Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2026 – 03:00 AM JST

PDB ID	:	45IZ / pdb_000045iz
Title	:	Crystal structure of N-terminally truncated caseinolytic protease proteolytic subunit ClpP from Pseudomonas syringae pv. actinidiae
Authors	:	Luo, X.; Li, X.Y.
Deposited on	:	2026-08-31
Resolution	:	2.22 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:

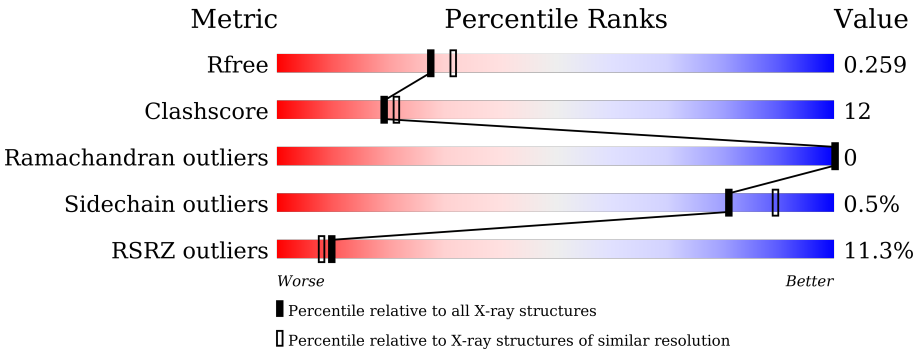
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	198	11% 77% 18%
1	B	198	11% 77% 18%
1	C	198	11% 80% 16%
1	D	198	11% 78% 18%
1	E	198	11% 82% 15%
1	F	198	11% 79% 16%

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Mol	Chain	Length	Quality of chain
1	G	198	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21125 atoms, of which 10339 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	B	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	C	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	D	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	E	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	F	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			
1	G	191	Total	C	H	N	O	S	0	0	0
			2962	930	1477	264	279	12			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
A	192	HIS	-	expression tag	UNP A0A2G9L4Z0
A	193	HIS	-	expression tag	UNP A0A2G9L4Z0
A	194	HIS	-	expression tag	UNP A0A2G9L4Z0
A	195	HIS	-	expression tag	UNP A0A2G9L4Z0
A	196	HIS	-	expression tag	UNP A0A2G9L4Z0
A	197	HIS	-	expression tag	UNP A0A2G9L4Z0
B	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
B	192	HIS	-	expression tag	UNP A0A2G9L4Z0
B	193	HIS	-	expression tag	UNP A0A2G9L4Z0
B	194	HIS	-	expression tag	UNP A0A2G9L4Z0
B	195	HIS	-	expression tag	UNP A0A2G9L4Z0
B	196	HIS	-	expression tag	UNP A0A2G9L4Z0
B	197	HIS	-	expression tag	UNP A0A2G9L4Z0
C	0	MET	-	initiating methionine	UNP A0A2G9L4Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	192	HIS	-	expression tag	UNP A0A2G9L4Z0
C	193	HIS	-	expression tag	UNP A0A2G9L4Z0
C	194	HIS	-	expression tag	UNP A0A2G9L4Z0
C	195	HIS	-	expression tag	UNP A0A2G9L4Z0
C	196	HIS	-	expression tag	UNP A0A2G9L4Z0
C	197	HIS	-	expression tag	UNP A0A2G9L4Z0
D	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
D	192	HIS	-	expression tag	UNP A0A2G9L4Z0
D	193	HIS	-	expression tag	UNP A0A2G9L4Z0
D	194	HIS	-	expression tag	UNP A0A2G9L4Z0
D	195	HIS	-	expression tag	UNP A0A2G9L4Z0
D	196	HIS	-	expression tag	UNP A0A2G9L4Z0
D	197	HIS	-	expression tag	UNP A0A2G9L4Z0
E	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
E	192	HIS	-	expression tag	UNP A0A2G9L4Z0
E	193	HIS	-	expression tag	UNP A0A2G9L4Z0
E	194	HIS	-	expression tag	UNP A0A2G9L4Z0
E	195	HIS	-	expression tag	UNP A0A2G9L4Z0
E	196	HIS	-	expression tag	UNP A0A2G9L4Z0
E	197	HIS	-	expression tag	UNP A0A2G9L4Z0
F	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
F	192	HIS	-	expression tag	UNP A0A2G9L4Z0
F	193	HIS	-	expression tag	UNP A0A2G9L4Z0
F	194	HIS	-	expression tag	UNP A0A2G9L4Z0
F	195	HIS	-	expression tag	UNP A0A2G9L4Z0
F	196	HIS	-	expression tag	UNP A0A2G9L4Z0
F	197	HIS	-	expression tag	UNP A0A2G9L4Z0
G	0	MET	-	initiating methionine	UNP A0A2G9L4Z0
G	192	HIS	-	expression tag	UNP A0A2G9L4Z0
G	193	HIS	-	expression tag	UNP A0A2G9L4Z0
G	194	HIS	-	expression tag	UNP A0A2G9L4Z0
G	195	HIS	-	expression tag	UNP A0A2G9L4Z0
G	196	HIS	-	expression tag	UNP A0A2G9L4Z0
G	197	HIS	-	expression tag	UNP A0A2G9L4Z0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	63	Total O 63 63	0	0
2	B	54	Total O 54 54	0	0

