Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2020 – 02:11 PM JST

PDB ID	:	7C1I
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 following versions of software and data (see references ⓘ) were used in the production of this report:

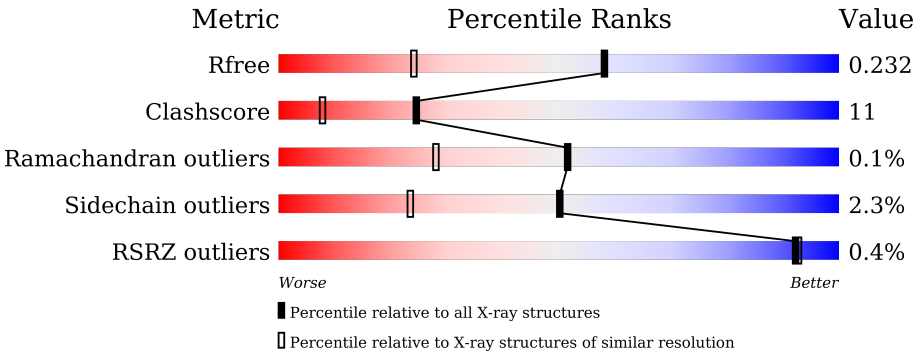
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 on 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 <=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	77% 19%
1	B	116	73% 22%
1	C	116	79% 18%
1	D	116	82% 14%
1	E	116	77% 20%
1	F	116	79% 16%

2 Entry composition (i)

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.

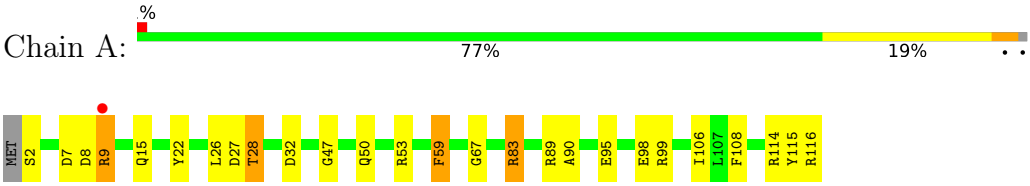
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	209	Total	O	0	0
			209	209		
2	B	189	Total	O	0	0
			189	189		
2	C	200	Total	O	0	0
			200	200		
2	D	215	Total	O	0	0
			215	215		
2	E	215	Total	O	0	0
			215	215		
2	F	201	Total	O	0	0
			201	201		

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.

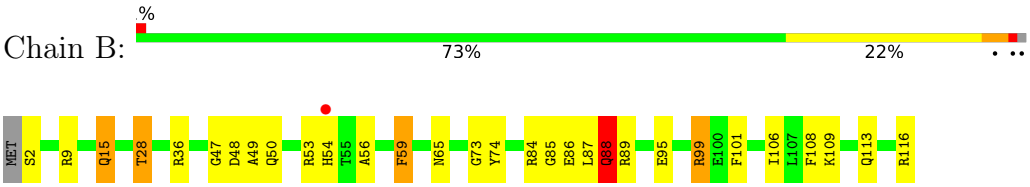
- Molecule 1: Histidine kinase

Chain A:



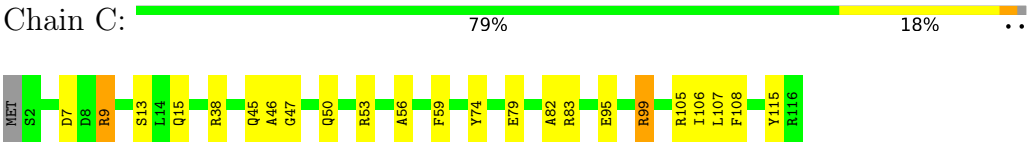
- Molecule 1: Histidine kinase

Chain B:



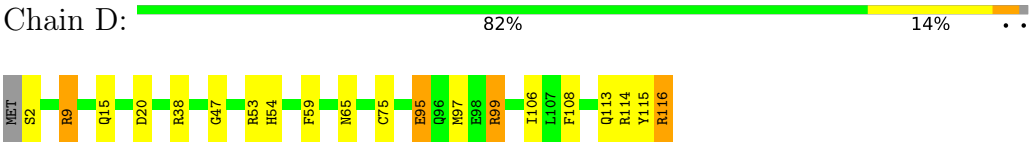
- Molecule 1: Histidine kinase

Chain C:



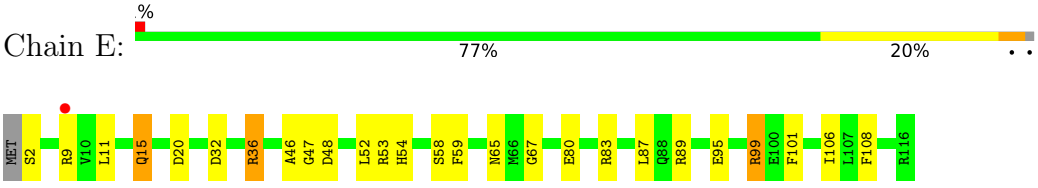
- Molecule 1: Histidine kinase

Chain D:



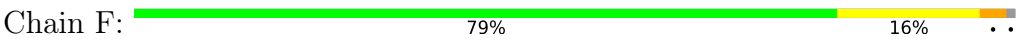
- Molecule 1: Histidine kinase

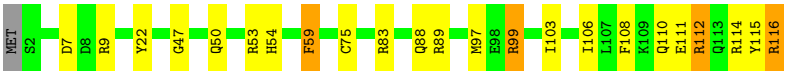
Chain E:



- Molecule 1: Histidine kinase

Chain F:




MET
S2
D7
D8
R9
Y22
G47
Q50
R53
H54
F59
C75
R83
Q88
R89
M97
E98
R99
I103
I106
L107
F108
K109
Q110
E111
R112
Q113
R114
Y115
R116

4 Data and refinement statistics (i)

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 29.36 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.37-1.58) 98.4 (29.36-1.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.193 , 0.225 0.202 , 0.232	Depositor DCC
R_{free} test set	8321 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.64	0/1103	1.68	21/1476 (1.4%)
1	B	0.65	0/1084	1.84	27/1453 (1.9%)
1	C	0.64	0/1031	1.75	16/1382 (1.2%)
1	D	0.64	0/1100	1.63	14/1472 (1.0%)
1	E	0.64	0/1066	1.77	19/1428 (1.3%)
1	F	0.64	0/1076	1.67	9/1442 (0.6%)
All	All	0.64	0/6460	1.72	106/8653 (1.2%)

