



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:37 PM UTC

PDB ID : 2HWJ / pdb_00002hwj
Title : Crystal structure of protein Atu1540 from Agrobacterium tumefaciens
Authors : Chang, C.; Xu, X.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-08-01
Resolution : 2.61 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:

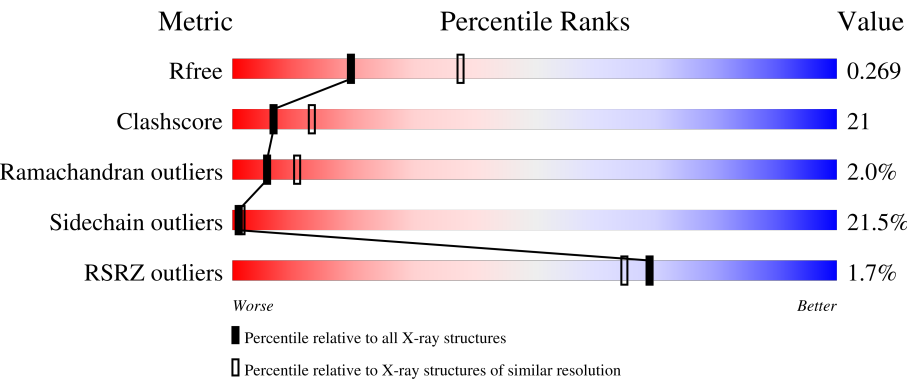
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	205	56%29%9% . .
1	B	205	% 43%35%13% . 8%
1	C	205	2% 46%35%11% . 5%
1	D	205	3% 40%36%17% . 6%
1	E	205	44%34%11% . 8%

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Mol	Chain	Length	Quality of chain
1	F	205	2% 45% 38% 8% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9380 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 Hypothetical protein Atu1540.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	Se	0	0	0
			1574	1000	289	281	1	3			
1	B	189	Total	C	N	O	S	Se	0	1	0
			1530	972	284	270	1	3			
1	C	195	Total	C	N	O	S	Se	0	2	0
			1579	1005	290	280	1	3			
1	D	193	Total	C	N	O	S	Se	0	1	0
			1555	987	286	278	1	3			
1	E	188	Total	C	N	O	S	Se	0	0	0
			1519	965	281	269	1	3			
1	F	190	Total	C	N	O	S	Se	0	0	0
			1528	970	283	271	1	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8UF59
A	103	MSE	MET	modified residue	UNP Q8UF59
A	145	MSE	MET	modified residue	UNP Q8UF59
A	186	MSE	MET	modified residue	UNP Q8UF59
B	1	MSE	MET	modified residue	UNP Q8UF59
B	103	MSE	MET	modified residue	UNP Q8UF59
B	145	MSE	MET	modified residue	UNP Q8UF59
B	186	MSE	MET	modified residue	UNP Q8UF59
C	1	MSE	MET	modified residue	UNP Q8UF59
C	103	MSE	MET	modified residue	UNP Q8UF59
C	145	MSE	MET	modified residue	UNP Q8UF59
C	186	MSE	MET	modified residue	UNP Q8UF59
D	1	MSE	MET	modified residue	UNP Q8UF59
D	103	MSE	MET	modified residue	UNP Q8UF59
D	145	MSE	MET	modified residue	UNP Q8UF59
D	186	MSE	MET	modified residue	UNP Q8UF59
E	1	MSE	MET	modified residue	UNP Q8UF59

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Chain	Residue	Modelled	Actual	Comment	Reference
E	103	MSE	MET	modified residue	UNP Q8UF59
E	145	MSE	MET	modified residue	UNP Q8UF59
E	186	MSE	MET	modified residue	UNP Q8UF59
F	1	MSE	MET	modified residue	UNP Q8UF59
F	103	MSE	MET	modified residue	UNP Q8UF59
F	145	MSE	MET	modified residue	UNP Q8UF59
F	186	MSE	MET	modified residue	UNP Q8UF59

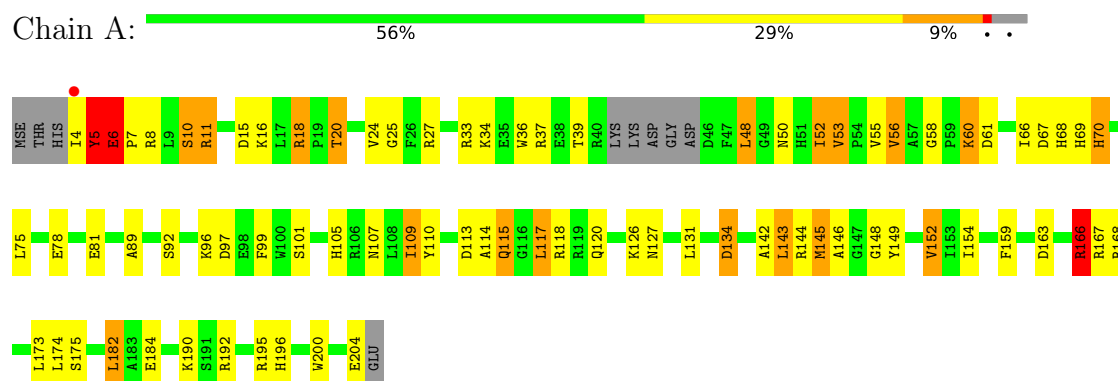
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	18	Total O 18 18	0	0
2	C	22	Total O 22 22	0	0
2	D	15	Total O 15 15	0	0
2	E	13	Total O 13 13	0	0
2	F	10	Total O 10 10	0	0

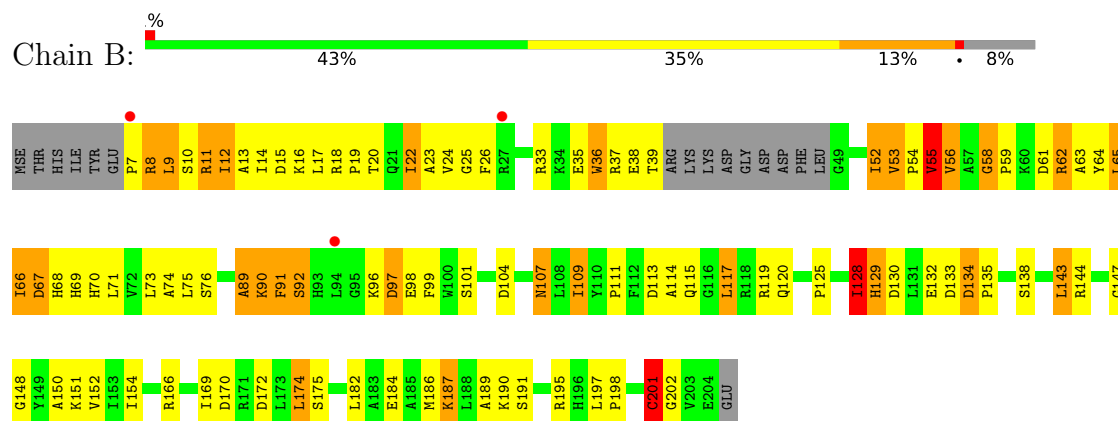
3 Residue-property plots

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.

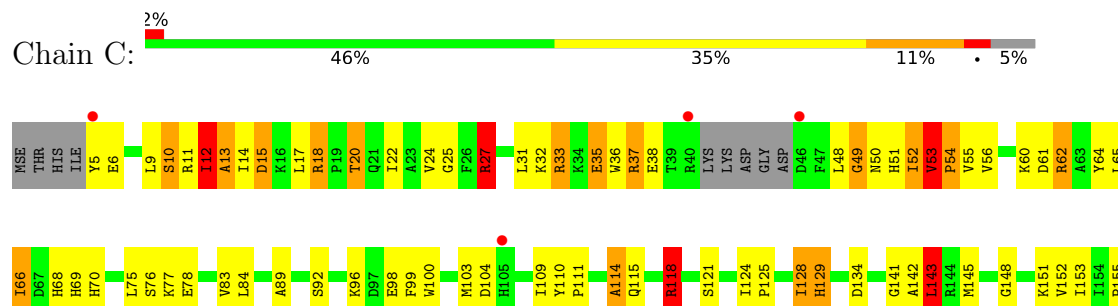
• Molecule 1: Hypothetical protein Atu1540



