Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 08:44 PM EST

PDB ID	:	2HWJ
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:

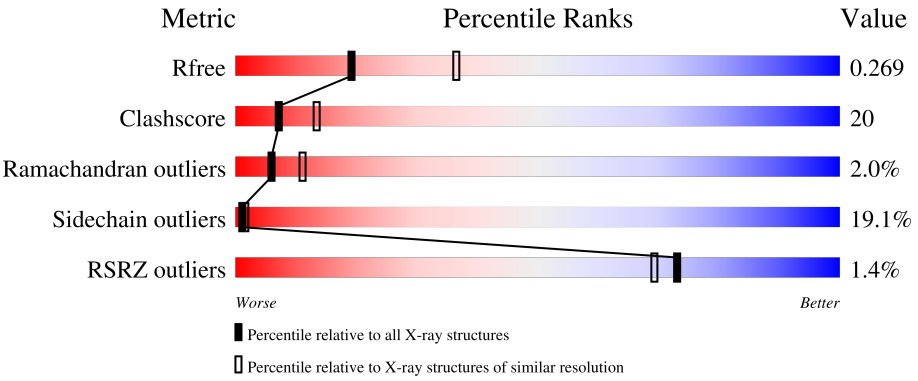
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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}	164625	4623 (2.64-2.60)
Clashscore	180529	5071 (2.64-2.60)
Ramachandran outliers	177936	5006 (2.64-2.60)
Sidechain outliers	177891	5006 (2.64-2.60)
RSRZ outliers	164620	4622 (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 <=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	59% 30% 6%
1	B	205	% 47% 35% 9% 8%
1	C	205	2% 52% 33% 8% 5%
1	D	205	2% 47% 33% 14% 6%
1	E	205	48% 33% 9% 8%

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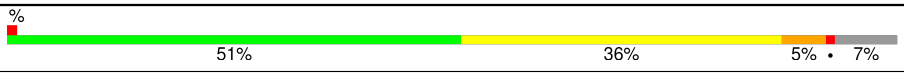
Mol	Chain	Length	Quality of chain
1	F	205	

2 Entry composition (i)

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.

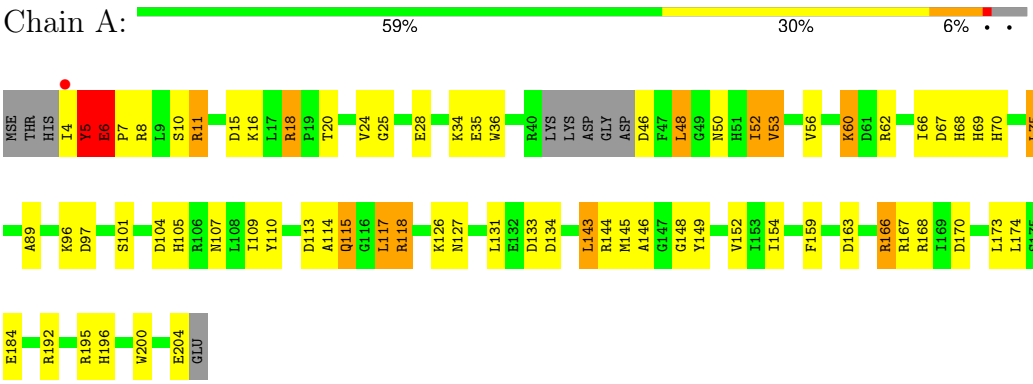
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	18	Total O 18 18	0	0
2	C	22	Total O 22 22	0	0
2	D	15	Total O 15 15	0	0
2	E	13	Total O 13 13	0	0
2	F	10	Total O 10 10	0	0

