



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:49 pm BST

PDB ID : 3AAE  
Title : Crystal structure of Actin capping protein in complex with CARMIL fragment  
Authors : Takeda, S.; Minakata, S.; Narita, A.; Kitazawa, M.; Yamakuni, T.; Maeda, Y.;  
Nitanai, Y.  
Deposited on : 2009-11-16  
Resolution : 3.30 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](mailto: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.

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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 : 2.11  
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) : 2.11

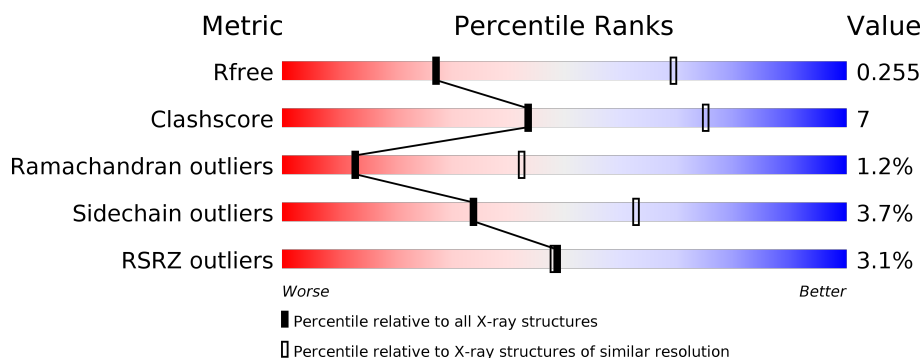
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>6%</div> </div> </div>
1	C	286	<div> <div></div> <div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>
1	E	286	<div> <div>6%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>6%</div> </div> </div>
1	G	286	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>6%</div> </div> </div>
1	I	286	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>6%</div> </div> </div>
2	B	277	<div> <div></div> <div> <div></div> <div>78%</div> <div>16%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	277	<p>%</p> <p>79% 14% • 5%</p>
2	F	277	<p>%</p> <p>76% 13% • 10%</p>
2	H	277	<p>2%</p> <p>73% 15% • 10%</p>
2	J	277	<p>2%</p> <p>75% 14% • 10%</p>
3	V	37	<p>3%</p> <p>49% 8% 43%</p>
3	W	37	<p>8%</p> <p>51% 16% • 30%</p>
3	X	37	<p>8%</p> <p>59% 14% 5% 22%</p>
3	Y	37	<p>22%</p> <p>70% 5% 24%</p>
3	Z	37	<p>3%</p> <p>62% 11% • 24%</p>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22177 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 F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2196	1384	385	422	5			
1	C	270	Total	C	N	O	S	0	0	0
			2196	1384	385	422	5			
1	E	270	Total	C	N	O	S	0	0	0
			2196	1384	385	422	5			
1	G	270	Total	C	N	O	S	0	0	0
			2196	1384	385	422	5			
1	I	270	Total	C	N	O	S	0	0	0
			2196	1384	385	422	5			

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	264	Total	C	N	O	S	0	0	0
			2090	1305	363	412	10			
2	D	264	Total	C	N	O	S	0	0	0
			2090	1305	363	412	10			
2	F	250	Total	C	N	O	S	0	0	0
			1967	1227	340	390	10			
2	H	249	Total	C	N	O	S	0	0	0
			1959	1223	338	388	10			
2	J	249	Total	C	N	O	S	0	0	0
			1959	1223	338	388	10			

- Molecule 3 is a protein called 32mer peptide from Leucine-rich repeat-containing protein 16A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	X	29	Total	C	N	O	0	0	0
			247	154	50	43			
3	Y	28	Total	C	N	O	0	0	0
			239	148	49	42			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	Z	28	Total	C	N	O	0	0	0
			239	148	49	42			
3	W	26	Total	C	N	O	0	0	0
			225	139	47	39			
3	V	21	Total	C	N	O	0	0	0
			182	113	39	30			

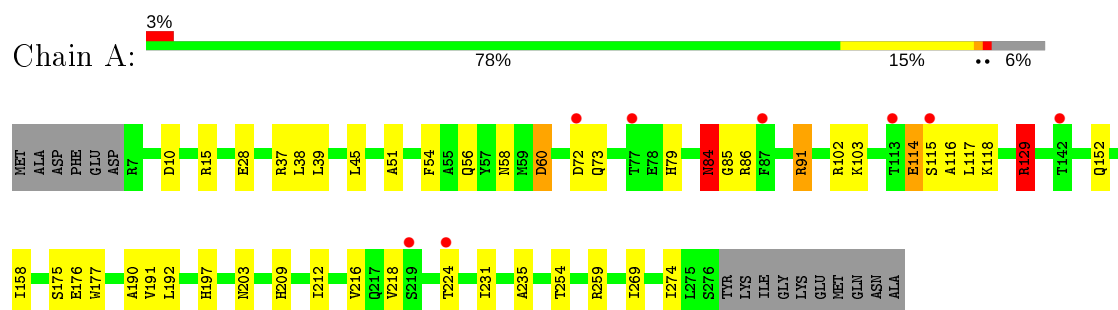
There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	966	GLY	-	EXPRESSION TAG	UNP Q6EDY6
X	967	PRO	-	EXPRESSION TAG	UNP Q6EDY6
X	968	LEU	-	EXPRESSION TAG	UNP Q6EDY6
X	969	GLY	-	EXPRESSION TAG	UNP Q6EDY6
X	970	SER	-	EXPRESSION TAG	UNP Q6EDY6
Y	966	GLY	-	EXPRESSION TAG	UNP Q6EDY6
Y	967	PRO	-	EXPRESSION TAG	UNP Q6EDY6
Y	968	LEU	-	EXPRESSION TAG	UNP Q6EDY6
Y	969	GLY	-	EXPRESSION TAG	UNP Q6EDY6
Y	970	SER	-	EXPRESSION TAG	UNP Q6EDY6
Z	966	GLY	-	EXPRESSION TAG	UNP Q6EDY6
Z	967	PRO	-	EXPRESSION TAG	UNP Q6EDY6
Z	968	LEU	-	EXPRESSION TAG	UNP Q6EDY6
Z	969	GLY	-	EXPRESSION TAG	UNP Q6EDY6
Z	970	SER	-	EXPRESSION TAG	UNP Q6EDY6
W	966	GLY	-	EXPRESSION TAG	UNP Q6EDY6
W	967	PRO	-	EXPRESSION TAG	UNP Q6EDY6
W	968	LEU	-	EXPRESSION TAG	UNP Q6EDY6
W	969	GLY	-	EXPRESSION TAG	UNP Q6EDY6
W	970	SER	-	EXPRESSION TAG	UNP Q6EDY6
V	966	GLY	-	EXPRESSION TAG	UNP Q6EDY6
V	967	PRO	-	EXPRESSION TAG	UNP Q6EDY6
V	968	LEU	-	EXPRESSION TAG	UNP Q6EDY6
V	969	GLY	-	EXPRESSION TAG	UNP Q6EDY6
V	970	SER	-	EXPRESSION TAG	UNP Q6EDY6

