Full wwPDB X-ray Structure Validation Report (i)

Jan 8, 2024 – 10:09 am GMT

PDB ID	:	5NSM
Title	:	unliganded Structure of Leucyl aminopeptidase from Trypanosoma brucei
Authors	:	Timm, J.; Wilson, K.
Deposited on	:	2017-04-26
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

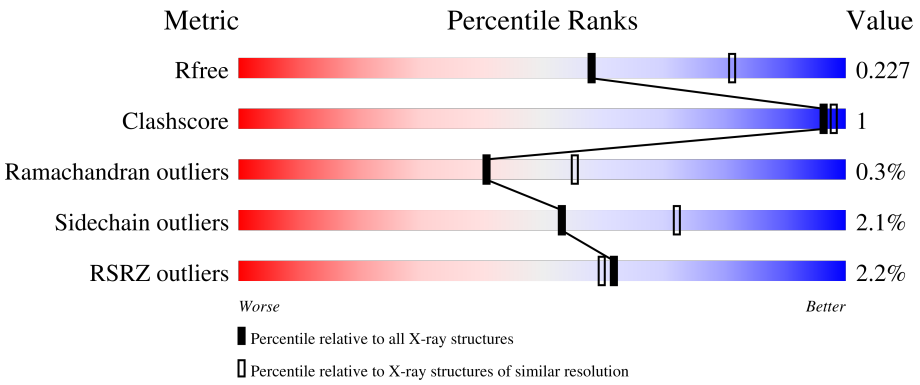
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	521	2% 95% 5%
1	B	521	2% 96% .
1	C	521	3% 96% .
1	D	521	2% 95% .
1	E	521	3% 96% .

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Mol	Chain	Length	Quality of chain
1	F	521	3% 95% 5%
1	G	521	% 96%
1	H	521	3% 96%
1	I	521	% 95% 5%
1	J	521	2% 95%
1	K	521	% 96%
1	L	521	2% 95%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 46357 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 Aminopeptidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3820	2418	646	734	22	0	2	0
1	B	519	3798	2402	643	731	22	0	0	0
1	C	519	3814	2415	643	734	22	0	2	0
1	D	519	3805	2409	643	731	22	0	1	0
1	E	519	3808	2408	647	731	22	0	0	0
1	F	519	3789	2401	637	729	22	0	1	0
1	G	519	3804	2409	643	730	22	0	1	0
1	H	519	3790	2397	642	729	22	0	0	0
1	I	519	3801	2407	643	729	22	0	1	0
1	J	519	3818	2418	644	734	22	0	2	0
1	K	519	3784	2393	639	730	22	0	0	0
1	L	519	3793	2403	637	731	22	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	THR	conflict	UNP Q385B0
A	139	THR	ALA	conflict	UNP Q385B0
B	32	ALA	THR	conflict	UNP Q385B0
B	139	THR	ALA	conflict	UNP Q385B0
C	32	ALA	THR	conflict	UNP Q385B0

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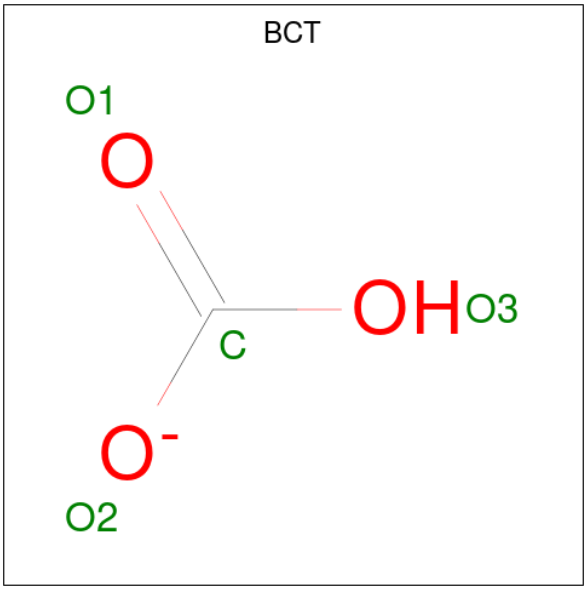
Chain	Residue	Modelled	Actual	Comment	Reference
C	139	THR	ALA	conflict	UNP Q385B0
D	32	ALA	THR	conflict	UNP Q385B0
D	139	THR	ALA	conflict	UNP Q385B0
E	32	ALA	THR	conflict	UNP Q385B0
E	139	THR	ALA	conflict	UNP Q385B0
F	32	ALA	THR	conflict	UNP Q385B0
F	139	THR	ALA	conflict	UNP Q385B0
G	32	ALA	THR	conflict	UNP Q385B0
G	139	THR	ALA	conflict	UNP Q385B0
H	32	ALA	THR	conflict	UNP Q385B0
H	139	THR	ALA	conflict	UNP Q385B0
I	32	ALA	THR	conflict	UNP Q385B0
I	139	THR	ALA	conflict	UNP Q385B0
J	32	ALA	THR	conflict	UNP Q385B0
J	139	THR	ALA	conflict	UNP Q385B0
K	32	ALA	THR	conflict	UNP Q385B0
K	139	THR	ALA	conflict	UNP Q385B0
L	32	ALA	THR	conflict	UNP Q385B0
L	139	THR	ALA	conflict	UNP Q385B0

- Molecule 2 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	4	1	3		0	0
			Total	C	O			
2	B	1	4	1	3		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	C	1	4	1	3	0	0
2	D	1	4	1	3	0	0
2	E	1	4	1	3	0	0
2	F	1	4	1	3	0	0
2	G	1	4	1	3	0	0
2	H	1	4	1	3	0	0
2	I	1	4	1	3	0	0
2	J	1	4	1	3	0	0
2	K	1	4	1	3	0	0
2	L	1	4	1	3	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0
3	E	2	2	2	0	0
3	F	2	2	2	0	0
3	G	2	2	2	0	0
3	H	2	2	2	0	0
3	I	2	2	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	2	Total Mn 2 2	0	0
3	K	2	Total Mn 2 2	0	0
3	L	2	Total Mn 2 2	0	0

- Molecule 4 is water.