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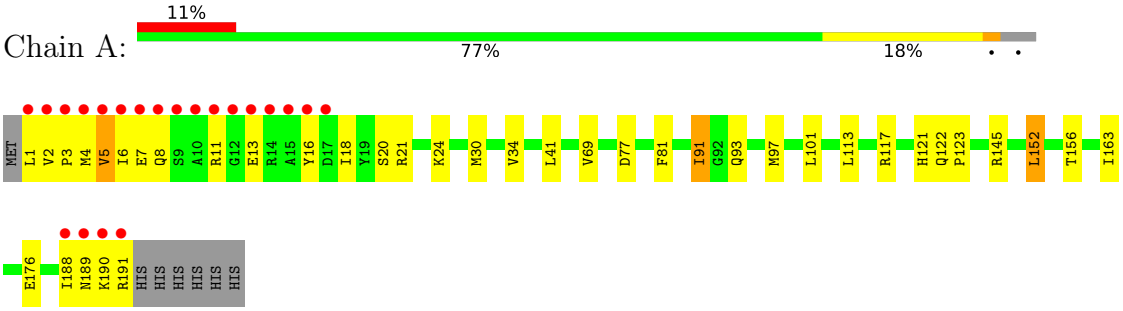
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	53	Total O 53 53	0	0
2	D	59	Total O 59 59	0	0
2	E	60	Total O 60 60	0	0
2	F	58	Total O 58 58	0	0
2	G	44	Total O 44 44	0	0

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.

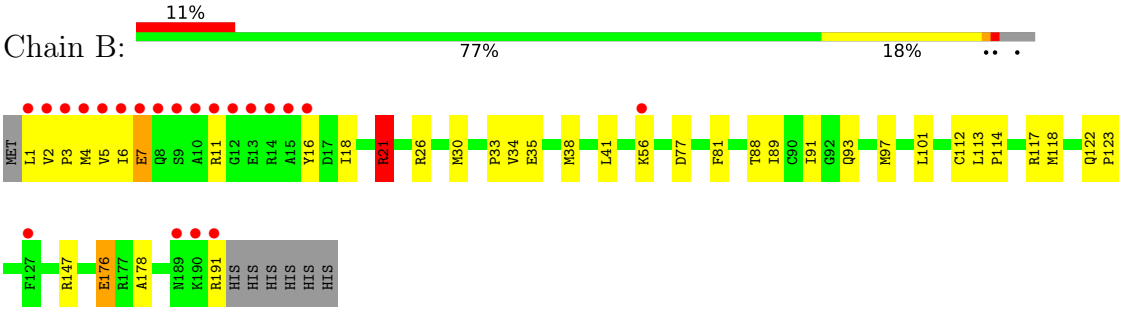
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain A:



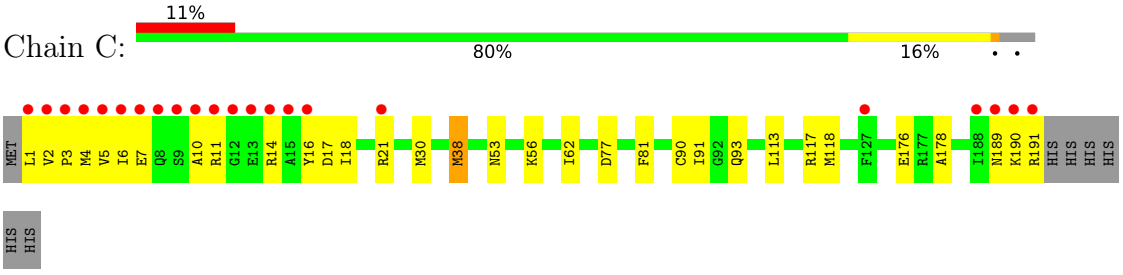
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain B:



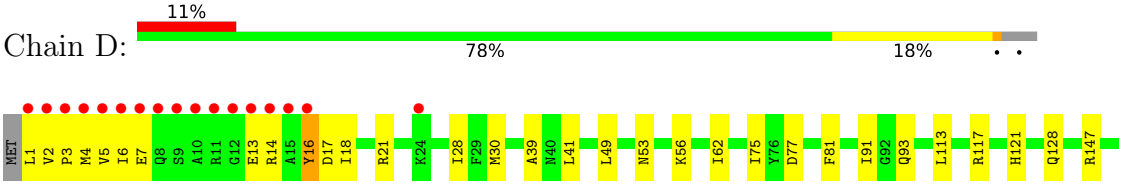
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

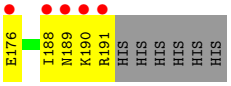
Chain C:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

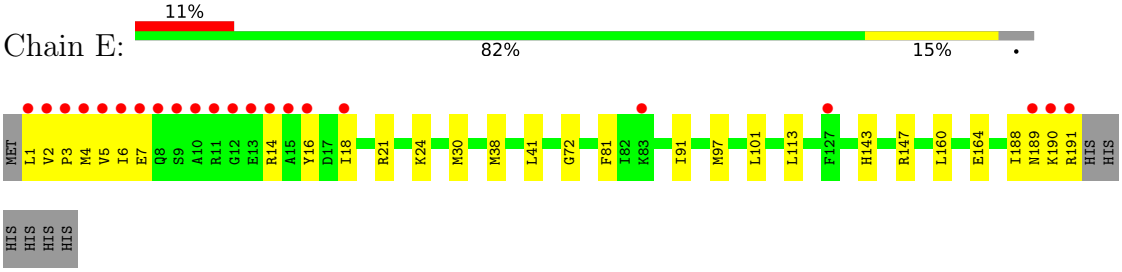
Chain D:





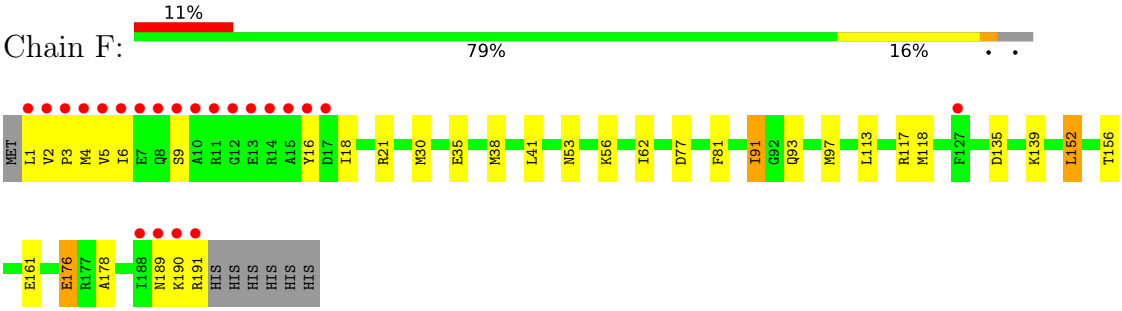
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain E:



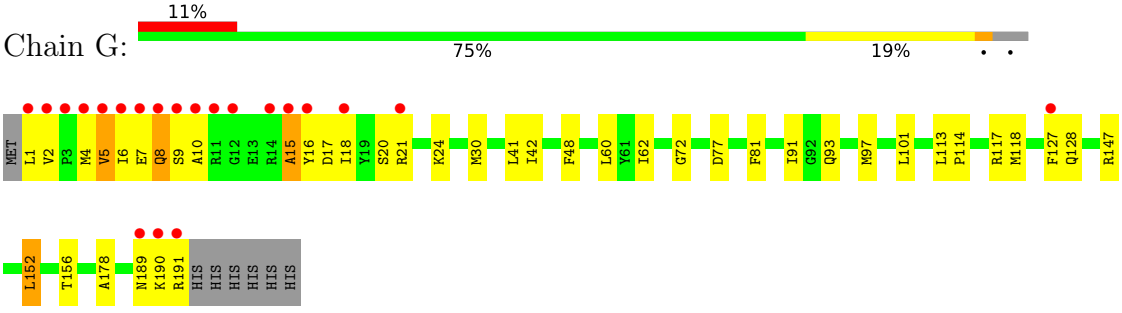
• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain F:



• Molecule 1: ATP-dependent Clp protease proteolytic subunit

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.06Å 181.66Å 157.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.87 – 2.22 31.87 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.87-2.22) 99.9 (31.87-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.217 , 0.259 0.218 , 0.259	Depositor DCC
R_{free} test set	4377 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 43.0	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	0.94	EDS
Total number of atoms	21125	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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	0.72	1/1511 (0.1%)	0.93	3/2037 (0.1%)
1	B	0.67	3/1511 (0.2%)	0.87	3/2037 (0.1%)
1	C	0.65	1/1511 (0.1%)	0.92	5/2037 (0.2%)
1	D	0.62	0/1511	0.86	2/2037 (0.1%)
1	E	0.60	0/1511	0.79	0/2037
1	F	0.74	3/1511 (0.2%)	0.90	5/2037 (0.2%)
1	G	0.67	1/1511 (0.1%)	0.92	6/2037 (0.3%)
All	All	0.67	9/10577 (0.1%)	0.89	24/14259 (0.2%)

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	B	0	2
1	D	0	1
1	E	0	1
1	G	0	1
All	All	0	5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	176	GLU	CG-CD	11.15	1.79	1.52
1	A	5	VAL	CB-CG1	-9.04	1.22	1.52
1	G	5	VAL	CB-CG1	-8.31	1.25	1.52
1	F	176	GLU	CD-OE2	7.17	1.39	1.25
1	B	21	ARG	CG-CD	-5.89	1.34	1.52
1	B	7	GLU	CB-CG	-5.81	1.35	1.52
1	B	176	GLU	CG-CD	5.58	1.66	1.52
1	C	176	GLU	CG-CD	5.58	1.66	1.52
1	F	161	GLU	CD-OE2	5.25	1.35	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	ILE	CA-C-N	-8.95	103.87	121.41
1	A	91	ILE	C-N-CA	-8.95	103.87	121.41
1	C	91	ILE	CA-C-N	-8.79	104.17	121.41
1	C	91	ILE	C-N-CA	-8.79	104.17	121.41
1	A	5	VAL	CA-CB-CG1	-8.50	95.94	110.40
1	F	161	GLU	CG-CD-OE1	-8.48	98.89	118.40
1	G	91	ILE	CA-C-N	-8.21	105.31	121.41
1	G	91	ILE	C-N-CA	-8.21	105.31	121.41
1	F	91	ILE	CA-C-N	-8.02	105.70	121.41
1	F	91	ILE	C-N-CA	-8.02	105.70	121.41
1	C	91	ILE	N-CA-C	7.92	121.30	113.53
1	G	5	VAL	CA-CB-CG1	-7.35	97.90	110.40
1	B	91	ILE	CA-C-N	-7.12	107.46	121.41
1	B	91	ILE	C-N-CA	-7.12	107.46	121.41
1	B	7	GLU	CB-CG-CD	-6.58	101.42	112.60
1	D	91	ILE	CA-C-N	-6.57	108.53	121.41
1	D	91	ILE	C-N-CA	-6.57	108.53	121.41
1	C	90	CYS	CA-C-N	-6.01	114.50	121.71
1	C	90	CYS	C-N-CA	-6.01	114.50	121.71
1	F	161	GLU	OE1-CD-OE2	5.73	136.66	122.90
1	G	15	ALA	CB-CA-C	5.68	118.89	110.14
1	G	8	GLN	CA-C-N	5.13	131.35	121.54
1	G	8	GLN	C-N-CA	5.13	131.35	121.54
1	F	176	GLU	CB-CG-CD	5.10	121.27	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	147	ARG	Sidechain
1	B	21	ARG	Sidechain
1	D	147	ARG	Sidechain
1	E	147	ARG	Sidechain
1	G	147	ARG	Sidechain

