63
1:D:93:VAL:HG22	1:D:111:GLU:HG2	1.80	0.62
1:C:95:GLU:HG2	1:C:109:ARG:HG3	1.81	0.62
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.82	0.62
1:C:75:PRO:HG2	1:C:78:MET:CG	2.30	0.62
1:C:204:GLN:OE1	1:D:144:ASN:HA	2.01	0.61
1:C:110:ALA:HB2	1:C:123:ILE:HG23	1.83	0.61
1:C:75:PRO:HG2	1:C:78:MET:HG2	1.83	0.60
1:D:71:PHE:HE2	1:D:119:LEU:HD22	1.67	0.59
1:C:71:PHE:HE2	1:C:119:LEU:HD22	1.66	0.59
1:C:66:CRO:CE1	1:C:203:THR:HG21	2.32	0.59
1:C:45:LYS:HE2	1:C:47:ILE:HD11	1.85	0.58
1:D:135:ASN:HA	1:D:140:LYS:HB2	1.85	0.58
1:A:214:LYS:HB2	2:A:242:HOH:O	2.03	0.58
1:C:72:SER:HA	1:C:224:VAL:HB	1.84	0.58
1:A:33:GLY:HA3	1:A:44:LEU:HD23	1.86	0.57
1:A:13:PRO:HB2	1:A:118:THR:HB	1.86	0.57
1:B:59:THR:HG23	1:B:141:LEU:HD11	1.87	0.57
1:B:161:ILE:HG13	1:B:185:ASN:HB2	1.87	0.57
1:D:72:SER:HA	1:D:224:VAL:HB	1.87	0.57
1:B:95:GLU:HG2	1:B:109:ARG:HG3	1.87	0.56
1:D:110:ALA:HB2	1:D:123:ILE:HG23	1.87	0.56
1:B:71:PHE:CE2	1:B:119:LEU:HD22	2.40	0.56
1:B:11:VAL:HB	1:D:157:GLN:HG3	1.89	0.55
1:C:135:ASN:HA	1:C:140:LYS:HB2	1.89	0.55
1:D:213:GLU:OE2	1:D:215:ARG:HB2	2.06	0.55
1:D:203:THR:HG23	1:D:224:VAL:HG13	1.88	0.55
1:C:141:LEU:HB3	2:C:328:HOH:O	2.07	0.55
1:C:205:SER:HB3	1:C:220:LEU:HD11	1.87	0.55
1:D:205:SER:HB3	1:D:220:LEU:HD11	1.88	0.55
1:A:42:LEU:HD13	1:A:66:CRO:HOG1	1.72	0.55
1:A:59:THR:HG23	1:A:141:LEU:HD11	1.88	0.55
1:A:71:PHE:CE2	1:A:119:LEU:HD22	2.42	0.55
1:C:169:HIS:HB2	1:C:177:GLN:O	2.06	0.55
1:B:13:PRO:HB2	1:B:118:THR:HB	1.88	0.54
1:D:78:MET:HE3	1:D:229:ILE:HD12	1.90	0.54
1:B:71:PHE:HE2	1:B:119:LEU:HD22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ASN:HB2	1:B:147:SER:OG	2.08	0.53
1:B:45:LYS:HE2	1:B:47:ILE:HD11	1.91	0.53
1:A:150:VAL:HB	1:A:201:LEU:HB2	1.91	0.53
1:B:29:VAL:HG21	1:B:64:PHE:CZ	2.44	0.52
1:A:71:PHE:HE2	1:A:119:LEU:HD22	1.73	0.52
1:C:66:CRO:OH	1:C:203:THR:HB	2.10	0.52
1:C:66:CRO:CZ	1:C:203:THR:HB	2.40	0.52
1:D:86:SER:HB3	1:D:194:LEU:HD12	1.91	0.52
1:A:59:THR:CG2	1:A:141:LEU:HD11	2.40	0.52
1:A:147:SER:OG	1:A:204:GLN:HG2	2.11	0.51
1:C:211:PRO:HD3	2:C:296:HOH:O	2.09	0.51
1:C:158:LYS:HD2	2:C:284:HOH:O	2.11	0.51
1:A:12:VAL:HB	1:A:71:PHE:CE1	2.46	0.51
