



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:34 PM UTC

PDB ID : 7C1I / pdb_00007c1i
Title : Crystal structure of histidine-containing phosphotransfer protein B (HptB) from *Pseudomonas aeruginosa* PAO1
Authors : Chen, S.K.; Guan, H.H.; Wu, P.H.; Lin, L.T.; Wu, M.C.; Chang, H.Y.; Chen, N.C.; Lin, C.C.; Chuankhayan, P.; Huang, Y.C.; Lin, P.J.; Chen, C.J.
Deposited on : 2020-05-04
Resolution : 1.58 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:

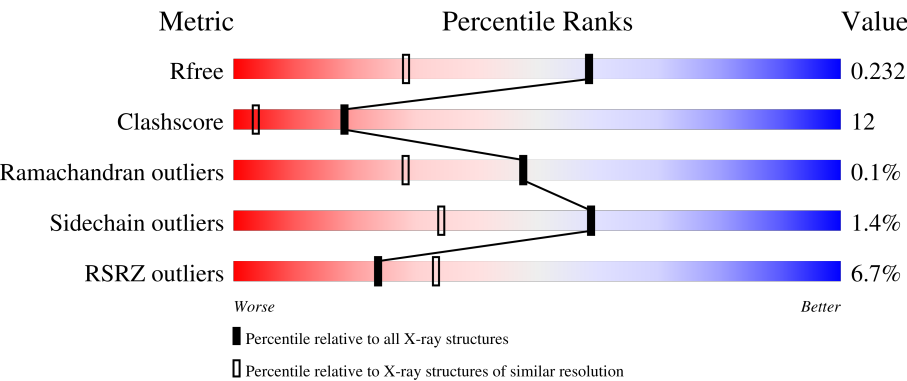
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	116	4% 71% 25% ..
1	B	116	13% 58% 34% 6% ..
1	C	116	8% 64% 34% ..
1	D	116	3% 75% 20% ..
1	E	116	4% 64% 32% ..

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Mol	Chain	Length	Quality of chain
1	F	116	7% 69% 25% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7604 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 Histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	20	0
			1090	664	209	211	6			
1	B	115	Total	C	N	O	S	0	18	0
			1070	654	205	206	5			
1	C	115	Total	C	N	O	S	0	11	0
			1017	623	194	196	4			
1	D	115	Total	C	N	O	S	0	20	0
			1084	663	212	204	5			
1	E	115	Total	C	N	O	S	0	15	0
			1052	642	202	204	4			
1	F	115	Total	C	N	O	S	0	16	0
			1062	650	207	200	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	0	0
			209	209		
2	B	189	Total	O	0	0
			189	189		
2	C	200	Total	O	0	0
			200	200		
2	D	215	Total	O	0	0
			215	215		
2	E	215	Total	O	0	0
			215	215		
2	F	201	Total	O	0	0
			201	201		

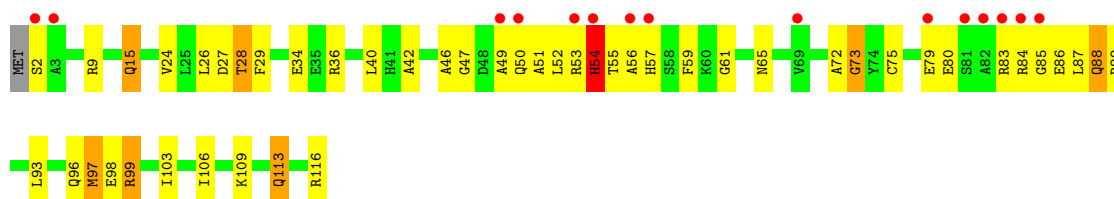
3 Residue-property plots [i](#)

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.

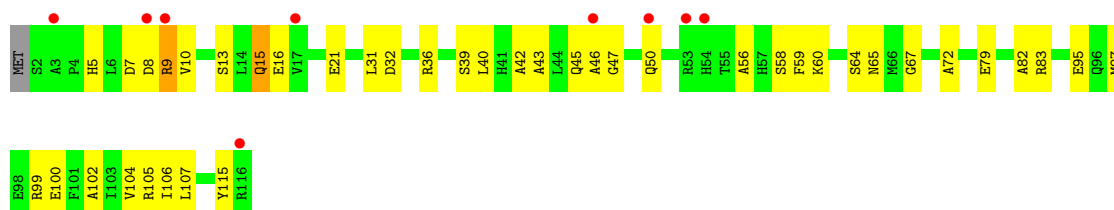
• Molecule 1: Histidine kinase



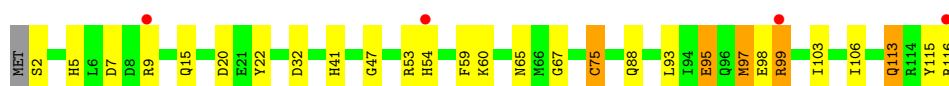
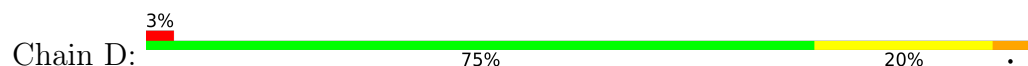
• Molecule 1: Histidine kinase