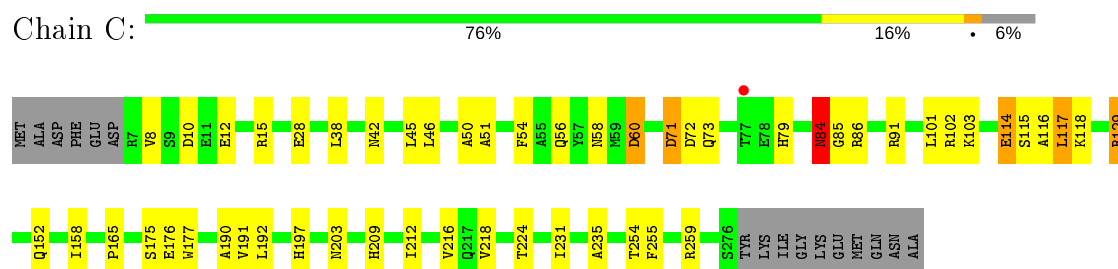
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

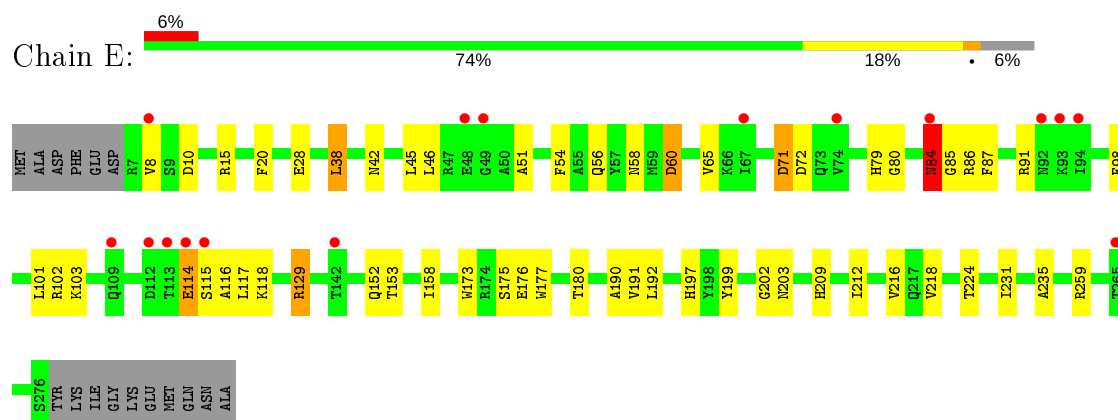
- Molecule 1: F-actin-capping protein subunit alpha-1



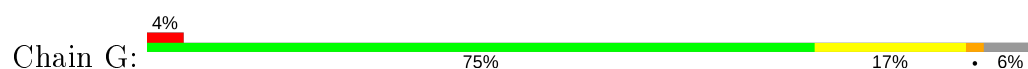
- Molecule 1: F-actin-capping protein subunit alpha-1

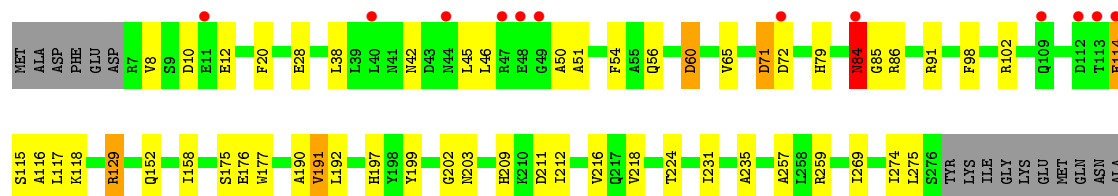


- Molecule 1: F-actin-capping protein subunit alpha-1

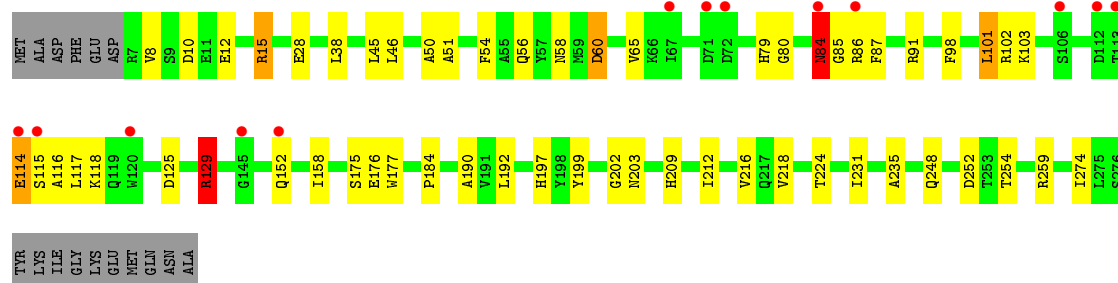


- Molecule 1: F-actin-capping protein subunit alpha-1

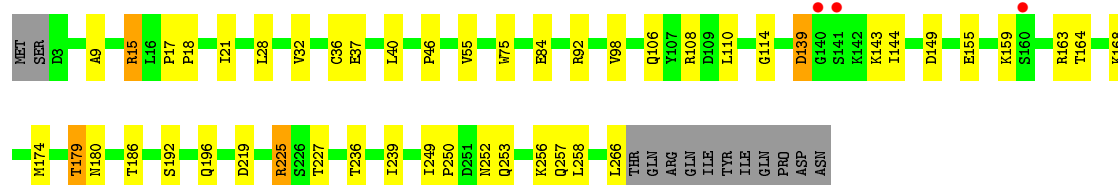
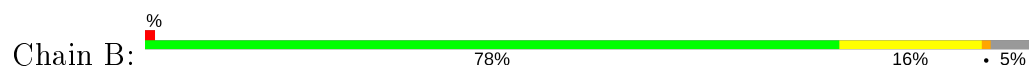




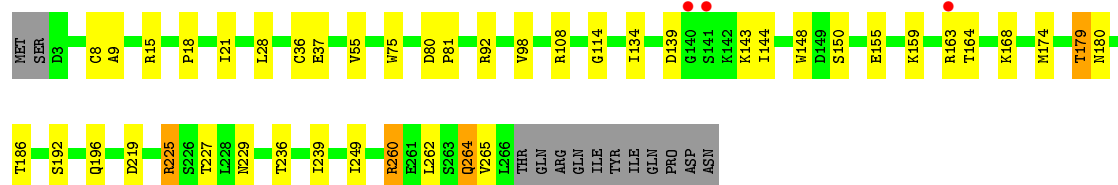
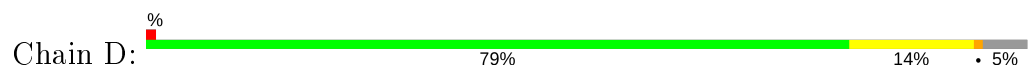
• Molecule 1: F-actin-capping protein subunit alpha-1



• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

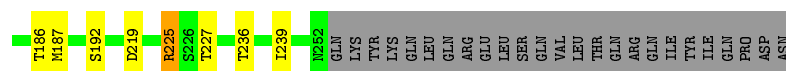


• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

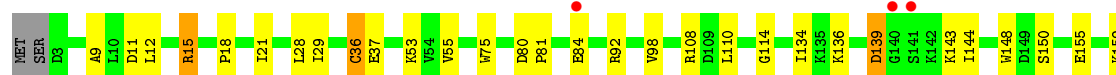
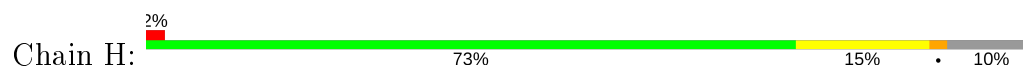


• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

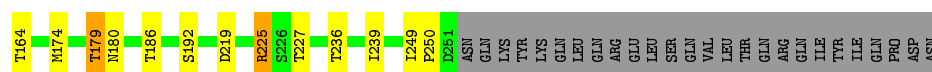
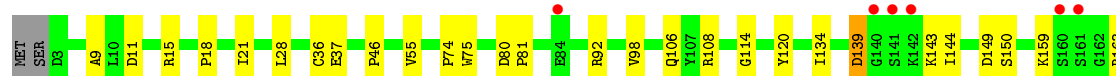
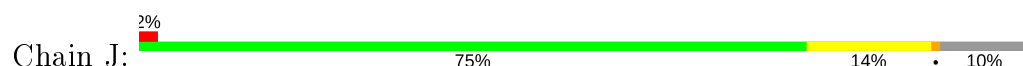




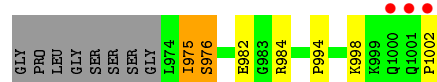
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



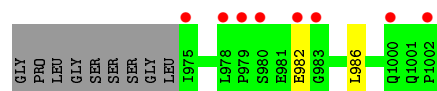
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



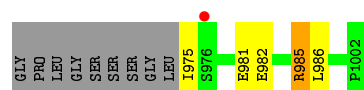
- Molecule 3: 32mer peptide from Leucine-rich repeat-containing protein 16A



- Molecule 3: 32mer peptide from Leucine-rich repeat-containing protein 16A

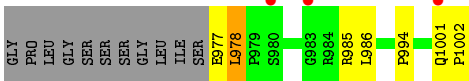


- Molecule 3: 32mer peptide from Leucine-rich repeat-containing protein 16A

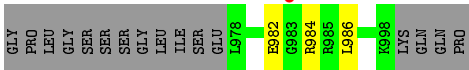


- Molecule 3: 32mer peptide from Leucine-rich repeat-containing protein 16A





- Molecule 3: 32mer peptide from Leucine-rich repeat-containing protein 16A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	231.15Å 104.36Å 186.63Å 90.00° 119.09° 90.00°	Depositor
Resolution (Å)	49.70 – 3.30 49.70 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.70-3.30) 99.5 (49.70-3.30)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.65 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.243 , 0.271 0.228 , 0.255	Depositor DCC
$R_{free}$ test set	2955 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 16.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22177	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.47	0/2247	0.90	8/3046 (0.3%)
1	C	0.47	0/2247	0.60	1/3046 (0.0%)
1	E	0.49	0/2247	0.63	1/3046 (0.0%)
1	G	0.48	0/2247	0.59	0/3046
1	I	0.49	0/2247	0.76	5/3046 (0.2%)
2	B	0.54	0/2125	0.63	4/2869 (0.1%)
2	D	0.51	1/2125 (0.0%)	0.77	5/2869 (0.2%)
2	F	0.48	0/2001	0.75	4/2704 (0.1%)
2	H	0.51	0/1993	0.62	3/2693 (0.1%)
2	J	0.52	0/1993	0.61	2/2693 (0.1%)
3	V	0.52	0/185	0.63	0/244
3	W	0.56	0/229	0.64	0/303
3	X	0.52	0/251	0.71	0/333
3	Y	0.49	0/243	0.62	0/322
3	Z	0.51	0/243	0.65	0/322
All	All	0.50	1/22623 (0.0%)	0.69	33/30582 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	CYS	CB-SG	-5.62	1.72	1.81

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	NE-CZ-NH1	-18.03	111.28	120.30
1	A	129	ARG	NE-CZ-NH2	17.82	129.21	120.30
1	A	91	ARG	NE-CZ-NH2	17.79	129.19	120.30
1	A	91	ARG	NE-CZ-NH1	-17.58	111.51	120.30
1	I	15	ARG	NE-CZ-NH2	-17.44	111.58	120.30
2	F	163	ARG	NE-CZ-NH1	-16.91	111.85	120.30
1	I	15	ARG	NE-CZ-NH1	16.90	128.75	120.30
2	D	15	ARG	NE-CZ-NH1	-16.88	111.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	15	ARG	NE-CZ-NH2	16.29	128.44	120.30
2	F	163	ARG	NE-CZ-NH2	14.66	127.63	120.30
1	A	129	ARG	CD-NE-CZ	8.85	135.99	123.60
1	A	91	ARG	CD-NE-CZ	8.69	135.76	123.60
1	I	15	ARG	CD-NE-CZ	8.36	135.30	123.60
2	F	163	ARG	CD-NE-CZ	8.04	134.85	123.60
2	D	15	ARG	CD-NE-CZ	7.48	134.07	123.60
2	H	15	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	C	15	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	E	15	ARG	NE-CZ-NH2	6.08	123.34	120.30
2	J	163	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	15	ARG	NE-CZ-NH2	5.73	123.17	120.30
2	D	163	ARG	NE-CZ-NH1	5.65	123.12	120.30
2	B	163	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	H	163	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	163	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	J	163	ARG	NE-CZ-NH2	-5.49	117.55	120.30
2	D	249	ILE	C-N-CD	5.49	139.93	128.40
2	F	15	ARG	NE-CZ-NH1	5.37	122.99	120.30
2	H	15	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	B	15	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	B	15	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	I	129	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	15	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	I	101	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2196	0	2117	36	0
1	C	2196	0	2117	31	0
1	E	2196	0	2117	33	0
1	G	2196	0	2117	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	2196	0	2117	35	0
2	B	2090	0	2076	37	0
2	D	2090	0	2076	24	0
2	F	1967	0	1943	24	0
2	H	1959	0	1937	29	0
2	J	1959	0	1937	27	0
3	V	182	0	192	1	0
3	W	225	0	234	3	0
3	X	247	0	261	14	0
3	Y	239	0	250	1	0
3	Z	239	0	250	3	0
All	All	22177	0	21741	295	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 7.