1:D:42:LEU:HD13	1:D:66:CRO:OG1	2.11	0.51
1:A:12:VAL:HB	1:A:71:PHE:HE1	1.76	0.51
1:C:33:GLY:HA3	1:C:43:THR:O	2.12	0.50
1:B:213:GLU:OE1	1:B:215:ARG:HD3	2.11	0.50
1:C:213:GLU:OE2	1:C:215:ARG:HB2	2.12	0.50
1:A:92:TYR:CE1	1:A:185:ASN:ND2	2.80	0.50
1:A:204:GLN:OE1	1:B:144:ASN:HA	2.12	0.50
1:B:12:VAL:HB	1:B:71:PHE:HE1	1.77	0.50
1:B:135:ASN:HA	1:B:140:LYS:HB2	1.92	0.50
1:C:144:ASN:HA	1:D:204:GLN:OE1	2.12	0.50
1:A:95:GLU:HG2	1:A:109:ARG:HG3	1.92	0.49
1:D:33:GLY:HA3	1:D:43:THR:O	2.11	0.49
1:B:147:SER:OG	1:B:204:GLN:HG2	2.11	0.49
1:D:12:VAL:HB	1:D:71:PHE:HE1	1.78	0.49
1:A:33:GLY:HA3	1:A:43:THR:O	2.11	0.49
1:A:105:ASN:O	1:A:127:GLY:HA2	2.13	0.48
1:A:155:ASP:OD2	1:A:158:LYS:HD3	2.13	0.48
1:B:12:VAL:HB	1:B:71:PHE:CE1	2.47	0.48
1:A:53:LEU:HD13	1:A:55:VAL:HG23	1.95	0.48
1:A:29:VAL:HG21	1:A:64:PHE:CE1	2.49	0.48
1:C:92:TYR:CD2	1:C:185:ASN:ND2	2.78	0.48
1:C:105:ASN:O	1:C:127:GLY:HA2	2.14	0.48
1:A:135:ASN:HA	1:A:140:LYS:HB2	1.96	0.48
1:B:33:GLY:HA3	1:B:43:THR:O	2.14	0.47
1:B:167:ILE:HB	1:B:179:ALA:HB3	1.96	0.47
1:B:41:LYS:HB3	1:B:223:PHE:CE1	2.49	0.47
1:C:144:ASN:HB2	1:D:147:SER:OG	2.14	0.47
1:B:33:GLY:HA3	1:B:44:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLN:HE21	1:B:157:GLN:HA	1.80	0.47
1:C:169:HIS:HE1	2:C:346:HOH:O	1.96	0.47
1:A:81:HIS:CD2	1:A:197:ASP:H	2.33	0.47
1:A:147:SER:OG	1:B:144:ASN:HB2	2.15	0.47
1:C:56:PRO:HD3	1:C:136:ILE:O	2.14	0.47
1:A:41:LYS:HB3	1:A:223:PHE:CE1	2.49	0.47
1:A:223:PHE:HB3	2:A:258:HOH:O	2.14	0.47
1:B:69:GLN:NE2	1:B:150:VAL:HG11	2.29	0.47
1:B:48:CYS:SG	1:B:53:LEU:HD23	2.55	0.46
1:D:171:ILE:HG22	1:D:172:GLU:N	2.30	0.46
1:A:63:THR:HG23	1:A:123:ILE:HG21	1.98	0.46
1:D:169:HIS:HD2	2:D:256:HOH:O	1.97	0.46
1:A:94:GLN:HE21	1:A:96:ARG:NH1	2.14	0.46
1:C:184:GLN:HG3	2:C:253:HOH:O	2.14	0.46
1:A:98:ILE:HG23	1:A:181:HIS:CE1	2.51	0.46
1:A:161:ILE:HG13	1:A:185:ASN:HB2	1.97	0.46
1:D:141:LEU:HB3	2:D:264:HOH:O	2.16	0.46
1:A:22:VAL:HG21	1:A:55:VAL:HG11	1.98	0.46
1:A:46:PHE:CZ	1:A:64:PHE:HB3	2.52	0.45
1:B:92:TYR:CE1	1:B:185:ASN:ND2	2.84	0.45
1:C:153:THR:HG22	1:C:162:LYS:HB2	1.99	0.45
1:D:92:TYR:CD2	1:D:185:ASN:ND2	2.81	0.45
