Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 09:45 pm BST

PDB ID	:	3H43
Title	:	N-terminal domain of the proteasome-activating nucleotidase of Methanocaldococcus jannaschii
Authors	:	Jeffrey, P.D.; Zhang, F.; Hu, M.; Tian, G.; Zhang, P.; Finley, D.; Shi, Y.
Deposited on	:	2009-04-17
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

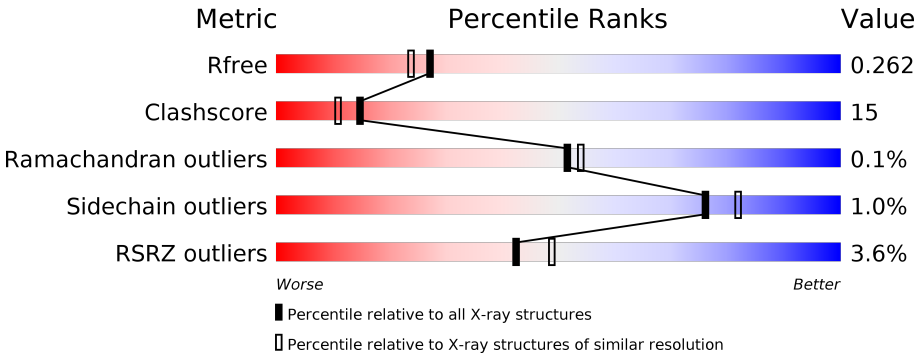
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	85	4% 71% 19% 11%
1	B	85	2% 62% 22% 6% 9%
1	C	85	% 79% 9% • 11%
1	D	85	2% 65% 25% 11%
1	E	85	4% 69% 19% • 11%
1	F	85	2% 61% 28% 11%