3 Residue-property plots (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.

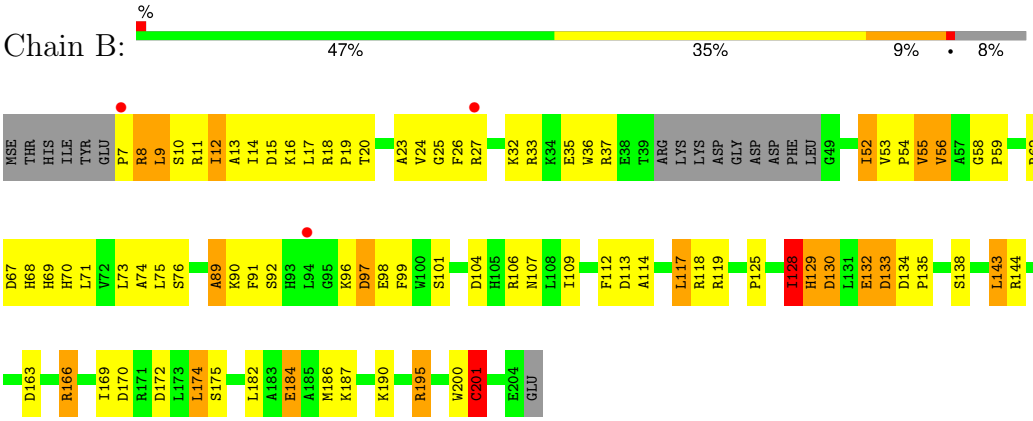
• Molecule 1: Hypothetical protein Atu1540

Chain A:



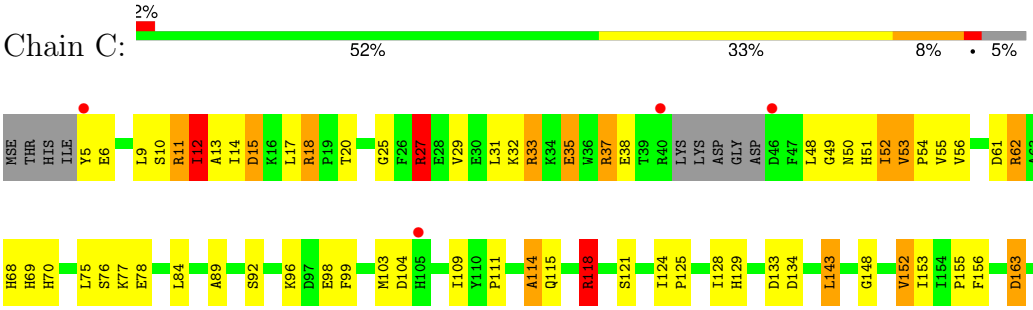
• Molecule 1: Hypothetical protein Atu1540

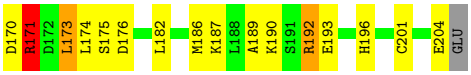
Chain B:



• Molecule 1: Hypothetical protein Atu1540

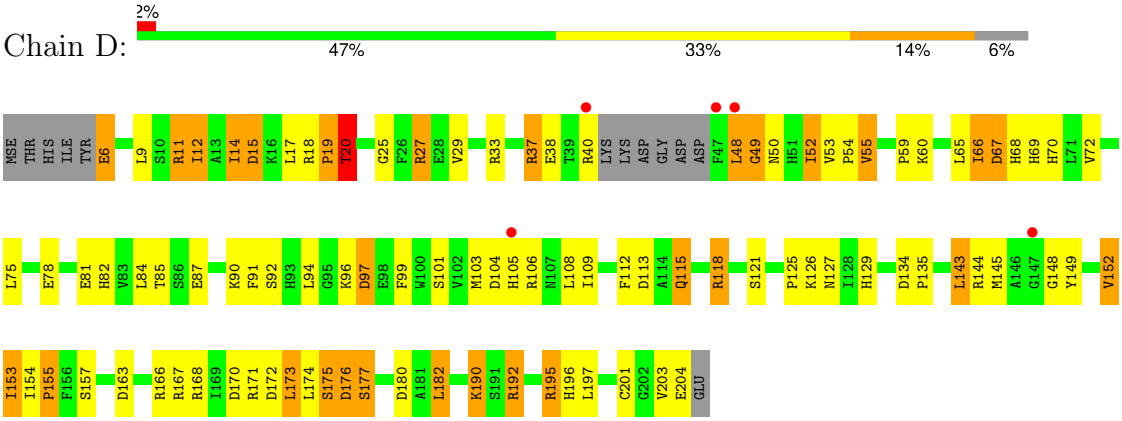
Chain C:





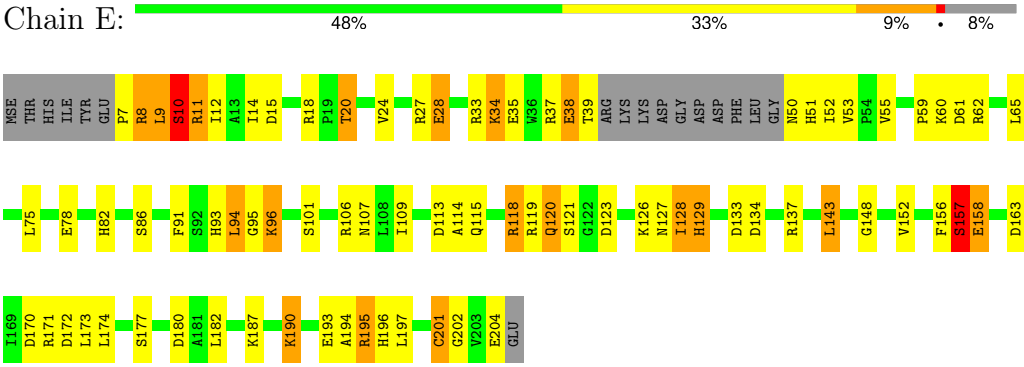
• Molecule 1: Hypothetical protein Atu1540

Chain D:



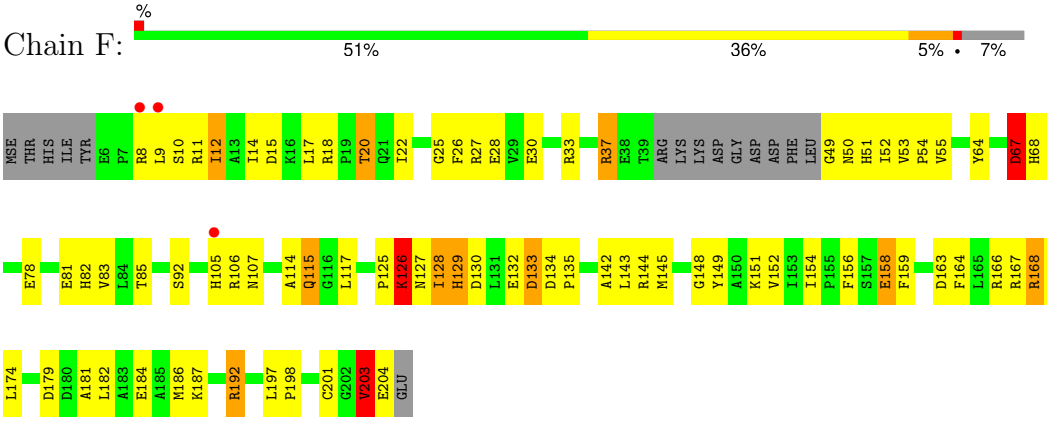
• Molecule 1: Hypothetical protein Atu1540

Chain E:



• Molecule 1: Hypothetical protein Atu1540

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	2481 reflections (5.07%)	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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[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	1.26	2/1608 (0.1%)	1.28	13/2164 (0.6%)
1	B	1.26	7/1567 (0.4%)	1.20	9/2107 (0.4%)
1	C	1.41	6/1620 (0.4%)	1.30	14/2180 (0.6%)
1	D	1.30	5/1591 (0.3%)	1.07	3/2141 (0.1%)
1	E	1.24	5/1552 (0.3%)	1.17	5/2087 (0.2%)
1	F	1.15	10/1561 (0.6%)	1.03	3/2100 (0.1%)
All	All	1.27	35/9499 (0.4%)	1.18	47/12779 (0.4%)