• Molecule 1: Histidine kinase

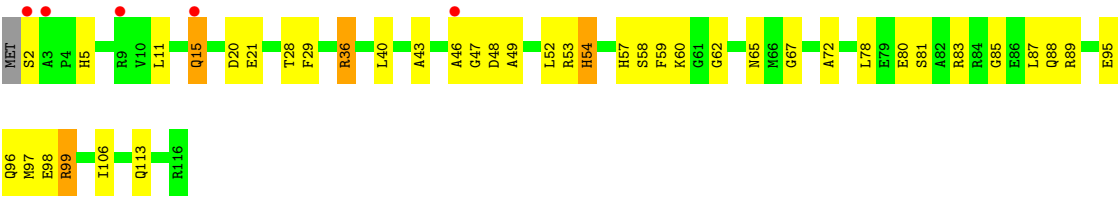


• Molecule 1: Histidine kinase



• Molecule 1: Histidine kinase





• Molecule 1: Histidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 119.17Å 171.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.37 – 1.58 29.37 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.37-1.58) 98.4 (29.37-1.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 1.58Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.225 0.202 , 0.232	Depositor DCC
R_{free} test set	8322 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2070e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.94	0/1103	1.94	33/1476 (2.2%)
1	B	0.95	0/1084	2.13	53/1453 (3.6%)
1	C	0.94	0/1031	2.15	48/1382 (3.5%)
1	D	0.94	0/1100	1.93	26/1472 (1.8%)
1	E	0.94	0/1066	2.06	43/1428 (3.0%)
1	F	0.94	0/1076	1.93	29/1442 (2.0%)
All	All	0.94	0/6460	2.02	232/8653 (2.7%)

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
1	B	0	2
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	2
All	All	0	9

There are no bond length outliers.

