



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 12:15 am GMT

PDB ID : 3MQ7
Title : Crystal Structure of Ectodomain Mutant of BST-2/Tetherin/CD317
Authors : Xiong, Y.; Yang, H.; Wang, J.; Meng, W.
Deposited on : 2010-04-27
Resolution : 2.28 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

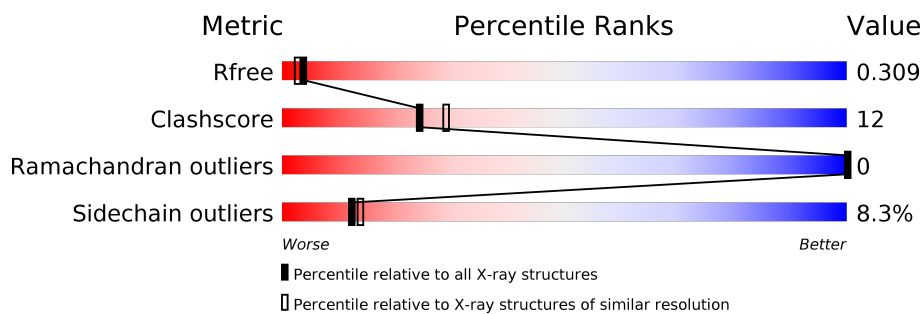
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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}	111664	6121 (2.30-2.26)
Clashscore	122126	6842 (2.30-2.26)
Ramachandran outliers	120053	6755 (2.30-2.26)
Sidechain outliers	120020	6755 (2.30-2.26)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	121	
1	B	121	
1	C	121	
1	D	121	
1	E	121	
1	F	121	
1	G	121	