All (295) 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)
3:X:975:ILE:HG23	3:X:976:SER:H	1.03	1.12
3:X:975:ILE:HG23	3:X:976:SER:N	1.64	1.06
2:H:174:MET:HG2	2:H:192:SER:HB3	1.42	1.01
2:B:174:MET:HG2	2:B:192:SER:HB3	1.44	0.99
2:D:174:MET:HG2	2:D:192:SER:HB3	1.42	0.98
2:F:174:MET:HG2	2:F:192:SER:HB3	1.46	0.97
2:J:174:MET:HG2	2:J:192:SER:HB3	1.43	0.97
1:E:28:GLU:OE1	1:E:197:HIS:HD2	1.50	0.93
1:A:28:GLU:OE1	1:A:197:HIS:HD2	1.55	0.88
1:I:28:GLU:OE1	1:I:197:HIS:HD2	1.57	0.86
1:G:28:GLU:OE1	1:G:197:HIS:HD2	1.59	0.84
1:C:28:GLU:OE1	1:C:197:HIS:HD2	1.60	0.84
3:X:975:ILE:CG2	3:X:976:SER:N	2.39	0.82
2:J:180:ASN:ND2	2:J:186:THR:HG22	1.96	0.81
2:J:249:ILE:HG23	2:J:250:PRO:HD2	1.63	0.78
1:G:275:LEU:HD11	2:H:211:ALA:HB2	1.65	0.77
1:A:37:ARG:NH1	3:X:975:ILE:HG21	2.00	0.77
2:H:180:ASN:ND2	2:H:186:THR:HG22	1.99	0.77
1:A:91:ARG:NH1	1:A:129:ARG:HG3	2.00	0.76
1:E:212:ILE:HD13	1:E:235:ALA:HB1	1.70	0.74
2:B:180:ASN:ND2	2:B:186:THR:HG22	2.02	0.74
2:D:180:ASN:ND2	2:D:186:THR:HG22	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:212:ILE:HD13	1:I:235:ALA:HB1	1.70	0.71
1:A:212:ILE:HD13	1:A:235:ALA:HB1	1.74	0.70
2:F:180:ASN:ND2	2:F:186:THR:HG22	2.05	0.70
1:C:212:ILE:HD13	1:C:235:ALA:HB1	1.75	0.67
1:G:212:ILE:HD13	1:G:235:ALA:HB1	1.78	0.66
2:B:144:ILE:HG12	2:B:179:THR:CG2	2.25	0.66
2:J:144:ILE:HG12	2:J:179:THR:CG2	2.26	0.66
2:J:9:ALA:HB1	2:J:28:LEU:HD21	1.81	0.63
2:D:260:ARG:O	2:D:264:GLN:HB2	1.98	0.63
2:F:144:ILE:HG12	2:F:179:THR:CG2	2.28	0.63
1:E:28:GLU:OE1	1:E:197:HIS:CD2	2.42	0.62
1:A:91:ARG:NH1	1:A:129:ARG:HD2	2.14	0.62
1:G:259:ARG:O	2:H:225:ARG:NH1	2.33	0.62
1:G:275:LEU:CD1	2:H:211:ALA:HB2	2.30	0.62
1:G:216:VAL:HG11	1:G:231:ILE:HD11	1.83	0.61
2:J:18:PRO:HA	2:J:21:ILE:HG13	1.83	0.61
1:C:216:VAL:HG11	1:C:231:ILE:HD11	1.83	0.61
1:E:84:ASN:HD22	1:E:86:ARG:HB2	1.66	0.60
2:H:144:ILE:HG12	2:H:179:THR:CG2	2.32	0.60
2:B:40:LEU:HD12	3:X:1002:PRO:HG2	1.82	0.60
1:I:259:ARG:O	2:J:225:ARG:NH1	2.35	0.60
2:J:180:ASN:HD22	2:J:186:THR:HG22	1.65	0.59
1:E:259:ARG:O	2:F:225:ARG:NH1	2.36	0.59
1:C:259:ARG:O	2:D:225:ARG:NH1	2.34	0.59
2:F:11:ASP:OD1	2:F:15:ARG:NH1	2.34	0.59
1:A:37:ARG:NH1	3:X:975:ILE:CG2	2.65	0.59
2:D:144:ILE:HG12	2:D:179:THR:CG2	2.33	0.58
1:I:56:GLN:O	1:I:60:ASP:HB2	2.04	0.58
1:E:117:LEU:HD11	1:E:152:GLN:HB3	1.84	0.58
2:D:108:ARG:HD2	2:D:114:GLY:O	2.03	0.58
1:I:212:ILE:CD1	1:I:235:ALA:HB1	2.34	0.58
2:B:9:ALA:HB1	2:B:28:LEU:HD21	1.85	0.57
1:C:197:HIS:HE1	1:C:203:ASN:OD1	1.87	0.57
2:H:236:THR:HA	2:H:239:ILE:HD12	1.85	0.57
1:E:46:LEU:HD23	3:Z:975:ILE:HD13	1.86	0.57
1:E:216:VAL:HG11	1:E:231:ILE:HD11	1.86	0.57
1:I:158:ILE:HB	1:I:175:SER:HB2	1.87	0.57
1:A:218:VAL:HA	1:A:224:THR:HG21	1.87	0.57
1:G:158:ILE:HB	1:G:175:SER:HB2	1.86	0.57
2:D:80:ASP:OD2	2:H:53:LYS:HD2	2.04	0.57
1:C:165:PRO:HB2	3:Y:982:GLU:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LEU:O	1:E:209:HIS:HA	2.05	0.56
1:C:91:ARG:HH12	1:C:129:ARG:HG3	1.70	0.56
2:J:144:ILE:HG12	2:J:179:THR:HG21	1.87	0.56
1:E:56:GLN:O	1:E:60:ASP:HB2	2.05	0.56
1:G:192:LEU:O	1:G:209:HIS:HA	2.06	0.56
1:A:91:ARG:HH12	1:A:129:ARG:HG3	1.67	0.56
1:A:216:VAL:HG11	1:A:231:ILE:HD11	1.88	0.56
1:I:84:ASN:HD22	1:I:86:ARG:HB2	1.69	0.56
2:D:18:PRO:HA	2:D:21:ILE:HG13	1.86	0.56
1:G:218:VAL:HA	1:G:224:THR:HG21	1.88	0.56
1:I:91:ARG:HH12	1:I:129:ARG:HG3	1.71	0.56
1:A:84:ASN:HD22	1:A:86:ARG:HB2	1.70	0.55
1:I:79:HIS:HE1	1:I:176:GLU:OE2	1.88	0.55
2:F:236:THR:HA	2:F:239:ILE:HD12	1.88	0.55
1:I:117:LEU:HD11	1:I:152:GLN:HB3	1.89	0.55
1:A:56:GLN:O	1:A:60:ASP:HB2	2.05	0.55
1:G:91:ARG:HH12	1:G:129:ARG:HG3	1.72	0.55
1:C:218:VAL:HA	1:C:224:THR:HG21	1.89	0.55
1:G:10:ASP:HB3	1:G:45:LEU:HD11	1.89	0.55
1:E:218:VAL:HA	1:E:224:THR:HG21	1.88	0.54
1:E:212:ILE:CD1	1:E:235:ALA:HB1	2.35	0.54
2:H:143:LYS:O	2:H:179:THR:HG22	2.07	0.54
2:H:18:PRO:HA	2:H:21:ILE:HG13	1.89	0.54
2:B:108:ARG:HD2	2:B:114:GLY:O	2.06	0.54
2:B:159:LYS:HG3	2:B:164:THR:HG23	1.90	0.54
1:C:84:ASN:HD22	1:C:86:ARG:HB2	1.73	0.54
2:D:236:THR:HA	2:D:239:ILE:HD12	1.90	0.54
2:H:9:ALA:HB1	2:H:28:LEU:HD21	1.90	0.54
1:C:91:ARG:NH1	1:C:129:ARG:HG3	2.23	0.54
2:F:18:PRO:HA	2:F:21:ILE:HG13	1.90	0.54
1:I:91:ARG:NH1	1:I:129:ARG:HG3	2.23	0.54
1:I:192:LEU:O	1:I:209:HIS:HA	2.08	0.54
1:A:91:ARG:NH1	1:A:129:ARG:CG	2.71	0.54
1:I:197:HIS:HE1	1:I:203:ASN:OD1	1.91	0.53
1:C:212:ILE:CD1	1:C:235:ALA:HB1	2.38	0.53
1:G:117:LEU:HD11	1:G:152:GLN:HB3	1.89	0.53
2:H:144:ILE:HG12	2:H:179:THR:HG21	1.91	0.53
2:B:18:PRO:HA	2:B:21:ILE:HG13	1.89	0.53
1:I:216:VAL:HG11	1:I:231:ILE:HD11	1.90	0.53
2:B:144:ILE:HG12	2:B:179:THR:HG21	1.88	0.53
1:A:197:HIS:HE1	1:A:203:ASN:OD1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:9:ALA:HB1	2:F:28:LEU:HD21	1.91	0.53
1:G:56:GLN:O	1:G:60:ASP:HB2	2.07	0.53
1:G:28:GLU:OE1	1:G:197:HIS:CD2	2.51	0.52
2:J:236:THR:HA	2:J:239:ILE:HD12	1.90	0.52
2:F:144:ILE:HG12	2:F:179:THR:HG21	1.89	0.52
2:B:155:GLU:HB2	3:X:994:PRO:HG3	1.90	0.52
2:B:236:THR:HA	2:B:239:ILE:HD12	1.91	0.52
1:E:10:ASP:HB3	1:E:45:LEU:HD11	1.92	0.52
2:H:180:ASN:HD22	2:H:186:THR:HG22	1.72	0.52
1:I:218:VAL:HA	1:I:224:THR:HG21	1.90	0.52
1:A:192:LEU:O	1:A:209:HIS:HA	2.09	0.52
1:G:84:ASN:HD22	1:G:86:ARG:HB2	1.75	0.52
1:E:79:HIS:HE1	1:E:176:GLU:OE2	1.92	0.52
2:H:159:LYS:HG3	2:H:164:THR:HG23	1.91	0.52
2:D:174:MET:HG2	2:D:192:SER:CB	2.29	0.51
2:J:108:ARG:HD2	2:J:114:GLY:O	2.10	0.51
2:B:252:ASN:HD21	2:B:256:LYS:NZ	2.07	0.51
1:C:10:ASP:HB3	1:C:45:LEU:HD11	1.91	0.51
2:B:15:ARG:HH22	3:X:982:GLU:CD	2.14	0.51
2:B:258:LEU:HD23	2:D:262:LEU:HD22	1.93	0.51
1:C:56:GLN:O	1:C:60:ASP:HB2	2.10	0.51
3:X:998:LYS:NZ	3:X:1002:PRO:HG3	2.26	0.51
2:D:143:LYS:O	2:D:179:THR:HG22	2.11	0.51
1:G:91:ARG:NH1	1:G:129:ARG:HG3	2.25	0.51
2:B:180:ASN:HD22	2:B:186:THR:HG22	1.72	0.51
2:F:174:MET:HG2	2:F:192:SER:CB	2.31	0.51
2:D:55:VAL:HG21	2:D:75:TRP:HB3	1.92	0.50
1:C:197:HIS:CE1	1:C:203:ASN:OD1	2.64	0.50
2:B:143:LYS:O	2:B:179:THR:HG22	2.12	0.50
2:F:55:VAL:HG21	2:F:75:TRP:HB3	1.93	0.50
3:X:975:ILE:CG2	3:X:976:SER:H	1.87	0.50
2:J:143:LYS:O	2:J:179:THR:HG22	2.11	0.50
1:A:117:LEU:HD11	1:A:152:GLN:HB3	1.94	0.50
2:D:9:ALA:HB1	2:D:28:LEU:HD21	1.94	0.50
2:H:55:VAL:HG21	2:H:75:TRP:HB3	1.94	0.50
2:B:174:MET:HG2	2:B:192:SER:CB	2.28	0.50
1:G:257:ALA:O	2:H:136:LYS:NZ	2.44	0.50
1:G:212:ILE:CD1	1:G:235:ALA:HB1	2.42	0.50
2:F:143:LYS:O	2:F:179:THR:HG22	2.12	0.49
2:J:159:LYS:HG3	2:J:164:THR:HG23	1.94	0.49
1:A:28:GLU:OE1	1:A:197:HIS:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HB	1:C:175:SER:HB2	1.95	0.49
2:D:180:ASN:HD22	2:D:186:THR:HG22	1.76	0.49
1:I:197:HIS:CE1	1:I:203:ASN:OD1	2.65	0.49
2:B:40:LEU:CD1	3:X:1002:PRO:HG2	2.43	0.49
1:I:274:ILE:HG23	2:J:106:GLN:HE21	1.77	0.49
2:D:159:LYS:HG3	2:D:164:THR:HG23	1.95	0.49
2:H:108:ARG:HD2	2:H:114:GLY:O	2.12	0.49
2:H:11:ASP:OD1	2:H:15:ARG:NH1	2.44	0.49
1:A:79:HIS:HE1	1:A:176:GLU:OE2	1.96	0.49