• Molecule 1: Hypothetical protein Atu1540

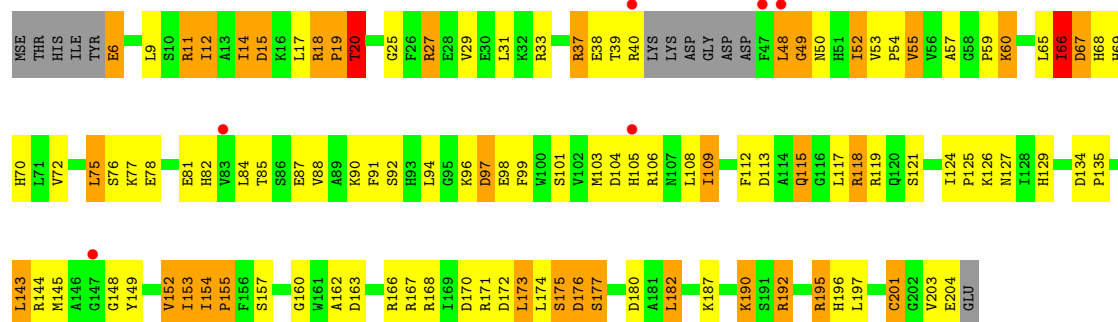


• Molecule 1: Hypothetical protein Atu1540

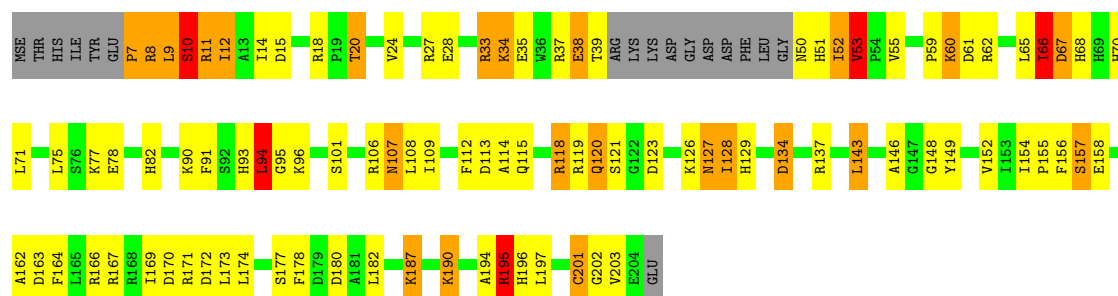
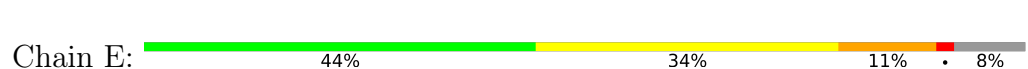




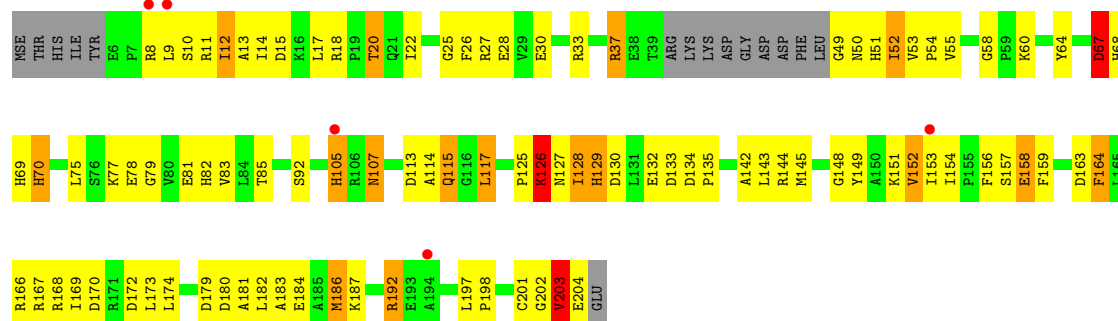
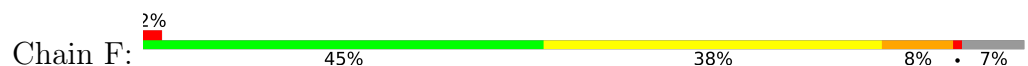
• Molecule 1: Hypothetical protein Atu1540



• Molecule 1: Hypothetical protein Atu1540



• Molecule 1: Hypothetical protein Atu1540



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	132.08Å 173.75Å 142.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.61 50.00 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.8 (50.00-2.61) 98.0 (50.00-2.61)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.273 0.196 , 0.269	Depositor DCC
R_{free} test set	2486 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.464	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.9	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	0.95	EDS
Total number of atoms	9380	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

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	1.51	6/1608 (0.4%)	1.57	18/2164 (0.8%)
1	B	1.47	9/1567 (0.6%)	1.49	23/2107 (1.1%)
1	C	1.68	21/1620 (1.3%)	1.59	22/2180 (1.0%)
1	D	1.43	9/1591 (0.6%)	1.41	16/2141 (0.7%)
1	E	1.44	10/1552 (0.6%)	1.49	20/2087 (1.0%)
1	F	1.43	12/1561 (0.8%)	1.34	16/2100 (0.8%)
All	All	1.50	67/9499 (0.7%)	1.49	115/12779 (0.9%)

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	3
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	ASP	CG-OD1	17.29	1.58	1.25
1	D	175	SER	CB-OG	15.10	1.72	1.42
1	F	179	ASP	C-N	12.36	1.50	1.33
1	F	181	ALA	C-O	12.23	1.38	1.24
1	D	40	ARG	C-O	11.67	1.46	1.23
1	D	176	ASP	CG-OD2	11.36	1.47	1.25
1	F	181	ALA	C-N	11.07	1.49	1.34
1	D	172	ASP	C-O	10.17	1.36	1.24
1	D	176	ASP	CG-OD1	9.73	1.43	1.25
1	F	179	ASP	CG-OD2	9.23	1.42	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	ASN	CA-C	-9.15	1.41	1.52
1	F	126	LYS	CE-NZ	7.79	1.72	1.49
1	A	109	ILE	C-O	-7.20	1.16	1.23
1	C	151	LYS	C-O	-7.14	1.15	1.23
1	C	128	ILE	CA-CB	-7.04	1.46	1.54
1	F	179	ASP	C-O	6.91	1.33	1.24
1	C	189	ALA	CA-CB	-6.78	1.42	1.53
1	C	181	ALA	CA-CB	-6.73	1.42	1.53
1	E	162	ALA	CA-CB	-6.64	1.42	1.53
1	A	99	PHE	N-CA	-6.60	1.38	1.46
1	D	172	ASP	C-N	6.60	1.43	1.33
1	E	155	PRO	CA-C	6.58	1.60	1.52
1	E	112	PHE	C-O	-6.37	1.16	1.24
1	C	159	PHE	C-O	-6.34	1.16	1.24
1	E	149	TYR	CA-CB	-6.30	1.43	1.53
1	D	201	CYS	C-O	-6.24	1.17	1.24
1	F	126	LYS	CG-CD	6.23	1.71	1.52
1	B	109	ILE	C-O	-6.20	1.17	1.24
1	F	186	MSE	C-O	6.18	1.31	1.24
1	C	27	ARG	CG-CD	6.11	1.70	1.52
1	B	55	VAL	CA-CB	-6.05	1.44	1.55
1	C	178	PHE	N-CA	-6.05	1.39	1.46
1	A	20	THR	CA-CB	5.98	1.62	1.53
1	C	13	ALA	CA-CB	-5.89	1.44	1.53
1	B	150	ALA	C-O	-5.86	1.17	1.24
1	A	92	SER	C-O	-5.82	1.15	1.24
1	C	200	TRP	C-O	-5.78	1.17	1.23
1	F	126	LYS	CD-CE	5.78	1.69	1.52
1	C	201	CYS	N-CA	-5.75	1.40	1.46
1	E	169	ILE	C-O	-5.75	1.17	1.24
1	E	187	LYS	CA-C	5.71	1.60	1.52
1	B	63	ALA	N-CA	5.71	1.53	1.46
1	F	186	MSE	C-N	5.63	1.41	1.33
1	F	183	ALA	C-O	5.62	1.30	1.24
1	A	10	SER	CA-C	-5.61	1.46	1.53
1	C	54	PRO	C-O	5.59	1.29	1.23
1	B	202	GLY	CA-C	-5.58	1.46	1.52
1	C	128	ILE	N-CA	-5.51	1.40	1.46
1	B	189	ALA	CA-CB	-5.50	1.44	1.53
1	C	83	VAL	CA-C	5.46	1.59	1.52
1	C	129	HIS	C-O	-5.46	1.17	1.24
1	B	187	LYS	N-CA	-5.42	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	166	ARG	CA-C	-5.41	1.45	1.52
1	C	186	MSE	N-CA	-5.33	1.39	1.46
1	C	145	MSE	CA-C	-5.32	1.45	1.52
1	C	118	ARG	C-O	-5.29	1.17	1.23
1	B	191	SER	C-O	-5.25	1.17	1.23
1	D	172	ASP	CG-OD1	5.25	1.35	1.25
1	B	134	ASP	CA-C	5.22	1.58	1.52
1	E	201	CYS	CB-SG	-5.18	1.64	1.81
1	C	20	THR	CA-CB	5.18	1.62	1.53
1	E	195	ARG	C-O	-5.11	1.17	1.24
1	C	100	TRP	N-CA	-5.09	1.40	1.46
1	D	57	ALA	CA-CB	-5.08	1.46	1.53
1	E	107	ASN	CA-C	-5.05	1.46	1.52
1	C	141	GLY	C-O	5.02	1.29	1.23
1	C	166	ARG	C-O	-5.01	1.17	1.24