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	1485	1477	1478	43	0
1	B	1485	1477	1478	44	0
1	C	1485	1477	1478	41	0
1	D	1485	1477	1478	47	0
1	E	1485	1477	1478	40	0
1	F	1485	1477	1478	38	0
1	G	1485	1477	1478	55	0
2	A	63	0	0	6	0
2	B	54	0	0	9	0
2	C	53	0	0	2	0
2	D	59	0	0	2	0
2	E	60	0	0	1	0
2	F	58	0	0	3	0
2	G	44	0	0	8	0
All	All	10786	10339	10346	242	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 (242) 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:176:GLU:CD	1:F:176:GLU:CG	1.79	1.55
1:D:5:VAL:HG11	1:D:21:ARG:HG3	1.54	0.90
1:B:35:GLU:HG3	2:B:201:HOH:O	1.76	0.82
1:C:30:MET:HE2	1:C:62:ILE:HG23	1.59	0.82
1:B:30:MET:HE3	1:B:34:VAL:HG22	1.64	0.80
1:A:7:GLU:HG2	1:A:21:ARG:NH1	1.97	0.79
1:B:33:PRO:O	2:B:201:HOH:O	2.00	0.79
1:C:2:VAL:HG21	1:G:1:LEU:HD21	1.65	0.79
1:D:191:ARG:HG3	1:E:81:PHE:CZ	2.17	0.78
1:E:1:LEU:HD21	1:G:2:VAL:HG21	1.65	0.77
1:C:189:ASN:C	1:C:190:LYS:HD2	2.09	0.77
1:A:176:GLU:OE1	2:A:201:HOH:O	2.03	0.76
1:C:11:ARG:HH12	1:G:10:ALA:HA	1.50	0.76
1:G:189:ASN:C	1:G:190:LYS:HD2	2.11	0.76
1:E:191:ARG:HG3	1:G:81:PHE:CZ	2.22	0.75
1:B:81:PHE:CZ	1:C:191:ARG:HG3	2.22	0.74
1:D:30:MET:HE2	1:D:62:ILE:HG23	1.68	0.74
1:G:128:GLN:O	2:G:201:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:GLU:HG2	1:G:21:ARG:NH1	2.03	0.73
1:A:81:PHE:CZ	1:F:191:ARG:HG3	2.24	0.72
1:G:30:MET:HE3	1:G:62:ILE:HG12	1.72	0.72
1:B:30:MET:HE1	1:B:101:LEU:HD12	1.73	0.71
1:G:5:VAL:HG11	1:G:21:ARG:HH11	1.55	0.71
1:C:16:TYR:CD2	1:G:6:ILE:HD12	2.27	0.70
1:A:16:TYR:CE1	1:F:6:ILE:HD12	2.27	0.70
1:F:189:ASN:C	1:F:190:LYS:HD2	2.16	0.69
1:E:5:VAL:CG2	1:E:18:ILE:HD12	2.23	0.68
1:G:60:LEU:HD21	2:G:238:HOH:O	1.92	0.68
1:B:191:ARG:HG3	1:F:81:PHE:CZ	2.28	0.68
1:B:38:MET:CG	2:B:201:HOH:O	2.42	0.68
1:D:2:VAL:HG11	2:D:208:HOH:O	1.93	0.67
1:F:30:MET:HE2	1:F:62:ILE:HG12	1.77	0.67
1:B:5:VAL:HG11	1:B:21:ARG:HH11	1.57	0.67
1:G:5:VAL:HG23	1:G:18:ILE:HD12	1.77	0.67
1:G:5:VAL:CG2	1:G:18:ILE:HD12	2.25	0.67
1:A:2:VAL:HG21	1:F:1:LEU:HD21	1.77	0.67
1:C:77:ASP:HB3	1:G:113:LEU:HD23	1.76	0.67
1:A:1:LEU:HD21	1:D:2:VAL:HG21	1.77	0.66
1:F:5:VAL:HG23	1:F:18:ILE:HD12	1.77	0.66
1:D:5:VAL:HG23	1:D:18:ILE:HD12	1.78	0.66
1:D:5:VAL:CG2	1:D:18:ILE:HD12	2.26	0.66
1:C:16:TYR:CE2	1:G:6:ILE:HD12	2.32	0.65
1:D:1:LEU:HD21	1:E:2:VAL:HG21	1.79	0.64
1:D:6:ILE:HD12	1:E:16:TYR:CE1	2.32	0.64
1:B:2:VAL:HG21	1:C:1:LEU:HD21	1.79	0.64
1:E:6:ILE:HD12	1:G:16:TYR:CE2	2.33	0.64
1:G:189:ASN:O	1:G:190:LYS:HD2	1.97	0.64
1:F:189:ASN:HB3	1:F:190:LYS:CD	2.28	0.63
1:E:189:ASN:C	1:E:190:LYS:HD2	2.24	0.63
1:A:21:ARG:HD3	2:A:249:HOH:O	1.99	0.63
1:B:97:MET:HE3	1:B:97:MET:O	1.99	0.62
1:E:5:VAL:HG23	1:E:18:ILE:HD12	1.80	0.62
1:F:30:MET:HE2	1:F:62:ILE:HG23	1.82	0.62
1:B:7:GLU:OE2	1:B:16:TYR:CE1	2.54	0.61
1:B:35:GLU:N	2:B:201:HOH:O	2.33	0.61
1:G:97:MET:HE3	1:G:97:MET:O	2.01	0.61
1:E:21:ARG:HG2	1:G:48:PHE:CE1	2.35	0.61
1:A:20:SER:O	1:A:24:LYS:HD3	2.01	0.61