1:A:212:ILE:CD1	1:A:235:ALA:HB1	2.42	0.49
1:A:254:THR:HG21	2:B:144:ILE:HB	1.95	0.49
1:A:274:ILE:HG23	2:B:106:GLN:HE21	1.77	0.49
1:C:192:LEU:O	1:C:209:HIS:HA	2.13	0.49
1:A:274:ILE:HG23	2:B:106:GLN:NE2	2.27	0.48
2:J:174:MET:HG2	2:J:192:SER:CB	2.30	0.48
1:A:91:ARG:HH11	1:A:129:ARG:HD2	1.79	0.48
2:H:174:MET:HG2	2:H:192:SER:CB	2.30	0.48
2:F:108:ARG:HD2	2:F:114:GLY:O	2.14	0.47
2:F:15:ARG:NH2	3:Z:982:GLU:OE2	2.47	0.47
1:I:274:ILE:HG23	2:J:106:GLN:NE2	2.28	0.47
2:B:55:VAL:HG21	2:B:75:TRP:HB3	1.96	0.47
2:H:155:GLU:HB2	3:W:994:PRO:HG3	1.96	0.47
1:C:79:HIS:HE1	1:C:176:GLU:OE2	1.97	0.47
1:A:259:ARG:O	2:B:225:ARG:NH1	2.46	0.47
2:D:144:ILE:HG12	2:D:179:THR:HG21	1.94	0.47
2:F:159:LYS:HG3	2:F:164:THR:HG23	1.95	0.47
1:A:197:HIS:CE1	1:A:203:ASN:OD1	2.68	0.47
1:E:158:ILE:HB	1:E:175:SER:HB2	1.96	0.47
2:J:139:ASP:N	2:J:139:ASP:OD1	2.46	0.47
1:A:158:ILE:HB	1:A:175:SER:HB2	1.96	0.47
2:J:55:VAL:HG21	2:J:75:TRP:HB3	1.96	0.47
1:G:71:ASP:HA	1:G:72:ASP:HA	1.42	0.47
1:E:71:ASP:HA	1:E:72:ASP:HA	1.42	0.47
2:F:180:ASN:HD22	2:F:186:THR:HG22	1.77	0.47
2:B:15:ARG:NH2	3:X:982:GLU:OE2	2.48	0.47
1:A:39:LEU:HD22	2:B:32:VAL:HG21	1.97	0.46
1:I:114:GLU:C	1:I:116:ALA:H	2.18	0.46
2:B:15:ARG:NH2	3:X:982:GLU:CD	2.69	0.46
2:F:46:PRO:HA	2:F:174:MET:HE3	1.97	0.46
2:H:139:ASP:OD1	2:H:139:ASP:N	2.45	0.46
1:A:114:GLU:C	1:A:116:ALA:H	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:PHE:CD2	2:F:12:LEU:HD21	2.51	0.46
1:E:91:ARG:NH1	1:E:129:ARG:HG3	2.31	0.45
2:F:139:ASP:OD1	2:F:139:ASP:N	2.45	0.45
3:Z:985:ARG:HB2	3:Z:985:ARG:HE	1.44	0.45
1:C:46:LEU:O	1:C:50:ALA:HB3	2.16	0.45
1:I:177:TRP:CE3	1:I:190:ALA:HB2	2.51	0.45
1:A:10:ASP:HB3	1:A:45:LEU:HD11	1.99	0.45
2:B:139:ASP:OD1	2:B:139:ASP:N	2.47	0.45
1:E:91:ARG:HH12	1:E:129:ARG:HG3	1.81	0.45
1:I:51:ALA:HA	1:I:54:PHE:CD2	2.52	0.45
1:C:51:ALA:HA	1:C:54:PHE:CD2	2.51	0.45
1:G:199:TYR:HA	1:G:202:GLY:O	2.16	0.45
2:H:155:GLU:HB3	2:H:168:LYS:HB2	1.98	0.45
1:A:91:ARG:NH1	1:A:129:ARG:CD	2.79	0.45
1:A:177:TRP:CE3	1:A:190:ALA:HB2	2.52	0.45
1:C:177:TRP:CE3	1:C:190:ALA:HB2	2.52	0.45
1:G:114:GLU:C	1:G:116:ALA:H	2.21	0.44
1:C:254:THR:HG21	2:D:144:ILE:HB	2.00	0.44
1:G:20:PHE:CD2	2:H:12:LEU:HD21	2.53	0.44
1:A:72:ASP:HB3	1:A:73:GLN:H	1.60	0.44
1:E:114:GLU:C	1:E:116:ALA:H	2.19	0.44
1:E:80:GLY:O	1:E:87:PHE:HA	2.17	0.44
1:I:28:GLU:OE1	1:I:197:HIS:CD2	2.50	0.44
2:D:134:ILE:HB	2:D:150:SER:HB2	1.98	0.44
2:H:80:ASP:HA	2:H:81:PRO:C	2.38	0.44
1:C:72:ASP:HB3	1:C:73:GLN:H	1.62	0.44
1:G:79:HIS:HE1	1:G:176:GLU:OE2	2.00	0.44
1:A:51:ALA:HA	1:A:54:PHE:CD2	2.53	0.44
3:X:998:LYS:HZ3	3:X:1002:PRO:HG3	1.82	0.44
2:J:249:ILE:CG2	2:J:250:PRO:HD2	2.40	0.44
1:C:114:GLU:C	1:C:116:ALA:H	2.21	0.43
1:G:65:VAL:HG21	1:G:98:PHE:HE1	1.84	0.43
1:I:10:ASP:HB3	1:I:45:LEU:HD11	1.98	0.43
1:I:254:THR:HG21	2:J:144:ILE:HB	2.00	0.43
2:J:149:ASP:HB2	2:J:174:MET:HB2	2.00	0.43
1:C:51:ALA:HA	1:C:54:PHE:HD2	1.84	0.43
1:E:197:HIS:HE1	1:E:203:ASN:OD1	2.01	0.43
1:E:51:ALA:HA	1:E:54:PHE:CD2	2.54	0.43
2:B:46:PRO:HA	2:B:174:MET:HE3	2.00	0.43
1:E:177:TRP:CE3	1:E:190:ALA:HB2	2.54	0.43
1:E:65:VAL:HG21	1:E:98:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:197:HIS:CE1	1:G:203:ASN:OD1	2.72	0.43
2:H:134:ILE:HB	2:H:150:SER:HB2	1.99	0.43
1:A:58:ASN:HD21	1:A:103:LYS:HE2	1.82	0.43
1:C:8:VAL:CG1	1:C:12:GLU:HG2	2.49	0.43
1:E:38:LEU:HD21	2:F:4:GLN:NE2	2.34	0.43
1:G:177:TRP:CE3	1:G:190:ALA:HB2	2.53	0.43
2:J:80:ASP:HA	2:J:81:PRO:C	2.39	0.43
3:V:982:GLU:HB2	3:V:984:ARG:HG2	2.01	0.43
3:W:1001:GLN:HA	3:W:1002:PRO:HD2	1.74	0.43
1:G:197:HIS:HE1	1:G:203:ASN:OD1	2.01	0.43
1:C:71:ASP:HA	1:C:72:ASP:HA	1.40	0.42
1:E:58:ASN:HD21	1:E:103:LYS:HE2	1.84	0.42
1:G:51:ALA:HA	1:G:54:PHE:CD2	2.54	0.42
1:I:248:GLN:NE2	1:I:252:ASP:OD2	2.41	0.42
1:C:58:ASN:HD21	1:C:103:LYS:HE2	1.83	0.42
2:H:148:TRP:CD1	2:H:148:TRP:C	2.92	0.42
1:I:51:ALA:HA	1:I:54:PHE:HD2	1.84	0.42
2:J:74:PRO:HD3	2:J:120:TYR:HE1	1.84	0.42
2:D:80:ASP:HA	2:D:81:PRO:C	2.40	0.42
1:I:46:LEU:O	1:I:50:ALA:HB3	2.19	0.42
2:B:17:PRO:HA	2:B:18:PRO:HD2	1.95	0.42
1:I:114:GLU:O	1:I:116:ALA:N	2.52	0.42
2:J:134:ILE:HB	2:J:150:SER:HB2	2.02	0.42
1:C:117:LEU:HD21	1:C:152:GLN:HB3	2.02	0.42
1:E:197:HIS:CE1	1:E:203:ASN:OD1	2.73	0.42
2:J:74:PRO:HD3	2:J:120:TYR:CE1	2.55	0.42
2:F:134:ILE:HB	2:F:150:SER:HB2	2.02	0.42
2:H:110:LEU:HG	1:I:184:PRO:HG2	2.01	0.42
1:I:80:GLY:O	1:I:87:PHE:HA	2.19	0.42
1:E:173:TRP:CD1	1:E:173:TRP:C	2.93	0.42
2:F:108:ARG:HB3	2:F:108:ARG:CZ	2.49	0.42
1:A:274:ILE:HA	2:B:106:GLN:HE22	1.85	0.42
1:I:58:ASN:HD21	1:I:103:LYS:HE2	1.84	0.42
1:I:8:VAL:CG1	1:I:12:GLU:HG2	2.50	0.42
1:A:269:ILE:HG12	2:B:110:LEU:HD13	2.02	0.41
2:B:196:GLN:HE21	2:B:196:GLN:HB2	1.66	0.41
1:G:117:LEU:O	1:G:118:LYS:C	2.58	0.41
2:B:253:GLN:O	2:B:257:GLN:HB2	2.19	0.41
2:D:196:GLN:HB2	2:D:196:GLN:HE21	1.60	0.41
2:J:11:ASP:OD1	2:J:15:ARG:NH1	2.50	0.41
2:D:148:TRP:CD1	2:D:148:TRP:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:ALA:HA	1:G:54:PHE:HD2	1.86	0.41
1:E:199:TYR:HA	1:E:202:GLY:O	2.20	0.41
1:G:269:ILE:HG21	1:G:274:ILE:HD12	2.03	0.41
1:G:8:VAL:CG1	1:G:12:GLU:HG2	2.49	0.41
2:D:155:GLU:HB3	2:D:168:LYS:HB2	2.02	0.41
1:A:117:LEU:O	1:A:118:LYS:C	2.59	0.41
2:B:249:ILE:HA	2:B:250:PRO:HD2	1.54	0.41
1:E:117:LEU:O	1:E:118:LYS:C	2.59	0.41
2:B:252:ASN:HD21	2:B:256:LYS:HZ1	1.68	0.41
1:C:114:GLU:O	1:C:116:ALA:N	2.54	0.41
1:E:114:GLU:O	1:E:116:ALA:N	2.54	0.41
1:G:46:LEU:O	1:G:50:ALA:HB3	2.20	0.41
1:I:199:TYR:HA	1:I:202:GLY:O	2.21	0.41
2:J:46:PRO:HA	2:J:174:MET:HE3	2.03	0.41
3:W:977:GLU:O	3:W:978:LEU:HD12	2.21	0.41
1:E:153:THR:OG1	1:E:180:THR:HG22	2.20	0.41
1:G:259:ARG:NH1	2:H:222:ASN:OD1	2.43	0.41
1:I:65:VAL:HG21	1:I:98:PHE:HE1	1.86	0.41
1:C:255:PHE:CE2	2:D:229:ASN:HB2	2.57	0.40
2:F:155:GLU:HB3	2:F:168:LYS:HB2	2.03	0.40
1:G:191:VAL:HG23	1:G:211:ASP:OD1	2.21	0.40
2:H:29:ILE:HG12	2:H:36:CYS:HA	2.03	0.40
2:B:149:ASP:HB2	2:B:174:MET:HB2	2.02	0.40
1:C:117:LEU:O	1:C:118:LYS:C	2.58	0.40
2:F:178:GLN:HA	2:F:187:MET:O	2.22	0.40
2:B:155:GLU:HB3	2:B:168:LYS:HB2	2.04	0.40
1:I:117:LEU:O	1:I:118:LYS:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/286 (94%)	247 (92%)	17 (6%)	4 (2%)	10	38
1	C	268/286 (94%)	247 (92%)	16 (6%)	5 (2%)	8	34
1	E	268/286 (94%)	246 (92%)	17 (6%)	5 (2%)	8	34
1	G	268/286 (94%)	247 (92%)	16 (6%)	5 (2%)	8	34
1	I	268/286 (94%)	247 (92%)	16 (6%)	5 (2%)	8	34
2	B	262/277 (95%)	249 (95%)	11 (4%)	2 (1%)	19	51
2	D	262/277 (95%)	247 (94%)	13 (5%)	2 (1%)	19	51
2	F	248/277 (90%)	233 (94%)	14 (6%)	1 (0%)	34	66
2	H	247/277 (89%)	235 (95%)	9 (4%)	3 (1%)	13	42
2	J	247/277 (89%)	232 (94%)	14 (6%)	1 (0%)	34	66
3	V	19/37 (51%)	17 (90%)	2 (10%)	0	100	100
3	W	24/37 (65%)	19 (79%)	5 (21%)	0	100	100
3	X	27/37 (73%)	24 (89%)	2 (7%)	1 (4%)	3	20
3	Y	26/37 (70%)	23 (88%)	3 (12%)	0	100	100
3	Z	26/37 (70%)	26 (100%)	0	0	100	100
All	All	2728/3000 (91%)	2539 (93%)	155 (6%)	34 (1%)	13	42