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Mol	Chain	Length	Quality of chain
1	H	121	 62% 16% • 18%
1	I	121	 60% 17% • • 18%
1	J	121	 67% 12% • • 18%
1	K	121	 65% 14% • 18%
1	L	121	 65% 15% • 18%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9314 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 Bone marrow stromal antigen 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	B	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	C	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	D	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	E	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	F	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	G	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	H	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	I	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	J	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	K	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			
1	L	99	Total	C	N	O	Se	0	0	0
			765	463	144	155	3			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	-	EXPRESSION TAG	UNP Q10589
A	42	GLY	-	EXPRESSION TAG	UNP Q10589
A	43	PHE	-	EXPRESSION TAG	UNP Q10589
A	44	SER	-	EXPRESSION TAG	UNP Q10589
A	45	MSE	-	EXPRESSION TAG	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASP	-	EXPRESSION TAG	UNP Q10589
A	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
A	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
A	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
B	41	ALA	-	EXPRESSION TAG	UNP Q10589
B	42	GLY	-	EXPRESSION TAG	UNP Q10589
B	43	PHE	-	EXPRESSION TAG	UNP Q10589
B	44	SER	-	EXPRESSION TAG	UNP Q10589
B	45	MSE	-	EXPRESSION TAG	UNP Q10589
B	46	ASP	-	EXPRESSION TAG	UNP Q10589
B	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
B	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
B	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
C	41	ALA	-	EXPRESSION TAG	UNP Q10589
C	42	GLY	-	EXPRESSION TAG	UNP Q10589
C	43	PHE	-	EXPRESSION TAG	UNP Q10589
C	44	SER	-	EXPRESSION TAG	UNP Q10589
C	45	MSE	-	EXPRESSION TAG	UNP Q10589
C	46	ASP	-	EXPRESSION TAG	UNP Q10589
C	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
C	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
C	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
D	41	ALA	-	EXPRESSION TAG	UNP Q10589
D	42	GLY	-	EXPRESSION TAG	UNP Q10589
D	43	PHE	-	EXPRESSION TAG	UNP Q10589
D	44	SER	-	EXPRESSION TAG	UNP Q10589
D	45	MSE	-	EXPRESSION TAG	UNP Q10589
D	46	ASP	-	EXPRESSION TAG	UNP Q10589
D	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
D	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
D	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
E	41	ALA	-	EXPRESSION TAG	UNP Q10589
E	42	GLY	-	EXPRESSION TAG	UNP Q10589
E	43	PHE	-	EXPRESSION TAG	UNP Q10589
E	44	SER	-	EXPRESSION TAG	UNP Q10589
E	45	MSE	-	EXPRESSION TAG	UNP Q10589
E	46	ASP	-	EXPRESSION TAG	UNP Q10589
E	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
E	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
E	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
F	41	ALA	-	EXPRESSION TAG	UNP Q10589
F	42	GLY	-	EXPRESSION TAG	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
F	43	PHE	-	EXPRESSION TAG	UNP Q10589
F	44	SER	-	EXPRESSION TAG	UNP Q10589
F	45	MSE	-	EXPRESSION TAG	UNP Q10589
F	46	ASP	-	EXPRESSION TAG	UNP Q10589
F	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
F	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
F	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
G	41	ALA	-	EXPRESSION TAG	UNP Q10589
G	42	GLY	-	EXPRESSION TAG	UNP Q10589
G	43	PHE	-	EXPRESSION TAG	UNP Q10589
G	44	SER	-	EXPRESSION TAG	UNP Q10589
G	45	MSE	-	EXPRESSION TAG	UNP Q10589
G	46	ASP	-	EXPRESSION TAG	UNP Q10589
G	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
G	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
G	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
H	41	ALA	-	EXPRESSION TAG	UNP Q10589
H	42	GLY	-	EXPRESSION TAG	UNP Q10589
H	43	PHE	-	EXPRESSION TAG	UNP Q10589
H	44	SER	-	EXPRESSION TAG	UNP Q10589
H	45	MSE	-	EXPRESSION TAG	UNP Q10589
H	46	ASP	-	EXPRESSION TAG	UNP Q10589
H	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
H	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
H	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
I	41	ALA	-	EXPRESSION TAG	UNP Q10589
I	42	GLY	-	EXPRESSION TAG	UNP Q10589
I	43	PHE	-	EXPRESSION TAG	UNP Q10589
I	44	SER	-	EXPRESSION TAG	UNP Q10589
I	45	MSE	-	EXPRESSION TAG	UNP Q10589
I	46	ASP	-	EXPRESSION TAG	UNP Q10589
I	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
I	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
I	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
J	41	ALA	-	EXPRESSION TAG	UNP Q10589
J	42	GLY	-	EXPRESSION TAG	UNP Q10589
J	43	PHE	-	EXPRESSION TAG	UNP Q10589
J	44	SER	-	EXPRESSION TAG	UNP Q10589
J	45	MSE	-	EXPRESSION TAG	UNP Q10589
J	46	ASP	-	EXPRESSION TAG	UNP Q10589
J	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
J	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
J	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
K	41	ALA	-	EXPRESSION TAG	UNP Q10589
K	42	GLY	-	EXPRESSION TAG	UNP Q10589
K	43	PHE	-	EXPRESSION TAG	UNP Q10589
K	44	SER	-	EXPRESSION TAG	UNP Q10589
K	45	MSE	-	EXPRESSION TAG	UNP Q10589
K	46	ASP	-	EXPRESSION TAG	UNP Q10589
K	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
K	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
K	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
L	41	ALA	-	EXPRESSION TAG	UNP Q10589
L	42	GLY	-	EXPRESSION TAG	UNP Q10589
L	43	PHE	-	EXPRESSION TAG	UNP Q10589
L	44	SER	-	EXPRESSION TAG	UNP Q10589
L	45	MSE	-	EXPRESSION TAG	UNP Q10589
L	46	ASP	-	EXPRESSION TAG	UNP Q10589
L	53	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
L	63	ALA	CYS	ENGINEERED MUTATION	UNP Q10589
L	91	ALA	CYS	ENGINEERED MUTATION	UNP Q10589

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	K	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	5	Total O 5 5	0	0
3	C	8	Total O 8 8	0	0
3	D	9	Total O 9 9	0	0
3	E	21	Total O 21 21	0	0
3	F	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	7	Total 7	O 7	0	0
3	H	7	Total 7	O 7	0	0
3	I	10	Total 10	O 10	0	0
3	J	9	Total 9	O 9	0	0
3	K	24	Total 24	O 24	0	0
3	L	8	Total 8	O 8	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. 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. 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.