1:D:169:HIS:HB2	1:D:177:GLN:O	2.16	0.45
1:D:171:ILE:HG22	1:D:172:GLU:HG2	1.97	0.45
1:A:48:CYS:SG	1:A:53:LEU:HD23	2.57	0.45
1:B:56:PRO:HD3	1:B:136:ILE:O	2.16	0.45
1:D:151:TYR:O	1:D:163:ALA:HA	2.17	0.45
1:D:92:TYR:CE2	1:D:185:ASN:ND2	2.85	0.45
1:D:148:HIS:CG	1:D:167:ILE:HD13	2.52	0.45
1:A:155:ASP:OD2	1:A:158:LYS:HB2	2.16	0.45
1:C:142:GLU:HG3	1:C:170:ASN:O	2.17	0.45
1:D:12:VAL:HB	1:D:71:PHE:CE1	2.52	0.45
1:A:163:ALA:HB3	1:A:183:GLN:HB3	1.98	0.45
1:B:59:THR:CG2	1:B:141:LEU:HD11	2.47	0.45
1:B:63:THR:HG23	1:B:123:ILE:HG21	1.98	0.45
1:C:169:HIS:HD2	2:C:330:HOH:O	1.99	0.45
1:B:18:LEU:HD23	1:B:123:ILE:HB	1.98	0.44
1:D:105:ASN:O	1:D:127:GLY:HA2	2.17	0.44
1:B:112:VAL:HG22	1:B:121:ASN:OD1	2.18	0.44
1:A:81:HIS:HD2	1:A:197:ASP:H	1.65	0.44
1:B:163:ALA:HB3	1:B:183:GLN:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:HIS:CD2	1:B:197:ASP:H	2.35	0.44
1:A:45:LYS:HE2	1:A:47:ILE:HD11	1.98	0.44
1:B:143:TYR:OH	1:B:218:MET:HA	2.18	0.44
1:D:83:PHE:CE1	1:D:160:GLY:HA2	2.53	0.44
1:A:18:LEU:HD23	1:A:123:ILE:HB	2.00	0.44
1:B:13:PRO:HB3	1:D:162:LYS:NZ	2.33	0.44
1:D:15:LEU:O	1:D:120:VAL:HA	2.17	0.44
1:D:25:HIS:HE1	2:D:285:HOH:O	2.00	0.44
1:C:15:LEU:O	1:C:120:VAL:HA	2.18	0.44
1:C:92:TYR:CE2	1:C:185:ASN:ND2	2.86	0.44
1:C:40:GLY:HA3	1:C:73:ARG:HB2	2.00	0.43
1:C:147:SER:OG	1:C:204:GLN:HG2	2.18	0.43
1:C:147:SER:HB2	1:D:146:ASN:OD1	2.18	0.43
1:A:144:ASN:HA	1:B:204:GLN:OE1	2.19	0.43
1:B:47:ILE:HD13	1:B:217:HIS:HB3	2.00	0.43
1:C:8:PHE:CE2	1:C:88:MET:HG3	2.54	0.43
1:C:12:VAL:HB	1:C:71:PHE:HE1	1.82	0.43
1:C:78:MET:O	1:C:81:HIS:HB2	2.19	0.43
1:D:169:HIS:HE1	2:D:246:HOH:O	2.02	0.43
1:B:22:VAL:HG23	1:B:27:PHE:HE1	1.82	0.43
1:C:160:GLY:HA3	1:C:185:ASN:O	2.18	0.43
1:A:143:TYR:OH	1:A:218:MET:HA	2.19	0.43
1:B:105:ASN:O	1:B:127:GLY:HA2	2.19	0.43
1:B:93:VAL:HA	1:B:110:ALA:O	2.19	0.43
1:C:42:LEU:HD13	1:C:66:CRO:OG1	2.18	0.43
1:C:62:THR:HG23	1:C:145:TYR:OH	2.17	0.43
1:D:63:THR:CG2	1:D:123:ILE:HG21	2.49	0.43
1:D:77:HIS:NE2	1:D:229:ILE:O	2.42	0.43
1:D:75:PRO:HG2	1:D:78:MET:HG2	2.01	0.43
1:A:157:GLN:HA	2:A:241:HOH:O	2.18	0.42
1:C:151:TYR:O	1:C:163:ALA:HA	2.19	0.42
1:D:150:VAL:O	1:D:200:TYR:HA	2.18	0.42