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	65	ASN	OD1-CG-ND2	16.32	138.92	122.60
1	B	65	ASN	CA-CB-CG	11.93	124.53	112.60
1	E	95[A]	GLU	O-C-N	9.42	132.27	122.09
1	E	95[B]	GLU	O-C-N	9.42	132.27	122.09
1	F	65	ASN	OD1-CG-ND2	9.19	131.79	122.60
1	B	116	ARG	CA-C-O	-9.12	105.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	65	ASN	CA-CB-CG	8.81	121.41	112.60
1	C	65	ASN	OD1-CG-ND2	8.57	131.17	122.60
1	C	5	HIS	CA-CB-CG	-8.50	105.30	113.80
1	E	65	ASN	OD1-CG-ND2	8.50	131.10	122.60
1	B	99[A]	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	B	99[B]	ARG	NE-CZ-NH2	-8.47	111.58	119.20
1	A	60	LYS	O-C-N	8.37	130.69	122.07
1	E	65	ASN	CB-CG-ND2	-8.17	104.14	116.40
1	F	60	LYS	O-C-N	8.12	130.43	122.07
1	C	16	GLU	CB-CG-CD	8.11	126.38	112.60
1	C	8	ASP	CA-CB-CG	-7.78	104.82	112.60
1	B	24	VAL	N-CA-C	-7.74	102.90	110.72
1	C	79	GLU	O-C-N	7.63	129.93	122.07
1	F	97[A]	MET	CA-C-O	7.55	128.42	120.42
1	F	97[B]	MET	CA-C-O	7.55	128.42	120.42
1	E	46	ALA	CA-C-N	7.49	131.42	120.11
1	E	46	ALA	C-N-CA	7.49	131.42	120.11
1	B	28[A]	THR	O-C-N	-7.43	112.47	122.43
1	B	28[B]	THR	O-C-N	-7.43	112.47	122.43
1	E	67	GLY	O-C-N	7.37	131.33	122.34
1	C	72	ALA	CA-C-N	7.33	128.27	119.99
1	C	72	ALA	C-N-CA	7.33	128.27	119.99
1	C	59	PHE	CA-C-N	7.31	129.95	120.44
1	C	59	PHE	C-N-CA	7.31	129.95	120.44
1	C	104	VAL	O-C-N	-7.31	114.72	121.89
1	F	101	PHE	CA-CB-CG	-7.26	106.54	113.80
1	E	60	LYS	O-C-N	7.03	129.31	122.07
1	E	85	GLY	CA-C-N	7.01	131.80	122.06
1	E	85	GLY	C-N-CA	7.01	131.80	122.06
1	B	113	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	A	11	LEU	CA-C-O	-6.99	111.94	119.97
1	C	72	ALA	CA-C-O	-6.98	113.02	120.42
1	F	10	VAL	N-CA-CB	6.98	118.70	110.53
1	D	41	HIS	CA-C-O	-6.91	113.22	120.55
1	C	79	GLU	CA-C-O	-6.91	113.57	120.82
1	A	28[A]	THR	O-C-N	-6.88	113.21	122.43
1	A	28[B]	THR	O-C-N	-6.88	113.21	122.43
1	B	59	PHE	CA-C-N	6.88	130.35	120.79
1	B	59	PHE	C-N-CA	6.88	130.35	120.79
1	E	57	HIS	ND1-CG-CD2	6.82	112.92	106.10
1	C	65	ASN	CA-CB-CG	6.79	119.39	112.60
1	E	81	SER	CA-C-N	6.78	129.36	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	81	SER	C-N-CA	6.78	129.36	120.28
1	A	65	ASN	OD1-CG-ND2	6.70	129.30	122.60
1	C	9	ARG	CG-CD-NE	6.67	126.67	112.00
1	B	72	ALA	CA-C-N	6.65	127.36	119.98
1	B	72	ALA	C-N-CA	6.65	127.36	119.98
1	C	32	ASP	CA-CB-CG	6.59	119.19	112.60
1	B	97[A]	MET	CA-C-O	6.58	127.47	119.31
1	B	97[B]	MET	CA-C-O	6.58	127.47	119.31
1	B	56	ALA	N-CA-CB	6.56	119.53	110.01
1	F	105	ARG	N-CA-C	-6.47	103.91	110.97
1	C	64	SER	CA-C-O	-6.46	113.70	120.55
1	A	11	LEU	O-C-N	6.45	130.20	122.27
1	C	60	LYS	N-CA-C	-6.44	104.17	111.07
1	D	93	LEU	O-C-N	-6.42	115.32	122.12
1	B	65	ASN	N-CA-C	-6.32	104.39	111.28
1	B	55	THR	CA-C-N	6.31	128.64	120.44
1	B	55	THR	C-N-CA	6.31	128.64	120.44
1	A	65	ASN	CA-CB-CG	6.29	118.89	112.60
1	C	13	SER	O-C-N	-6.28	115.60	122.07
1	A	13	SER	O-C-N	-6.28	115.46	122.12
1	A	97[A]	MET	CA-C-O	6.27	127.09	119.31
1	A	97[B]	MET	CA-C-O	6.27	127.09	119.31
1	E	49	ALA	N-CA-C	-6.25	104.50	111.25
1	C	100	GLU	N-CA-C	-6.25	104.55	111.23
1	C	60	LYS	O-C-N	6.25	128.51	122.07
1	D	65	ASN	N-CA-C	-6.24	104.58	111.82
1	E	62	GLY	N-CA-C	-6.23	105.27	112.50
1	D	98	GLU	CB-CG-CD	6.19	123.12	112.60
1	D	32	ASP	CA-CB-CG	6.14	118.74	112.60
1	C	105	ARG	CA-C-O	-6.13	114.57	121.00