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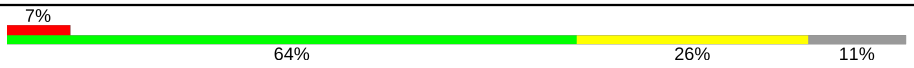
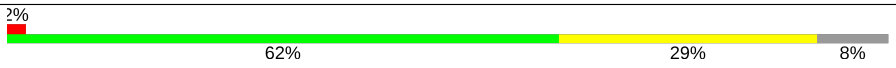
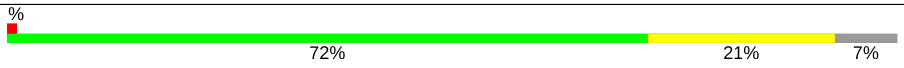
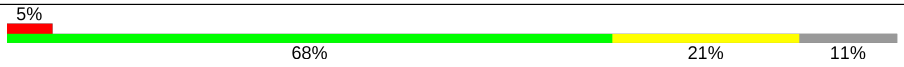
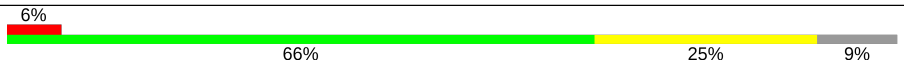
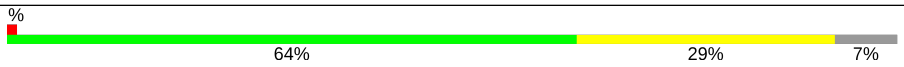
Mol	Chain	Length	Quality of chain
1	G	85	
1	H	85	
1	I	85	
1	J	85	
1	K	85	
1	L	85	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7312 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 Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	B	77	Total	C	N	O	S	Se	0	0	0
			600	378	108	111	1	2			
1	C	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	D	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	E	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	F	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	G	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	H	78	Total	C	N	O	S	Se	0	0	0
			608	384	109	112	1	2			
1	I	79	Total	C	N	O	S	Se	0	0	0
			617	389	110	115	1	2			
1	J	76	Total	C	N	O	S	Se	0	0	0
			591	373	107	108	1	2			
1	K	77	Total	C	N	O	S	Se	0	0	0
			600	379	108	111	1	1			
1	L	79	Total	C	N	O	S	Se	0	0	0
			617	389	110	115	1	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	151	LEU	-	EXPRESSION TAG	UNP Q58576
A	152	GLU	-	EXPRESSION TAG	UNP Q58576
A	153	HIS	-	EXPRESSION TAG	UNP Q58576
A	154	HIS	-	EXPRESSION TAG	UNP Q58576
A	155	HIS	-	EXPRESSION TAG	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
A	156	HIS	-	EXPRESSION TAG	UNP Q58576
A	157	HIS	-	EXPRESSION TAG	UNP Q58576
A	158	HIS	-	EXPRESSION TAG	UNP Q58576
B	151	LEU	-	EXPRESSION TAG	UNP Q58576
B	152	GLU	-	EXPRESSION TAG	UNP Q58576
B	153	HIS	-	EXPRESSION TAG	UNP Q58576
B	154	HIS	-	EXPRESSION TAG	UNP Q58576
B	155	HIS	-	EXPRESSION TAG	UNP Q58576
B	156	HIS	-	EXPRESSION TAG	UNP Q58576
B	157	HIS	-	EXPRESSION TAG	UNP Q58576
B	158	HIS	-	EXPRESSION TAG	UNP Q58576
C	151	LEU	-	EXPRESSION TAG	UNP Q58576
C	152	GLU	-	EXPRESSION TAG	UNP Q58576
C	153	HIS	-	EXPRESSION TAG	UNP Q58576
C	154	HIS	-	EXPRESSION TAG	UNP Q58576
C	155	HIS	-	EXPRESSION TAG	UNP Q58576
C	156	HIS	-	EXPRESSION TAG	UNP Q58576
C	157	HIS	-	EXPRESSION TAG	UNP Q58576
C	158	HIS	-	EXPRESSION TAG	UNP Q58576
D	151	LEU	-	EXPRESSION TAG	UNP Q58576
D	152	GLU	-	EXPRESSION TAG	UNP Q58576
D	153	HIS	-	EXPRESSION TAG	UNP Q58576
D	154	HIS	-	EXPRESSION TAG	UNP Q58576
D	155	HIS	-	EXPRESSION TAG	UNP Q58576
D	156	HIS	-	EXPRESSION TAG	UNP Q58576
D	157	HIS	-	EXPRESSION TAG	UNP Q58576
D	158	HIS	-	EXPRESSION TAG	UNP Q58576
E	151	LEU	-	EXPRESSION TAG	UNP Q58576
E	152	GLU	-	EXPRESSION TAG	UNP Q58576
E	153	HIS	-	EXPRESSION TAG	UNP Q58576
E	154	HIS	-	EXPRESSION TAG	UNP Q58576
E	155	HIS	-	EXPRESSION TAG	UNP Q58576
E	156	HIS	-	EXPRESSION TAG	UNP Q58576
E	157	HIS	-	EXPRESSION TAG	UNP Q58576
E	158	HIS	-	EXPRESSION TAG	UNP Q58576
F	151	LEU	-	EXPRESSION TAG	UNP Q58576
F	152	GLU	-	EXPRESSION TAG	UNP Q58576
F	153	HIS	-	EXPRESSION TAG	UNP Q58576
F	154	HIS	-	EXPRESSION TAG	UNP Q58576
F	155	HIS	-	EXPRESSION TAG	UNP Q58576
F	156	HIS	-	EXPRESSION TAG	UNP Q58576
F	157	HIS	-	EXPRESSION TAG	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
F	158	HIS	-	EXPRESSION TAG	UNP Q58576
G	151	LEU	-	EXPRESSION TAG	UNP Q58576
G	152	GLU	-	EXPRESSION TAG	UNP Q58576
G	153	HIS	-	EXPRESSION TAG	UNP Q58576
G	154	HIS	-	EXPRESSION TAG	UNP Q58576
G	155	HIS	-	EXPRESSION TAG	UNP Q58576
G	156	HIS	-	EXPRESSION TAG	UNP Q58576
G	157	HIS	-	EXPRESSION TAG	UNP Q58576
G	158	HIS	-	EXPRESSION TAG	UNP Q58576
H	151	LEU	-	EXPRESSION TAG	UNP Q58576
H	152	GLU	-	EXPRESSION TAG	UNP Q58576
H	153	HIS	-	EXPRESSION TAG	UNP Q58576
H	154	HIS	-	EXPRESSION TAG	UNP Q58576
H	155	HIS	-	EXPRESSION TAG	UNP Q58576
H	156	HIS	-	EXPRESSION TAG	UNP Q58576
H	157	HIS	-	EXPRESSION TAG	UNP Q58576
H	158	HIS	-	EXPRESSION TAG	UNP Q58576
I	151	LEU	-	EXPRESSION TAG	UNP Q58576
I	152	GLU	-	EXPRESSION TAG	UNP Q58576
I	153	HIS	-	EXPRESSION TAG	UNP Q58576
I	154	HIS	-	EXPRESSION TAG	UNP Q58576
I	155	HIS	-	EXPRESSION TAG	UNP Q58576
I	156	HIS	-	EXPRESSION TAG	UNP Q58576
I	157	HIS	-	EXPRESSION TAG	UNP Q58576
I	158	HIS	-	EXPRESSION TAG	UNP Q58576
J	151	LEU	-	EXPRESSION TAG	UNP Q58576
J	152	GLU	-	EXPRESSION TAG	UNP Q58576
J	153	HIS	-	EXPRESSION TAG	UNP Q58576
J	154	HIS	-	EXPRESSION TAG	UNP Q58576
J	155	HIS	-	EXPRESSION TAG	UNP Q58576
J	156	HIS	-	EXPRESSION TAG	UNP Q58576
J	157	HIS	-	EXPRESSION TAG	UNP Q58576
J	158	HIS	-	EXPRESSION TAG	UNP Q58576
K	151	LEU	-	EXPRESSION TAG	UNP Q58576
K	152	GLU	-	EXPRESSION TAG	UNP Q58576
K	153	HIS	-	EXPRESSION TAG	UNP Q58576
K	154	HIS	-	EXPRESSION TAG	UNP Q58576
K	155	HIS	-	EXPRESSION TAG	UNP Q58576
K	156	HIS	-	EXPRESSION TAG	UNP Q58576
K	157	HIS	-	EXPRESSION TAG	UNP Q58576
K	158	HIS	-	EXPRESSION TAG	UNP Q58576
L	151	LEU	-	EXPRESSION TAG	UNP Q58576

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Chain	Residue	Modelled	Actual	Comment	Reference
L	152	GLU	-	EXPRESSION TAG	UNP Q58576
L	153	HIS	-	EXPRESSION TAG	UNP Q58576
L	154	HIS	-	EXPRESSION TAG	UNP Q58576
L	155	HIS	-	EXPRESSION TAG	UNP Q58576
L	156	HIS	-	EXPRESSION TAG	UNP Q58576
L	157	HIS	-	EXPRESSION TAG	UNP Q58576
L	158	HIS	-	EXPRESSION TAG	UNP Q58576

- Molecule 2 is water.