1:A:22:VAL:HG23	1:A:27:PHE:HE1	1.84	0.42
1:A:78:MET:HE2	1:A:226:ALA:HB1	2.01	0.42
1:B:69:GLN:HE22	1:B:150:VAL:HG11	1.83	0.42
1:C:45:LYS:HD3	2:C:303:HOH:O	2.20	0.42
1:A:56:PRO:HG2	1:A:141:LEU:HG	2.01	0.42
1:A:93:VAL:O	1:A:185:ASN:HA	2.19	0.42
1:B:150:VAL:HB	1:B:201:LEU:HB2	2.01	0.42
1:C:58:PRO:HG3	1:C:207:LEU:CD1	2.49	0.42
1:A:14:ILE:HB	1:A:44:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:CYS:SG	1:D:53:LEU:HD23	2.59	0.42
1:A:53:LEU:HA	1:A:54:PRO:HD2	1.93	0.42
1:C:150:VAL:HB	1:C:201:LEU:HB2	2.01	0.42
1:D:153:THR:HG22	1:D:162:LYS:HB2	2.01	0.42
1:D:85:LYS:NZ	2:D:297:HOH:O	2.52	0.42
1:D:98:ILE:HD11	2:D:317:HOH:O	2.19	0.42
1:A:66:CRO:N2	1:A:66:CRO:HD1	2.35	0.42
1:B:8:PHE:CE2	1:B:88:MET:HG3	2.55	0.42
1:C:93:VAL:O	1:C:185:ASN:HA	2.20	0.42
1:A:69:GLN:HE22	1:A:150:VAL:HG11	1.85	0.41
1:B:14:ILE:HB	1:B:44:LEU:HD21	2.02	0.41
1:B:53:LEU:HD13	1:B:55:VAL:HG23	2.01	0.41
1:A:26:LYS:H	1:A:26:LYS:HG3	1.65	0.41
1:A:46:PHE:CE1	1:A:64:PHE:HB3	2.56	0.41
1:C:63:THR:HA	2:C:246:HOH:O	2.20	0.41
1:C:153:THR:CG2	1:C:162:LYS:HB2	2.51	0.41
1:C:83:PHE:CE1	1:C:160:GLY:HA2	2.56	0.41
1:C:98:ILE:HB	1:C:106:TYR:HB2	2.02	0.41
1:D:70:CYS:HB3	1:D:84:PHE:HB3	2.03	0.41
1:A:62:THR:HA	1:A:66:CRO:CA2	2.51	0.41
1:D:171:ILE:HD11	1:D:177:GLN:CB	2.40	0.41
1:A:213:GLU:OE1	1:A:215:ARG:HD3	2.20	0.41
1:C:223:PHE:HD2	1:D:206:ALA:HB1	1.85	0.41
1:D:53:LEU:HA	1:D:54:PRO:HD2	1.88	0.41
1:A:167:ILE:HB	1:A:179:ALA:HB3	2.03	0.41
1:B:22:VAL:HG21	1:B:55:VAL:HG11	2.03	0.41
1:B:93:VAL:O	1:B:185:ASN:HA	2.21	0.41
1:A:56:PRO:HD3	1:A:136:ILE:O	2.20	0.41
1:B:53:LEU:HD11	1:B:60:LEU:CD1	2.51	0.41
1:B:66:CRO:N2	1:B:66:CRO:HD1	2.36	0.41
1:B:130:PHE:HB3	1:B:137:LEU:HD23	2.04	0.40
1:C:135:ASN:HD22	1:C:140:LYS:HD2	1.85	0.40
1:C:135:ASN:HD22	1:C:140:LYS:CD	2.34	0.40
1:A:93:VAL:HA	1:A:110:ALA:O	2.21	0.40
1:A:42:LEU:HB2	1:A:222:GLU:HB3	2.03	0.40
1:A:74:TYR:HA	1:A:226:ALA:HB3	2.02	0.40
1:C:12:VAL:HB	1:C:71:PHE:CE1	2.56	0.40
1:C:207:LEU:O	1:D:204:GLN:NE2	2.50	0.40
1:A:69:GLN:NE2	1:A:150:VAL:HG11	2.35	0.40
1:C:6:GLU:HA	1:C:9:THR:HG23	2.03	0.40
1:D:78:MET:O	1:D:81:HIS:HB2	2.22	0.40

There are no symmetry-related clashes.