1	E	78	LEU	N-CA-C	-6.12	104.53	111.14
1	A	99[A]	ARG	CA-C-O	-6.12	113.93	120.42
1	A	99[B]	ARG	CA-C-O	-6.12	113.93	120.42
1	E	113	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	B	29	PHE	CA-CB-CG	-6.11	107.69	113.80
1	B	40	LEU	CA-C-O	-6.11	114.01	120.48
1	A	28[A]	THR	CA-C-O	6.10	126.88	119.38
1	A	28[B]	THR	CA-C-O	6.10	126.88	119.38
1	B	80	GLU	CB-CG-CD	6.10	122.97	112.60
1	B	103	ILE	N-CA-C	-6.09	104.69	110.42
1	F	98	GLU	CB-CG-CD	6.08	122.94	112.60
1	C	46	ALA	CA-C-N	6.08	133.32	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ALA	C-N-CA	6.08	133.32	121.41
1	B	57	HIS	CA-C-O	-6.07	114.25	120.69
1	B	34	GLU	N-CA-C	-6.05	104.58	111.17
1	B	9	ARG	CB-CG-CD	6.05	125.21	111.30
1	F	60	LYS	CA-C-O	-6.04	114.48	120.82
1	F	29	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	46	ALA	O-C-N	-6.01	113.88	122.41
1	B	52	LEU	N-CA-CB	6.00	118.71	110.01
1	C	65	ASN	N-CA-C	-6.00	104.74	111.28
1	D	99[A]	ARG	CG-CD-NE	-5.99	98.82	112.00
1	D	99[B]	ARG	CG-CD-NE	-5.99	98.82	112.00
1	E	99[A]	ARG	CA-C-O	5.98	126.84	119.97
1	E	99[B]	ARG	CA-C-O	5.98	126.84	119.97
1	D	22	TYR	O-C-N	-5.90	115.23	120.48
1	B	54[A]	HIS	CA-C-O	5.89	126.75	119.79
1	B	54[B]	HIS	CA-C-O	5.89	126.75	119.79
1	C	104	VAL	CA-C-N	5.87	128.39	120.65
1	C	104	VAL	C-N-CA	5.87	128.39	120.65
1	B	61	GLY	CA-C-O	-5.85	114.68	121.00
1	B	98	GLU	CB-CG-CD	5.85	122.54	112.60
1	D	5	HIS	O-C-N	5.84	128.81	122.15
1	B	98	GLU	N-CA-C	-5.84	104.86	111.10
1	C	67	GLY	O-C-N	5.83	128.95	122.31
1	D	75	CYS	N-CA-C	-5.82	104.85	111.07
1	B	75	CYS	CA-C-O	-5.81	114.39	120.55
1	B	99[A]	ARG	CA-C-O	5.81	126.65	119.97
1	B	99[B]	ARG	CA-C-O	5.81	126.65	119.97
1	E	36	ARG	N-CA-CB	5.81	118.43	110.01
1	C	39[A]	SER	CA-C-O	5.80	126.57	120.42
1	C	39[B]	SER	CA-C-O	5.80	126.57	120.42
1	F	111	GLU	N-CA-C	-5.80	104.16	111.23
1	E	54[A]	HIS	O-C-N	5.79	128.06	122.03
1	E	54[B]	HIS	O-C-N	5.79	128.06	122.03
1	F	111	GLU	CA-C-N	5.78	128.03	120.28
1	F	111	GLU	C-N-CA	5.78	128.03	120.28
1	F	105	ARG	CA-C-O	-5.78	114.93	121.00
1	B	59	PHE	O-C-N	-5.78	114.72	122.23
1	E	48	ASP	CA-C-N	5.77	128.21	120.37
1	E	48	ASP	C-N-CA	5.77	128.21	120.37
1	D	95[A]	GLU	O-C-N	5.76	128.31	122.09
1	D	95[B]	GLU	O-C-N	5.76	128.31	122.09
1	E	46	ALA	O-C-N	-5.74	114.25	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	97[A]	MET	O-C-N	-5.71	115.25	122.27
1	D	97[B]	MET	O-C-N	-5.71	115.25	122.27
1	A	59	PHE	CA-CB-CG	5.69	119.49	113.80
1	C	42	ALA	N-CA-C	-5.68	105.09	111.28
1	F	103	ILE	N-CA-C	-5.66	104.81	110.30
1	E	96	GLN	N-CA-C	-5.65	105.12	111.28
1	B	40	LEU	O-C-N	5.65	128.10	122.12
1	A	111	GLU	N-CA-C	-5.64	105.14	111.28
1	B	96	GLN	N-CA-C	-5.63	105.40	111.48
1	A	86	GLU	CA-C-O	-5.63	115.08	121.39
1	B	9	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	C	31	LEU	N-CA-C	-5.63	105.05	111.07
1	B	75	CYS	N-CA-C	-5.62	105.15	111.28
1	C	105	ARG	N-CA-C	-5.62	104.84	110.97
1	A	10	VAL	O-C-N	-5.60	116.34	121.94
1	D	65	ASN	CB-CG-ND2	-5.60	108.00	116.40
1	A	10	VAL	N-CA-CB	5.60	116.73	110.52
1	D	65	ASN	CA-CB-CG	5.56	118.16	112.60
1	C	105	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	A	57	HIS	CA-C-O	-5.55	114.66	120.55
1	B	28[A]	THR	CA-C-O	5.53	126.18	119.38
1	B	28[B]	THR	CA-C-O	5.53	126.18	119.38
1	B	56	ALA	N-CA-C	-5.53	105.16	111.07
1	E	28[A]	THR	O-C-N	-5.52	115.48	122.27