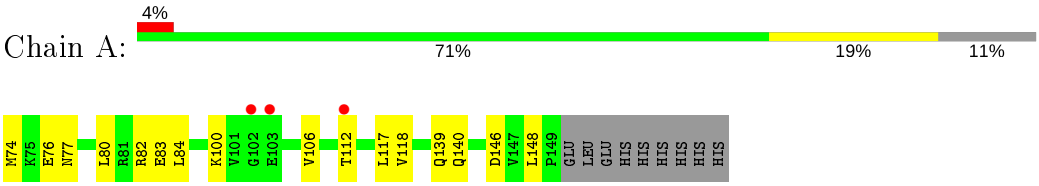
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	8	Total O 8 8	0	0
2	C	18	Total O 18 18	0	0
2	D	21	Total O 21 21	0	0
2	E	8	Total O 8 8	0	0
2	F	6	Total O 6 6	0	0
2	G	12	Total O 12 12	0	0
2	H	11	Total O 11 11	0	0
2	I	10	Total O 10 10	0	0
2	J	8	Total O 8 8	0	0
2	K	11	Total O 11 11	0	0
2	L	10	Total O 10 10	0	0

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.

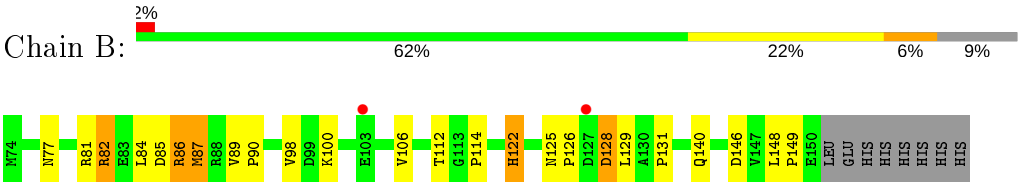
- Molecule 1: Proteasome-activating nucleotidase

Chain A:



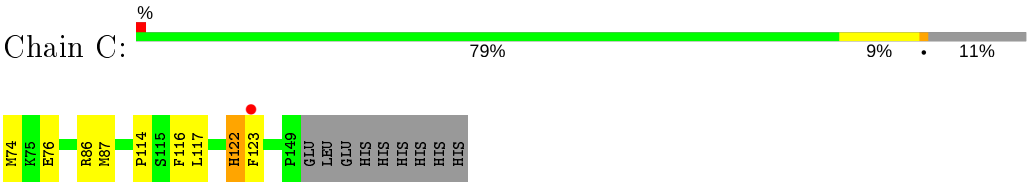
- Molecule 1: Proteasome-activating nucleotidase

Chain B:



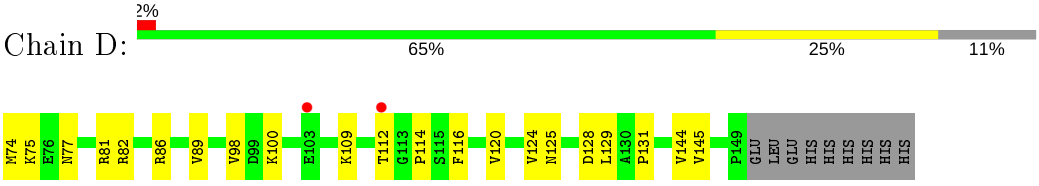
- Molecule 1: Proteasome-activating nucleotidase

Chain C:



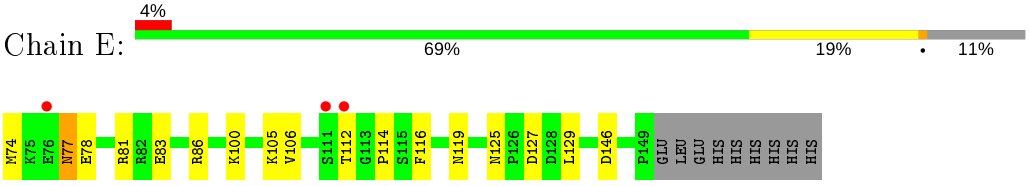
- Molecule 1: Proteasome-activating nucleotidase

Chain D:



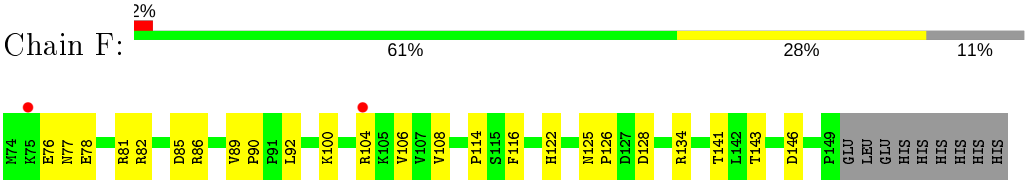
- Molecule 1: Proteasome-activating nucleotidase

Chain E:



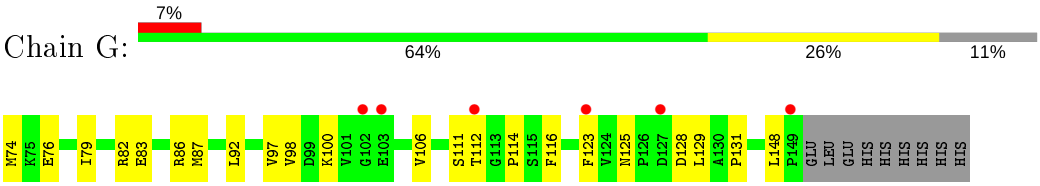
- Molecule 1: Proteasome-activating nucleotidase

Chain F:



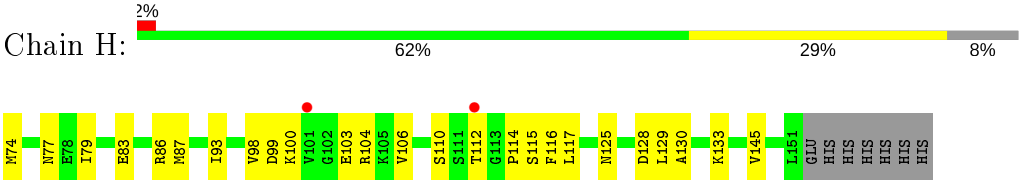
• Molecule 1: Proteasome-activating nucleotidase