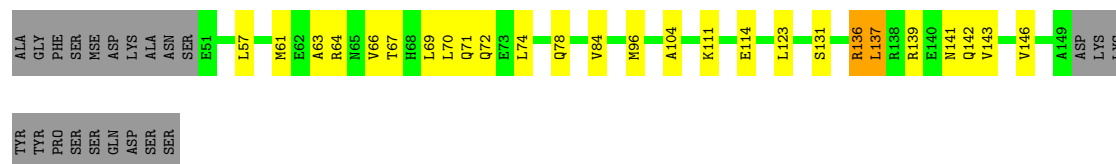
• Molecule 1: Bone marrow stromal antigen 2

Chain A: 



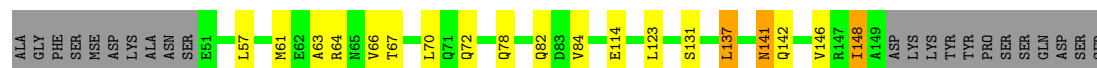
• Molecule 1: Bone marrow stromal antigen 2

Chain B: 



• Molecule 1: Bone marrow stromal antigen 2

Chain C: 



• Molecule 1: Bone marrow stromal antigen 2

Chain D: 



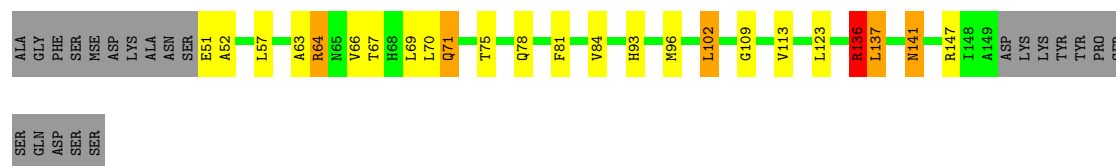
• Molecule 1: Bone marrow stromal antigen 2

Chain E: 



• Molecule 1: Bone marrow stromal antigen 2

Chain F: 



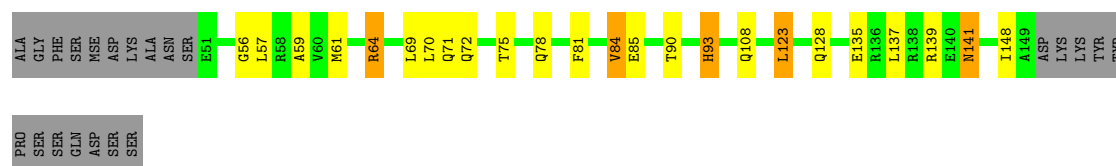
• Molecule 1: Bone marrow stromal antigen 2

Chain G: 



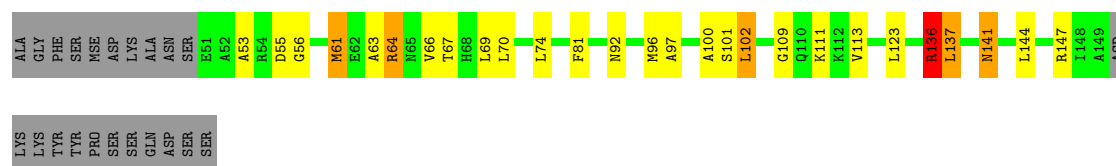
• Molecule 1: Bone marrow stromal antigen 2

Chain H: 



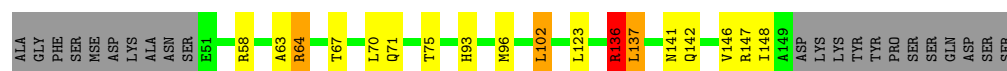
• Molecule 1: Bone marrow stromal antigen 2

Chain I: 



• Molecule 1: Bone marrow stromal antigen 2

Chain J: 



• Molecule 1: Bone marrow stromal antigen 2

Chain K: 



• Molecule 1: Bone marrow stromal antigen 2

Chain L: 

ALA	GLY	PHE	SER	ASN	ASP	LYS	ALA	ASN	SER	E51	L57	A63	R64	N65	Y66	T67	H68	L69	L70	E73	L74	T75	F81	V84	H93	N96	V134	L137	R138	R139	V143	R147	T148	A149	ASP	LYS	LYS	TYR	PRO	SER	SER	GLN	ASP	SER	SER
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.00Å 97.16Å 117.40Å 90.00° 105.86° 90.00°	Depositor
Resolution (Å)	38.68 – 2.28 38.58 – 2.29	Depositor EDS
% Data completeness (in resolution range)	96.0 (38.68-2.28) 97.6 (38.58-2.29)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.236 , 0.270 0.281 , 0.309	Depositor DCC
R_{free} test set	3142 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.893 for H, K, L 0.107 for -H, -K, H+L	Depositor
Outliers	3 of 63326 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9314	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2414e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