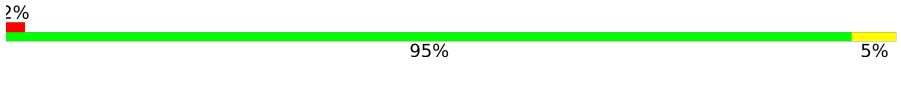
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	56	Total O 56 56	0	0
4	B	40	Total O 40 40	0	0
4	C	54	Total O 54 54	0	0
4	D	59	Total O 59 59	0	0
4	E	54	Total O 54 54	0	0
4	F	26	Total O 26 26	0	0
4	G	55	Total O 55 55	0	0
4	H	51	Total O 51 51	0	0
4	I	46	Total O 46 46	0	0
4	J	92	Total O 92 92	0	0
4	K	67	Total O 67 67	0	0
4	L	61	Total O 61 61	0	0

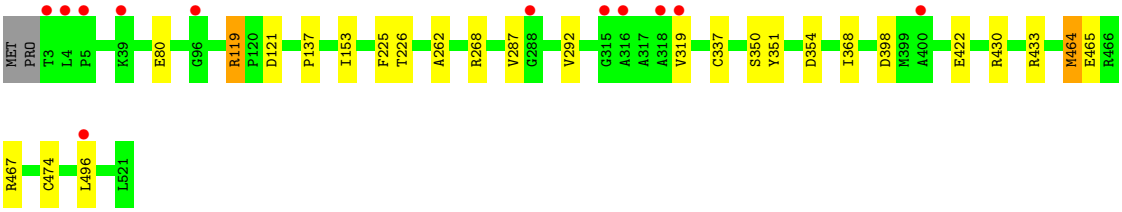
3 Residue-property plots (i)

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: Aminopeptidase, putative

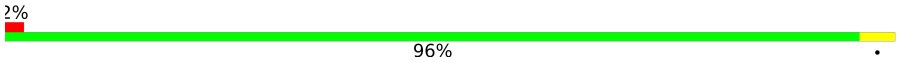
Chain A:

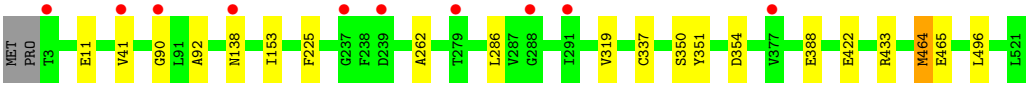




- Molecule 1: Aminopeptidase, putative

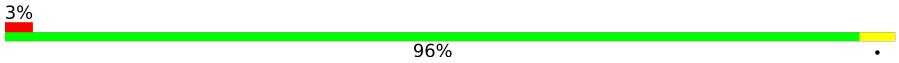
Chain B:

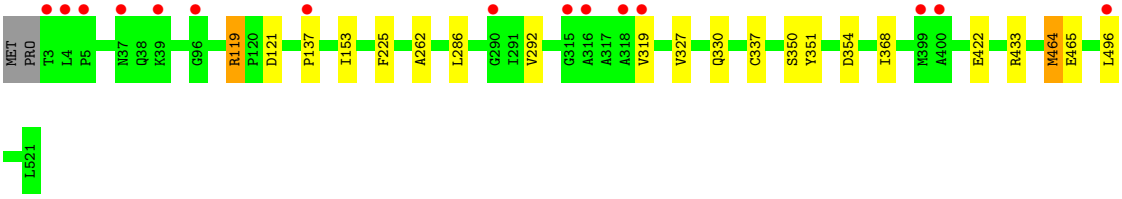




- Molecule 1: Aminopeptidase, putative

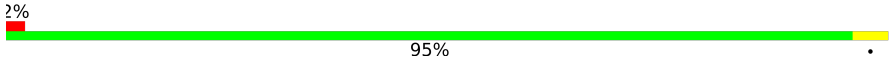
Chain C:

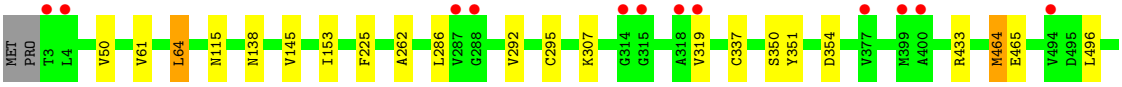




- Molecule 1: Aminopeptidase, putative

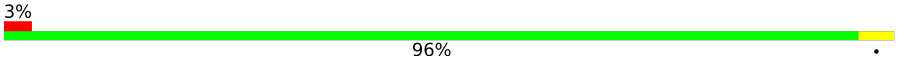
Chain D:

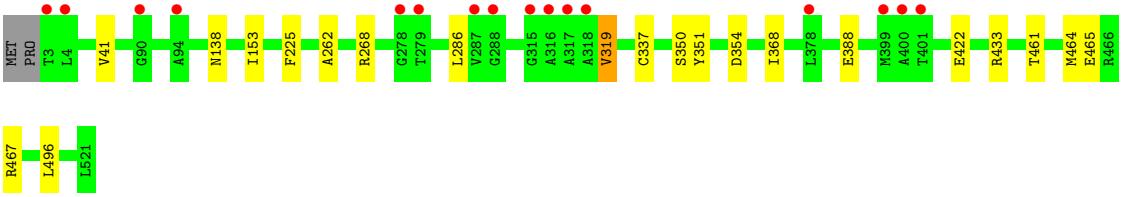




• Molecule 1: Aminopeptidase, putative

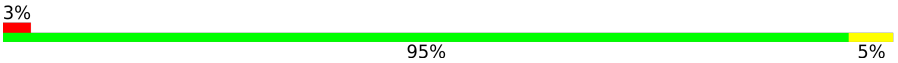
Chain E:

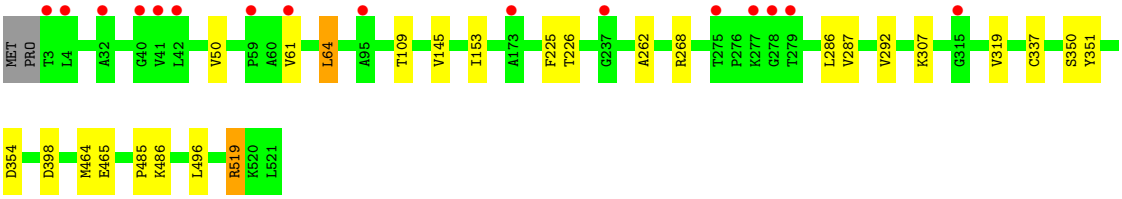




• Molecule 1: Aminopeptidase, putative

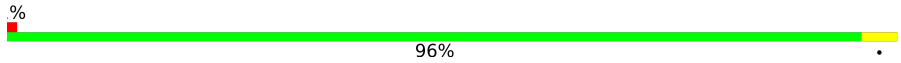
Chain F:

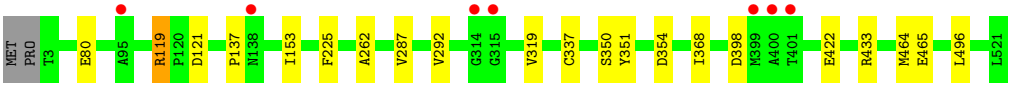




• Molecule 1: Aminopeptidase, putative

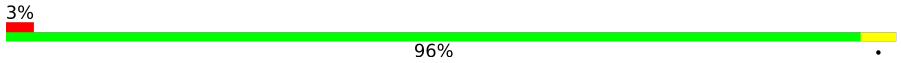
Chain G:

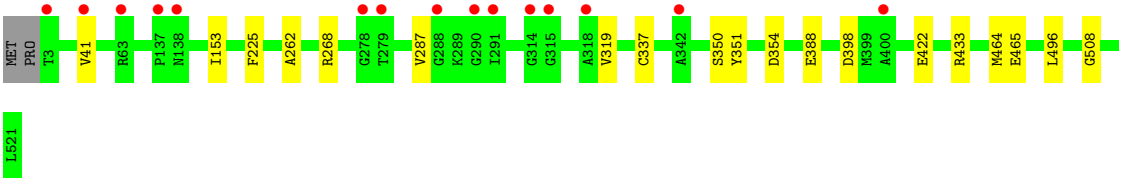




• Molecule 1: Aminopeptidase, putative

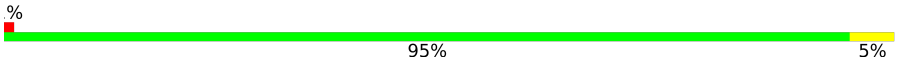
Chain H:

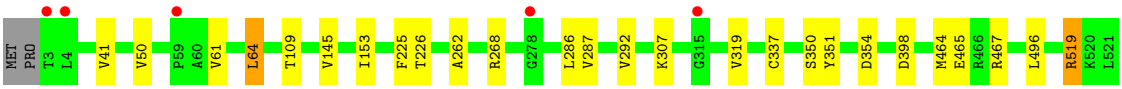




• Molecule 1: Aminopeptidase, putative

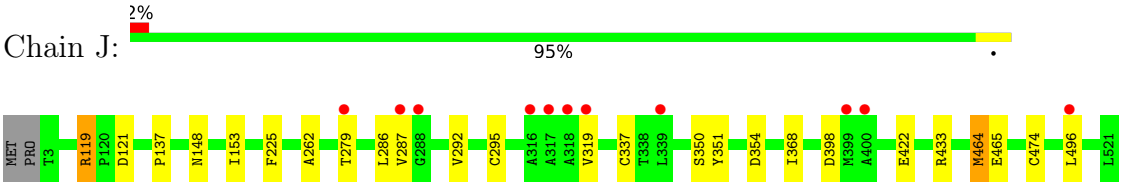
Chain I:





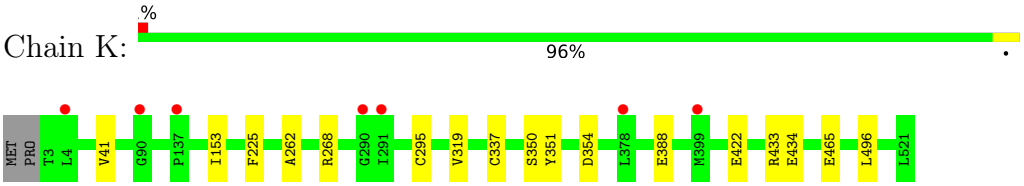
• Molecule 1: Aminopeptidase, putative

Chain J:



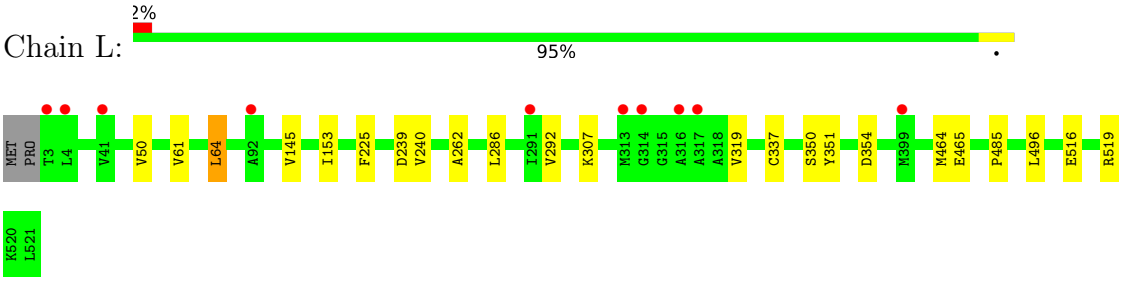
- Molecule 1: Aminopeptidase, putative

Chain K:



- Molecule 1: Aminopeptidase, putative

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.37Å 143.76Å 270.08Å 90.00° 95.47° 90.00°	Depositor
Resolution (Å)	32.73 – 2.40 32.73 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (32.73-2.40) 94.3 (32.73-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.206 , 0.225 0.209 , 0.227	Depositor DCC
R_{free} test set	11981 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	46357	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, MN

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	0.70	0/3900	0.76	5/5323 (0.1%)
1	B	0.72	1/3876 (0.0%)	0.75	4/5295 (0.1%)
1	C	0.71	0/3894	0.75	3/5316 (0.1%)
1	D	0.71	0/3886	0.74	1/5306 (0.0%)
1	E	0.71	0/3886	0.76	6/5306 (0.1%)
1	F	0.71	0/3870	0.74	2/5287 (0.0%)
1	G	0.71	1/3881 (0.0%)	0.76	4/5299 (0.1%)
1	H	0.71	0/3868	0.76	5/5286 (0.1%)
1	I	0.71	0/3882	0.75	2/5301 (0.0%)
1	J	0.72	0/3898	0.77	4/5320 (0.1%)
1	K	0.74	0/3862	0.77	5/5278 (0.1%)
1	L	0.72	0/3874	0.73	1/5292 (0.0%)
All	All	0.71	2/46577 (0.0%)	0.75	42/63609 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	GLU	CD-OE2	5.65	1.31	1.25
1	G	80	GLU	CD-OE1	-5.39	1.19	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	119	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	119	ARG	NE-CZ-NH2	-8.81	115.90	120.30
1	C	119	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	G	119	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	J	119	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	E	464	MET	CA-CB-CG	7.04	125.26	113.30
1	E	433	ARG	NE-CZ-NH2	-6.96	116.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	464	MET	CA-CB-CG	6.75	124.78	113.30
1	A	119	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	H	433	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	J	433	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	433	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	G	119	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	433	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	I	519	ARG	CG-CD-NE	6.15	124.72	111.80
1	H	388	GLU	CG-CD-OE2	-6.03	106.24	118.30
1	E	388	GLU	CG-CD-OE1	6.03	130.36	118.30
1	A	433	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	K	433	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	H	388	GLU	CG-CD-OE1	5.86	130.02	118.30
1	B	388	GLU	CG-CD-OE1	5.84	129.97	118.30
1	B	388	GLU	CG-CD-OE2	-5.80	106.70	118.30
1	E	388	GLU	CG-CD-OE2	-5.77	106.76	118.30
1	K	388	GLU	CG-CD-OE1	5.72	129.74	118.30
1	K	388	GLU	CG-CD-OE2	-5.71	106.87	118.30
1	I	64	LEU	CB-CG-CD1	5.60	120.51	111.00
1	B	433	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	C	119	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	H	268	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	G	433	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	433	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	H	433	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	64	LEU	CB-CG-CD1	5.42	120.22	111.00
1	F	64	LEU	CB-CG-CD1	5.42	120.21	111.00
1	K	433	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	L	64	LEU	CB-CG-CD1	5.40	120.19	111.00
1	K	268	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	J	433	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	430	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	F	519	ARG	CD-NE-CZ	5.08	130.72	123.60
1	E	268	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	80	GLU	CG-CD-OE2	5.01	128.31	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3820	0	3732	8	0
1	B	3798	0	3693	13	0
1	C	3814	0	3721	7	0
1	D	3805	0	3715	9	1
1	E	3808	0	3715	4	0
1	F	3789	0	3689	18	0
1	G	3804	0	3711	5	0
1	H	3790	0	3678	4	0
1	I	3801	0	3711	10	0
1	J	3818	0	3732	9	1
1	K	3784	0	3659	3	0
1	L	3793	0	3693	10	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	4	0	0	0	0
2	K	4	0	0	0	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	56	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	0	1	0
4	C	54	0	0	1	0
4	D	59	0	0	0	0
4	E	54	0	0	0	0
4	F	26	0	0	0	0
4	G	55	0	0	0	0
4	H	51	0	0	1	0
4	I	46	0	0	0	0
4	J	92	0	0	2	0
4	K	67	0	0	1	0
4	L	61	0	0	0	0
All	All	46357	0	44449	86	1

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 1.