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	LYS	CA-C-N	-11.21	104.68	122.73
1	A	60	LYS	C-N-CA	-11.21	104.68	122.73
1	D	66	ILE	CA-C-N	-10.02	108.93	122.16
1	D	66	ILE	C-N-CA	-10.02	108.93	122.16
1	D	154	ILE	CA-C-N	9.40	131.59	119.84
1	D	154	ILE	C-N-CA	9.40	131.59	119.84
1	A	5	TYR	N-CA-C	8.93	129.82	110.80
1	B	62	ARG	N-CA-C	8.44	122.65	110.24
1	C	143	LEU	N-CA-C	-8.27	101.81	112.23
1	E	202	GLY	N-CA-C	-8.07	97.79	111.27
1	D	124	ILE	CA-C-N	8.01	128.03	119.78
1	D	124	ILE	C-N-CA	8.01	128.03	119.78
1	B	67	ASP	N-CA-C	8.00	118.52	108.45
1	F	180	ASP	N-CA-C	-7.72	102.80	111.14
1	B	53	VAL	CA-C-N	-7.66	112.02	120.14
1	B	53	VAL	C-N-CA	-7.66	112.02	120.14
1	B	107	ASN	CB-CA-C	-7.65	101.03	111.89
1	B	63	ALA	N-CA-C	7.61	121.06	108.96
1	F	153	ILE	N-CA-C	7.58	119.26	110.62
1	C	52	ILE	CB-CA-C	-7.56	98.85	110.50
1	A	58	GLY	CA-C-N	7.54	127.54	119.78
1	A	58	GLY	C-N-CA	7.54	127.54	119.78
1	E	66	ILE	CB-CA-C	-7.05	101.39	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	VAL	N-CA-CB	-7.04	101.35	111.21
1	A	134	ASP	CB-CA-C	7.01	116.75	110.44
1	E	108	LEU	N-CA-C	-6.94	104.81	112.72
1	F	181	ALA	O-C-N	6.81	129.33	122.12
1	C	61	ASP	N-CA-C	6.78	120.24	112.57
1	A	6	GLU	N-CA-C	6.77	124.78	109.81
1	C	60	LYS	CA-C-N	-6.74	112.46	122.83
1	C	60	LYS	C-N-CA	-6.74	112.46	122.83
1	F	105	HIS	N-CA-C	6.66	120.28	111.75
1	B	128	ILE	N-CA-C	6.65	118.20	110.62
1	A	61	ASP	N-CA-C	6.63	120.28	112.72
1	E	60	LYS	CA-C-N	-6.58	109.84	122.61
1	E	60	LYS	C-N-CA	-6.58	109.84	122.61
1	B	147	GLY	N-CA-C	-6.39	105.52	116.01
1	F	157	SER	N-CA-C	-6.33	104.46	111.36
1	C	141	GLY	N-CA-C	-6.28	105.19	112.73
1	F	58	GLY	CA-C-N	6.17	126.52	119.92
1	F	58	GLY	C-N-CA	6.17	126.52	119.92
1	D	162	ALA	N-CA-C	-6.12	104.53	111.14
1	B	198	PRO	CB-CA-C	-6.07	103.99	111.64
1	C	61	ASP	CB-CA-C	6.07	120.47	111.06
1	E	7	PRO	CA-C-N	6.07	132.62	121.70
1	E	7	PRO	C-N-CA	6.07	132.62	121.70
1	F	179	ASP	CA-C-N	-6.02	112.25	120.44
1	F	179	ASP	C-N-CA	-6.02	112.25	120.44
1	A	37	ARG	N-CA-C	-5.97	104.84	111.71
1	D	172	ASP	O-C-N	5.97	129.20	122.22
1	F	70	HIS	N-CA-C	-5.86	104.53	111.03
1	A	145	MSE	N-CA-C	-5.85	105.41	112.54
1	E	146	ALA	N-CA-C	-5.83	105.93	113.16
1	B	61	ASP	N-CA-C	-5.77	106.22	113.20
1	F	179	ASP	O-C-N	5.77	130.37	122.46
1	C	181	ALA	N-CA-C	-5.76	105.08	111.36
1	F	60	LYS	CA-C-N	-5.72	114.64	122.87
1	F	60	LYS	C-N-CA	-5.72	114.64	122.87
1	A	70	HIS	N-CA-C	-5.71	104.96	111.07
1	B	16	LYS	CD-CE-NZ	-5.70	93.65	111.90
1	C	110	TYR	CA-C-N	-5.70	112.72	119.84
1	C	110	TYR	C-N-CA	-5.70	112.72	119.84
1	A	6	GLU	CA-C-N	-5.69	114.40	120.03
1	A	6	GLU	C-N-CA	-5.69	114.40	120.03
1	D	60	LYS	CA-C-N	-5.68	113.57	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	LYS	C-N-CA	-5.68	113.57	122.65
1	A	142	ALA	N-CA-C	-5.67	105.24	111.82
1	B	65	LEU	CA-C-N	-5.64	112.50	121.02
1	B	65	LEU	C-N-CA	-5.64	112.50	121.02
1	E	155	PRO	N-CA-C	5.63	120.43	111.26
1	E	53	VAL	CA-C-N	-5.62	113.42	120.51
1	E	53	VAL	C-N-CA	-5.62	113.42	120.51
1	F	164	PHE	N-CA-C	-5.62	105.07	111.14
1	B	58	GLY	CA-C-N	5.58	126.82	119.84
1	B	58	GLY	C-N-CA	5.58	126.82	119.84
1	F	202	GLY	N-CA-C	5.58	118.72	110.63
1	C	142	ALA	N-CA-C	-5.53	105.40	111.82
1	C	49	GLY	N-CA-C	-5.48	107.96	114.48
1	E	77	LYS	N-CA-C	-5.48	106.55	113.18
1	D	39	THR	N-CA-C	5.45	119.82	108.53
1	C	192	ARG	N-CA-C	-5.44	106.14	112.89
1	B	91	PHE	N-CA-C	-5.44	104.53	113.50
1	B	189	ALA	N-CA-C	5.43	117.90	111.33
1	E	71	LEU	N-CA-C	5.41	117.61	111.11
1	E	52	ILE	CB-CA-C	-5.39	102.28	110.95
1	B	197	LEU	N-CA-C	5.38	117.50	110.08
1	B	22	ILE	N-CA-C	5.37	116.86	111.00
1	C	22	ILE	N-CA-C	5.37	116.44	111.45
1	E	201	CYS	N-CA-C	5.36	117.81	108.76
1	F	107	ASN	CB-CA-C	-5.34	104.30	111.89
1	E	178	PHE	N-CA-C	-5.34	105.54	111.36
1	A	166	ARG	N-CA-C	-5.34	106.27	112.89
1	C	202	GLY	N-CA-C	5.33	119.87	112.57
1	B	11	ARG	N-CA-C	5.31	116.69	107.93
1	D	160	GLY	N-CA-C	-5.29	106.27	113.37
1	C	24	VAL	CA-C-N	-5.28	117.59	122.29
1	C	24	VAL	C-N-CA	-5.28	117.59	122.29
1	C	53	VAL	N-CA-CB	-5.22	103.90	111.21
1	E	12	ILE	CB-CA-C	5.22	119.04	110.69
1	B	201	CYS	CA-C-N	-5.18	115.40	122.03
1	B	201	CYS	C-N-CA	-5.18	115.40	122.03
1	A	182	LEU	N-CA-C	-5.17	105.72	111.36
1	B	53	VAL	N-CA-CB	-5.17	103.98	111.21
1	C	10	SER	N-CA-C	5.16	115.10	108.34
1	C	33	ARG	CB-CG-CD	-5.16	99.44	111.30
1	D	98	GLU	N-CA-C	-5.15	105.75	111.36
1	C	118	ARG	CG-CD-NE	-5.14	100.70	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLN	N-CA-C	5.12	117.13	110.53
1	E	134	ASP	CA-C-N	-5.09	113.68	119.28
1	E	134	ASP	C-N-CA	-5.09	113.68	119.28
1	E	94	LEU	N-CA-C	5.07	117.71	109.24
1	D	18	ARG	CA-C-N	5.07	126.18	119.84
1	D	18	ARG	C-N-CA	5.07	126.18	119.84
1	C	175	SER	CA-CB-OG	-5.06	100.99	111.10
1	D	97	ASP	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	TRP	Peptide
1	A	4	ILE	Peptide
1	A	6	GLU	Peptide
1	C	12	ILE	Peptide
1	E	156	PHE	Peptide
1	F	67	ASP	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	1574	0	1549	60	0
1	B	1530	0	1521	73	0
1	C	1579	0	1558	67	0
1	D	1555	0	1538	96	0
1	E	1519	0	1512	63	0
1	F	1528	0	1516	68	0
2	A	17	0	0	2	0
2	B	18	0	0	1	0
2	C	22	0	0	0	0
2	D	15	0	0	2	0
2	E	13	0	0	2	0
2	F	10	0	0	2	0
All	All	9380	0	9194	395	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 21.