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

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	0.62	0/765	0.67	0/1023
1	B	0.61	0/765	0.69	2/1023 (0.2%)
1	C	0.61	0/765	0.68	0/1023
1	D	0.60	0/765	0.67	0/1023
1	E	0.77	0/765	0.86	1/1023 (0.1%)
1	F	0.67	0/765	0.82	2/1023 (0.2%)
1	G	0.79	1/765 (0.1%)	0.78	0/1023
1	H	0.65	0/765	0.69	0/1023
1	I	0.71	0/765	0.83	3/1023 (0.3%)
1	J	0.60	0/765	0.76	2/1023 (0.2%)
1	K	0.75	0/765	0.78	0/1023
1	L	0.70	0/765	0.72	0/1023
All	All	0.68	1/9180 (0.0%)	0.75	10/12276 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	60	VAL	CB-CG2	-6.54	1.39	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	58	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	F	102	LEU	CA-CB-CG	6.54	130.34	115.30
1	B	136	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	B	136	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	I	136	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	E	83	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	F	136	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	I	136	ARG	NE-CZ-NH1	5.14	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	136	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	I	55	ASP	CB-CG-OD1	-5.09	113.72	118.30

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	765	0	766	25	0
1	B	765	0	766	31	0
1	C	765	0	766	27	0
1	D	765	0	766	25	0
1	E	765	0	766	32	0
1	F	765	0	766	35	0
1	G	765	0	766	35	0
1	H	765	0	766	43	0
1	I	765	0	766	32	0
1	J	765	0	766	14	0
1	K	765	0	766	26	0
1	L	765	0	766	25	0
2	E	1	0	0	0	0
2	K	1	0	0	0	0
3	A	7	0	0	0	0
3	B	5	0	0	0	0
3	C	8	0	0	0	0
3	D	9	0	0	0	0
3	E	21	0	0	1	0
3	F	17	0	0	2	0
3	G	7	0	0	8	0
3	H	7	0	0	2	0
3	I	10	0	0	2	0
3	J	9	0	0	1	0
3	K	24	0	0	6	0
3	L	8	0	0	0	0
All	All	9314	0	9192	216	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (216) 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:A:84:VAL:CG1	1:B:84:VAL:HG11	1.73	1.19
1:C:70:LEU:HD21	1:D:70:LEU:HD21	1.28	1.15
1:K:70:LEU:HD21	1:L:70:LEU:HD21	1.21	1.14
1:A:84:VAL:HG11	1:B:84:VAL:CG1	1.78	1.12
1:G:84:VAL:HG11	1:H:84:VAL:HG11	1.31	1.11
1:G:70:LEU:HD21	1:H:70:LEU:HD21	1.32	1.11
1:A:70:LEU:HD21	1:B:70:LEU:HD21	1.15	1.07
1:C:84:VAL:HG11	1:D:84:VAL:HG11	1.27	1.07
1:A:66:VAL:HG13	1:D:66:VAL:HG13	1.38	1.06
1:E:84:VAL:HG11	1:F:84:VAL:HG11	1.39	1.05
1:E:78:GLN:OE1	1:G:64:ARG:NH1	1.92	1.00
1:I:70:LEU:CD2	1:J:70:LEU:HD21	1.93	0.99
1:F:51:GLU:HG3	1:F:52:ALA:H	1.27	0.99