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	220/236 (93%)	214 (97%)	5 (2%)	1 (0%)	24	37
1	B	220/236 (93%)	215 (98%)	4 (2%)	1 (0%)	24	37
1	C	220/236 (93%)	203 (92%)	16 (7%)	1 (0%)	24	37
1	D	220/236 (93%)	204 (93%)	15 (7%)	1 (0%)	24	37
All	All	880/944 (93%)	836 (95%)	40 (4%)	4 (0%)	24	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	191	GLY
1	D	189	GLY
1	A	198	ASN
1	B	198	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/204 (96%)	174 (89%)	21 (11%)	6	9
1	B	195/204 (96%)	175 (90%)	20 (10%)	7	11
1	C	195/204 (96%)	173 (89%)	22 (11%)	5	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	195/204 (96%)	171 (88%)	24 (12%)	4	6
All	All	780/816 (96%)	693 (89%)	87 (11%)	6	9

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	15	LEU
1	A	26	LYS
1	A	29	VAL
1	A	52	LYS
1	A	53	LEU
1	A	58	PRO
1	A	76	ASP
1	A	90	GLU
1	A	103	ASP
1	A	115	GLU
1	A	118	THR
1	A	119	LEU
1	A	125	LEU
1	A	156	LYS
1	A	157	GLN
1	A	161	ILE
1	A	180	ASP
1	A	214	LYS
1	A	215	ARG
1	A	221	LEU
1	B	6	GLU
1	B	15	LEU
1	B	29	VAL
1	B	53	LEU
1	B	58	PRO
1	B	90	GLU
1	B	107	LYS
1	B	117	ASP
1	B	118	THR
1	B	119	LEU
1	B	133	ASP
1	B	157	GLN
1	B	161	ILE
1	B	172	GLU
1	B	180	ASP

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Mol	Chain	Res	Type
1	B	203	THR
1	B	212	ASN
1	B	214	LYS
1	B	215	ARG
1	B	221	LEU
1	C	6	GLU
1	C	15	LEU
1	C	18	LEU
1	C	29	VAL
1	C	43	THR
1	C	52	LYS
1	C	53	LEU
1	C	80	GLN
1	C	118	THR
1	C	119	LEU
1	C	123	ILE
1	C	126	LYS
1	C	132	GLU
1	C	147	SER
1	C	176	VAL
1	C	178	LEU
1	C	180	ASP
1	C	184	GLN
1	C	205	SER
1	C	208	SER
1	C	214	LYS
1	C	224	VAL
1	D	6	GLU
1	D	15	LEU
1	D	18	LEU
1	D	29	VAL
1	D	43	THR
1	D	52	LYS
1	D	53	LEU
1	D	80	GLN
1	D	118	THR
1	D	119	LEU
1	D	123	ILE
1	D	126	LYS
1	D	132	GLU
1	D	147	SER
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	178	LEU
1	D	180	ASP
1	D	190	ASP
1	D	196	PRO
1	D	203	THR
1	D	205	SER
1	D	208	SER
1	D	214	LYS
1	D	224	VAL

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

Mol	Chain	Res	Type
1	A	149	ASN
1	A	157	GLN
1	A	169	HIS
1	A	212	ASN
1	B	69	GLN
1	B	94	GLN
1	B	149	ASN
1	B	157	GLN
1	B	159	ASN
1	B	183	GLN
1	B	185	ASN
1	B	212	ASN
1	C	81	HIS
1	C	135	ASN
1	C	157	GLN
1	C	169	HIS
1	C	212	ASN
1	D	25	HIS
1	D	81	HIS
1	D	105	ASN
1	D	135	ASN
1	D	169	HIS
1	D	170	ASN

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	A	66	1	20,22,24	2.08	6 (30%)	25,30,34	2.67	8 (32%)
1	CRO	C	66	1	20,22,24	2.48	6 (30%)	25,30,34	3.18	13 (52%)