All (395) 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:F:126:LYS:CE	1:F:126:LYS:NZ	1.72	1.50
1:A:5:TYR:CB	1:C:32:LYS:HE2	1.43	1.44
1:D:175:SER:OG	1:D:175:SER:CB	1.72	1.36
1:A:11:ARG:HG2	1:A:11:ARG:HH11	1.05	1.09
1:F:128:ILE:H	1:F:128:ILE:HD13	1.11	1.09
1:A:5:TYR:CB	1:C:32:LYS:CE	2.33	1.06
1:F:128:ILE:H	1:F:128:ILE:CD1	1.67	1.05
1:E:195:ARG:HG2	1:E:195:ARG:HH11	1.15	1.04
1:E:128:ILE:HD12	1:E:128:ILE:H	1.22	1.02
1:B:25:GLY:H	1:B:70:HIS:CE1	1.80	0.99
1:E:66:ILE:O	1:E:67:ASP:HB2	1.57	0.98
1:E:128:ILE:H	1:E:128:ILE:CD1	1.76	0.98
1:B:25:GLY:H	1:B:70:HIS:HE1	1.08	0.97
1:F:126:LYS:NZ	1:F:126:LYS:HG2	1.79	0.97
1:D:25:GLY:H	1:D:70:HIS:HE1	1.15	0.94
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.32	0.93
1:F:67:ASP:HB3	1:F:68:HIS:CD2	2.05	0.91
1:C:186:MSE:HE2	1:C:190:LYS:HG2	1.51	0.90
1:C:12:ILE:HD13	1:C:17:LEU:HG	1.55	0.89
1:A:154:ILE:CD1	1:D:153:ILE:HD11	2.03	0.89
1:D:25:GLY:H	1:D:70:HIS:CE1	1.92	0.87
1:A:11:ARG:HG2	1:A:11:ARG:NH1	1.84	0.87
1:E:127:ASN:HB3	1:E:129:HIS:HD2	1.40	0.86
1:F:128:ILE:HD13	1:F:128:ILE:N	1.90	0.86
1:F:126:LYS:HG2	1:F:126:LYS:HZ2	1.37	0.84
1:F:126:LYS:NZ	1:F:126:LYS:CG	2.41	0.83
1:D:11:ARG:HD2	1:D:82:HIS:HB3	1.63	0.81
1:C:186:MSE:CE	1:C:190:LYS:HE2	2.11	0.79
1:C:134:ASP:CG	1:C:166:ARG:HH22	1.90	0.79
1:D:12:ILE:CD1	1:D:85:THR:HG21	2.11	0.79
1:E:33:ARG:HD2	1:E:78:GLU:OE1	1.82	0.79
1:F:67:ASP:HB3	1:F:68:HIS:CG	2.19	0.78
1:E:128:ILE:HD12	1:E:128:ILE:N	1.99	0.78
1:E:195:ARG:HH11	1:E:195:ARG:CG	1.96	0.78
1:D:12:ILE:HD11	1:D:85:THR:HG21	1.66	0.77
1:E:9:LEU:O	1:E:10:SER:HB2	1.83	0.77
1:E:70:HIS:HB2	2:E:210:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:ASP:CB	1:F:68:HIS:CD2	2.67	0.77
1:D:127:ASN:HB3	1:D:129:HIS:CD2	2.20	0.76
1:E:66:ILE:O	1:E:67:ASP:CB	2.26	0.76
1:D:81:GLU:OE1	1:D:82:HIS:CE1	2.37	0.76
1:A:25:GLY:H	1:A:70:HIS:HE1	1.32	0.76
1:E:53:VAL:CG1	1:E:65:LEU:HD11	2.15	0.75
1:B:8:ARG:NH1	1:D:49:GLY:O	2.20	0.75
1:A:107:ASN:HD21	1:B:107:ASN:HD21	1.32	0.74
1:B:143:LEU:HD22	1:B:148:GLY:HA3	1.70	0.73
1:D:163[A]:ASP:OD1	1:D:166:ARG:NH1	2.21	0.73
1:A:6:GLU:HB3	1:A:7:PRO:HD3	1.70	0.73
1:E:170:ASP:OD1	1:E:172:ASP:N	2.19	0.72
1:E:53:VAL:HG11	1:E:65:LEU:HD11	1.71	0.72
1:E:120:GLN:H	1:E:120:GLN:HE21	1.38	0.72
1:E:11:ARG:HD3	1:E:82:HIS:HB3	1.72	0.71
1:D:68:HIS:O	1:D:72:VAL:HG23	1.90	0.71
1:A:146:ALA:O	1:D:203:VAL:HG22	1.91	0.71
1:E:7:PRO:HA	1:E:8:ARG:HB2	1.73	0.71
1:D:173:LEU:HD11	1:D:180:ASP:HB3	1.73	0.70
1:F:163:ASP:O	1:F:167:ARG:HG3	1.90	0.70
1:A:18:ARG:HD2	2:A:208:HOH:O	1.89	0.70
1:A:154:ILE:HD11	1:D:153:ILE:HD11	1.71	0.70
1:F:33:ARG:HD2	1:F:78:GLU:OE1	1.92	0.69
1:C:104:ASP:OD2	1:D:118:ARG:NH1	2.25	0.69
1:C:76:SER:OG	1:C:129:HIS:NE2	2.25	0.69
1:B:12:ILE:HD13	1:B:12:ILE:H	1.56	0.69
1:E:53:VAL:HG11	1:E:65:LEU:CD1	2.23	0.69
1:E:53:VAL:CG1	1:E:65:LEU:CD1	2.71	0.68
1:F:142:ALA:O	1:F:145:MSE:HB2	1.93	0.68
1:E:127:ASN:HD22	1:E:129:HIS:CD2	2.12	0.68
1:E:118:ARG:O	1:E:119:ARG:HD2	1.94	0.68
1:A:11:ARG:HH11	1:A:11:ARG:CG	1.92	0.68
1:C:186:MSE:HE1	1:C:190:LYS:HE2	1.75	0.67
1:F:158:GLU:CD	1:F:158:GLU:H	2.01	0.67
1:B:134:ASP:CG	1:B:166:ARG:HH22	2.02	0.67
1:E:195:ARG:HG2	1:E:195:ARG:NH1	1.96	0.67
1:A:25:GLY:H	1:A:70:HIS:CE1	2.12	0.67
1:E:106:ARG:O	1:E:107:ASN:HB2	1.94	0.67
1:C:186:MSE:HE2	1:C:190:LYS:HE2	1.75	0.67
1:F:143:LEU:HD12	1:F:149:TYR:CE2	2.29	0.67
1:D:134:ASP:OD2	1:D:166:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ASP:CG	1:B:68:HIS:H	2.04	0.66
1:C:118:ARG:NH1	1:D:104:ASP:OD2	2.28	0.66
1:D:11:ARG:HD2	1:D:82:HIS:CB	2.25	0.65
1:B:19:PRO:HG2	1:B:125:PRO:O	1.96	0.65
1:F:49:GLY:HA3	2:F:210:HOH:O	1.95	0.65
1:A:20:THR:H	1:A:69:HIS:HE1	1.42	0.65
1:C:186:MSE:HE3	1:C:189:ALA:HB3	1.78	0.65
1:A:107:ASN:ND2	1:B:107:ASN:HD21	1.95	0.65
1:C:143:LEU:HD22	1:C:148:GLY:HA3	1.77	0.65
1:D:144:ARG:HB2	1:D:149:TYR:CZ	2.31	0.65
1:B:58:GLY:O	1:B:92:SER:HB3	1.96	0.65
1:B:12:ILE:HD13	1:B:12:ILE:N	2.13	0.64
1:E:128:ILE:CD1	1:E:128:ILE:N	2.57	0.64
1:A:8:ARG:HD3	1:C:49:GLY:O	1.96	0.64
1:A:20:THR:H	1:A:69:HIS:CE1	2.15	0.64
1:C:171:ARG:HG2	1:C:171:ARG:NH1	2.03	0.64
1:B:12:ILE:HG12	1:B:13:ALA:O	1.98	0.64
1:E:177:SER:HB3	1:E:180:ASP:HB2	1.79	0.64
1:A:67:ASP:HB3	1:A:68:HIS:CD2	2.33	0.63
1:A:113:ASP:OD2	1:A:117:LEU:HB2	1.98	0.63
1:D:20:THR:HG23	1:D:108:LEU:O	1.98	0.63
1:C:25:GLY:H	1:C:70:HIS:HE1	1.45	0.62
1:F:144:ARG:NH1	1:F:151:LYS:HE3	2.14	0.62
1:D:127:ASN:HB3	1:D:129:HIS:HD2	1.62	0.62
1:C:25:GLY:H	1:C:70:HIS:CE1	2.18	0.61
1:C:186:MSE:HE2	1:C:190:LYS:CG	2.25	0.61
1:A:36:TRP:CD1	1:A:78:GLU:HG3	2.35	0.61
1:E:127:ASN:HB3	1:E:129:HIS:CD2	2.30	0.61
1:E:7:PRO:HG3	1:E:8:ARG:HH21	1.65	0.61
1:A:196:HIS:H	1:A:196:HIS:CD2	2.15	0.61
1:E:113:ASP:OD1	1:E:113:ASP:C	2.43	0.61
1:B:59:PRO:O	1:B:62:ARG:HB2	2.00	0.61
1:C:56:VAL:HG22	1:C:89:ALA:HB3	1.81	0.61
1:E:137:ARG:NH1	1:E:158:GLU:CB	2.64	0.61
1:F:30:GLU:O	1:F:33:ARG:HB2	2.00	0.60
1:C:186:MSE:CE	1:C:190:LYS:HG2	2.29	0.60
1:D:19:PRO:HG2	1:D:125:PRO:O	2.01	0.60
1:E:120:GLN:O	1:E:123:ASP:HB2	2.02	0.60
1:E:67:ASP:HB3	1:E:68:HIS:CD2	2.36	0.60
1:F:126:LYS:NZ	1:F:126:LYS:CD	2.64	0.60
1:B:129:HIS:CD2	1:B:129:HIS:H	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:ASN:CB	1:E:129:HIS:HD2	2.14	0.60
1:F:26:PHE:HB2	1:F:133:ASP:CG	2.26	0.60
1:F:12:ILE:HD12	1:F:85:THR:HG21	1.84	0.60
1:B:12:ILE:N	1:B:12:ILE:CD1	2.65	0.60
1:C:15:ASP:OD1	1:C:15:ASP:N	2.33	0.59
1:C:148:GLY:HA2	1:C:186:MSE:HE1	1.83	0.59
1:D:12:ILE:HD13	1:D:85:THR:HG21	1.83	0.59
1:C:167:ARG:NH2	1:D:97:ASP:HB3	2.16	0.59
1:A:113:ASP:C	1:A:113:ASP:OD1	2.45	0.59
1:A:204:GLU:OE2	1:D:144:ARG:NH1	2.35	0.59
1:A:6:GLU:HB3	1:A:7:PRO:CD	2.31	0.59
1:F:163:ASP:OD2	1:F:167:ARG:NH1	2.35	0.59
1:E:196:HIS:H	1:E:196:HIS:CD2	2.20	0.59
1:F:12:ILE:HD12	1:F:85:THR:CG2	2.32	0.59
1:D:176:ASP:O	1:D:177:SER:HB3	2.02	0.59
1:E:157:SER:HB3	2:E:218:HOH:O	2.03	0.58
1:B:20:THR:H	1:B:69:HIS:HE1	1.52	0.58