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	115	SER
1	E	115	SER
1	G	84	ASN
1	I	115	SER
2	J	36	CYS
3	X	975	ILE
1	A	84	ASN
1	A	85	GLY
1	A	115	SER
1	C	84	ASN
1	C	85	GLY
1	C	114	GLU
2	D	36	CYS
2	D	265	VAL
1	E	84	ASN
1	E	85	GLY
1	G	85	GLY
1	G	115	SER

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Mol	Chain	Res	Type
2	H	36	CYS
1	I	84	ASN
1	I	85	GLY
1	I	114	GLU
2	B	36	CYS
2	B	84	GLU
1	E	114	GLU
2	F	36	CYS
1	A	114	GLU
1	C	42	ASN
1	E	42	ASN
1	G	42	ASN
1	G	114	GLU
2	H	84	GLU
1	I	125	ASP
2	H	208	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	239/252 (95%)	233 (98%)	6 (2%)	47	72
1	C	239/252 (95%)	230 (96%)	9 (4%)	33	62
1	E	239/252 (95%)	230 (96%)	9 (4%)	33	62
1	G	239/252 (95%)	232 (97%)	7 (3%)	42	69
1	I	239/252 (95%)	232 (97%)	7 (3%)	42	69
2	B	235/248 (95%)	226 (96%)	9 (4%)	33	62
2	D	235/248 (95%)	225 (96%)	10 (4%)	29	59
2	F	221/248 (89%)	213 (96%)	8 (4%)	35	63
2	H	220/248 (89%)	212 (96%)	8 (4%)	35	63
2	J	220/248 (89%)	212 (96%)	8 (4%)	35	63
3	V	20/33 (61%)	19 (95%)	1 (5%)	24	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W	25/33 (76%)	22 (88%)	3 (12%)	5	20
3	X	28/33 (85%)	26 (93%)	2 (7%)	14	42
3	Y	27/33 (82%)	26 (96%)	1 (4%)	34	63
3	Z	27/33 (82%)	24 (89%)	3 (11%)	6	23
All	All	2453/2665 (92%)	2362 (96%)	91 (4%)	34	63