1	E	28[B]	THR	O-C-N	-5.52	115.48	122.27
1	C	21	GLU	N-CA-C	-5.51	106.05	112.89
1	E	36	ARG	CA-CB-CG	-5.51	103.09	114.10
1	F	31	LEU	CA-C-O	-5.50	115.05	120.82
1	F	11	LEU	CA-C-O	-5.49	114.60	120.42
1	C	102	ALA	CA-C-O	-5.48	113.66	119.97
1	E	29	PHE	CA-CB-CG	-5.48	108.32	113.80
1	A	67	GLY	O-C-N	5.48	129.03	122.34
1	C	13	SER	CA-C-O	5.46	126.55	120.82
1	D	97[A]	MET	CA-C-O	-5.45	115.07	121.07
1	D	97[B]	MET	CA-C-O	-5.45	115.07	121.07
1	F	42	ALA	N-CA-C	-5.44	105.43	111.36
1	D	103	ILE	N-CA-C	-5.44	105.03	110.30
1	E	83	ARG	O-C-N	5.43	127.87	122.12
1	A	26	LEU	CA-C-N	5.41	127.47	120.44
1	A	26	LEU	C-N-CA	5.41	127.47	120.44
1	A	3	ALA	CA-C-O	-5.40	115.08	120.64
1	D	88	GLN	CA-C-O	-5.39	114.01	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	GLY	O-C-N	-5.37	117.03	122.19
1	A	60	LYS	CA-C-O	-5.37	115.18	120.82
1	E	59	PHE	CA-C-N	5.37	127.42	120.44
1	E	59	PHE	C-N-CA	5.37	127.42	120.44
1	E	98	GLU	CB-CG-CD	5.36	121.71	112.60
1	A	34	GLU	CA-C-O	-5.35	114.84	120.46
1	B	83	ARG	CA-C-O	-5.35	114.88	120.55
1	C	36	ARG	N-CA-C	-5.33	105.40	111.10
1	B	26	LEU	N-CA-C	-5.32	105.38	111.07
1	C	15	GLN	O-C-N	5.32	128.22	122.15
1	E	59	PHE	O-C-N	-5.30	115.34	122.23
1	E	5	HIS	CA-CB-CG	-5.29	108.51	113.80
1	F	46	ALA	CA-C-N	5.27	130.63	120.66
1	F	46	ALA	C-N-CA	5.27	130.63	120.66
1	C	10	VAL	N-CA-C	-5.26	105.37	110.42
1	F	10	VAL	N-CA-C	-5.26	105.34	110.39
1	C	59	PHE	O-C-N	-5.25	116.56	122.12
1	B	51	ALA	N-CA-C	-5.25	105.64	111.36
1	D	67	GLY	O-C-N	5.24	128.74	122.34
1	C	56	ALA	N-CA-CB	5.24	117.60	110.01
1	F	64	SER	N-CA-C	-5.23	105.58	111.28
1	C	60	LYS	CA-C-O	-5.23	115.33	120.82
1	E	81	SER	O-C-N	-5.19	116.49	122.09
1	B	42	ALA	N-CA-C	-5.18	105.63	111.28
1	B	46	ALA	CA-C-N	5.17	130.12	120.87
1	B	46	ALA	C-N-CA	5.17	130.12	120.87
1	B	75	CYS	O-C-N	5.15	127.58	122.12
1	C	58	SER	N-CA-CB	5.14	117.47	110.01
1	A	10	VAL	N-CA-C	-5.14	105.20	110.59
1	C	43	ALA	N-CA-C	-5.14	105.68	111.28
1	F	50[A]	GLN	CA-C-O	5.14	125.68	119.31
1	F	50[B]	GLN	CA-C-O	5.14	125.68	119.31
1	E	43	ALA	N-CA-C	-5.13	105.69	111.28
1	D	60	LYS	CA-C-O	-5.12	115.12	120.55
1	E	72	ALA	CA-C-N	5.12	125.77	120.03
1	E	72	ALA	C-N-CA	5.12	125.77	120.03
1	D	59	PHE	CA-C-N	5.11	127.13	120.28
1	D	59	PHE	C-N-CA	5.11	127.13	120.28
1	F	68	ALA	CA-C-O	-5.11	116.50	122.37
1	C	59	PHE	CA-CB-CG	5.09	118.89	113.80
1	F	50[A]	GLN	O-C-N	-5.08	115.44	122.46
1	F	50[B]	GLN	O-C-N	-5.08	115.44	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	13	SER	CA-C-O	5.06	125.92	120.55
1	A	42	ALA	N-CA-C	-5.06	105.84	111.36
1	B	113	GLN	CA-C-O	-5.06	113.36	119.49
1	B	79	GLU	N-CA-C	-5.05	105.67	111.07
1	C	21	GLU	CA-C-O	-5.05	113.42	119.32
1	F	51	ALA	N-CA-C	-5.04	106.03	111.53
1	E	57	HIS	ND1-CE1-NE2	5.04	113.44	108.40
1	A	97[A]	MET	O-C-N	-5.03	115.52	122.46
1	A	97[B]	MET	O-C-N	-5.03	115.52	122.46
1	C	43	ALA	O-C-N	-5.03	116.79	122.12
1	B	27	ASP	N-CA-C	-5.02	105.70	111.17
1	E	49	ALA	CA-C-O	-5.02	115.39	120.56
1	E	21	GLU	N-CA-C	-5.01	107.12	113.18
1	A	96	GLN	N-CA-C	-5.00	105.82	111.17
1	A	60	LYS	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	GLY	Mainchain
1	B	113	GLN	Sidechain
1	B	73	GLY	Mainchain
1	C	82	ALA	Mainchain
1	D	113	GLN	Sidechain
1	E	20	ASP	Mainchain
1	E	52	LEU	Mainchain
1	F	103	ILE	Mainchain
1	F	7	ASP	Mainchain