1:D:11:ARG:CB	1:D:11:ARG:HH11	2.17	0.58
1:D:15:ASP:OD1	1:D:15:ASP:N	2.27	0.58
1:D:144:ARG:HB2	1:D:149:TYR:CE1	2.39	0.58
1:D:155:PRO:HA	2:D:218:HOH:O	2.04	0.58
1:F:51:HIS:C	1:F:52:ILE:HD13	2.29	0.57
1:A:163:ASP:O	1:A:167:ARG:HG3	2.05	0.57
1:C:134:ASP:OD1	1:C:166:ARG:NH2	2.37	0.57
1:D:18:ARG:HH11	1:D:126:LYS:HB3	1.70	0.57
1:B:15:ASP:OD1	1:B:15:ASP:C	2.47	0.57
1:B:170:ASP:OD1	1:B:172:ASP:HB2	2.03	0.57
1:C:104:ASP:OD1	1:C:104:ASP:C	2.47	0.57
1:E:7:PRO:HA	1:E:8:ARG:CB	2.35	0.57
1:F:197:LEU:HB3	1:F:198:PRO:HD2	1.87	0.57
1:A:52:ILE:HD11	1:C:9:LEU:HA	1.85	0.57
1:D:11:ARG:HH11	1:D:11:ARG:HB3	1.69	0.57
1:E:134:ASP:OD2	1:E:166:ARG:NH2	2.37	0.56
1:E:137:ARG:NH1	1:E:158:GLU:HB3	2.19	0.56
1:F:163:ASP:HA	1:F:166:ARG:HD2	1.87	0.56
1:B:9:LEU:O	1:D:49:GLY:HA2	2.05	0.56
1:B:98:GLU:O	1:B:101:SER:HB3	2.05	0.56
1:C:37:ARG:HD2	1:C:78:GLU:OE2	2.06	0.56
1:D:14:ILE:HD12	1:D:14:ILE:O	2.06	0.56
1:D:143:LEU:HD13	1:D:149:TYR:CD2	2.41	0.56
1:F:143:LEU:HD12	1:F:149:TYR:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:ARG:HD2	1:C:78:GLU:OE1	2.06	0.55
1:E:34:LYS:O	1:E:38:GLU:OE2	2.25	0.55
1:E:195:ARG:CG	1:E:195:ARG:NH1	2.63	0.55
1:B:17:LEU:HD22	1:B:65:LEU:HB2	1.89	0.55
1:C:12:ILE:HD13	1:C:17:LEU:CG	2.34	0.55
1:D:20:THR:CG2	1:D:108:LEU:O	2.54	0.55
1:F:148:GLY:HA2	1:F:186:MSE:HE1	1.87	0.55
1:A:134:ASP:CG	1:A:166:ARG:HH22	2.14	0.55
1:E:120:GLN:NE2	1:E:123:ASP:OD1	2.39	0.55
1:E:91:PHE:HB3	1:E:94:LEU:HD12	1.89	0.55
1:E:14:ILE:HD12	1:E:15:ASP:N	2.21	0.54
1:C:104:ASP:HB2	1:C:109:ILE:HD11	1.89	0.54
1:F:174:LEU:C	1:F:174:LEU:HD23	2.33	0.54
1:D:9:LEU:HD11	1:D:84:LEU:HB3	1.89	0.54
1:B:54:PRO:HD2	1:B:68:HIS:CD2	2.42	0.54
1:B:12:ILE:H	1:B:12:ILE:CD1	2.22	0.53
1:D:11:ARG:HG3	1:D:84:LEU:HD23	1.91	0.53
1:D:9:LEU:HD21	1:D:84:LEU:HD22	1.90	0.53
1:A:52:ILE:HD11	1:C:9:LEU:CA	2.38	0.53
1:F:127:ASN:OD1	1:F:129:HIS:CE1	2.61	0.53
1:B:54:PRO:HD2	1:B:68:HIS:HD2	1.72	0.53
1:B:67:ASP:OD1	1:B:68:HIS:N	2.40	0.53
1:D:192:ARG:O	1:D:195:ARG:HG2	2.08	0.53
1:A:20:THR:HB	1:A:109:ILE:HG22	1.89	0.52
1:B:54:PRO:HB2	1:B:66:ILE:HD11	1.92	0.52
1:E:53:VAL:HG13	1:E:65:LEU:HD11	1.90	0.52
1:E:127:ASN:CB	1:E:129:HIS:CD2	2.92	0.52
1:E:120:GLN:H	1:E:120:GLN:NE2	2.05	0.52
1:F:156:PHE:HB3	1:F:159:PHE:HB2	1.92	0.52
1:C:20:THR:H	1:C:69:HIS:HE1	1.57	0.52
1:B:71:LEU:HD22	1:D:6:GLU:HB3	1.92	0.52
1:F:182:LEU:HD23	1:F:182:LEU:O	2.10	0.52
1:D:53:VAL:HG22	1:D:54:PRO:HD2	1.92	0.51
1:A:11:ARG:NH1	1:A:11:ARG:CG	2.58	0.51
1:B:135:PRO:HB2	1:B:174:LEU:HD13	1.92	0.51
1:A:48:LEU:HD21	1:C:11:ARG:HG3	1.92	0.51
1:D:163[B]:ASP:OD1	1:D:167:ARG:NH1	2.42	0.51
1:D:67:ASP:O	1:D:68:HIS:HB2	2.10	0.51
1:D:106:ARG:NH2	2:D:214:HOH:O	2.44	0.51
1:B:52:ILE:HD11	1:D:9:LEU:CA	2.40	0.51
1:F:54:PRO:HG2	1:F:67:ASP:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:LEU:HD22	1:E:148:GLY:HA3	1.92	0.51
1:A:114:ALA:HA	1:A:134:ASP:HB2	1.92	0.51
1:A:192:ARG:HB3	1:A:195:ARG:NH1	2.26	0.51
1:B:54:PRO:HB2	1:B:66:ILE:CD1	2.40	0.51
1:B:114:ALA:HA	1:B:134:ASP:HB2	1.93	0.51
1:F:152:VAL:HG13	1:F:154:ILE:HD12	1.92	0.51
1:F:81:GLU:HG3	1:F:82:HIS:ND1	2.26	0.51
1:B:9:LEU:HB2	1:D:52:ILE:HG12	1.93	0.50
1:B:9:LEU:HG	1:B:10:SER:N	2.26	0.50
1:F:52:ILE:HD13	1:F:52:ILE:N	2.27	0.50
1:A:36:TRP:HD1	1:A:78:GLU:HG3	1.76	0.50
1:A:107:ASN:HD21	1:B:107:ASN:ND2	2.05	0.50
1:B:18:ARG:HH11	1:B:62:ARG:NH1	2.10	0.50
1:C:18:ARG:HB3	1:C:64:TYR:CD2	2.47	0.50
1:D:112:PHE:CE2	1:D:118:ARG:HB2	2.46	0.50
1:A:144:ARG:NH1	1:D:204:GLU:OE2	2.44	0.50
1:B:14:ILE:HG21	1:B:76:SER:HB2	1.93	0.50
1:C:14:ILE:HG21	1:C:76:SER:HB2	1.94	0.50
1:D:65:LEU:HD21	1:D:72:VAL:HG21	1.93	0.50
1:F:15:ASP:OD1	1:F:15:ASP:C	2.54	0.50
1:A:24:VAL:HB	1:A:70:HIS:CE1	2.47	0.49
1:F:14:ILE:HG12	1:F:83:VAL:HG12	1.94	0.49
1:A:167:ARG:NH2	1:B:97:ASP:HB3	2.27	0.49
1:F:67:ASP:HB2	1:F:68:HIS:CD2	2.45	0.49
1:A:113:ASP:OD1	1:A:115:GLN:N	2.46	0.49
1:D:135:PRO:HB2	1:D:174:LEU:HD13	1.95	0.49
1:B:104:ASP:HB2	1:B:109:ILE:HD11	1.94	0.49
1:D:37:ARG:HB3	1:D:38:GLU:CD	2.38	0.49
1:B:125:PRO:HB3	1:B:130:ASP:HB3	1.95	0.49
1:C:163:ASP:O	1:C:167:ARG:HG3	2.12	0.49
1:F:143:LEU:HD12	1:F:149:TYR:HE2	1.75	0.48
1:B:20:THR:H	1:B:69:HIS:CE1	2.32	0.48
1:F:115:GLN:HG2	1:F:117:LEU:HD23	1.95	0.48
1:B:26:PHE:CG	1:B:133:ASP:HB2	2.48	0.48
1:F:126:LYS:CG	1:F:126:LYS:HZ3	2.22	0.48
1:B:33:ARG:HG2	1:B:74:ALA:HB1	1.94	0.48
1:D:67:ASP:HB3	1:D:68:HIS:CD2	2.48	0.48
1:A:15:ASP:C	1:A:15:ASP:OD1	2.57	0.48
1:B:55:VAL:HA	1:B:64:TYR:O	2.13	0.48
1:E:170:ASP:OD1	1:E:170:ASP:C	2.56	0.48
1:F:20:THR:H	1:F:69:HIS:HE1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:PRO:O	1:E:62:ARG:HB2	2.13	0.48
1:C:99:PHE:O	1:C:103:MSE:HG2	2.13	0.47
1:E:38:GLU:CD	1:E:38:GLU:H	2.22	0.47
1:B:96:LYS:O	1:B:99:PHE:HB3	2.13	0.47
1:C:62:ARG:HD2	1:C:62:ARG:HA	1.60	0.47
1:C:196:HIS:H	1:C:196:HIS:CD2	2.31	0.47
1:C:13:ALA:HB1	1:C:15:ASP:OD1	2.13	0.47
1:D:113:ASP:OD1	1:D:113:ASP:C	2.56	0.47
1:E:95:GLY:O	1:E:96:LYS:C	2.57	0.47
1:C:66:ILE:HD13	1:C:66:ILE:HA	1.71	0.47
1:F:37:ARG:HH11	1:F:37:ARG:HB2	1.78	0.47
1:A:143:LEU:HD22	1:A:148:GLY:HA3	1.96	0.47
1:B:8:ARG:HB2	1:D:50:ASN:O	2.14	0.47
1:F:67:ASP:O	1:F:69:HIS:CD2	2.68	0.47
1:A:110:TYR:OH	1:A:159:PHE:HB3	2.14	0.47
1:A:154:ILE:HD12	1:D:153:ILE:HD11	1.93	0.47
1:B:26:PHE:CD1	1:B:133:ASP:HB2	2.50	0.47
1:D:65:LEU:CD2	1:D:72:VAL:HG21	2.45	0.47
1:A:15:ASP:OD1	1:A:16:LYS:HG2	2.15	0.46
1:B:25:GLY:N	1:B:70:HIS:CE1	2.65	0.46
1:A:56:VAL:HG22	1:A:89:ALA:HB3	1.96	0.46
1:C:54:PRO:HD2	1:C:68:HIS:HD2	1.80	0.46
1:B:190:LYS:NZ	2:B:222:HOH:O	2.44	0.46
1:F:125:PRO:HB3	1:F:130:ASP:HB2	1.97	0.46
1:B:25:GLY:N	1:B:70:HIS:HE1	1.92	0.46
1:F:129:HIS:CD2	2:F:206:HOH:O	2.69	0.46
1:B:134:ASP:OD1	1:B:134:ASP:C	2.58	0.46
1:E:107:ASN:HD21	1:F:107:ASN:HD21	1.63	0.46
1:B:23:ALA:HA	1:B:132:GLU:O	2.16	0.46
1:B:90:LYS:O	1:B:91:PHE:CD1	2.69	0.46
1:F:11:ARG:HD3	1:F:82:HIS:HB3	1.98	0.46
1:F:164:PHE:CE1	1:F:168:ARG:CZ	2.98	0.46