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	60	ASP
1	A	84	ASN
1	A	102	ARG
1	A	129	ARG
1	A	191	VAL
2	B	37	GLU
2	B	92	ARG
2	B	98	VAL
2	B	139	ASP
2	B	179	THR
2	B	219	ASP
2	B	225	ARG
2	B	227	THR
2	B	266	LEU
1	C	38	LEU
1	C	60	ASP
1	C	71	ASP
1	C	84	ASN
1	C	101	LEU
1	C	102	ARG
1	C	117	LEU
1	C	129	ARG
1	C	191	VAL
2	D	37	GLU
2	D	92	ARG
2	D	98	VAL
2	D	139	ASP
2	D	179	THR
2	D	219	ASP
2	D	225	ARG
2	D	227	THR

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Mol	Chain	Res	Type
2	D	260	ARG
2	D	264	GLN
1	E	8	VAL
1	E	38	LEU
1	E	60	ASP
1	E	71	ASP
1	E	84	ASN
1	E	101	LEU
1	E	102	ARG
1	E	129	ARG
1	E	191	VAL
2	F	37	GLU
2	F	92	ARG
2	F	98	VAL
2	F	108	ARG
2	F	179	THR
2	F	219	ASP
2	F	225	ARG
2	F	227	THR
1	G	38	LEU
1	G	60	ASP
1	G	71	ASP
1	G	84	ASN
1	G	102	ARG
1	G	129	ARG
1	G	191	VAL
2	H	37	GLU
2	H	92	ARG
2	H	98	VAL
2	H	139	ASP
2	H	179	THR
2	H	219	ASP
2	H	225	ARG
2	H	227	THR
1	I	15	ARG
1	I	38	LEU
1	I	60	ASP
1	I	84	ASN
1	I	101	LEU
1	I	102	ARG
1	I	129	ARG
2	J	37	GLU