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 (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	99[A]	ARG	NE-CZ-NH1	-15.58	112.51	120.30
1	E	99[B]	ARG	NE-CZ-NH1	-15.58	112.51	120.30
1	B	99[A]	ARG	NE-CZ-NH2	13.87	127.23	120.30
1	B	99[B]	ARG	NE-CZ-NH2	13.87	127.23	120.30
1	F	99[A]	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	F	99[B]	ARG	NE-CZ-NH1	12.59	126.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	TYR	CB-CG-CD2	11.69	128.01	121.00
1	A	115	TYR	CB-CG-CD1	-10.46	114.73	121.00
1	C	108	PHE	CB-CG-CD1	10.44	128.11	120.80
1	E	32	ASP	CB-CG-OD2	-9.25	109.97	118.30
1	C	99[A]	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	C	99[B]	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	E	108	PHE	CB-CG-CD1	9.12	127.18	120.80
1	A	32	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	F	99[A]	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	F	99[B]	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	108	PHE	CB-CG-CD2	-8.85	114.61	120.80
1	C	105	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	C	108	PHE	CB-CG-CD2	-8.30	114.99	120.80
1	A	116	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	108	PHE	CB-CG-CD2	-7.95	115.23	120.80
1	B	9	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	E	83	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	F	108	PHE	CB-CG-CD2	-7.51	115.54	120.80
1	E	108	PHE	CB-CG-CD2	-7.48	115.56	120.80
1	F	59	PHE	CB-CG-CD2	-7.47	115.57	120.80
1	F	108	PHE	CB-CG-CD1	7.46	126.02	120.80
1	D	65	ASN	OD1-CG-ND2	7.40	138.92	121.90
1	B	99[A]	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	B	99[B]	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	C	9	ARG	CG-CD-NE	7.08	126.67	111.80
1	B	116	ARG	CA-C-O	-7.05	105.30	120.10
1	B	101	PHE	CB-CG-CD2	6.95	125.67	120.80
1	E	95[A]	GLU	O-C-N	-6.87	111.71	122.70
1	E	95[B]	GLU	O-C-N	-6.87	111.71	122.70
1	B	101	PHE	CG-CD2-CE2	6.75	128.22	120.80
1	B	56	ALA	N-CA-CB	6.74	119.53	110.10
1	A	108	PHE	CB-CG-CD1	6.56	125.39	120.80
1	D	116[A]	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	D	116[B]	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	A	114	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	C	74	TYR	CB-CG-CD1	6.43	124.86	121.00
1	A	83[A]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	83[B]	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	28[A]	THR	O-C-N	-6.39	112.47	122.70
1	B	28[B]	THR	O-C-N	-6.39	112.47	122.70
1	F	22	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	B	53[A]	ARG	NE-CZ-NH1	-6.33	117.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53[B]	ARG	NE-CZ-NH1	-6.33	117.13	120.30
1	B	48	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	D	95[A]	GLU	O-C-N	-6.24	112.72	122.70
1	D	95[B]	GLU	O-C-N	-6.24	112.72	122.70
1	B	108	PHE	CB-CG-CD1	6.21	125.15	120.80
1	C	79	GLU	OE1-CD-OE2	6.20	130.74	123.30
1	D	99[A]	ARG	CG-CD-NE	-6.18	98.82	111.80
1	D	99[B]	ARG	CG-CD-NE	-6.18	98.82	111.80
1	E	48	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	E	36	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	101	PHE	CD1-CE1-CZ	5.94	127.23	120.10
1	A	28[A]	THR	O-C-N	-5.93	113.21	122.70
1	A	28[B]	THR	O-C-N	-5.93	113.21	122.70
1	E	99[A]	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	E	99[B]	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	A	26	LEU	CB-CG-CD2	5.90	121.03	111.00
1	A	59	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	C	38	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	38	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	48	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	89	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	D	114[A]	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	D	114[B]	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	48	ASP	OD1-CG-OD2	5.73	134.18	123.30
1	B	88[A]	GLN	CB-CA-C	-5.71	98.98	110.40
1	B	88[B]	GLN	CB-CA-C	-5.71	98.98	110.40
1	B	74	TYR	CB-CG-CD1	5.70	124.42	121.00
1	C	99[A]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	99[B]	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	89	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	F	112	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	95[A]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	E	95[B]	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	A	22	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	C	46	ALA	O-C-N	-5.48	113.88	123.20
1	C	53	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	98	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	D	108	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	E	67	GLY	O-C-N	5.39	131.33	122.70
1	E	101	PHE	CZ-CE2-CD2	-5.36	113.67	120.10
1	C	56	ALA	N-CA-CB	5.36	117.60	110.10
1	A	90	ALA	N-CA-CB	5.33	117.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	E	46	ALA	O-C-N	-5.26	114.25	123.20
1	C	46	ALA	C-N-CA	5.25	133.32	122.30
1	B	95[A]	GLU	CB-CA-C	5.24	120.87	110.40
1	B	95[B]	GLU	CB-CA-C	5.24	120.87	110.40
1	B	9	ARG	CB-CG-CD	5.23	125.21	111.60
1	E	65	ASN	CB-CG-ND2	-5.23	104.14	116.70
1	B	59	PHE	CB-CG-CD2	-5.21	117.16	120.80
1	D	9[A]	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	9[B]	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	D	59	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	A	83[A]	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	A	83[B]	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	65	ASN	CA-CB-CG	5.06	124.53	113.40
1	C	13	SER	N-CA-CB	-5.03	102.96	110.50
1	E	46	ALA	CA-C-N	5.03	126.25	116.20

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1090	0	1056	22	0
1	B	1070	0	1037	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1017	0	987	16	0
1	D	1084	0	1064	25	0
1	E	1052	0	1016	26	0
1	F	1062	0	1036	37	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	139	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 11.