1:F:5:VAL:CG2	1:F:18:ILE:HD12	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:PHE:CZ	1:G:191:ARG:HG3	2.36	0.60
1:F:189:ASN:HB3	1:F:190:LYS:HD2	1.81	0.60
1:C:11:ARG:HH12	1:G:10:ALA:CA	2.15	0.59
1:F:5:VAL:HG11	1:F:21:ARG:HG3	1.85	0.59
1:B:1:LEU:HD21	1:F:2:VAL:HG21	1.84	0.59
1:G:5:VAL:HG11	1:G:21:ARG:NH1	2.17	0.58
1:F:189:ASN:HB3	1:F:190:LYS:NZ	2.18	0.58
1:A:191:ARG:HG3	1:D:81:PHE:CZ	2.37	0.58
1:G:4:MET:HA	1:G:16:TYR:O	2.03	0.58
1:A:16:TYR:CE1	1:A:24:LYS:HE3	2.39	0.58
1:F:97:MET:HE2	2:F:258:HOH:O	2.04	0.57
1:A:91:ILE:O	2:A:202:HOH:O	2.18	0.56
1:C:93:GLN:HA	1:C:117:ARG:O	2.05	0.56
1:F:4:MET:HA	1:F:16:TYR:O	2.05	0.56
1:E:3:PRO:HD3	1:G:41:LEU:HD21	1.85	0.56
1:B:30:MET:CE	1:B:34:VAL:HG22	2.34	0.56
1:E:30:MET:HG3	1:E:38:MET:HE2	1.87	0.56
1:D:53:ASN:ND2	1:D:56:LYS:HD2	2.20	0.56
1:G:42:ILE:HG21	2:G:238:HOH:O	2.05	0.56
1:C:53:ASN:ND2	1:C:56:LYS:HD2	2.21	0.55
1:A:16:TYR:HB2	2:A:249:HOH:O	2.05	0.55
1:C:11:ARG:NH1	1:G:9:SER:O	2.38	0.55
1:E:30:MET:HG3	1:E:38:MET:CE	2.36	0.55
1:G:4:MET:HE2	1:G:15:ALA:HB1	1.89	0.55
1:C:30:MET:HG3	1:C:38:MET:CE	2.36	0.55
1:A:5:VAL:CG2	1:A:18:ILE:HD13	2.37	0.54
1:G:127:PHE:CZ	2:G:201:HOH:O	2.60	0.54
1:B:11:ARG:HH12	1:C:10:ALA:HA	1.72	0.54
1:C:7:GLU:OE2	1:C:21:ARG:HD3	2.07	0.54
1:E:113:LEU:HD13	1:G:77:ASP:HB3	1.90	0.53
1:B:1:LEU:HD11	1:F:2:VAL:HG21	1.88	0.53
1:B:16:TYR:CE2	1:C:6:ILE:HD12	2.43	0.53
1:A:189:ASN:C	1:A:190:LYS:HD2	2.34	0.53
1:D:6:ILE:HD12	1:E:16:TYR:CD1	2.43	0.53
1:F:53:ASN:ND2	1:F:56:LYS:HD2	2.24	0.53
1:B:7:GLU:OE2	1:B:16:TYR:CZ	2.62	0.53
1:A:30:MET:HE3	1:A:34:VAL:HG22	1.91	0.52
1:A:152:LEU:HD22	1:A:156:THR:HG23	1.90	0.52
1:D:7:GLU:OE2	1:D:16:TYR:CE2	2.62	0.52
1:G:72:GLY:HA3	1:G:97:MET:HE2	1.91	0.52
1:A:3:PRO:HD2	1:D:41:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ILE:HD12	1:G:16:TYR:CD2	2.44	0.52
1:A:7:GLU:HG2	1:A:21:ARG:CZ	2.40	0.51
1:B:77:ASP:HB3	1:C:113:LEU:HD13	1.91	0.51
1:C:5:VAL:CG2	1:C:18:ILE:HD12	2.40	0.51
1:C:7:GLU:OE2	1:C:16:TYR:CE1	2.64	0.51
1:D:2:VAL:CG1	2:D:208:HOH:O	2.57	0.51
1:B:97:MET:CE	1:B:101:LEU:HG	2.41	0.51
1:C:5:VAL:HG23	1:C:18:ILE:HD12	1.92	0.51
1:D:189:ASN:C	1:D:190:LYS:HD2	2.36	0.51
1:G:16:TYR:HE2	1:G:24:LYS:HZ3	1.57	0.51
1:C:7:GLU:CD	1:C:21:ARG:HD3	2.35	0.50
1:G:97:MET:CE	1:G:101:LEU:HG	2.41	0.50
1:B:26:ARG:CD	1:B:56:LYS:HD3	2.42	0.50
1:D:6:ILE:HG21	1:E:14:ARG:CD	2.41	0.50
1:C:30:MET:HG3	1:C:38:MET:HE1	1.94	0.50
1:D:13:GLU:HB3	1:E:14:ARG:CZ	2.41	0.50
1:G:118:MET:HE3	1:G:178:ALA:HB2	1.93	0.50
1:C:11:ARG:NH1	1:G:10:ALA:HA	2.21	0.50
1:D:6:ILE:HG23	1:E:14:ARG:NH1	2.27	0.49
1:B:5:VAL:CG2	1:B:18:ILE:HD13	2.42	0.49
1:C:7:GLU:OE1	1:C:21:ARG:CZ	2.60	0.49
1:B:41:LEU:HD11	1:C:3:PRO:HD2	1.94	0.49
1:E:143:HIS:HB2	2:E:237:HOH:O	2.12	0.49
1:D:6:ILE:HG23	1:E:14:ARG:HH11	1.76	0.49
1:E:30:MET:HE1	1:E:101:LEU:HD12	1.93	0.49
1:G:60:LEU:CD2	2:G:238:HOH:O	2.55	0.49
1:A:6:ILE:HD12	1:D:16:TYR:CD1	2.48	0.49
1:A:152:LEU:HD13	1:A:163:ILE:HD12	1.94	0.49