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Mol	Chain	Res	Type
2	J	92	ARG
2	J	98	VAL
2	J	139	ASP
2	J	179	THR
2	J	219	ASP
2	J	225	ARG
2	J	227	THR
3	X	976	SER
3	X	984	ARG
3	Y	986	LEU
3	Z	981	GLU
3	Z	985	ARG
3	Z	986	LEU
3	W	978	LEU
3	W	985	ARG
3	W	986	LEU
3	V	986	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	58	ASN
1	A	73	GLN
1	A	79	HIS
1	A	84	ASN
1	A	164	GLN
1	A	167	ASN
1	A	187	GLN
1	A	197	HIS
1	A	246	ASN
2	B	4	GLN
2	B	106	GLN
2	B	180	ASN
2	B	196	GLN
2	B	252	ASN
2	B	264	GLN
1	C	34	ASN
1	C	58	ASN
1	C	73	GLN
1	C	79	HIS
1	C	84	ASN

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Mol	Chain	Res	Type
1	C	164	GLN
1	C	167	ASN
1	C	197	HIS
1	C	205	GLN
1	C	246	ASN
2	D	4	GLN
2	D	106	GLN
2	D	180	ASN
2	D	196	GLN
1	E	34	ASN
1	E	58	ASN
1	E	73	GLN
1	E	79	HIS
1	E	84	ASN
1	E	197	HIS
1	E	246	ASN
2	F	4	GLN
2	F	106	GLN
2	F	180	ASN
2	F	196	GLN
1	G	34	ASN
1	G	58	ASN
1	G	73	GLN
1	G	79	HIS
1	G	84	ASN
1	G	92	ASN
1	G	164	GLN
1	G	167	ASN
1	G	197	HIS
1	G	217	GLN
2	H	4	GLN
2	H	180	ASN
2	H	196	GLN
1	I	34	ASN
1	I	58	ASN
1	I	73	GLN
1	I	79	HIS
1	I	84	ASN
1	I	164	GLN
1	I	167	ASN
1	I	197	HIS
1	I	246	ASN

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Mol	Chain	Res	Type
2	J	4	GLN
2	J	106	GLN
2	J	180	ASN
2	J	196	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 carbohydrates 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	270/286 (94%)	0.45	8 (2%)	50	49	31, 51, 85, 98	0
1	C	270/286 (94%)	0.42	1 (0%)	92	93	31, 51, 85, 98	0
1	E	270/286 (94%)	0.47	16 (5%)	22	22	31, 51, 85, 98	0
1	G	270/286 (94%)	0.41	12 (4%)	34	33	31, 51, 85, 98	0
1	I	270/286 (94%)	0.46	13 (4%)	30	28	31, 51, 85, 98	0
2	B	264/277 (95%)	0.35	3 (1%)	80	81	29, 44, 68, 81	0
2	D	264/277 (95%)	0.30	3 (1%)	80	81	29, 44, 69, 81	0
2	F	250/277 (90%)	0.08	3 (1%)	79	78	30, 43, 63, 72	0
2	H	249/277 (89%)	0.19	5 (2%)	65	64	30, 43, 62, 72	0
2	J	249/277 (89%)	0.20	6 (2%)	59	56	30, 43, 62, 72	0
3	V	21/37 (56%)	0.75	1 (4%)	30	28	56, 65, 79, 80	0
3	W	26/37 (70%)	0.83	3 (11%)	4	4	56, 70, 83, 85	0
3	X	29/37 (78%)	0.85	3 (10%)	6	6	56, 70, 79, 82	0
3	Y	28/37 (75%)	1.16	8 (28%)	0	0	56, 73, 82, 83	0
3	Z	28/37 (75%)	0.57	1 (3%)	42	40	56, 72, 81, 82	0
All	All	2758/3000 (91%)	0.36	86 (3%)	49	48	29, 47, 79, 98	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	1001	GLN	6.2
2	H	141	SER	5.6
2	J	141	SER	5.1
1	E	112	ASP	4.9
2	B	141	SER	4.8
3	V	983	GLY	4.3
3	X	1002	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	113	THR	4.1
2	F	141	SER	4.0
3	Z	976	SER	3.8
3	W	980	SER	3.6
1	I	114	GLU	3.5
2	J	160	SER	3.5
2	D	141	SER	3.5
1	I	84	ASN	3.4
2	J	161	SER	3.3
1	I	120	TRP	3.3
1	I	72	ASP	3.3
1	G	113	THR	3.2
1	I	106	SER	3.2
2	D	163	ARG	3.2
2	D	140	GLY	3.2
1	E	8	VAL	3.1
3	Y	980	SER	3.1
1	E	114	GLU	3.1
1	I	112	ASP	3.1
1	I	67	ILE	3.0
1	A	115	SER	3.0
2	J	140	GLY	2.9
3	W	983	GLY	2.9
2	H	140	GLY	2.9
1	E	93	LYS	2.9
2	B	160	SER	2.8
2	J	84	GLU	2.8
2	F	140	GLY	2.7
1	G	109	GLN	2.7
1	E	115	SER	2.7
1	E	74	VAL	2.7
1	A	87	PHE	2.6
3	Y	983	GLY	2.6
3	Y	975	ILE	2.6
1	I	71	ASP	2.6
1	A	219	SER	2.6
1	G	11	GLU	2.6
1	I	113	THR	2.6
1	E	49	GLY	2.6
1	G	48	GLU	2.6
1	G	49	GLY	2.6
3	Y	982	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	H	251	ASP	2.5
1	A	224	THR	2.5
1	E	67	ILE	2.4
3	Y	1002	PRO	2.4
1	G	112	ASP	2.4
1	A	77	THR	2.4
2	H	182	THR	2.4
1	E	109	GLN	2.4
1	G	47	ARG	2.3
1	A	113	THR	2.3
1	G	84	ASN	2.3
1	G	44	ASN	2.3
1	I	152	GLN	2.3
3	W	1001	GLN	2.3
2	J	142	LYS	2.3
3	X	1000	GLN	2.3
1	I	115	SER	2.3
3	Y	1000	GLN	2.2
1	A	72	ASP	2.2
1	E	92	ASN	2.2
3	Y	979	PRO	2.2
2	H	84	GLU	2.2
1	I	145	GLY	2.2
2	B	140	GLY	2.2
2	F	163	ARG	2.1
1	G	40	LEU	2.1
1	I	86	ARG	2.1
3	Y	978	LEU	2.1
1	C	77	THR	2.1
1	E	84	ASN	2.1
1	E	265	THR	2.1
1	G	114	GLU	2.1
1	G	72	ASP	2.0
1	A	142	THR	2.0
1	E	142	THR	2.0
1	E	48	GLU	2.0
1	E	94	ILE	2.0

## 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 [i](#)

There are no carbohydrates 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.