1:A:154:ILE:CD1	1:A:154:ILE:H	2.29	0.46
1:B:73:LEU:HD13	1:B:128:ILE:HG23	1.97	0.46
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.77	0.46
1:B:67:ASP:CG	1:B:68:HIS:N	2.71	0.46
1:B:113:ASP:OD1	1:B:117:LEU:HB2	2.16	0.46
1:C:53:VAL:HG13	1:C:65:LEU:CD1	2.46	0.46
1:D:37:ARG:HD2	1:D:78:GLU:OE2	2.16	0.46
1:E:20:THR:HG23	1:E:109:ILE:HA	1.97	0.46
1:C:20:THR:H	1:C:69:HIS:CE1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PRO:HB2	1:C:156:PHE:CD1	2.51	0.45
1:D:27:ARG:HE	1:D:27:ARG:HB3	1.43	0.45
1:E:60:LYS:HE3	1:E:96:LYS:NZ	2.31	0.45
1:E:66:ILE:HD13	1:E:66:ILE:N	2.31	0.45
1:C:173:LEU:HD22	1:C:173:LEU:O	2.15	0.45
1:F:134:ASP:HA	1:F:135:PRO:HD2	1.80	0.45
1:C:124:ILE:O	1:C:125:PRO:C	2.55	0.45
1:D:175:SER:CB	1:D:175:SER:HG	2.15	0.45
1:F:127:ASN:CG	1:F:129:HIS:CE1	2.94	0.45
1:A:143:LEU:HD13	1:A:149:TYR:CE2	2.51	0.45
1:E:163:ASP:OD2	1:E:167:ARG:NH1	2.46	0.45
1:C:103:MSE:HB3	1:C:109:ILE:HG23	1.99	0.45
1:F:127:ASN:OD1	1:F:129:HIS:ND1	2.50	0.45
1:C:134:ASP:OD1	1:C:134:ASP:C	2.56	0.45
1:F:169:ILE:HG22	1:F:170:ASP:O	2.17	0.45
1:B:144:ARG:HD2	1:C:204:GLU:OE2	2.17	0.45
1:C:35:GLU:O	1:C:38:GLU:N	2.46	0.45
1:D:113:ASP:OD1	1:D:115:GLN:N	2.44	0.45
1:D:127:ASN:CB	1:D:129:HIS:CD2	2.97	0.45
1:D:148:GLY:HA2	1:D:190:LYS:NZ	2.31	0.45
1:E:60:LYS:HE3	1:E:96:LYS:HZ1	1.82	0.45
1:F:13:ALA:O	1:F:14:ILE:C	2.58	0.45
1:B:9:LEU:HB2	1:D:52:ILE:CG1	2.47	0.44
1:A:6:GLU:OE2	1:A:6:GLU:HA	2.15	0.44
1:A:68:HIS:HD1	1:C:5:TYR:N	2.15	0.44
1:D:174:LEU:HD23	1:D:174:LEU:HA	1.73	0.44
1:E:9:LEU:N	1:E:9:LEU:HD12	2.32	0.44
1:C:11:ARG:HD3	1:C:84:LEU:HD23	2.00	0.44
1:D:66:ILE:HD13	1:D:66:ILE:HA	1.65	0.44
1:D:175:SER:OG	1:D:175:SER:CA	2.60	0.44
1:E:33:ARG:HB3	1:E:78:GLU:OE1	2.17	0.44
1:F:114:ALA:HB2	1:F:132:GLU:HB3	1.99	0.44
1:F:25:GLY:H	1:F:70:HIS:CE1	2.35	0.44
1:C:50:ASN:N	1:C:50:ASN:HD22	2.15	0.44
1:C:98[B]:GLU:OE2	1:D:168:ARG:NH2	2.46	0.44
1:C:114:ALA:HA	1:C:134:ASP:HB2	1.99	0.44
1:F:20:THR:N	1:F:69:HIS:HE1	2.15	0.43
1:D:18:ARG:NH1	1:D:126:LYS:HB3	2.32	0.43
1:F:12:ILE:HD11	1:F:17:LEU:HD21	2.00	0.43
1:E:190:LYS:HE3	1:E:201:CYS:O	2.18	0.43
1:B:24:VAL:HB	1:B:70:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:HD3	1:C:62:ARG:NH1	2.34	0.43
1:C:186:MSE:CE	1:C:190:LYS:CE	2.91	0.43
1:D:29:VAL:O	1:D:33:ARG:HG3	2.19	0.43
1:D:152:VAL:HG13	1:D:154:ILE:HG12	2.00	0.43
1:D:20:THR:HG23	1:D:109:ILE:HA	2.00	0.43
1:E:164:PHE:CZ	1:E:194:ALA:HB2	2.53	0.43
1:C:35:GLU:O	1:C:36:TRP:C	2.62	0.43
1:C:128:ILE:HD12	1:C:128:ILE:HG23	1.66	0.43
1:B:134:ASP:CG	1:B:166:ARG:NH2	2.76	0.43
1:F:25:GLY:H	1:F:70:HIS:HE1	1.66	0.43
1:F:134:ASP:OD1	1:F:134:ASP:C	2.61	0.43
1:D:134:ASP:CG	1:D:166:ARG:NH2	2.76	0.43
1:B:190:LYS:HE2	1:B:201:CYS:O	2.19	0.42
1:D:182:LEU:HD23	1:D:182:LEU:HA	1.76	0.42
1:A:10:SER:HB2	1:A:11:ARG:H	1.60	0.42
1:F:64:TYR:CD1	1:F:64:TYR:N	2.85	0.42
1:F:144:ARG:HB2	1:F:149:TYR:CZ	2.55	0.42
1:B:22:ILE:HD12	1:B:111:PRO:C	2.43	0.42
1:B:35:GLU:O	1:B:36:TRP:C	2.62	0.42
1:B:169:ILE:HG12	1:B:184:GLU:OE1	2.19	0.42
1:C:51:HIS:O	1:C:84:LEU:HB2	2.18	0.42
1:D:104:ASP:HB2	1:D:109:ILE:HD11	2.01	0.42
1:F:142:ALA:C	1:F:145:MSE:HB2	2.44	0.42
1:A:101:SER:O	1:A:105:HIS:HB2	2.20	0.42
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.75	0.42
1:A:50:ASN:HB3	2:A:222:HOH:O	2.18	0.42
1:B:35:GLU:O	1:B:37:ARG:N	2.53	0.42
1:D:134:ASP:CG	1:D:166:ARG:HH21	2.27	0.42
1:D:143:LEU:HD13	1:D:149:TYR:HD2	1.82	0.42
1:A:20:THR:N	1:A:69:HIS:HE1	2.15	0.42
1:B:18:ARG:HA	1:B:19:PRO:HD2	1.93	0.42
1:D:12:ILE:HG13	1:D:17:LEU:HG	2.00	0.42
1:D:103:MSE:HB3	1:D:109:ILE:HG23	2.02	0.42
1:F:203:VAL:HG12	1:F:204:GLU:H	1.84	0.42
1:B:56:VAL:HG22	1:B:89:ALA:HB3	2.00	0.42
1:C:18:ARG:NH1	1:C:62:ARG:CZ	2.83	0.42
1:D:87:GLU:OE1	1:D:90:LYS:HD2	2.19	0.42
1:D:81:GLU:OE1	1:D:82:HIS:HE1	2.00	0.41
1:E:114:ALA:HB3	1:E:115:GLN:HE21	1.84	0.41
1:D:55:VAL:HG12	1:D:87:GLU:HA	2.03	0.41
1:D:69:HIS:O	1:D:70:HIS:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:LEU:CD1	1:F:149:TYR:CD2	3.03	0.41
1:D:154:ILE:HA	1:D:155:PRO:HD2	1.61	0.41
1:D:197:LEU:HD23	1:D:197:LEU:HA	1.79	0.41
1:E:50:ASN:HB3	1:E:51:HIS:H	1.50	0.41
1:A:144:ARG:HH11	1:A:144:ARG:HD2	1.69	0.41
1:C:27:ARG:NH2	1:C:31:LEU:HD11	2.36	0.41
1:C:186:MSE:HE1	1:C:190:LYS:CE	2.47	0.41
1:B:65:LEU:HD11	1:B:67:ASP:O	2.21	0.41
1:B:113:ASP:OD1	1:B:113:ASP:C	2.64	0.41
1:C:186:MSE:HE2	1:C:190:LYS:CE	2.48	0.41
1:D:118:ARG:C	1:D:119:ARG:HD2	2.45	0.41
1:D:143:LEU:HD22	1:D:148:GLY:HA3	2.02	0.41
1:C:156:PHE:O	1:C:157:SER:C	2.64	0.41
1:D:20:THR:N	1:D:69:HIS:HE1	2.19	0.41
1:A:8:ARG:HD3	1:A:8:ARG:HH11	1.73	0.41
1:B:52:ILE:HD11	1:D:9:LEU:HA	2.02	0.41
1:D:91:PHE:HB3	1:D:94:LEU:HD12	2.02	0.41
1:D:196:HIS:CD2	1:D:196:HIS:H	2.38	0.41
1:F:113:ASP:OD1	1:F:113:ASP:C	2.64	0.41
1:B:18:ARG:HD3	1:B:62:ARG:HH11	1.86	0.40
1:D:75:LEU:O	1:D:76:SER:C	2.63	0.40
1:D:154:ILE:HG12	1:D:154:ILE:H	1.68	0.40
1:D:60:LYS:HA	1:D:60:LYS:HD3	1.76	0.40
1:A:152:VAL:HG12	1:A:154:ILE:HB	2.04	0.40
1:D:59:PRO:HD3	1:D:99:PHE:CD1	2.56	0.40
1:F:77:LYS:C	1:F:79:GLY:H	2.29	0.40
1:A:154:ILE:HD12	1:A:154:ILE:H	1.85	0.40
1:A:168:ARG:NH2	1:B:98:GLU:OE1	2.40	0.40
1:E:164:PHE:CG	1:E:197:LEU:HD11	2.56	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	192/205 (94%)	179 (93%)	11 (6%)	2 (1%)	12	26
1	B	186/205 (91%)	170 (91%)	14 (8%)	2 (1%)	11	23
1	C	193/205 (94%)	181 (94%)	8 (4%)	4 (2%)	5	10
1	D	190/205 (93%)	166 (87%)	17 (9%)	7 (4%)	2	3
1	E	184/205 (90%)	162 (88%)	16 (9%)	6 (3%)	3	4
1	F	186/205 (91%)	162 (87%)	22 (12%)	2 (1%)	11	23
All	All	1131/1230 (92%)	1020 (90%)	88 (8%)	23 (2%)	6	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	6	GLU
1	D	19	PRO
1	D	48	LEU
1	D	177	SER
1	E	10	SER
1	F	192	ARG
1	E	157	SER
1	B	36	TRP
1	C	6	GLU
1	C	114	ALA
1	D	155	PRO
1	E	93	HIS
1	B	89	ALA
1	D	20	THR
1	D	49	GLY
1	D	195	ARG
1	E	8	ARG
1	E	9	LEU
1	E	121	SER
1	C	121	SER
1	C	111	PRO
1	F	203	VAL