1	CRO	B	66	1	20,22,24	2.04	6 (30%)	25,30,34	2.39	7 (28%)
1	CRO	D	66	1	20,22,24	1.91	6 (30%)	25,30,34	3.26	11 (44%)

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	-	2/10/29/32	0/2/2/2
1	CRO	C	66	1	-	2/10/29/32	0/2/2/2
1	CRO	B	66	1	-	1/10/29/32	0/2/2/2
1	CRO	D	66	1	-	2/10/29/32	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	CRO	CB2-CA2	5.40	1.40	1.35
1	C	66	CRO	CG2-CB2	-5.22	1.37	1.46
1	A	66	CRO	CG2-CB2	-5.17	1.37	1.46
1	C	66	CRO	CA2-N2	4.59	1.48	1.38
1	D	66	CRO	CG2-CB2	-4.27	1.39	1.46
1	B	66	CRO	CB2-CA2	4.18	1.39	1.35
1	B	66	CRO	CG2-CB2	-4.03	1.39	1.46
1	D	66	CRO	CB2-CA2	3.67	1.38	1.35
1	A	66	CRO	C2-N3	-3.50	1.31	1.40
1	B	66	CRO	CA2-N2	3.48	1.46	1.38
1	B	66	CRO	C2-N3	-3.45	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	CRO	CA2-N2	3.42	1.45	1.38
1	B	66	CRO	C1-N2	3.41	1.37	1.32
1	C	66	CRO	C1-N2	3.39	1.37	1.32
1	C	66	CRO	CA2-C2	3.36	1.52	1.48
1	A	66	CRO	C1-N2	3.34	1.37	1.32
1	C	66	CRO	C2-N3	-3.34	1.32	1.40
1	D	66	CRO	C2-N3	-3.17	1.32	1.40
1	D	66	CRO	CA2-N2	2.89	1.44	1.38
1	A	66	CRO	CA3-N3	-2.83	1.42	1.47
1	A	66	CRO	CB2-CA2	2.62	1.37	1.35
1	D	66	CRO	C1-N2	2.53	1.35	1.32
1	D	66	CRO	CA3-N3	-2.32	1.43	1.47
1	B	66	CRO	CA2-C2	2.27	1.51	1.48

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	CRO	O2-C2-CA2	-9.01	125.27	131.02
1	C	66	CRO	O2-C2-CA2	-8.86	125.36	131.02
1	A	66	CRO	C3-CA3-N3	6.49	127.21	112.43
1	B	66	CRO	CA2-N2-C1	-6.42	100.78	105.80
1	A	66	CRO	CA2-N2-C1	-6.26	100.91	105.80
1	D	66	CRO	N3-C1-N2	6.14	116.33	111.48
1	B	66	CRO	N3-C1-N2	6.01	116.22	111.48
1	D	66	CRO	C3-CA3-N3	5.97	126.02	112.43
1	D	66	CRO	CA2-N2-C1	-5.89	101.20	105.80
1	C	66	CRO	CA2-N2-C1	-5.49	101.51	105.80
1	C	66	CRO	N3-C1-N2	5.35	115.70	111.48
1	A	66	CRO	N3-C1-N2	5.31	115.67	111.48
1	C	66	CRO	C2-N3-C1	5.20	110.47	108.07
1	A	66	CRO	C2-N3-C1	4.79	110.28	108.07
1	C	66	CRO	CB2-CA2-C2	4.28	127.55	122.36
1	B	66	CRO	O2-C2-CA2	-3.93	128.51	131.02
1	D	66	CRO	CA1-C1-N2	-3.72	116.31	123.57
1	B	66	CRO	C2-N3-C1	3.48	109.68	108.07
1	D	66	CRO	CB2-CA2-C2	3.43	126.52	122.36
1	A	66	CRO	O2-C2-CA2	-3.28	128.93	131.02
1	C	66	CRO	CD2-CG2-CB2	-3.05	110.72	121.22
1	C	66	CRO	C2-CA2-N2	-3.04	106.78	108.95
1	B	66	CRO	CB2-CA2-C2	2.94	125.92	122.36
1	A	66	CRO	CB2-CA2-C2	2.81	125.76	122.36
1	B	66	CRO	CA1-C1-N3	-2.72	121.30	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	66	CRO	C2-N3-C1	2.71	109.32	108.07
1	C	66	CRO	C3-CA3-N3	2.70	118.58	112.43