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 (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	SER	CB-OG	23.15	1.72	1.42
1	F	179	ASP	CG-OD1	14.28	1.58	1.25
1	D	40	ARG	C-O	12.39	1.46	1.23
1	E	201	CYS	CB-SG	-10.64	1.64	1.82
1	F	126	LYS	CE-NZ	9.47	1.72	1.49
1	D	176	ASP	CG-OD2	9.38	1.47	1.25
1	C	201	CYS	CB-SG	-9.23	1.66	1.82
1	A	28	GLU	CG-CD	8.24	1.64	1.51
1	D	176	ASP	CG-OD1	8.03	1.43	1.25
1	F	181	ALA	C-O	7.99	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	179	ASP	CG-OD2	7.62	1.42	1.25
1	C	27	ARG	CG-CD	7.53	1.70	1.51
1	F	126	LYS	CD-CE	7.42	1.69	1.51
1	A	35	GLU	CG-CD	7.10	1.62	1.51
1	D	172	ASP	C-O	7.08	1.36	1.23
1	F	179	ASP	C-N	7.07	1.50	1.34
1	F	181	ALA	C-N	6.60	1.49	1.34
1	B	112	PHE	CD2-CE2	6.11	1.51	1.39
1	B	200	TRP	CG-CD1	6.05	1.45	1.36
1	E	28	GLU	CG-CD	5.82	1.60	1.51
1	C	192	ARG	CG-CD	5.80	1.66	1.51
1	B	195	ARG	CG-CD	5.76	1.66	1.51
1	C	29	VAL	CB-CG1	-5.55	1.41	1.52
1	E	158	GLU	CG-CD	5.54	1.60	1.51
1	E	193	GLU	CD-OE2	5.51	1.31	1.25
1	F	126	LYS	CG-CD	5.50	1.71	1.52
1	B	201	CYS	CB-SG	-5.30	1.73	1.81
1	B	184	GLU	CG-CD	5.30	1.59	1.51
1	B	16	LYS	CE-NZ	5.26	1.62	1.49
1	C	152	VAL	CB-CG1	-5.23	1.41	1.52
1	E	204	GLU	CG-CD	5.22	1.59	1.51
1	F	179	ASP	C-O	5.19	1.33	1.23
1	B	132	GLU	CB-CG	5.19	1.62	1.52
1	C	77	LYS	CE-NZ	5.17	1.61	1.49
1	F	187	LYS	CB-CG	5.15	1.66	1.52

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	179	ASP	CB-CG-OD1	-9.58	109.67	118.30
1	A	176	ASP	CB-CG-OD1	9.15	126.54	118.30
1	A	118	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	B	133	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	B	16	LYS	CD-CE-NZ	-7.85	93.65	111.70
1	A	118	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	A	176	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	133	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	62	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	C	170	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	C	171	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	5	TYR	N-CA-C	6.97	129.82	111.00
1	A	60	LYS	C-N-CA	-6.81	104.68	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	170	ASP	CB-CG-OD1	6.52	124.17	118.30
1	F	106	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	104	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	A	133	ASP	CB-CG-OD1	6.45	124.10	118.30
1	E	133	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	163	ASP	CB-CG-OD1	6.39	124.05	118.30
1	C	52	ILE	CB-CA-C	-6.37	98.85	111.60
1	B	27	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	E	202	GLY	N-CA-C	-6.12	97.79	113.10
1	C	77	LYS	CD-CE-NZ	5.97	125.43	111.70
1	A	170	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	75	LEU	CA-CB-CG	5.75	128.53	115.30
1	B	130	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	F	133	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	32	LYS	CD-CE-NZ	-5.55	98.93	111.70
1	C	27	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	C	33	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	168	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	53	VAL	CG1-CB-CG2	5.34	119.45	110.90
1	E	157	SER	N-CA-CB	-5.30	102.56	110.50
1	C	118	ARG	CG-CD-NE	-5.29	100.70	111.80
1	D	176	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	C	133	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	118	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	D	66	ILE	C-N-CA	-5.11	108.93	121.70
1	E	66	ILE	CB-CA-C	-5.10	101.39	111.60
1	A	6	GLU	N-CA-C	5.10	124.78	111.00
1	B	128	ILE	CG1-CB-CG2	-5.08	100.22	111.40
1	C	176	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	E	168	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	C	61	ASP	CB-CA-C	5.03	120.47	110.40
1	D	176	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	C	168	ARG	NE-CZ-NH1	5.00	122.80	120.30

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

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Mol	Chain	Res	Type	Group
1	C	12	ILE	Peptide
1	E	156	PHE	Peptide
1	F	67	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1574	0	1549	60	0
1	B	1530	0	1521	68	0
1	C	1579	0	1558	65	0
1	D	1555	0	1538	91	0
1	E	1519	0	1512	63	0
1	F	1528	0	1516	63	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	378	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 20.