1:D:4:MET:O	1:E:24:LYS:NZ	2.45	0.49
1:D:30:MET:HE2	1:D:62:ILE:CG2	2.42	0.49
1:D:128:GLN:N	1:D:128:GLN:OE1	2.45	0.49
1:F:118:MET:HE3	1:F:178:ALA:CB	2.43	0.49
1:A:5:VAL:HB	2:A:249:HOH:O	2.13	0.48
1:F:93:GLN:HA	1:F:117:ARG:O	2.13	0.48
1:B:41:LEU:HD21	1:C:3:PRO:HD3	1.95	0.48
1:E:4:MET:HA	1:E:16:TYR:O	2.13	0.48
1:A:69:VAL:HA	1:A:97:MET:HE3	1.95	0.48
1:A:6:ILE:HD12	1:D:16:TYR:CE1	2.48	0.48
1:A:41:LEU:HD21	1:F:3:PRO:HD3	1.95	0.48
1:D:30:MET:HE2	1:D:62:ILE:HG12	1.95	0.48
1:D:93:GLN:HA	1:D:117:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:PRO:HD2	1:G:41:LEU:HD11	1.95	0.48
1:D:189:ASN:HB3	1:D:190:LYS:HD2	1.95	0.47
1:C:11:ARG:HH22	1:G:10:ALA:HA	1.77	0.47
1:B:93:GLN:HA	1:B:117:ARG:O	2.14	0.47
1:B:112:CYS:SG	1:B:118:MET:HE1	2.55	0.47
1:B:30:MET:HG3	1:B:38:MET:HE1	1.96	0.47
1:E:4:MET:HE1	1:G:17:ASP:CG	2.39	0.47
1:A:11:ARG:NH1	1:F:9:SER:O	2.48	0.47
1:E:160:LEU:O	1:E:164:GLU:HG3	2.15	0.47
1:A:113:LEU:HD13	1:D:77:ASP:HB3	1.95	0.47
1:D:113:LEU:HD23	1:D:188:ILE:HG13	1.96	0.47
1:A:2:VAL:HG21	1:F:1:LEU:HD11	1.97	0.47
1:B:16:TYR:CD2	1:C:6:ILE:HD12	2.49	0.47
1:G:7:GLU:OE2	1:G:16:TYR:CE1	2.68	0.47
1:F:152:LEU:HD22	1:F:156:THR:HG23	1.97	0.46
1:A:30:MET:HE1	1:A:101:LEU:HD12	1.98	0.46
1:D:4:MET:HA	1:D:16:TYR:O	2.15	0.46
1:D:39:ALA:HA	1:D:75:ILE:HD11	1.96	0.46
1:G:16:TYR:HE2	1:G:24:LYS:HE2	1.79	0.46
1:A:4:MET:HA	1:A:16:TYR:O	2.16	0.46
1:E:7:GLU:OE2	1:E:21:ARG:HD3	2.15	0.46
1:A:3:PRO:CD	1:D:41:LEU:HD11	2.45	0.46
1:G:127:PHE:CD1	2:G:201:HOH:O	2.67	0.46
1:F:35:GLU:HB3	2:F:213:HOH:O	2.15	0.46
1:G:118:MET:HE3	1:G:178:ALA:CB	2.45	0.46
1:A:8:GLN:HG2	1:D:14:ARG:HH22	1.80	0.46
1:C:189:ASN:O	1:C:190:LYS:HD2	2.15	0.45
1:B:26:ARG:HD3	1:B:56:LYS:NZ	2.32	0.45
1:B:118:MET:HE2	1:B:178:ALA:CB	2.46	0.45
1:B:26:ARG:HD3	1:B:56:LYS:HD3	1.99	0.45
1:B:176:GLU:CD	1:B:176:GLU:H	2.25	0.45
1:C:2:VAL:HG12	1:C:17:ASP:HB2	1.99	0.45
1:D:6:ILE:HG21	1:E:14:ARG:HD2	1.99	0.45
1:E:91:ILE:HG22	1:E:113:LEU:HD12	1.99	0.45
1:A:113:LEU:HD23	1:A:188:ILE:CG1	2.48	0.44
1:G:113:LEU:HB3	1:G:114:PRO:CD	2.47	0.44
1:A:5:VAL:HG11	1:A:21:ARG:HH11	1.83	0.44
1:F:30:MET:HE2	1:F:62:ILE:CG2	2.47	0.44
1:E:72:GLY:HA3	1:E:97:MET:HE2	1.99	0.44
1:G:127:PHE:CE1	2:G:201:HOH:O	2.57	0.44
2:B:241:HOH:O	1:C:3:PRO:CB	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:HIS:CD2	1:D:121:HIS:C	2.96	0.44
1:A:77:ASP:HB3	1:F:113:LEU:HD13	2.00	0.44
1:B:30:MET:HE3	1:B:34:VAL:CG2	2.42	0.44
1:B:3:PRO:HD3	1:F:41:LEU:HD21	1.99	0.43
1:C:14:ARG:HH22	1:G:8:GLN:HG2	1.82	0.43
1:G:60:LEU:HD11	2:G:238:HOH:O	2.16	0.43
1:E:113:LEU:HD23	1:E:188:ILE:HG13	2.00	0.43
1:A:16:TYR:CD1	1:F:6:ILE:HD12	2.54	0.43
1:A:93:GLN:HA	1:A:117:ARG:O	2.18	0.43
1:B:113:LEU:HD13	1:F:77:ASP:HB3	2.00	0.43
1:C:17:ASP:O	2:C:201:HOH:O	2.21	0.43
1:F:135:ASP:HB2	2:F:233:HOH:O	2.18	0.43
1:G:16:TYR:CE2	1:G:24:LYS:HE2	2.54	0.43
1:B:5:VAL:CG1	1:B:21:ARG:HH11	2.30	0.43
1:C:2:VAL:HG21	1:G:1:LEU:HD11	2.01	0.43
1:G:20:SER:O	1:G:24:LYS:HD3	2.18	0.43