All (86) 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:B:92:ALA:HB2	1:F:485:PRO:HB2	1.37	1.05
1:B:92:ALA:CB	1:F:485:PRO:HB2	1.87	1.04
1:B:90:GLY:O	1:F:486:LYS:HG2	1.81	0.80
1:B:92:ALA:HB1	1:F:485:PRO:HB2	1.71	0.72
1:B:90:GLY:O	1:F:486:LYS:CG	2.41	0.68
1:C:119:ARG:NH1	1:C:121:ASP:OD2	2.32	0.62
1:A:119:ARG:NH1	1:A:121:ASP:OD2	2.33	0.62
1:J:119:ARG:NH1	1:J:121:ASP:OD2	2.33	0.62
1:L:516:GLU:OE1	1:L:519:ARG:NH1	2.33	0.61
1:G:119:ARG:NH1	1:G:121:ASP:OD2	2.34	0.61
1:L:61:VAL:HA	1:L:64:LEU:HD23	1.84	0.60
1:I:61:VAL:HA	1:I:64:LEU:HD23	1.86	0.57
1:D:61:VAL:HA	1:D:64:LEU:HD23	1.86	0.57
1:F:61:VAL:HA	1:F:64:LEU:HD23	1.85	0.57
1:F:319:VAL:HG13	1:F:337:CYS:SG	2.45	0.57
1:H:319:VAL:HG13	1:H:337:CYS:SG	2.45	0.56
1:K:319:VAL:HG13	1:K:337:CYS:SG	2.45	0.56
1:D:319:VAL:HG13	1:D:337:CYS:SG	2.45	0.56
1:J:319:VAL:HG13	1:J:337:CYS:SG	2.46	0.56
1:I:319:VAL:HG13	1:I:337:CYS:SG	2.46	0.56
1:G:319:VAL:HG13	1:G:337:CYS:SG	2.46	0.56
1:B:92:ALA:HB1	1:F:485:PRO:CB	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:VAL:HG13	1:B:337:CYS:SG	2.46	0.55
1:E:319:VAL:HG13	1:E:337:CYS:SG	2.45	0.55
1:I:41:VAL:CG2	1:L:485:PRO:HB2	2.36	0.55
1:L:319:VAL:HG13	1:L:337:CYS:SG	2.47	0.55
1:A:319:VAL:HG13	1:A:337:CYS:SG	2.46	0.55
1:C:319:VAL:HG13	1:C:337:CYS:SG	2.46	0.55
1:K:434:GLU:HG3	4:K:739:HOH:O	2.08	0.53
1:B:90:GLY:O	1:F:486:LYS:CB	2.58	0.52
1:H:508:GLY:N	4:H:701:HOH:O	2.43	0.52
1:B:92:ALA:CB	1:F:485:PRO:CB	2.75	0.52
1:B:464:MET:HG2	4:B:738:HOH:O	2.11	0.51
1:C:368:ILE:HD13	1:F:307:LYS:HE2	1.93	0.50
1:J:464:MET:HE1	1:J:474:CYS:HB2	1.93	0.50
1:A:368:ILE:HD13	1:D:307:LYS:HE2	1.92	0.50
1:A:464:MET:HE3	4:A:755:HOH:O	2.12	0.50
1:J:368:ILE:HD13	1:L:307:LYS:HE2	1.94	0.49
1:J:148:ASN:OD1	4:J:701:HOH:O	2.19	0.49
1:L:61:VAL:HA	1:L:64:LEU:CD2	2.41	0.49
1:D:61:VAL:HA	1:D:64:LEU:CD2	2.43	0.49
1:F:61:VAL:HA	1:F:64:LEU:CD2	2.43	0.48
1:I:61:VAL:HA	1:I:64:LEU:CD2	2.43	0.48
1:L:239[B]:ASP:OD1	1:L:240:VAL:N	2.49	0.45
1:B:90:GLY:O	1:F:486:LYS:HB3	2.16	0.45
1:G:368:ILE:HD13	1:I:307:LYS:HE2	1.99	0.44
1:L:50:VAL:CG2	1:L:145:VAL:HG12	2.48	0.44
1:D:50:VAL:CG2	1:D:145:VAL:HG12	2.47	0.44
1:C:327:VAL:O	1:C:330:GLN:NE2	2.50	0.44
1:I:50:VAL:CG2	1:I:145:VAL:HG12	2.48	0.44
1:J:262:ALA:HB2	1:J:350:SER:HA	2.00	0.44
1:K:262:ALA:HB2	1:K:350:SER:HA	2.00	0.44
1:E:286:LEU:HB3	1:E:319:VAL:HG22	2.00	0.43
1:F:50:VAL:CG2	1:F:145:VAL:HG12	2.48	0.43
1:D:262:ALA:HB2	1:D:350:SER:HA	2.00	0.43
1:I:262:ALA:HB2	1:I:350:SER:HA	2.01	0.43
1:A:262:ALA:HB2	1:A:350:SER:HA	2.01	0.43
1:G:262:ALA:HB2	1:G:350:SER:HA	2.01	0.43
1:L:262:ALA:HB2	1:L:350:SER:HA	2.01	0.43
1:E:262:ALA:HB2	1:E:350:SER:HA	2.00	0.42
1:B:286:LEU:HB3	1:B:319:VAL:HG22	2.02	0.42
1:H:262:ALA:HB2	1:H:350:SER:HA	2.02	0.42
1:F:287:VAL:O	1:F:398:ASP:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:MET:HG2	4:C:746:HOH:O	2.20	0.42
1:F:262:ALA:HB2	1:F:350:SER:HA	2.01	0.42
1:I:287:VAL:O	1:I:398:ASP:HA	2.20	0.42
1:A:287:VAL:O	1:A:398:ASP:HA	2.20	0.41
1:D:115:ASN:O	1:D:433:ARG:NH2	2.52	0.41
1:F:226:THR:OG1	1:F:268:ARG:HD3	2.21	0.41
1:J:464:MET:HG2	4:J:791:HOH:O	2.20	0.41
1:L:286:LEU:HB3	1:L:319:VAL:HG22	2.01	0.41
1:A:226:THR:OG1	1:A:268:ARG:HD3	2.21	0.41
1:C:286:LEU:HB3	1:C:319:VAL:HG22	2.03	0.41
1:D:464:MET:H	1:D:464:MET:HG2	1.80	0.41
1:C:262:ALA:HB2	1:C:350:SER:HA	2.02	0.41
1:G:287:VAL:O	1:G:398:ASP:HA	2.20	0.41
1:H:287:VAL:O	1:H:398:ASP:HA	2.21	0.41
1:A:464:MET:CE	1:A:474:CYS:HB2	2.51	0.41
1:J:286:LEU:HB3	1:J:319:VAL:HG22	2.02	0.41
1:D:286:LEU:HB3	1:D:319:VAL:HG22	2.04	0.40
1:I:286:LEU:HB3	1:I:319:VAL:HG22	2.03	0.40
1:B:262:ALA:HB2	1:B:350:SER:HA	2.02	0.40
1:E:368:ILE:HG12	1:E:461:THR:HB	2.04	0.40
1:J:287:VAL:O	1:J:398:ASP:HA	2.21	0.40
1:F:286:LEU:HB3	1:F:319:VAL:HG22	2.02	0.40
1:I:226:THR:OG1	1:I:268:ARG:HD3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:519:ARG:O	1:J:279:THR:CG2[2_848]	1.63	0.57