All (378) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:134:ASP:CG	1:C:166:ARG:HH22	1.90	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:158:GLU:CD	1:F:158:GLU:H	2.01	0.63
1:B:134:ASP:CG	1:B:166:ARG:HH22	2.02	0.62
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:B:59:PRO:O	1:B:62:ARG:HB2	2.00	0.61
1:B:67:ASP:CG	1:B:68:HIS:H	2.04	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
1:E:127:ASN:CB	1:E:129:HIS:HD2	2.14	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: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:D:176:ASP:O	1:D:177:SER:HB3	2.02	0.59
1:F:12:ILE:HD12	1:F:85:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:170:ASP:OD1	1:B:172:ASP:HB2	2.03	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:E:113:ASP:OD1	1:E:113:ASP:C	2.43	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
1:C:33:ARG:HD2	1:C:78:GLU:OE1	2.06	0.55
1:F:26:PHE:HB2	1:F:133:ASP:CG	2.26	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:E:120:GLN:NE2	1:E:123:ASP:OD1	2.39	0.55
1:A:113:ASP:C	1:A:113:ASP:OD1	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:51:HIS:C	1:F:52:ILE:HD13	2.29	0.53
1:B:15:ASP:OD1	1:B:15:ASP:C	2.47	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:C:104:ASP:OD1	1:C:104:ASP:C	2.47	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:175:SER:CB	1:D:175:SER:HG	2.15	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
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:A:134:ASP:CG	1:A:166:ARG:HH22	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:174:LEU:C	1:F:174:LEU:HD23	2.33	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: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:B:55:VAL:HA	1:B:64:TYR:O	2.13	0.48
1:F:20:THR:H	1:F:69:HIS:HE1	1.61	0.48
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:F:15:ASP:OD1	1:F:15:ASP:C	2.54	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HD1	1:C:5:TYR:N	2.15	0.44
1:D:37:ARG:HB3	1:D:38:GLU:CD	2.38	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:C:134:ASP:OD1	1:C:134:ASP:C	2.56	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:B:67:ASP:CG	1:B:68:HIS:N	2.71	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
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:A:15:ASP:OD1	1:A:15:ASP:C	2.57	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:E:170:ASP:OD1	1:E:170:ASP:C	2.56	0.43
1:C:128:ILE:HD12	1:C:128:ILE:HG23	1.66	0.43
1:D:113:ASP:OD1	1:D:113:ASP:C	2.56	0.43
1:F:25:GLY:H	1:F:70:HIS:HE1	1.66	0.43
1:E:95:GLY:O	1:E:96:LYS:C	2.57	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: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:E:38:GLU:CD	1:E:38:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:134:ASP:OD1	1:B:134:ASP:C	2.58	0.41
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:C:186:MSE:HE2	1:C:190:LYS:CE	2.48	0.41
1:D:143:LEU:HD22	1:D:148:GLY:HA3	2.02	0.41
1:D:20:THR:N	1:D:69:HIS:HE1	2.19	0.41
1:F:127:ASN:CG	1:F:129:HIS:CE1	2.94	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:B:18:ARG:HD3	1:B:62:ARG:HH11	1.86	0.40
1:C:124:ILE:O	1:C:125:PRO:C	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:PHE:CG	1:E:197:LEU:HD11	2.56	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	192/205 (94%)	179 (93%)	11 (6%)	2 (1%)	13	26
1	B	186/205 (91%)	170 (91%)	14 (8%)	2 (1%)	12	24
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%)	12	24
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

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Mol	Chain	Res	Type
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 (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	163/170 (96%)	138 (85%)	25 (15%)	2	3
1	B	160/170 (94%)	131 (82%)	29 (18%)	1	2
1	C	164/170 (96%)	132 (80%)	32 (20%)	1	1
1	D	162/170 (95%)	129 (80%)	33 (20%)	1	1
1	E	159/170 (94%)	122 (77%)	37 (23%)	0	1
1	F	159/170 (94%)	131 (82%)	28 (18%)	1	2
All	All	967/1020 (95%)	783 (81%)	184 (19%)	1	2