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	1090	0	1056	24	0
1	B	1070	0	1037	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1017	0	987	18	0
1	D	1084	0	1064	27	0
1	E	1052	0	1016	28	0
1	F	1062	0	1036	40	0
2	A	209	0	0	12	0
2	B	189	0	0	10	0
2	C	200	0	0	8	0
2	D	215	0	0	12	0
2	E	215	0	0	15	0
2	F	201	0	0	15	0
All	All	7604	0	6196	154	0

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

All (154) 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:53[B]:ARG:HH21	1:F:83[B]:ARG:NH2	1.25	1.31
1:F:53[B]:ARG:NH2	1:F:83[B]:ARG:NH2	1.80	1.29
1:D:95[B]:GLU:HG2	2:E:211:HOH:O	1.36	1.24
1:B:84[B]:ARG:O	1:B:86[B]:GLU:OE2	1.60	1.19
1:E:2:SER:HA	2:E:204:HOH:O	1.57	1.04
1:B:86[B]:GLU:OE2	1:B:86[B]:GLU:N	1.92	1.03
1:E:99[B]:ARG:N	1:E:99[B]:ARG:HD2	1.75	1.00
1:F:116:ARG:HA	2:F:213:HOH:O	1.62	0.99
1:F:53[B]:ARG:NH2	1:F:83[B]:ARG:HH21	1.49	0.96
1:F:9[B]:ARG:CZ	2:F:204:HOH:O	2.16	0.92
1:D:9[A]:ARG:NE	2:D:201:HOH:O	2.07	0.88
1:C:45[A]:GLN:HG2	2:C:217:HOH:O	1.71	0.88
1:B:36[B]:ARG:CG	1:B:36[B]:ARG:HH11	1.90	0.84
1:F:116:ARG:CA	2:F:213:HOH:O	2.22	0.81
1:F:53[B]:ARG:NH2	1:F:83[B]:ARG:HH22	1.77	0.81
1:D:9[A]:ARG:CG	2:D:201:HOH:O	2.27	0.81
1:A:95[A]:GLU:OE2	1:A:99[A]:ARG:NE	2.14	0.80
1:E:80[B]:GLU:HG2	2:E:335:HOH:O	1.80	0.79
1:C:99[B]:ARG:HD2	2:C:335:HOH:O	1.83	0.78
1:B:28[A]:THR:HG22	2:B:341:HOH:O	1.85	0.77
1:F:9[B]:ARG:NH2	2:F:204:HOH:O	2.17	0.77
1:F:99[B]:ARG:HD3	2:F:295:HOH:O	1.85	0.76
1:C:15:GLN:HG2	2:C:303:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54[B]:HIS:ND1	2:E:201:HOH:O	2.20	0.74
1:B:36[B]:ARG:NH1	2:B:201:HOH:O	1.88	0.74
1:A:7:ASP:OD1	1:A:9[B]:ARG:HG2	1.88	0.73
1:D:9[A]:ARG:CD	2:D:201:HOH:O	2.35	0.73
1:F:88[B]:GLN:NE2	2:F:201:HOH:O	1.94	0.73
1:B:36[B]:ARG:HH11	1:B:36[B]:ARG:HG3	1.52	0.73
1:A:106:ILE:CD1	1:C:47:GLY:HA2	2.20	0.70
1:F:53[B]:ARG:HE	1:F:54[B]:HIS:CE1	2.09	0.69
1:D:116[B]:ARG:NE	2:D:203:HOH:O	2.22	0.69
1:A:50[B]:GLN:OE1	2:A:201:HOH:O	2.10	0.69
1:E:54[B]:HIS:HD2	2:E:352:HOH:O	1.78	0.67
1:B:99[B]:ARG:HD3	2:B:291:HOH:O	1.94	0.67
1:D:47:GLY:HA2	1:E:106:ILE:CD1	2.25	0.66
1:E:99[A]:ARG:HD3	2:E:350:HOH:O	1.95	0.66
1:D:9[A]:ARG:HG2	2:D:201:HOH:O	1.91	0.65
1:F:75:CYS:HA	1:F:97[B]:MET:HE2	1.78	0.65
1:E:47:GLY:HA2	1:F:106:ILE:CD1	2.27	0.65
1:D:47:GLY:HA2	1:E:106:ILE:HD11	1.79	0.65
1:D:9[A]:ARG:NH1	2:D:204:HOH:O	2.29	0.64
1:A:50[B]:GLN:HG3	2:A:259:HOH:O	1.96	0.64
1:E:47:GLY:HA2	1:F:106:ILE:HD11	1.80	0.64
1:A:99[B]:ARG:HD3	2:A:310:HOH:O	1.99	0.62
1:E:99[B]:ARG:HD2	1:E:99[B]:ARG:H	1.60	0.62
1:D:75:CYS:HA	1:D:97[B]:MET:HE3	1.81	0.61
1:A:47:GLY:HA2	1:B:106:ILE:CD1	2.31	0.60
1:B:50:GLN:OE1	2:B:202:HOH:O	2.16	0.60
1:D:106:ILE:CD1	1:F:47:GLY:HA2	2.31	0.60
1:F:111:GLU:OE2	2:F:203:HOH:O	2.16	0.60
1:A:106:ILE:HD11	1:C:47:GLY:HA2	1.84	0.59
1:C:40:LEU:CD1	1:C:97:MET:HE1	2.32	0.59
1:E:54[B]:HIS:CD2	2:E:352:HOH:O	2.53	0.59
1:D:20[B]:ASP:CG	2:D:210:HOH:O	2.45	0.59
1:B:84[A]:ARG:NH1	1:B:86[A]:GLU:CD	2.61	0.58
1:B:36[B]:ARG:HH11	1:B:36[B]:ARG:HG2	1.68	0.58
1:D:99[A]:ARG:HH12	1:E:99[A]:ARG:NH1	2.02	0.58
1:D:106:ILE:HD11	1:F:47:GLY:HA2	1.86	0.57
1:C:50:GLN:NE2	2:C:204:HOH:O	2.36	0.57
1:A:2:SER:OG	1:A:8[A]:ASP:OD1	2.20	0.57
1:B:84[A]:ARG:HH11	1:B:86[A]:GLU:CD	2.14	0.56
1:F:53[B]:ARG:HH22	1:F:83[B]:ARG:NH2	1.93	0.56
1:A:99[B]:ARG:HD2	2:A:213:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84[A]:ARG:NH1	1:B:86[A]:GLU:OE1	2.39	0.55
1:B:93:LEU:O	1:B:97[B]:MET:HE3	2.06	0.55
1:E:99[A]:ARG:HD2	2:E:301:HOH:O	2.04	0.55
1:C:7:ASP:OD1	1:C:9:ARG:HB2	2.07	0.55
1:E:99[A]:ARG:CD	2:E:350:HOH:O	2.53	0.55
1:B:84[B]:ARG:HH21	1:B:84[B]:ARG:HG2	1.72	0.55
1:A:47:GLY:HA2	1:B:106:ILE:HD11	1.89	0.54
1:E:15[B]:GLN:HG3	2:E:326:HOH:O	2.07	0.54
1:E:89:ARG:HD3	2:E:209:HOH:O	2.07	0.54
1:B:88[A]:GLN:HG3	1:C:107:LEU:HD21	1.90	0.54
1:D:9[B]:ARG:HD3	2:D:227:HOH:O	2.07	0.54
1:B:36[B]:ARG:CG	1:B:36[B]:ARG:NH1	2.58	0.53