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	163/170 (96%)	131 (80%)	32 (20%)	1	2
1	B	160/170 (94%)	126 (79%)	34 (21%)	1	1
1	C	164/170 (96%)	133 (81%)	31 (19%)	1	2
1	D	162/170 (95%)	123 (76%)	39 (24%)	1	1
1	E	159/170 (94%)	120 (76%)	39 (24%)	1	1
1	F	159/170 (94%)	127 (80%)	32 (20%)	1	2
All	All	967/1020 (95%)	760 (79%)	207 (21%)	1	1

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	11	ARG
1	A	18	ARG
1	A	27	ARG
1	A	33	ARG
1	A	34	LYS
1	A	39	THR
1	A	48	LEU
1	A	52	ILE
1	A	53	VAL
1	A	55	VAL
1	A	56	VAL
1	A	66	ILE
1	A	75	LEU
1	A	81	GLU
1	A	96	LYS
1	A	97	ASP
1	A	115	GLN
1	A	117	LEU
1	A	118	ARG
1	A	126	LYS
1	A	127	ASN
1	A	143	LEU
1	A	145	MSE
1	A	152	VAL
1	A	166	ARG
1	A	173	LEU

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Mol	Chain	Res	Type
1	A	174	LEU
1	A	175	SER
1	A	182	LEU
1	A	184	GLU
1	A	190	LYS
1	B	7	PRO
1	B	8	ARG
1	B	9	LEU
1	B	11	ARG
1	B	12	ILE
1	B	38	GLU
1	B	39	THR
1	B	52	ILE
1	B	53	VAL
1	B	55	VAL
1	B	56	VAL
1	B	66	ILE
1	B	75	LEU
1	B	90	LYS
1	B	92	SER
1	B	97	ASP
1	B	115	GLN
1	B	117	LEU
1	B	119	ARG
1	B	120	GLN
1	B	128	ILE
1	B	129	HIS
1	B	138	SER
1	B	143	LEU
1	B	151	LYS
1	B	152	VAL
1	B	154	ILE
1	B	174	LEU
1	B	175	SER
1	B	182	LEU
1	B	186	MSE
1	B	187	LYS
1	B	195	ARG
1	B	201	CYS
1	C	10	SER
1	C	12	ILE
1	C	15	ASP