All (139) 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:HD2	1:E:99[B]:ARG:N	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:HH11	1:B:36[B]:ARG:CG	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: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: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:E:54[B]:HIS:CD2	2:E:352:HOH:O	2.53	0.59
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:D:75:CYS:HA	1:D:97[B]:MET:HE3	1.87	0.57
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
1:B:84[A]:ARG:NH1	1:B:86[A]:GLU:OE1	2.39	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:HG2	1:B:84[B]:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA2	1:B:106:ILE:HD11	1.89	0.54
1:D:20[B]:ASP:CG	2:D:210:HOH:O	2.45	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:84[A]:ARG:NH1	1:B:86[A]:GLU:CD	2.61	0.54
1:B:36[B]:ARG:NH1	1:B:36[B]:ARG:CG	2.58	0.53
1:D:54[A]:HIS:CD2	2:D:206:HOH:O	2.61	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: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:B:84[A]:ARG:HH11	1:B:86[A]:GLU:CD	2.14	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: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: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:84[B]:ARG:NH2	1:B:84[B]:ARG:HG2	2.28	0.47
1:B:47:GLY:HA2	1:C:106:ILE:CD1	2.45	0.47
1:F:112:ARG:HH22	1:F:116:ARG:HG2	1.79	0.47
1:F:9[B]:ARG:HA	1:F:9[B]:ARG:NE	2.29	0.46
1:D:99[A]:ARG:HH12	1:E:99[A]:ARG:HH12	1.62	0.46
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:B:109:LYS:NZ	2:B:215:HOH:O	2.49	0.46
1:F:75:CYS:HA	1:F:97[B]:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLN:NE2	1:D:115:TYR:OH	2.49	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:116:ARG:HA	1:F:116:ARG:HD2	1.65	0.45
1:F:53[B]:ARG:HH22	1:F:83[B]:ARG:HH22	1.60	0.45
1:F:50[B]:GLN:CD	1:F:54[B]:HIS:HD2	2.20	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: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:D:99[A]:ARG:HD3	2:D:388:HOH:O	2.18	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: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:84[B]:ARG:C	1:B:86[B]:GLU:OE2	2.50	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:F:53[A]:ARG:O	1:F:54[A]:HIS:C	2.57	0.42
1:A:8[B]:ASP:CG	1:A:8[B]:ASP:O	2.57	0.42
1:B:49:ALA:HB2	1:B:87:LEU:HD11	2.01	0.41
1:F:114[B]:ARG:CZ	2:F:216:HOH:O	2.68	0.41
1:F:115:TYR:O	1:F:116:ARG:HB2	2.20	0.41
1:F:53[B]:ARG:HH21	1:F:83[B]:ARG:HH21	1.16	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:A:99[A]:ARG:HD2	2:A:327:HOH:O	2.20	0.40
1:D:75:CYS:SG	1:D:97[B]:MET:HE3	2.61	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%)	19 5
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%)	51 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	GLY

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	115/96 (120%)	112 (97%)	3 (3%)	46 19
1	B	113/96 (118%)	106 (94%)	7 (6%)	18 3
1	C	106/96 (110%)	103 (97%)	3 (3%)	43 17
1	D	114/96 (119%)	114 (100%)	0	100 100
1	E	110/96 (115%)	105 (96%)	5 (4%)	27 6
1	F	111/96 (116%)	109 (98%)	2 (2%)	59 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	669/576 (116%)	649 (97%)	20 (3%)	50 15

All (20) 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	59	PHE
1	B	15[A]	GLN
1	B	15[B]	GLN
1	B	54[A]	HIS
1	B	54[B]	HIS
1	B	59	PHE
1	B	88[A]	GLN
1	B	88[B]	GLN
1	C	59	PHE
1	C	83[A]	ARG
1	C	83[B]	ARG
1	E	9[A]	ARG
1	E	9[B]	ARG
1	E	15[A]	GLN
1	E	15[B]	GLN
1	E	59	PHE
1	F	59	PHE
1	F	116	ARG

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

Mol	Chain	Res	Type
1	C	15	GLN
1	D	15	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 monosaccharides 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, 95^{th} 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%)	-0.17	1 (0%) 84 85	13, 20, 37, 50	0
1	B	115/116 (99%)	-0.01	1 (0%) 84 85	14, 23, 42, 51	0
1	C	115/116 (99%)	-0.14	0 100 100	14, 22, 43, 51	0
1	D	115/116 (99%)	-0.32	0 100 100	13, 19, 32, 51	0
1	E	115/116 (99%)	-0.20	1 (0%) 84 85	13, 20, 33, 51	0
1	F	115/116 (99%)	-0.20	0 100 100	13, 20, 35, 61	0
All	All	690/696 (99%)	-0.17	3 (0%) 92 93	13, 21, 38, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54[A]	HIS	2.7
1	A	9[A]	ARG	2.4
1	E	9[A]	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.