1:E:97:MET:HE3	1:E:97:MET:O	2.17	0.43
1:E:38:MET:SD	1:E:38:MET:C	3.01	0.43
1:A:13:GLU:HB3	1:D:14:ARG:CZ	2.49	0.43
1:B:30:MET:CE	1:B:34:VAL:CG2	2.97	0.43
1:D:16:TYR:CD1	1:D:16:TYR:N	2.85	0.43
1:G:5:VAL:CG1	1:G:21:ARG:HH11	2.28	0.43
1:B:122:GLN:HB2	1:B:123:PRO:HD2	2.01	0.42
1:D:6:ILE:CG2	1:E:14:ARG:NH1	2.83	0.42
1:D:16:TYR:CD2	1:D:21:ARG:HG2	2.53	0.42
1:B:88:THR:C	1:B:89:ILE:HG13	2.44	0.42
1:B:176:GLU:HG3	2:B:249:HOH:O	2.18	0.42
1:G:7:GLU:OE2	1:G:21:ARG:HD3	2.19	0.42
1:A:176:GLU:HB2	2:A:201:HOH:O	2.19	0.42
2:B:241:HOH:O	1:C:3:PRO:HB3	2.19	0.42
1:D:3:PRO:HD3	1:E:41:LEU:HD21	2.01	0.42
1:E:16:TYR:HE1	1:E:24:LYS:HE2	1.84	0.42
1:F:30:MET:HG3	1:F:38:MET:HE1	2.01	0.42
1:F:118:MET:HE3	1:F:178:ALA:HB2	2.02	0.42
1:G:152:LEU:HD22	1:G:156:THR:HG23	2.02	0.42
1:C:30:MET:CG	1:C:38:MET:HE1	2.50	0.42
1:A:121:HIS:CD2	1:A:121:HIS:C	2.97	0.41
1:D:13:GLU:HB3	1:E:14:ARG:NH1	2.35	0.41
1:A:5:VAL:HG11	1:A:21:ARG:NH1	2.35	0.41
1:D:2:VAL:HG12	1:D:17:ASP:HB2	2.01	0.41
1:D:28:ILE:HD11	1:D:49:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:MET:HE3	1:C:178:ALA:HB2	2.01	0.41
1:D:113:LEU:HD23	1:D:188:ILE:CG1	2.51	0.41
1:D:176:GLU:H	1:D:176:GLU:CD	2.29	0.41
1:E:4:MET:HE1	1:G:17:ASP:OD2	2.19	0.41
1:G:93:GLN:HA	1:G:117:ARG:O	2.20	0.41
1:B:113:LEU:HB3	1:B:114:PRO:CD	2.51	0.41
1:F:135:ASP:OD1	1:F:139:LYS:HE2	2.21	0.41
1:F:91:ILE:HG22	1:F:113:LEU:CD1	2.50	0.41
1:A:123:PRO:HG2	1:A:145:ARG:HB2	2.02	0.40
1:C:38:MET:HG2	2:C:218:HOH:O	2.20	0.40
1:F:91:ILE:HG22	1:F:113:LEU:HD12	2.02	0.40
1:A:13:GLU:HB3	1:D:14:ARG:NH1	2.37	0.40
1:E:7:GLU:CD	1:E:21:ARG:HD3	2.47	0.40
1:B:2:VAL:O	1:B:4:MET:HE2	2.21	0.40
1:B:38:MET:HG2	2:B:201:HOH:O	2.14	0.40
1:B:176:GLU:CG	2:B:249:HOH:O	2.69	0.40
1:A:122:GLN:HB2	1:A:123:PRO:HD2	2.02	0.40
1:C:4:MET:HA	1:C:16:TYR:O	2.22	0.40
1:F:189:ASN:OD1	1:F:190:LYS:NZ	2.55	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	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
1	B	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
1	C	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
1	D	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
1	E	189/198 (96%)	186 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
1	G	189/198 (96%)	187 (99%)	2 (1%)	0	100	100
All	All	1323/1386 (96%)	1308 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	159/166 (96%)	158 (99%)	1 (1%)	78	88
1	B	159/166 (96%)	158 (99%)	1 (1%)	78	88
1	C	159/166 (96%)	158 (99%)	1 (1%)	78	88
1	D	159/166 (96%)	158 (99%)	1 (1%)	78	88
1	E	159/166 (96%)	159 (100%)	0	100	100
1	F	159/166 (96%)	158 (99%)	1 (1%)	78	88
1	G	159/166 (96%)	158 (99%)	1 (1%)	78	88
All	All	1113/1162 (96%)	1107 (100%)	6 (0%)	81	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	B	6	ILE
1	C	38	MET
1	D	16	TYR
1	F	152	LEU
1	G	152	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	B	8	GLN
1	D	40	ASN
1	D	189	ASN
1	E	40	ASN
1	E	93	GLN
1	F	8	GLN
1	G	40	ASN