1:D:54[A]:HIS:CD2	2:D:206:HOH:O	2.61	0.53
1:C:40:LEU:HD13	1:C:97:MET:HE1	1.91	0.53
1:E:54[A]:HIS:CE1	2:E:221:HOH:O	2.61	0.53
1:B:15[B]:GLN:NE2	2:B:205:HOH:O	2.34	0.52
1:A:18[B]:MET:HE2	1:A:25:LEU:HD11	1.91	0.52
1:A:9[A]:ARG:HG3	1:A:9[A]:ARG:O	2.09	0.52
1:F:50[B]:GLN:NE2	2:F:205:HOH:O	2.28	0.52
1:F:53[B]:ARG:NE	1:F:54[B]:HIS:CE1	2.78	0.51
1:E:36:ARG:NH2	1:E:58[A]:SER:OG	2.45	0.50
1:F:50[B]:GLN:CD	1:F:54[B]:HIS:HD2	2.20	0.49
1:B:99[A]:ARG:HD3	2:B:292:HOH:O	2.11	0.49
1:C:15:GLN:NE2	1:C:115:TYR:OH	2.40	0.49
1:B:84[B]:ARG:C	1:B:86[B]:GLU:OE2	2.50	0.49
1:F:116:ARG:N	2:F:213:HOH:O	2.42	0.49
1:B:89:ARG:HD3	2:B:217:HOH:O	2.14	0.48
1:E:53[B]:ARG:CZ	2:E:217:HOH:O	2.61	0.48
1:B:36[B]:ARG:NH1	1:B:36[B]:ARG:HG3	2.25	0.48
1:A:15[B]:GLN:NE2	2:A:209:HOH:O	2.45	0.48
1:E:11:LEU:O	1:E:15[B]:GLN:HG2	2.13	0.48
1:D:2:SER:OG	2:D:202:HOH:O	2.13	0.48
1:A:95[B]:GLU:HG2	2:A:254:HOH:O	2.14	0.47
1:C:95[B]:GLU:HG2	2:C:228:HOH:O	2.13	0.47
1:E:87:LEU:HD12	1:F:110[A]:GLN:CG	2.45	0.47
1:F:89:ARG:HD3	2:F:253:HOH:O	2.13	0.47
1:B:47:GLY:HA2	1:C:106:ILE:CD1	2.45	0.47
1:B:84[B]:ARG:HG2	1:B:84[B]:ARG:NH2	2.28	0.47
1:F:112:ARG:HH22	1:F:116:ARG:HG2	1.79	0.47
1:F:9[B]:ARG:NE	1:F:9[B]:ARG:HA	2.29	0.46
1:D:99[A]:ARG:HH12	1:E:99[A]:ARG:HH12	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114[B]:ARG:NH1	2:F:216:HOH:O	2.48	0.46
1:C:99[B]:ARG:NE	2:C:201:HOH:O	1.99	0.46
1:E:54[B]:HIS:CE1	2:E:201:HOH:O	2.68	0.46
1:A:18[B]:MET:HE3	1:A:21:GLU:HB3	1.98	0.46
1:D:75:CYS:SG	1:D:97[B]:MET:CE	3.04	0.46
1:C:7:ASP:OD2	1:C:9:ARG:HD3	2.16	0.45
1:D:15:GLN:NE2	1:D:115:TYR:OH	2.49	0.45
1:A:8[B]:ASP:O	1:A:8[B]:ASP:CG	2.57	0.45
1:E:40:LEU:CD1	1:E:97:MET:HE1	2.46	0.45
1:A:83[B]:ARG:NH2	2:A:206:HOH:O	2.38	0.45
1:A:99[B]:ARG:NE	2:A:213:HOH:O	2.49	0.45
1:B:50:GLN:NE2	2:B:202:HOH:O	2.49	0.45
1:F:53[B]:ARG:HH22	1:F:83[B]:ARG:HH22	1.60	0.45
1:F:116:ARG:HA	1:F:116:ARG:HD2	1.65	0.45
1:C:45[A]:GLN:CG	2:C:217:HOH:O	2.46	0.45
1:A:99[B]:ARG:CD	2:A:213:HOH:O	2.64	0.44
1:B:15[B]:GLN:CD	1:B:15[B]:GLN:O	2.60	0.44
1:E:99[A]:ARG:NH1	2:E:211:HOH:O	2.50	0.44
1:B:2:SER:HA	2:B:242:HOH:O	2.17	0.44
1:F:7:ASP:OD1	1:F:7:ASP:C	2.60	0.44
1:F:15:GLN:CD	1:F:15:GLN:C	2.86	0.44
1:B:53[B]:ARG:O	1:B:54[B]:HIS:C	2.60	0.44
1:D:99[A]:ARG:HD3	2:D:388:HOH:O	2.18	0.44
1:F:53[A]:ARG:O	1:F:54[A]:HIS:C	2.57	0.44
1:A:50[B]:GLN:NE2	2:A:216:HOH:O	2.51	0.43
1:D:2:SER:HB3	2:F:201:HOH:O	2.18	0.43
1:F:112:ARG:HH12	1:F:116:ARG:HD3	1.83	0.43
1:A:28[A]:THR:HG23	2:A:351:HOH:O	2.18	0.43
1:C:45[B]:GLN:HG2	2:C:305:HOH:O	2.19	0.43
1:F:75:CYS:HA	1:F:97[B]:MET:CE	2.46	0.43
1:F:110[A]:GLN:NE2	2:F:210:HOH:O	2.30	0.43
1:F:116:ARG:HB3	2:F:357:HOH:O	2.18	0.43
1:B:15[B]:GLN:CD	1:B:15[B]:GLN:C	2.87	0.42
1:D:53[A]:ARG:HE	1:D:53[A]:ARG:HB3	1.63	0.42
1:F:9[B]:ARG:NE	1:F:9[B]:ARG:CA	2.81	0.42
1:D:53[A]:ARG:O	1:D:54[A]:HIS:C	2.63	0.42
1:B:49:ALA:HB2	1:B:87:LEU:HD11	2.01	0.41
1:D:7:ASP:OD1	1:D:7:ASP:C	2.62	0.41
1:F:114[B]:ARG:CZ	2:F:216:HOH:O	2.68	0.41
1:B:109:LYS:NZ	2:B:215:HOH:O	2.49	0.41
1:D:75:CYS:SG	1:D:97[B]:MET:HE2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53[B]:ARG:HH21	1:F:83[B]:ARG:HH21	1.16	0.41
1:F:115:TYR:O	1:F:116:ARG:HB2	2.20	0.41
1:B:47:GLY:HA2	1:C:106:ILE:HD11	2.01	0.41
1:E:53[B]:ARG:HE	1:E:54[B]:HIS:CE1	2.39	0.41
1:E:88[A]:GLN:H	1:E:88[A]:GLN:CD	2.28	0.41
1:A:99[A]:ARG:HD2	2:A:327:HOH:O	2.20	0.40
1:D:95[A]:GLU:HG2	2:D:236:HOH:O	2.21	0.40
1:A:50[A]:GLN:NE2	1:A:53:ARG:HE	2.19	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	133/116 (115%)	130 (98%)	3 (2%)	0	100	100
1	B	131/116 (113%)	121 (92%)	9 (7%)	1 (1%)	16	4
1	C	124/116 (107%)	120 (97%)	4 (3%)	0	100	100
1	D	132/116 (114%)	132 (100%)	0	0	100	100
1	E	128/116 (110%)	126 (98%)	2 (2%)	0	100	100
1	F	129/116 (111%)	127 (98%)	2 (2%)	0	100	100
All	All	777/696 (112%)	756 (97%)	20 (3%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	GLY