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	518/521 (99%)	507 (98%)	9 (2%)	2 (0%)	34	48
1	B	517/521 (99%)	507 (98%)	8 (2%)	2 (0%)	34	48
1	C	518/521 (99%)	506 (98%)	10 (2%)	2 (0%)	34	48
1	D	518/521 (99%)	505 (98%)	11 (2%)	2 (0%)	34	48
1	E	517/521 (99%)	506 (98%)	9 (2%)	2 (0%)	34	48
1	F	518/521 (99%)	507 (98%)	10 (2%)	1 (0%)	47	62
1	G	517/521 (99%)	504 (98%)	11 (2%)	2 (0%)	34	48
1	H	517/521 (99%)	505 (98%)	11 (2%)	1 (0%)	47	62
1	I	518/521 (99%)	507 (98%)	10 (2%)	1 (0%)	47	62
1	J	518/521 (99%)	506 (98%)	10 (2%)	2 (0%)	34	48
1	K	517/521 (99%)	505 (98%)	11 (2%)	1 (0%)	47	62
1	L	518/521 (99%)	506 (98%)	11 (2%)	1 (0%)	47	62
All	All	6211/6252 (99%)	6071 (98%)	121 (2%)	19 (0%)	41	55

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	354	ASP
1	C	354	ASP
1	D	354	ASP
1	E	354	ASP
1	F	354	ASP
1	G	354	ASP
1	H	354	ASP
1	I	354	ASP
1	J	354	ASP
1	K	354	ASP
1	L	354	ASP
1	A	137	PRO
1	C	137	PRO
1	G	137	PRO
1	J	137	PRO
1	D	138	ASN
1	E	138	ASN
1	B	138	ASN

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	395/411 (96%)	386 (98%)	9 (2%)	50	70
1	B	391/411 (95%)	383 (98%)	8 (2%)	55	74
1	C	394/411 (96%)	386 (98%)	8 (2%)	55	74
1	D	393/411 (96%)	385 (98%)	8 (2%)	55	74
1	E	393/411 (96%)	384 (98%)	9 (2%)	50	70
1	F	390/411 (95%)	381 (98%)	9 (2%)	50	70
1	G	392/411 (95%)	385 (98%)	7 (2%)	59	76
1	H	389/411 (95%)	381 (98%)	8 (2%)	53	72
1	I	392/411 (95%)	382 (97%)	10 (3%)	46	66
1	J	395/411 (96%)	386 (98%)	9 (2%)	50	70
1	K	387/411 (94%)	379 (98%)	8 (2%)	53	72
1	L	391/411 (95%)	384 (98%)	7 (2%)	59	76
All	All	4702/4932 (95%)	4602 (98%)	100 (2%)	53	72

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ILE
1	A	225	PHE
1	A	292	VAL
1	A	351	TYR
1	A	422	GLU
1	A	464	MET
1	A	465	GLU
1	A	467	ARG
1	A	496	LEU
1	B	41	VAL
1	B	153	ILE
1	B	225	PHE
1	B	351	TYR
1	B	422	GLU

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Mol	Chain	Res	Type
1	B	464	MET
1	B	465	GLU
1	B	496	LEU
1	C	153	ILE
1	C	225	PHE
1	C	292	VAL
1	C	351	TYR
1	C	422	GLU
1	C	464	MET
1	C	465	GLU
1	C	496	LEU
1	D	153	ILE
1	D	225	PHE
1	D	292	VAL
1	D	295	CYS
1	D	351	TYR
1	D	464	MET
1	D	465	GLU
1	D	496	LEU
1	E	41	VAL
1	E	153	ILE
1	E	225	PHE
1	E	319	VAL
1	E	351	TYR
1	E	422	GLU
1	E	465	GLU
1	E	467	ARG
1	E	496	LEU
1	F	109	THR
1	F	153	ILE
1	F	225	PHE
1	F	292	VAL
1	F	351	TYR
1	F	464	MET
1	F	465	GLU
1	F	496	LEU
1	F	519	ARG
1	G	153	ILE
1	G	225	PHE
1	G	292	VAL
1	G	351	TYR
1	G	422	GLU