Chain G:



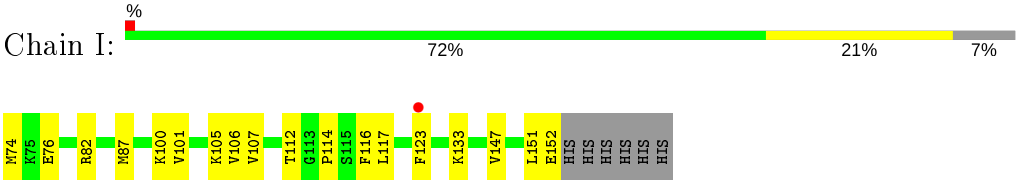
• Molecule 1: Proteasome-activating nucleotidase

Chain H:



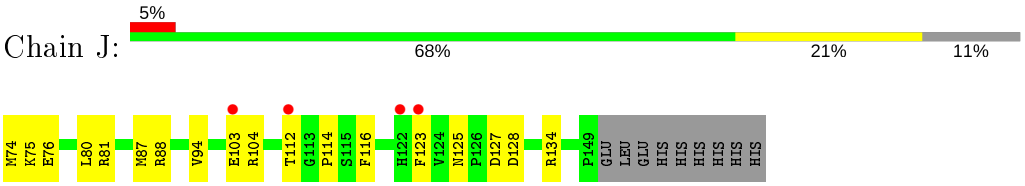
• Molecule 1: Proteasome-activating nucleotidase

Chain I:



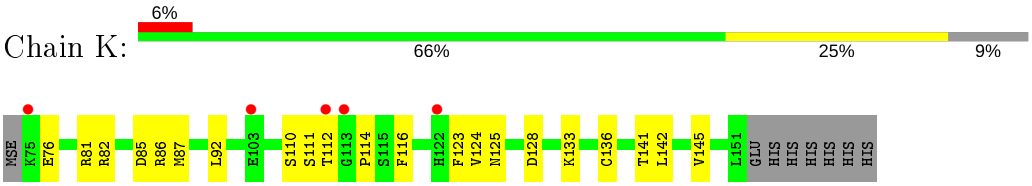
• Molecule 1: Proteasome-activating nucleotidase

Chain J:



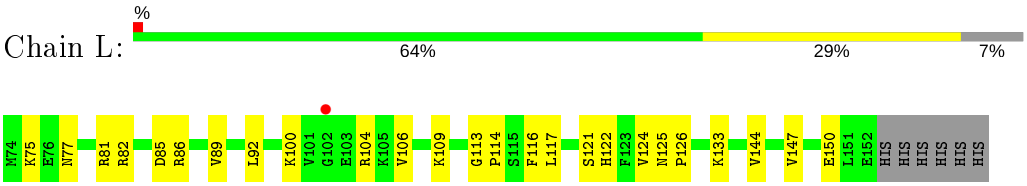
• Molecule 1: Proteasome-activating nucleotidase

Chain K:



• Molecule 1: Proteasome-activating nucleotidase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	126.64Å 129.62Å 60.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.89 – 2.10 40.89 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.89-2.10) 98.8 (40.89-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.217 , 0.262 0.217 , 0.262	Depositor DCC
R_{free} test set	2931 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 61.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7312	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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	0.45	0/598	0.69	0/810
1	B	0.42	0/607	0.66	0/822
1	C	0.46	0/598	0.70	0/810
1	D	0.45	0/598	0.72	0/810
1	E	0.40	0/598	0.69	0/810
1	F	0.39	0/598	0.68	0/810
1	G	0.39	0/598	0.66	0/810
1	H	0.44	0/615	0.70	0/833
1	I	0.43	0/624	0.69	0/845
1	J	0.41	0/598	0.70	0/810
1	K	0.41	0/607	0.77	0/823
1	L	0.43	0/624	0.69	0/845
All	All	0.42	0/7263	0.70	0/9838

There are no bond length outliers.

There are no bond angle outliers.

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	591	0	626	19	0
1	B	600	0	632	35	0
1	C	591	0	626	12	0
1	D	591	0	626	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	591	0	626	21	0
1	F	591	0	626	34	0
1	G	591	0	626	31	0
1	H	608	0	643	26	0
1	I	617	0	649	29	0
1	J	591	0	626	21	0
1	K	600	0	634	22	0
1	L	617	0	649	29	0
2	A	10	0	0	0	0
2	B	8	0	0	1	0
2	C	18	0	0	1	0
2	D	21	0	0	2	0
2	E	8	0	0	0	0
2	F	6	0	0	0	0
2	G	12	0	0	1	0
2	H	11	0	0	0	0
2	I	10	0	0	0	0
2	J	8	0	0	0	0
2	K	11	0	0	1	0
2	L	10	0	0	2	0
All	All	7312	0	7589	224	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 15.