1	C	66	CRO	CD1-CG2-CB2	2.63	130.24	121.22
1	D	66	CRO	O2-C2-N3	2.61	129.75	124.31
1	C	66	CRO	CA1-C1-N2	-2.60	118.50	123.57
1	D	66	CRO	CB2-CA2-N2	-2.53	125.33	128.76
1	A	66	CRO	O3-C3-CA3	-2.41	114.61	125.47
1	C	66	CRO	CA2-C2-N3	2.40	105.51	103.50
1	D	66	CRO	CD2-CG2-CB2	-2.30	113.33	121.22
1	C	66	CRO	O2-C2-N3	2.29	129.09	124.31
1	C	66	CRO	CB2-CA2-N2	-2.27	125.68	128.76
1	B	66	CRO	CA2-C2-N3	2.18	105.33	103.50
1	D	66	CRO	CE1-CD1-CG2	-2.14	118.46	121.22
1	A	66	CRO	CB2-CA2-N2	-2.04	125.99	128.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	66	CRO	N1-CA1-CB1-OG1
1	C	66	CRO	N1-CA1-CB1-OG1
1	C	66	CRO	C1-CA1-CB1-OG1
1	D	66	CRO	N1-CA1-CB1-OG1
1	D	66	CRO	C1-CA1-CB1-OG1
1	A	66	CRO	C1-CA1-CB1-OG1
1	B	66	CRO	N1-CA1-CB1-OG1

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	CRO	4	0
1	C	66	CRO	4	0
1	B	66	CRO	1	0
1	D	66	CRO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	224/236 (94%)	0.82	19 (8%) 16 13	18, 38, 61, 77	0
1	B	224/236 (94%)	0.84	22 (9%) 13 10	14, 40, 61, 72	0
1	C	224/236 (94%)	0.10	4 (1%) 67 63	10, 21, 36, 57	0
1	D	224/236 (94%)	0.20	7 (3%) 51 47	5, 21, 43, 57	0
All	All	896/944 (94%)	0.49	52 (5%) 29 25	5, 30, 58, 77	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	TYR	5.7
1	B	133	ASP	4.2
1	A	179	ALA	3.9
1	B	4	GLY	3.7
1	A	4	GLY	3.6
1	A	133	ASP	3.6
1	A	171	ILE	3.6
1	B	172	GLU	3.4
1	B	134	GLY	3.3
1	D	4	GLY	2.9
1	A	80	GLN	2.8
1	A	230	THR	2.8
1	B	230	THR	2.8
1	A	6	GLU	2.8
1	B	132	GLU	2.7
1	B	164	ASN	2.7
1	C	133	ASP	2.6
1	B	140	LYS	2.6
1	C	182	TYR	2.6
1	A	182	TYR	2.6
1	D	39	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	133	ASP	2.5
1	A	163	ALA	2.5
1	A	191	GLY	2.4
1	D	132	GLU	2.4
1	A	190	ASP	2.4
1	A	164	ASN	2.4
1	C	6	GLU	2.4
1	B	157	GLN	2.4
1	A	132	GLU	2.4
1	B	53	LEU	2.3
1	B	131	LYS	2.3
1	A	102	ASP	2.3
1	B	163	ALA	2.2
1	A	194	LEU	2.1
1	A	22	VAL	2.1
1	B	137	LEU	2.1
1	C	230	THR	2.1
1	D	230	THR	2.1
1	B	138	GLY	2.1
1	A	90	GLU	2.1
1	D	28	SER	2.1
1	B	184	GLN	2.1
1	B	151	TYR	2.1
1	B	180	ASP	2.1
1	D	211	PRO	2.1
1	A	160	GLY	2.0
1	B	174	GLY	2.0
1	A	156	LYS	2.0
1	B	171	ILE	2.0
1	B	99	SER	2.0
1	B	6	GLU	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	C	66	21/23	0.81	0.17	8,22,29,46	0
1	CRO	B	66	21/23	0.87	0.12	22,28,43,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CRO	A	66	21/23	0.90	0.12	18,30,48,55	0
1	CRO	D	66	21/23	0.91	0.10	2,16,21,36	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.