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Mol	Chain	Res	Type
1	G	465	GLU
1	G	496	LEU
1	H	41	VAL
1	H	153	ILE
1	H	225	PHE
1	H	351	TYR
1	H	422	GLU
1	H	464	MET
1	H	465	GLU
1	H	496	LEU
1	I	109	THR
1	I	153	ILE
1	I	225	PHE
1	I	292	VAL
1	I	351	TYR
1	I	464	MET
1	I	465	GLU
1	I	467	ARG
1	I	496	LEU
1	I	519	ARG
1	J	153	ILE
1	J	225	PHE
1	J	292	VAL
1	J	295	CYS
1	J	351	TYR
1	J	422	GLU
1	J	464	MET
1	J	465	GLU
1	J	496	LEU
1	K	41	VAL
1	K	153	ILE
1	K	225	PHE
1	K	295	CYS
1	K	351	TYR
1	K	422	GLU
1	K	465	GLU
1	K	496	LEU
1	L	153	ILE
1	L	225	PHE
1	L	292	VAL
1	L	351	TYR
1	L	464	MET

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Mol	Chain	Res	Type
1	L	465	GLU
1	L	496	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	148	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BCT	E	601	-	2,3,3	0.75	0	2,3,3	1.25	0
2	BCT	J	601	-	2,3,3	0.85	0	2,3,3	0.88	0
2	BCT	D	601	-	2,3,3	0.56	0	2,3,3	1.94	1 (50%)
2	BCT	A	601	-	2,3,3	0.81	0	2,3,3	1.10	0
2	BCT	F	601	-	2,3,3	0.98	0	2,3,3	1.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BCT	K	601	-	2,3,3	0.75	0	2,3,3	1.46	1 (50%)
2	BCT	B	601	-	2,3,3	0.70	0	2,3,3	1.28	0
2	BCT	I	601	-	2,3,3	1.16	0	2,3,3	0.56	0
2	BCT	C	601	-	2,3,3	0.84	0	2,3,3	2.22	1 (50%)
2	BCT	G	601	-	2,3,3	0.83	0	2,3,3	1.76	1 (50%)
2	BCT	L	601	-	2,3,3	0.69	0	2,3,3	0.92	0
2	BCT	H	601	-	2,3,3	0.64	0	2,3,3	1.22	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	BCT	O2-C-O1	3.04	127.44	119.55
2	G	601	BCT	O2-C-O1	2.45	125.89	119.55
2	D	601	BCT	O2-C-O1	2.20	125.25	119.55
2	K	601	BCT	O2-C-O1	2.01	124.77	119.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	519/521 (99%)	-0.19	12 (2%)	60	58	23, 33, 53, 85	0
1	B	519/521 (99%)	-0.09	10 (1%)	66	64	27, 35, 54, 83	0
1	C	519/521 (99%)	-0.20	15 (2%)	51	50	22, 32, 52, 90	0
1	D	519/521 (99%)	-0.22	13 (2%)	57	55	24, 33, 51, 74	0
1	E	519/521 (99%)	-0.15	16 (3%)	49	47	23, 33, 53, 82	0
1	F	519/521 (99%)	0.15	16 (3%)	49	47	26, 39, 58, 78	0
1	G	519/521 (99%)	-0.20	7 (1%)	77	75	22, 32, 53, 83	0
1	H	519/521 (99%)	-0.11	15 (2%)	51	50	24, 35, 55, 112	0
1	I	519/521 (99%)	-0.20	5 (0%)	82	80	23, 32, 50, 78	0
1	J	519/521 (99%)	-0.28	11 (2%)	63	61	21, 29, 51, 83	0
1	K	519/521 (99%)	-0.27	7 (1%)	77	75	20, 29, 48, 92	0
1	L	519/521 (99%)	-0.18	10 (1%)	66	64	23, 33, 53, 73	0
All	All	6228/6252 (99%)	-0.16	137 (2%)	62	60	20, 33, 54, 112	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	THR	5.1
1	F	41	VAL	4.3
1	F	278	GLY	4.3
1	B	90	GLY	4.2
1	E	317	ALA	4.0
1	B	279	THR	3.9
1	K	137	PRO	3.8
1	K	90	GLY	3.6
1	J	279	THR	3.6
1	G	95	ALA	3.5
1	H	138	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	4	LEU	3.5
1	H	137	PRO	3.5
1	E	279	THR	3.4
1	K	4	LEU	3.4
1	B	41	VAL	3.3
1	C	319	VAL	3.2
1	C	96	GLY	3.1
1	A	4	LEU	3.1
1	A	3	THR	3.0
1	F	4	LEU	3.0
1	F	279	THR	3.0
1	F	237	GLY	2.9
1	J	319	VAL	2.9
1	F	277	LYS	2.9
1	A	5	PRO	2.9
1	E	288	GLY	2.9
1	L	4	LEU	2.8
1	J	288	GLY	2.8
1	A	316	ALA	2.8
1	C	316	ALA	2.8
1	D	314	GLY	2.8
1	D	3	THR	2.7
1	L	41	VAL	2.7
1	H	41	VAL	2.7
1	B	3	THR	2.7
1	F	173	ALA	2.7
1	C	318	ALA	2.6
1	L	3	THR	2.6
1	H	63	ARG	2.6
1	A	315	GLY	2.6
1	B	138	ASN	2.6
1	F	275	THR	2.6
1	A	96	GLY	2.6
1	H	291	ILE	2.6