All (184) 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	34	LYS
1	A	46	ASP
1	A	48	LEU

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Mol	Chain	Res	Type
1	A	52	ILE
1	A	53	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	166	ARG
1	A	173	LEU
1	A	174	LEU
1	A	182	LEU
1	A	184	GLU
1	B	7	PRO
1	B	8	ARG
1	B	9	LEU
1	B	11	ARG
1	B	12	ILE
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	97	ASP
1	B	106	ARG
1	B	117	LEU
1	B	118	ARG
1	B	119	ARG
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	174	LEU

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Mol	Chain	Res	Type
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	11	ARG
1	C	12	ILE
1	C	15	ASP
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	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	163	ASP
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

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Mol	Chain	Res	Type
1	D	15	ASP
1	D	20	THR
1	D	27	ARG
1	D	37	ARG
1	D	48	LEU
1	D	52	ILE
1	D	55	VAL
1	D	67	ASP
1	D	75	LEU
1	D	92	SER
1	D	96	LYS
1	D	97	ASP
1	D	101	SER
1	D	105	HIS
1	D	115	GLN
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	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	34	LYS
1	E	35	GLU
1	E	37	ARG
1	E	38	GLU
1	E	39	THR

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Mol	Chain	Res	Type
1	E	52	ILE
1	E	55	VAL
1	E	61	ASP
1	E	66	ILE
1	E	67	ASP
1	E	75	LEU
1	E	86	SER
1	E	94	LEU
1	E	96	LYS
1	E	101	SER
1	E	118	ARG
1	E	120	GLN
1	E	126	LYS
1	E	128	ILE
1	E	129	HIS
1	E	143	LEU
1	E	152	VAL
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	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	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

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Mol	Chain	Res	Type
1	F	126	LYS
1	F	128	ILE
1	F	129	HIS
1	F	158	GLU
1	F	168	ARG
1	F	173	LEU
1	F	184	GLU
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 (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	69	HIS
1	A	70	HIS
1	A	107	ASN
1	A	120	GLN
1	A	196	HIS
1	B	68	HIS
1	B	69	HIS
1	B	70	HIS
1	B	129	HIS
1	C	50	ASN
1	C	68	HIS
1	C	69	HIS
1	C	70	HIS
1	C	196	HIS
1	D	68	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	69	HIS
1	E	115	GLN
1	E	120	GLN
1	E	196	HIS
1	F	51	HIS

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Mol	Chain	Res	Type
1	F	68	HIS
1	F	69	HIS
1	F	105	HIS
1	F	107	ASN
1	F	196	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	193/205 (94%)	-0.28	1 (0%) 87 85	48, 60, 75, 82	0
1	B	186/205 (90%)	0.03	3 (1%) 70 66	42, 70, 84, 112	1 (0%)
1	C	192/205 (93%)	-0.36	4 (2%) 63 59	38, 59, 81, 94	2 (1%)
1	D	190/205 (92%)	0.45	5 (2%) 57 52	43, 71, 85, 93	1 (0%)
1	E	185/205 (90%)	-0.23	0 100 100	49, 65, 78, 96	0
1	F	187/205 (91%)	0.25	3 (1%) 70 66	57, 77, 88, 94	0
All	All	1133/1230 (92%)	-0.02	16 (1%) 73 69	38, 68, 84, 112	4 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ILE	3.5
1	B	7	PRO	3.4
1	D	40	ARG	3.2
1	C	5	TYR	3.2
1	D	105	HIS	3.1
1	D	147	GLY	2.6
1	C	40	ARG	2.6
1	D	47	PHE	2.5
1	C	105[A]	HIS	2.4
1	C	46	ASP	2.4
1	F	9	LEU	2.4
1	D	48	LEU	2.3
1	F	8	ARG	2.2
1	B	94	LEU	2.2
1	F	105	HIS	2.1
1	B	27	ARG	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 monosaccharides 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.