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	115/96 (120%)	111 (96%)	4 (4%)	32	6
1	B	113/96 (118%)	107 (95%)	6 (5%)	20	2
1	C	106/96 (110%)	104 (98%)	2 (2%)	50	21
1	D	114/96 (119%)	114 (100%)	0	100	100
1	E	110/96 (115%)	108 (98%)	2 (2%)	51	23
1	F	111/96 (116%)	110 (99%)	1 (1%)	70	52
All	All	669/576 (116%)	654 (98%)	15 (2%)	59	15

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9[A]	ARG
1	A	9[B]	ARG
1	A	35[A]	GLU
1	A	35[B]	GLU
1	B	15[A]	GLN
1	B	15[B]	GLN
1	B	54[A]	HIS
1	B	54[B]	HIS
1	B	88[A]	GLN
1	B	88[B]	GLN
1	C	83[A]	ARG
1	C	83[B]	ARG
1	E	15[A]	GLN
1	E	15[B]	GLN
1	F	116	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	15	GLN
1	E	45	GLN

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	115/116 (99%)	0.52	5 (4%)	40 52	6, 19, 35, 50	20 (17%)
1	B	115/116 (99%)	0.91	15 (13%)	7 12	7, 21, 40, 51	18 (15%)
1	C	115/116 (99%)	0.66	9 (7%)	19 28	9, 20, 43, 51	11 (9%)
1	D	115/116 (99%)	0.23	4 (3%)	47 59	7, 17, 32, 51	20 (17%)
1	E	115/116 (99%)	0.46	5 (4%)	40 52	8, 19, 32, 51	15 (13%)
1	F	115/116 (99%)	0.49	8 (6%)	22 32	7, 18, 35, 61	16 (13%)
All	All	690/696 (99%)	0.54	46 (6%)	24 33	6, 19, 36, 61	100 (14%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9[A]	ARG	5.8
1	B	54[A]	HIS	5.5
1	B	82	ALA	4.2
1	F	116	ARG	4.0
1	F	114[A]	ARG	3.7
1	E	9[A]	ARG	3.6
1	F	54[A]	HIS	3.3
1	D	116[A]	ARG	3.2
1	D	54[A]	HIS	3.0
1	C	3	ALA	2.9
1	F	9[A]	ARG	2.9
1	F	2	SER	2.9
1	B	84[A]	ARG	2.9
1	F	115	TYR	2.9
1	B	2	SER	2.8
1	C	8	ASP	2.8
1	B	81[A]	SER	2.8
1	E	15[A]	GLN	2.7
1	E	46	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	53[A]	ARG	2.5
1	A	20[A]	ASP	2.5
1	A	21	GLU	2.4
1	C	17	VAL	2.4
1	B	3	ALA	2.4
1	D	9[A]	ARG	2.4
1	B	79	GLU	2.4
1	B	85	GLY	2.3
1	C	53	ARG	2.3
1	A	2	SER	2.3
1	A	15[A]	GLN	2.3
1	C	54[A]	HIS	2.3
1	B	56	ALA	2.2
1	F	8	ASP	2.2
1	B	69[A]	VAL	2.2
1	E	2	SER	2.2
1	C	46	ALA	2.2
1	B	83	ARG	2.2
1	B	49	ALA	2.2
1	C	9	ARG	2.1
1	D	99[A]	ARG	2.1
1	C	116	ARG	2.1
1	B	50	GLN	2.1
1	E	3	ALA	2.1
1	C	50	GLN	2.0
1	B	57	HIS	2.0
1	F	15	GLN	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.