1	D	399	MET	2.5
1	E	287	VAL	2.5
1	A	288	GLY	2.5
1	G	400	ALA	2.5
1	C	39	LYS	2.5
1	E	3	THR	2.5
1	H	3	THR	2.5
1	F	40	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	138	ASN	2.5
1	B	377	VAL	2.5
1	G	401	THR	2.5
1	I	4	LEU	2.4
1	C	4	LEU	2.4
1	F	42	LEU	2.4
1	D	494	VAL	2.4
1	F	95	ALA	2.4
1	I	3	THR	2.4
1	D	4	LEU	2.4
1	C	37	ASN	2.4
1	G	399	MET	2.4
1	C	3	THR	2.4
1	J	316	ALA	2.4
1	C	315	GLY	2.4
1	G	314	GLY	2.4
1	E	400	ALA	2.4
1	H	318	ALA	2.4
1	J	318	ALA	2.4
1	L	317	ALA	2.4
1	A	319	VAL	2.3
1	I	59	PRO	2.3
1	A	496	LEU	2.3
1	I	315	GLY	2.3
1	K	378	LEU	2.3
1	E	318	ALA	2.3
1	E	401	THR	2.3
1	H	314	GLY	2.3
1	D	318	ALA	2.3
1	C	400	ALA	2.3
1	D	287	VAL	2.3
1	E	399	MET	2.3
1	D	377	VAL	2.2
1	H	315	GLY	2.2
1	B	291	ILE	2.2
1	L	92	ALA	2.2
1	J	287	VAL	2.2
1	K	291	ILE	2.2
1	D	288	GLY	2.2
1	H	288	GLY	2.2
1	D	319	VAL	2.2
1	I	278	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	61	VAL	2.2
1	L	316	ALA	2.2
1	G	315	GLY	2.2
1	A	318	ALA	2.2
1	F	315	GLY	2.2
1	D	511	PRO	2.2
1	J	339	LEU	2.2
1	H	400	ALA	2.1
1	H	278	GLY	2.1
1	J	400	ALA	2.1
1	E	378	LEU	2.1
1	A	400	ALA	2.1
1	J	317	ALA	2.1
1	B	239	ASP	2.1
1	B	237	GLY	2.1
1	B	288	GLY	2.1
1	E	90	GLY	2.1
1	E	278	GLY	2.1
1	H	290	GLY	2.1
1	D	400	ALA	2.1
1	F	32	ALA	2.1
1	E	315	GLY	2.1
1	C	399	MET	2.1
1	C	137	PRO	2.1
1	L	291	ILE	2.1
1	C	496	LEU	2.1
1	D	315	GLY	2.1
1	E	94	ALA	2.0
1	E	316	ALA	2.0
1	F	59	PRO	2.0
1	J	496	LEU	2.0
1	C	290	GLY	2.0
1	K	290	GLY	2.0
1	L	314	GLY	2.0
1	L	399	MET	2.0
1	H	279	THR	2.0
1	L	313	MET	2.0
1	A	39	LYS	2.0
1	H	342	ALA	2.0
1	C	5	PRO	2.0
1	J	399	MET	2.0
1	K	399	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BCT	D	601	4/4	0.92	0.19	37,39,40,44	0
3	MN	B	602	1/1	0.93	0.08	36,36,36,36	0
2	BCT	E	601	4/4	0.94	0.23	38,42,43,48	0
3	MN	F	603	1/1	0.94	0.10	38,38,38,38	0
3	MN	B	603	1/1	0.95	0.10	32,32,32,32	0
3	MN	F	602	1/1	0.95	0.07	38,38,38,38	0
2	BCT	H	601	4/4	0.95	0.19	30,33,34,37	0
2	BCT	I	601	4/4	0.96	0.19	35,36,36,42	0
2	BCT	J	601	4/4	0.96	0.14	33,37,40,40	0
2	BCT	F	601	4/4	0.96	0.17	40,41,46,46	0
3	MN	L	602	1/1	0.96	0.09	30,30,30,30	0
3	MN	L	603	1/1	0.96	0.12	26,26,26,26	0
2	BCT	B	601	4/4	0.97	0.18	39,39,42,42	0
3	MN	E	602	1/1	0.97	0.09	33,33,33,33	0
3	MN	E	603	1/1	0.97	0.09	31,31,31,31	0
2	BCT	G	601	4/4	0.97	0.18	35,35,37,39	0
2	BCT	K	601	4/4	0.97	0.17	27,31,31,33	0
3	MN	G	603	1/1	0.97	0.10	28,28,28,28	0
3	MN	I	603	1/1	0.97	0.11	30,30,30,30	0
3	MN	A	602	1/1	0.97	0.09	31,31,31,31	0
2	BCT	C	601	4/4	0.97	0.21	32,37,42,44	0
3	MN	A	603	1/1	0.98	0.08	29,29,29,29	0
2	BCT	L	601	4/4	0.98	0.15	37,39,39,45	0
3	MN	J	603	1/1	0.98	0.12	25,25,25,25	0
3	MN	K	603	1/1	0.98	0.15	26,26,26,26	0
2	BCT	A	601	4/4	0.98	0.15	32,33,34,34	0
3	MN	D	602	1/1	0.98	0.09	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MN	H	603	1/1	0.99	0.09	28,28,28,28	0
3	MN	I	602	1/1	0.99	0.11	32,32,32,32	0
3	MN	D	603	1/1	0.99	0.15	31,31,31,31	0
3	MN	J	602	1/1	0.99	0.07	27,27,27,27	0
3	MN	C	603	1/1	0.99	0.10	29,29,29,29	0
3	MN	K	602	1/1	0.99	0.08	26,26,26,26	0
3	MN	G	602	1/1	0.99	0.07	30,30,30,30	0
3	MN	C	602	1/1	0.99	0.09	31,31,31,31	0
3	MN	H	602	1/1	0.99	0.08	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.