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Mol	Chain	Res	Type
1	C	18	ARG
1	C	27	ARG
1	C	35	GLU
1	C	37	ARG
1	C	48	LEU
1	C	52	ILE
1	C	53	VAL
1	C	55	VAL
1	C	62	ARG
1	C	66	ILE
1	C	75	LEU
1	C	77	LYS
1	C	92	SER
1	C	96	LYS
1	C	115	GLN
1	C	118	ARG
1	C	143	LEU
1	C	152	VAL
1	C	153	ILE
1	C	166	ARG
1	C	171	ARG
1	C	173	LEU
1	C	174	LEU
1	C	175	SER
1	C	182	LEU
1	C	187	LYS
1	C	192	ARG
1	C	193	GLU
1	D	6	GLU
1	D	11	ARG
1	D	12	ILE
1	D	14	ILE
1	D	15	ASP
1	D	20	THR
1	D	27	ARG
1	D	31	LEU
1	D	37	ARG
1	D	48	LEU
1	D	52	ILE
1	D	55	VAL
1	D	66	ILE
1	D	67	ASP

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Mol	Chain	Res	Type
1	D	75	LEU
1	D	77	LYS
1	D	88	VAL
1	D	92	SER
1	D	96	LYS
1	D	101	SER
1	D	105	HIS
1	D	109	ILE
1	D	115	GLN
1	D	117	LEU
1	D	118	ARG
1	D	121	SER
1	D	143	LEU
1	D	145	MSE
1	D	152	VAL
1	D	153	ILE
1	D	157	SER
1	D	170	ASP
1	D	171	ARG
1	D	173	LEU
1	D	182	LEU
1	D	187	LYS
1	D	190	LYS
1	D	192	ARG
1	D	201	CYS
1	E	10	SER
1	E	11	ARG
1	E	12	ILE
1	E	18	ARG
1	E	20	THR
1	E	24	VAL
1	E	27	ARG
1	E	28	GLU
1	E	33	ARG
1	E	34	LYS
1	E	35	GLU
1	E	37	ARG
1	E	38	GLU
1	E	39	THR
1	E	52	ILE
1	E	53	VAL
1	E	55	VAL

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Mol	Chain	Res	Type
1	E	61	ASP
1	E	66	ILE
1	E	67	ASP
1	E	75	LEU
1	E	90	LYS
1	E	94	LEU
1	E	101	SER
1	E	118	ARG
1	E	120	GLN
1	E	126	LYS
1	E	128	ILE
1	E	143	LEU
1	E	152	VAL
1	E	154	ILE
1	E	171	ARG
1	E	173	LEU
1	E	174	LEU
1	E	182	LEU
1	E	187	LYS
1	E	190	LYS
1	E	195	ARG
1	E	203	VAL
1	F	8	ARG
1	F	9	LEU
1	F	10	SER
1	F	12	ILE
1	F	18	ARG
1	F	20	THR
1	F	22	ILE
1	F	27	ARG
1	F	28	GLU
1	F	37	ARG
1	F	50	ASN
1	F	52	ILE
1	F	53	VAL
1	F	55	VAL
1	F	67	ASP
1	F	75	LEU
1	F	92	SER
1	F	105	HIS
1	F	115	GLN
1	F	117	LEU

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Mol	Chain	Res	Type
1	F	126	LYS
1	F	128	ILE
1	F	129	HIS
1	F	152	VAL
1	F	158	GLU
1	F	172	ASP
1	F	173	LEU
1	F	184	GLU
1	F	187	LYS
1	F	192	ARG
1	F	201	CYS
1	F	203	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	69	HIS
1	A	70	HIS
1	A	120	GLN
1	A	127	ASN
1	A	196	HIS
1	B	68	HIS
1	B	69	HIS
1	B	70	HIS
1	B	107	ASN
1	B	127	ASN
1	B	129	HIS
1	C	21	GLN
1	C	50	ASN
1	C	68	HIS
1	C	69	HIS
1	C	70	HIS
1	C	196	HIS
1	D	69	HIS
1	D	70	HIS
1	D	82	HIS
1	D	129	HIS
1	D	196	HIS
1	E	50	ASN
1	E	68	HIS
1	E	115	GLN

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Mol	Chain	Res	Type
1	E	120	GLN
1	E	196	HIS
1	F	51	HIS
1	F	68	HIS
1	F	69	HIS
1	F	105	HIS
1	F	107	ASN
1	F	129	HIS
1	F	196	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	193/205 (94%)	-0.15	1 (0%) 87 85	48, 60, 75, 82	0
1	B	186/205 (90%)	0.16	3 (1%) 70 67	42, 70, 84, 112	1 (0%)
1	C	192/205 (93%)	-0.22	4 (2%) 63 59	38, 59, 81, 94	2 (1%)
1	D	190/205 (92%)	0.58	6 (3%) 50 45	43, 71, 85, 93	1 (0%)
1	E	185/205 (90%)	-0.10	0 100 100	49, 65, 78, 96	0
1	F	187/205 (91%)	0.38	5 (2%) 56 51	57, 77, 88, 94	0
All	All	1133/1230 (92%)	0.11	19 (1%) 69 65	38, 68, 84, 112	4 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	3.6
1	B	7	PRO	3.5
1	C	5	TYR	3.3
1	D	40	ARG	3.2
1	D	105	HIS	3.2
1	D	147	GLY	2.8
1	D	47	PHE	2.7
1	C	40	ARG	2.6
1	C	105[A]	HIS	2.5
1	C	46	ASP	2.5
1	F	9	LEU	2.5
1	D	48	LEU	2.4
1	B	94	LEU	2.3
1	F	8	ARG	2.3
1	F	105	HIS	2.2
1	B	27	ARG	2.1
1	D	83	VAL	2.1
1	F	194	ALA	2.1
1	F	153	ILE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.