All (224) 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:I:100:LYS:HG2	1:I:106:VAL:HG12	1.53	0.90
1:D:112:THR:HG22	1:G:114:PRO:HG3	1.53	0.89
1:J:103:GLU:HG3	1:J:104:ARG:HG3	1.53	0.88
1:I:133:LYS:HE3	1:I:147:VAL:HG11	1.55	0.88
1:I:82:ARG:NH1	1:K:81:ARG:HG2	1.90	0.86
1:L:77:ASN:O	1:L:81:ARG:HG3	1.78	0.83
1:J:88:ARG:HD3	1:J:123:PHE:CE2	2.16	0.80
1:I:82:ARG:HH12	1:K:81:ARG:HG2	1.48	0.79
1:I:133:LYS:HE3	1:I:147:VAL:CG1	2.13	0.78
1:A:112:THR:HA	1:B:114:PRO:HB3	1.67	0.77
1:B:86:ARG:HH11	1:B:86:ARG:HB3	1.48	0.77
1:F:77:ASN:HD21	1:F:81:ARG:HH12	1.35	0.74
1:F:100:LYS:NZ	1:F:126:PRO:HB2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MSE:HE3	1:A:77:ASN:HD21	1.56	0.70
1:E:146:ASP:OD2	1:H:74:MSE:HG3	1.92	0.70
1:E:81:ARG:HH21	1:F:76:GLU:HG2	1.57	0.70
1:D:82:ARG:HD3	2:D:161:HOH:O	1.92	0.69
1:B:86:ARG:HH22	1:B:87:MSE:HE3	1.58	0.69
1:G:100:LYS:HA	1:G:106:VAL:HG12	1.73	0.69
1:A:148:LEU:HD23	1:D:74:MSE:HE1	1.75	0.68
1:B:86:ARG:HH12	1:B:87:MSE:HG2	1.59	0.68
1:B:77:ASN:HD21	1:B:81:ARG:HH11	1.41	0.68
1:I:123:PHE:HE1	1:L:82:ARG:HH11	1.41	0.67
1:L:133:LYS:HE3	1:L:147:VAL:CG1	2.25	0.66
1:F:82:ARG:HH21	1:F:86:ARG:HH22	1.44	0.65
1:D:100:LYS:HE3	1:D:129:LEU:O	1.98	0.64
1:G:112:THR:HA	1:H:114:PRO:HB3	1.80	0.64
1:G:79:ILE:O	1:G:83:GLU:HG3	1.98	0.64
1:I:123:PHE:CD2	1:L:75:LYS:HE2	2.33	0.64
1:F:82:ARG:HD2	1:G:123:PHE:HE1	1.62	0.64
1:B:82:ARG:NH2	1:C:123:PHE:HZ	1.96	0.64
1:B:82:ARG:CZ	1:C:123:PHE:HZ	2.11	0.64
1:G:86:ARG:HH22	1:H:104:ARG:HB3	1.64	0.64
1:D:112:THR:HG22	1:G:114:PRO:CG	2.25	0.63
1:A:74:MSE:HE1	1:B:77:ASN:HB2	1.81	0.63
1:G:86:ARG:NH2	1:H:104:ARG:HB3	2.12	0.63
1:E:83:GLU:HG2	1:F:122:HIS:CE1	2.34	0.62
1:F:100:LYS:HZ1	1:F:126:PRO:HB2	1.65	0.62
1:J:114:PRO:HG2	1:J:116:PHE:CE1	2.34	0.62
1:I:101:VAL:CG2	1:I:117:LEU:HD11	2.30	0.62
1:I:100:LYS:HG2	1:I:106:VAL:CG1	2.27	0.62
1:B:100:LYS:HE3	1:B:129:LEU:O	2.00	0.61
1:H:86:ARG:NH1	1:H:87:MSE:HE3	2.15	0.61
1:E:86:ARG:CZ	1:F:104:ARG:HD3	2.31	0.61
1:J:125:ASN:HB3	1:J:128:ASP:OD2	2.01	0.61
1:E:106:VAL:HG11	1:E:129:LEU:HD13	1.82	0.61
1:I:82:ARG:NH1	1:K:85:ASP:OD2	2.34	0.60
1:H:86:ARG:HH11	1:H:87:MSE:HE3	1.66	0.60
1:F:86:ARG:HG3	1:F:86:ARG:HH11	1.66	0.60
1:H:100:LYS:HD2	1:H:129:LEU:O	2.01	0.59
1:K:110:SER:HB2	2:K:162:HOH:O	2.01	0.59
1:G:74:MSE:HE2	1:G:74:MSE:HA	1.85	0.59
1:E:105:LYS:HE2	1:E:119:ASN:OD1	2.03	0.59
1:B:86:ARG:NH2	1:B:140:GLN:HE22	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:85:ASP:O	1:L:89:VAL:HG13	2.02	0.59
1:J:125:ASN:HD21	1:J:127:ASP:HB3	1.68	0.58
1:E:114:PRO:HG2	1:E:116:PHE:CE1	2.39	0.58
1:I:112:THR:HA	1:J:114:PRO:HB3	1.86	0.58
1:E:100:LYS:HE2	1:E:129:LEU:O	2.04	0.57
1:E:114:PRO:HG3	1:J:112:THR:HG22	1.87	0.57
1:F:78:GLU:HG2	1:G:123:PHE:HE2	1.69	0.57
1:C:86:ARG:NH2	1:D:120:VAL:O	2.38	0.57
1:L:133:LYS:NZ	1:L:150:GLU:HG3	2.19	0.56
1:L:133:LYS:NZ	1:L:150:GLU:CG	2.67	0.56
1:J:75:LYS:HE3	1:K:124:VAL:HG22	1.87	0.56
1:B:90:PRO:CG	1:I:105:LYS:HE3	2.36	0.56
1:E:112:THR:HG22	1:F:114:PRO:HB3	1.87	0.56
1:J:74:MSE:HE1	1:L:117:LEU:CD2	2.36	0.56
1:F:82:ARG:HE	1:F:86:ARG:NH1	2.04	0.56
1:F:82:ARG:HH21	1:F:86:ARG:NH2	2.03	0.56
1:K:76:GLU:HG2	1:L:77:ASN:ND2	2.20	0.55
1:J:74:MSE:HE1	1:L:117:LEU:HD21	1.89	0.55
1:F:77:ASN:ND2	1:F:81:ARG:HH12	2.03	0.55
1:E:100:LYS:HG2	1:E:106:VAL:HG12	1.88	0.55
1:L:77:ASN:OD1	1:L:81:ARG:HD2	2.07	0.55
1:I:87:MSE:O	1:J:87:MSE:HE1	2.06	0.54
1:F:141:THR:OG1	1:F:143:THR:HG22	2.08	0.54
1:F:77:ASN:OD1	1:F:81:ARG:NH1	2.41	0.54
1:G:114:PRO:HG2	1:G:116:PHE:CE1	2.43	0.54