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, 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	191/198 (96%)	0.23	21 (10%)	10	8	29, 38, 158, 189	0
1	B	191/198 (96%)	0.31	21 (10%)	10	8	33, 44, 163, 188	0
1	C	191/198 (96%)	0.32	22 (11%)	9	8	33, 43, 153, 180	0
1	D	191/198 (96%)	0.27	22 (11%)	9	8	30, 40, 156, 189	0
1	E	191/198 (96%)	0.33	22 (11%)	9	8	32, 42, 158, 181	0
1	F	191/198 (96%)	0.32	22 (11%)	9	8	31, 42, 164, 200	0
1	G	191/198 (96%)	0.33	21 (10%)	10	8	33, 43, 149, 184	0
All	All	1337/1386 (96%)	0.30	151 (11%)	10	8	29, 42, 163, 200	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	8.7
1	A	5	VAL	7.7
1	D	10	ALA	7.6
1	F	10	ALA	7.6
1	A	6	ILE	7.3
1	E	5	VAL	7.2
1	B	15	ALA	7.0
1	D	3	PRO	7.0
1	C	10	ALA	7.0
1	A	10	ALA	6.9
1	G	10	ALA	6.9
1	B	3	PRO	6.8
1	A	4	MET	6.8
1	B	4	MET	6.7
1	E	3	PRO	6.7
1	E	10	ALA	6.7
1	A	3	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	3	PRO	6.5
1	G	3	PRO	6.4
1	F	3	PRO	6.2
1	D	189	ASN	6.2
1	G	5	VAL	6.1
1	G	4	MET	6.1
1	A	1	LEU	6.1
1	A	2	VAL	5.9
1	B	2	VAL	5.7
1	C	4	MET	5.7
1	F	191	ARG	5.7
1	A	15	ALA	5.6
1	E	1	LEU	5.6
1	E	6	ILE	5.6
1	E	16	TYR	5.6
1	D	1	LEU	5.5
1	C	6	ILE	5.5
1	E	2	VAL	5.5
1	G	15	ALA	5.4
1	D	15	ALA	5.4
1	C	2	VAL	5.4
1	E	15	ALA	5.3
1	F	6	ILE	5.1
1	A	16	TYR	5.1
1	D	190	LYS	5.0
1	C	15	ALA	5.0
1	F	15	ALA	5.0
1	C	5	VAL	5.0
1	F	5	VAL	5.0
1	G	6	ILE	5.0
1	F	2	VAL	4.9
1	A	191	ARG	4.9
1	G	2	VAL	4.9
1	G	1	LEU	4.8
1	D	5	VAL	4.8
1	B	191	ARG	4.8
1	C	1	LEU	4.8
1	D	4	MET	4.8
1	E	191	ARG	4.8
1	D	191	ARG	4.7
1	F	1	LEU	4.7
1	G	191	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	12	GLY	4.6
1	C	191	ARG	4.5
1	E	4	MET	4.5
1	B	5	VAL	4.5
1	D	2	VAL	4.5
1	B	16	TYR	4.4
1	B	6	ILE	4.3
1	F	189	ASN	4.3
1	D	6	ILE	4.3
1	G	9	SER	4.2
1	D	12	GLY	4.1
1	D	16	TYR	4.0
1	A	12	GLY	4.0
1	F	4	MET	4.0
1	E	189	ASN	3.9
1	C	9	SER	3.8
1	E	9	SER	3.7
1	A	190	LYS	3.7
1	C	16	TYR	3.7
1	F	7	GLU	3.7
1	E	12	GLY	3.6
1	B	190	LYS	3.6
1	C	7	GLU	3.6
1	F	12	GLY	3.5
1	C	189	ASN	3.5
1	G	16	TYR	3.5
1	B	1	LEU	3.4
1	F	16	TYR	3.4
1	B	9	SER	3.3
1	A	9	SER	3.3
1	C	190	LYS	3.3
1	C	14	ARG	3.3
1	G	7	GLU	3.3
1	G	8	GLN	3.2
1	B	189	ASN	3.2
1	G	190	LYS	3.1
1	A	189	ASN	3.1
1	F	190	LYS	3.1
1	C	127	PHE	3.1
1	D	11	ARG	3.1
1	B	12	GLY	3.1
1	D	13	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	127	PHE	3.0
1	F	13	GLU	3.0
1	C	12	GLY	3.0
1	E	7	GLU	2.9
1	D	7	GLU	2.9
1	F	127	PHE	2.8
1	F	9	SER	2.8
1	B	127	PHE	2.7
1	D	176	GLU	2.6
1	F	188	ILE	2.6
1	B	8	GLN	2.6
1	C	8	GLN	2.6
1	A	7	GLU	2.5
1	B	11	ARG	2.5
1	D	9	SER	2.5
1	G	11	ARG	2.5
1	E	127	PHE	2.5
1	F	11	ARG	2.5
1	A	11	ARG	2.4
1	E	11	ARG	2.4
1	E	190	LYS	2.4
1	B	14	ARG	2.4
1	A	14	ARG	2.4
1	C	13	GLU	2.4
1	A	188	ILE	2.3
1	A	13	GLU	2.3
1	F	8	GLN	2.3
1	D	188	ILE	2.3
1	D	8	GLN	2.3
1	E	83	LYS	2.3
1	G	14	ARG	2.2
1	E	13	GLU	2.2
1	E	8	GLN	2.2
1	B	7	GLU	2.2
1	B	56	LYS	2.2
1	G	21	ARG	2.1
1	A	8	GLN	2.1
1	C	21	ARG	2.1
1	D	14	ARG	2.1
1	B	13	GLU	2.1
1	D	24	LYS	2.1
1	A	17	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	ASP	2.1
1	G	189	ASN	2.1
1	E	14	ARG	2.1
1	E	18	ILE	2.0
1	F	14	ARG	2.0
1	C	11	ARG	2.0
1	C	188	ILE	2.0
1	G	18	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.