1:I:114:PRO:HG2	1:I:116:PHE:CZ	2.42	0.54
1:E:125:ASN:OD1	1:E:127:ASP:HB2	2.08	0.53
1:L:124:VAL:HG21	1:L:144:VAL:HG12	1.90	0.53
1:A:84:LEU:HD13	1:B:84:LEU:HD23	1.91	0.53
1:F:106:VAL:HG23	1:F:108:VAL:HG13	1.90	0.53
1:L:133:LYS:HE3	1:L:147:VAL:HG11	1.90	0.53
1:D:112:THR:CA	1:G:114:PRO:HB3	2.39	0.52
1:K:125:ASN:HB3	1:K:128:ASP:OD2	2.09	0.52
1:B:82:ARG:NH1	1:B:82:ARG:HG2	2.24	0.52
1:D:124:VAL:HG21	1:D:144:VAL:HG12	1.92	0.52
1:D:98:VAL:O	1:D:131:PRO:HB3	2.10	0.51
1:B:86:ARG:NH1	1:B:87:MSE:HG2	2.24	0.51
2:C:163:HOH:O	1:D:77:ASN:HB2	2.09	0.51
1:B:100:LYS:HA	1:B:106:VAL:HG12	1.93	0.51
1:C:114:PRO:HG2	1:C:116:PHE:CZ	2.46	0.51
1:B:148:LEU:HD22	1:B:149:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:HIS:H	1:C:122:HIS:CD2	2.28	0.51
1:F:100:LYS:HZ2	1:F:126:PRO:HB2	1.76	0.51
1:L:121:SER:HA	2:L:160:HOH:O	2.10	0.51
1:K:76:GLU:CG	1:L:77:ASN:ND2	2.74	0.51
1:D:112:THR:HA	1:G:114:PRO:HB3	1.93	0.50
1:F:114:PRO:HG2	1:F:116:PHE:CE1	2.46	0.50
1:I:74:MSE:HE1	1:I:82:ARG:HH21	1.75	0.50
1:F:134:ARG:HG2	1:F:134:ARG:HH11	1.76	0.50
1:J:75:LYS:HD2	1:K:145:VAL:O	2.12	0.50
1:K:128:ASP:O	1:K:133:LYS:HD3	2.11	0.50
1:G:125:ASN:HB3	1:G:128:ASP:OD2	2.12	0.50
1:I:123:PHE:HD2	1:L:75:LYS:HE2	1.75	0.50
1:A:148:LEU:HD23	1:D:74:MSE:CE	2.41	0.49
1:F:77:ASN:HD21	1:F:81:ARG:NH1	2.07	0.49
1:D:86:ARG:O	1:D:89:VAL:HG22	2.12	0.49
1:L:114:PRO:HG2	1:L:116:PHE:CE1	2.46	0.49
1:B:125:ASN:HB3	1:B:128:ASP:OD1	2.12	0.49
1:C:87:MSE:HE3	1:D:145:VAL:HG12	1.95	0.49
1:I:112:THR:HG22	1:J:114:PRO:HG3	1.94	0.49
1:F:78:GLU:HG2	1:G:123:PHE:CE2	2.47	0.49
1:G:111:SER:CB	1:H:115:SER:H	2.26	0.49
1:D:114:PRO:HG2	1:D:116:PHE:CE1	2.48	0.48
1:A:117:LEU:HD23	1:F:92:LEU:HD12	1.94	0.48
1:A:74:MSE:CE	1:B:77:ASN:HB2	2.42	0.48
1:B:112:THR:HA	1:I:114:PRO:HB3	1.95	0.48
1:I:101:VAL:HG21	1:I:117:LEU:HD11	1.95	0.48
1:B:82:ARG:CG	1:B:82:ARG:HH11	2.27	0.48
1:D:112:THR:N	1:G:114:PRO:HB3	2.28	0.47
1:E:100:LYS:HA	1:E:106:VAL:HG12	1.97	0.47
1:J:94:VAL:HG12	1:J:134:ARG:NH1	2.29	0.47
1:H:100:LYS:HA	1:H:106:VAL:HG23	1.96	0.47
1:H:125:ASN:HB3	1:H:128:ASP:OD2	2.14	0.47
1:I:114:PRO:HG2	1:I:116:PHE:CE1	2.49	0.47
1:E:112:THR:CG2	1:F:114:PRO:HB3	2.44	0.47
1:F:82:ARG:NH2	1:F:86:ARG:NH2	2.63	0.47
1:E:77:ASN:HD21	1:F:76:GLU:CG	2.28	0.47
1:I:107:VAL:CG2	1:I:117:LEU:HD13	2.45	0.47
1:J:125:ASN:HD22	1:J:128:ASP:CG	2.18	0.47
1:A:112:THR:CA	1:B:114:PRO:HB3	2.42	0.47
1:A:146:ASP:OD2	1:D:74:MSE:HB3	2.15	0.47
1:E:81:ARG:HB3	1:G:82:ARG:NH2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ARG:HH11	1:B:82:ARG:HG2	1.80	0.46
1:L:86:ARG:O	1:L:89:VAL:HG22	2.16	0.46
1:A:100:LYS:HG2	1:A:106:VAL:HG12	1.96	0.46
1:E:74:MSE:O	1:E:78:GLU:HG2	2.15	0.46
1:I:151:LEU:O	1:I:152:GLU:HB2	2.16	0.46
1:A:140:GLN:HE22	1:D:86:ARG:CZ	2.28	0.46
1:K:141:THR:O	1:K:142:LEU:HB2	2.16	0.46
1:F:125:ASN:HB3	1:F:128:ASP:OD2	2.16	0.46
1:J:114:PRO:HG2	1:J:116:PHE:HE1	1.80	0.46
1:I:76:GLU:OE2	1:J:81:ARG:NH2	2.49	0.46
1:C:122:HIS:CD2	1:C:122:HIS:N	2.84	0.46
1:B:85:ASP:O	1:B:89:VAL:HG13	2.15	0.45
1:L:133:LYS:HE3	1:L:147:VAL:HG12	1.97	0.45
1:B:86:ARG:NH1	2:B:159:HOH:O	2.48	0.45
1:D:112:THR:HG22	1:G:114:PRO:CB	2.46	0.45
1:G:92:LEU:HD12	1:H:117:LEU:HD23	1.98	0.45
1:A:82:ARG:NH2	1:C:74:MSE:CG	2.80	0.45
1:G:98:VAL:O	1:G:131:PRO:HB3	2.17	0.45
1:L:133:LYS:HZ3	1:L:150:GLU:CG	2.29	0.45
1:K:86:ARG:CD	1:L:104:ARG:HH22	2.29	0.45
1:B:82:ARG:NH2	1:C:123:PHE:CZ	2.82	0.45
1:D:114:PRO:HG2	1:D:116:PHE:HE1	1.81	0.45
1:F:82:ARG:CD	1:G:123:PHE:HE1	2.30	0.45
1:E:146:ASP:OD2	1:H:74:MSE:CG	2.61	0.44
1:H:112:THR:HA	1:K:114:PRO:HB3	1.98	0.44
1:K:86:ARG:CD	1:L:104:ARG:NH2	2.80	0.44
1:G:86:ARG:CZ	1:H:104:ARG:HD3	2.48	0.44
1:B:148:LEU:CD2	1:B:149:PRO:HD2	2.47	0.44
1:K:112:THR:CG2	1:L:113:GLY:C	2.86	0.44
1:E:77:ASN:HD21	1:F:76:GLU:HG3	1.81	0.44
1:C:76:GLU:OE2	1:D:81:ARG:NH2	2.47	0.44
1:D:125:ASN:HB3	1:D:128:ASP:OD2	2.17	0.44
1:D:74:MSE:O	1:D:75:LYS:HD3	2.18	0.44
1:J:76:GLU:O	1:J:80:LEU:HG	2.18	0.44
1:K:87:MSE:HG3	2:L:160:HOH:O	2.18	0.44
1:H:103:GLU:CD	1:H:103:GLU:H	2.20	0.44
1:I:74:MSE:HE3	1:K:82:ARG:NH2	2.33	0.44
1:K:111:SER:OG	1:L:109:LYS:HE3	2.18	0.43
1:I:107:VAL:HG22	1:I:117:LEU:HD13	2.00	0.43
1:A:140:GLN:HE22	1:D:86:ARG:NE	2.17	0.43
1:H:114:PRO:HG2	1:H:116:PHE:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NH2	1:C:74:MSE:HG3	2.33	0.43
1:D:109:LYS:HE2	2:D:160:HOH:O	2.19	0.43
1:E:77:ASN:OD1	1:F:77:ASN:HB2	2.18	0.43
1:B:98:VAL:O	1:B:131:PRO:HB3	2.19	0.43
1:K:92:LEU:HD13	1:K:136:CYS:HB3	1.99	0.43
1:H:110:SER:C	1:H:112:THR:N	2.71	0.43
1:B:100:LYS:HE2	1:B:126:PRO:O	2.18	0.43
1:B:86:ARG:HH21	1:B:140:GLN:HE22	1.66	0.43
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.83	0.43
1:F:85:ASP:O	1:F:89:VAL:HG13	2.19	0.43
1:B:90:PRO:HG2	1:I:105:LYS:HE3	2.01	0.43
1:E:146:ASP:OD2	1:H:74:MSE:HA	2.19	0.42
1:L:104:ARG:CZ	1:L:122:HIS:NE2	2.82	0.42
1:A:76:GLU:O	1:A:80:LEU:HG	2.19	0.42
1:G:100:LYS:HD3	1:G:129:LEU:O	2.19	0.42
1:L:100:LYS:HA	1:L:106:VAL:HG12	2.01	0.42
1:A:76:GLU:H	1:A:76:GLU:CD	2.23	0.42
1:B:86:ARG:HH11	1:B:86:ARG:CB	2.26	0.42
1:C:117:LEU:HD23	1:L:92:LEU:HD12	2.02	0.42
1:F:125:ASN:HA	1:F:126:PRO:HD2	1.89	0.42
1:I:100:LYS:HA	1:I:106:VAL:HG12	2.01	0.42
1:J:88:ARG:HD3	1:J:123:PHE:CD2	2.55	0.42
1:F:134:ARG:HG2	1:F:134:ARG:NH1	2.35	0.41
1:D:112:THR:CG2	1:G:114:PRO:HB3	2.50	0.41
1:G:86:ARG:NE	2:G:46:HOH:O	2.34	0.41
1:A:83:GLU:HG2	1:B:122:HIS:CG	2.55	0.41
1:L:125:ASN:HA	1:L:126:PRO:HD2	1.93	0.41
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.83	0.41
1:G:148:LEU:HA	1:G:148:LEU:HD23	1.93	0.41
1:H:114:PRO:HG2	1:H:116:PHE:HE1	1.85	0.41
1:H:130:ALA:O	1:H:133:LYS:HB2	2.20	0.41
1:H:79:ILE:O	1:H:83:GLU:HG2	2.21	0.41
1:B:86:ARG:NH2	1:B:87:MSE:HE3	2.30	0.41
1:G:87:MSE:HE3	1:H:145:VAL:HG12	2.02	0.41
1:H:98:VAL:HG12	1:H:99:ASP:OD1	2.21	0.41
1:J:88:ARG:HD3	1:J:123:PHE:CZ	2.56	0.41
1:G:76:GLU:OE2	1:H:77:ASN:HB2	2.20	0.41
1:G:97:VAL:O	1:G:131:PRO:HA	2.21	0.40
1:I:74:MSE:HE3	1:K:82:ARG:CZ	2.50	0.40
1:G:74:MSE:CE	1:G:74:MSE:HA	2.51	0.40
1:K:123:PHE:HE1	1:K:145:VAL:O	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:SER:C	1:H:112:THR:H	2.24	0.40
1:I:112:THR:HG22	1:J:114:PRO:CB	2.51	0.40
1:A:118:VAL:HA	1:F:90:PRO:HB3	2.03	0.40
1:L:133:LYS:HZ2	1:L:150:GLU:CG	2.34	0.40
1:B:100:LYS:HE2	1:B:129:LEU:HB2	2.03	0.40
1:H:93:ILE:HG12	1:K:116:PHE:CE2	2.56	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	74/85 (87%)	71 (96%)	2 (3%)	1 (1%)	11 6
1	B	75/85 (88%)	72 (96%)	3 (4%)	0	100 100
1	C	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
1	D	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
1	E	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
1	F	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
1	G	74/85 (87%)	72 (97%)	2 (3%)	0	100 100
1	H	76/85 (89%)	73 (96%)	3 (4%)	0	100 100
1	I	77/85 (91%)	74 (96%)	3 (4%)	0	100 100
1	J	74/85 (87%)	73 (99%)	1 (1%)	0	100 100
1	K	75/85 (88%)	73 (97%)	2 (3%)	0	100 100
1	L	77/85 (91%)	74 (96%)	3 (4%)	0	100 100
All	All	898/1020 (88%)	872 (97%)	25 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLN

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	71/78 (91%)	71 (100%)	0	100 100
1	B	72/78 (92%)	66 (92%)	6 (8%)	11 7
1	C	71/78 (91%)	70 (99%)	1 (1%)	67 73
1	D	71/78 (91%)	71 (100%)	0	100 100
1	E	71/78 (91%)	70 (99%)	1 (1%)	67 73
1	F	71/78 (91%)	70 (99%)	1 (1%)	67 73
1	G	71/78 (91%)	71 (100%)	0	100 100
1	H	73/78 (94%)	73 (100%)	0	100 100
1	I	74/78 (95%)	74 (100%)	0	100 100
1	J	71/78 (91%)	71 (100%)	0	100 100
1	K	72/78 (92%)	72 (100%)	0	100 100
1	L	74/78 (95%)	74 (100%)	0	100 100
All	All	862/936 (92%)	853 (99%)	9 (1%)	76 82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	82	ARG
1	B	86	ARG
1	B	87	MSE
1	B	122	HIS
1	B	128	ASP
1	B	146	ASP
1	C	122	HIS
1	E	77	ASN
1	F	146	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	GLN
1	B	77	ASN
1	B	140	GLN
1	C	122	HIS
1	J	125	ASN

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 carbohydrates 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	74/85 (87%)	0.01	3 (4%)	37	43	20, 32, 58, 72	0
1	B	75/85 (88%)	0.08	2 (2%)	54	60	19, 34, 61, 81	0
1	C	74/85 (87%)	-0.15	1 (1%)	75	78	18, 27, 46, 64	0
1	D	74/85 (87%)	0.06	2 (2%)	54	60	18, 31, 50, 63	0
1	E	74/85 (87%)	0.19	3 (4%)	37	43	18, 33, 59, 88	0
1	F	74/85 (87%)	0.17	2 (2%)	54	60	21, 38, 69, 91	0
1	G	74/85 (87%)	0.16	6 (8%)	12	15	20, 35, 61, 74	0
1	H	76/85 (89%)	0.09	2 (2%)	56	61	19, 34, 58, 67	0
1	I	77/85 (90%)	-0.12	1 (1%)	77	80	16, 30, 56, 78	0
1	J	74/85 (87%)	0.16	4 (5%)	25	31	21, 38, 61, 74	0
1	K	76/85 (89%)	0.05	5 (6%)	18	23	20, 33, 58, 76	0
1	L	77/85 (90%)	0.11	1 (1%)	77	80	18, 33, 64, 82	0
All	All	899/1020 (88%)	0.07	32 (3%)	42	49	16, 33, 60, 91	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	112	THR	6.7
1	H	112	THR	5.0
1	D	112	THR	4.4
1	F	75	LYS	4.3
1	A	103	GLU	4.0
1	B	103	GLU	3.7
1	G	112	THR	3.6
1	K	75	LYS	3.3
1	J	112	THR	3.1
1	G	103	GLU	3.1
1	K	112	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	J	103	GLU	2.9
1	E	111	SER	2.9
1	E	76	GLU	2.8
1	H	101	VAL	2.8
1	J	122	HIS	2.7
1	K	113	GLY	2.6
1	G	127	ASP	2.6
1	G	102	GLY	2.6
1	A	102	GLY	2.5
1	K	122	HIS	2.4
1	A	112	THR	2.3
1	C	123	PHE	2.3
1	I	123	PHE	2.2
1	J	123	PHE	2.2
1	L	102	GLY	2.2
1	G	123	PHE	2.2
1	D	103	GLU	2.1
1	B	127	ASP	2.0
1	K	103	GLU	2.0
1	G	149	PRO	2.0
1	F	104	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 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.