1:H:135:GLU:HG3	1:L:143:VAL:HG22	1.51	0.93
1:C:84:VAL:CG1	1:D:84:VAL:HG11	2.01	0.91
1:F:67:THR:OG1	1:H:71:GLN:NE2	2.04	0.89
1:A:70:LEU:HD21	1:B:70:LEU:CD2	2.01	0.89
1:G:71:GLN:OE1	3:G:162:HOH:O	1.89	0.89
1:G:141:ASN:HD22	1:H:141:ASN:HD22	1.20	0.89
1:B:66:VAL:HG13	1:C:66:VAL:HG13	1.51	0.89
1:B:96:MSE:CE	1:L:57:LEU:HD23	2.03	0.88
1:I:64:ARG:HD2	3:I:168:HOH:O	1.76	0.85
1:E:84:VAL:CG1	1:F:84:VAL:HG11	2.06	0.84
1:A:66:VAL:CG1	1:D:66:VAL:HG13	2.09	0.83
1:A:84:VAL:HG11	1:B:84:VAL:HG11	0.87	0.83
1:B:96:MSE:HE3	1:L:57:LEU:HD23	1.60	0.82
1:F:71:GLN:HE22	1:H:64:ARG:CG	1.94	0.81
1:G:84:VAL:CG1	1:H:84:VAL:HG11	2.10	0.81
1:K:78:GLN:OE1	3:K:5:HOH:O	1.99	0.79
1:G:64:ARG:NE	3:G:168:HOH:O	2.14	0.79
1:E:53:ALA:HB2	1:H:84:VAL:HG23	1.65	0.78
1:K:78:GLN:CD	3:K:5:HOH:O	2.21	0.78
1:A:84:VAL:CG1	1:B:84:VAL:CG1	2.46	0.78
1:I:70:LEU:HD21	1:J:70:LEU:HD21	1.64	0.77
1:E:111:LYS:NZ	1:I:97:ALA:O	2.18	0.76
1:I:141:ASN:HD22	1:J:141:ASN:HD22	1.30	0.76
1:I:102:LEU:HD23	1:J:102:LEU:HD23	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:LEU:HD23	1:J:70:LEU:HD21	1.67	0.76
1:B:66:VAL:HG13	1:C:66:VAL:CG1	2.15	0.75
1:E:78:GLN:CD	1:G:61:MSE:HE1	2.07	0.75
1:F:93:HIS:HA	1:F:96:MSE:HE3	1.69	0.75
1:F:51:GLU:HG3	1:F:52:ALA:N	2.02	0.74
1:G:141:ASN:HD22	1:H:141:ASN:ND2	1.85	0.74
1:I:56:GLY:HA3	1:K:81:PHE:CZ	2.23	0.74
1:E:84:VAL:HG11	1:F:84:VAL:CG1	2.14	0.73
1:F:71:GLN:HE22	1:H:64:ARG:HG3	1.52	0.73
1:K:70:LEU:CD2	1:L:70:LEU:HD21	2.11	0.72
1:G:84:VAL:HG11	1:H:84:VAL:CG1	2.15	0.72
1:E:78:GLN:OE1	1:G:61:MSE:HE1	1.90	0.72
1:E:136:ARG:HE	1:E:137:LEU:HD13	1.55	0.72
1:F:71:GLN:NE2	1:H:64:ARG:HG3	2.06	0.71
1:A:64:ARG:NH1	1:C:78:GLN:OE1	2.25	0.70
1:E:84:VAL:CG1	1:F:84:VAL:CG1	2.70	0.70
1:E:53:ALA:HB2	1:H:84:VAL:CG2	2.23	0.69
1:B:66:VAL:CG1	1:C:66:VAL:HG13	2.23	0.68
1:I:61:MSE:HE1	1:K:78:GLN:NE2	2.08	0.68
1:A:66:VAL:HG13	1:D:66:VAL:CG1	2.20	0.67
1:F:64:ARG:NH2	1:H:75:THR:OG1	2.27	0.67
1:I:61:MSE:HE1	1:K:78:GLN:CD	2.14	0.67
1:H:139:ARG:NH2	1:L:143:VAL:O	2.28	0.67
1:J:93:HIS:HA	1:J:96:MSE:HE3	1.77	0.67
1:G:84:VAL:CG1	1:H:84:VAL:HG21	2.26	0.65
1:E:56:GLY:HA3	1:G:81:PHE:CZ	2.32	0.65
1:A:78:GLN:OE1	1:C:64:ARG:NH1	2.30	0.65
1:I:63:ALA:O	1:I:67:THR:HG23	1.97	0.65
1:F:67:THR:HG1	1:H:71:GLN:NE2	1.94	0.64
1:I:136:ARG:HE	1:I:137:LEU:HD13	1.62	0.63
1:B:66:VAL:CG1	1:C:66:VAL:CG1	2.76	0.63
1:J:64:ARG:NH2	1:L:75:THR:OG1	2.31	0.63
1:G:71:GLN:HG3	3:G:162:HOH:O	1.99	0.63
1:H:81:PHE:O	1:H:84:VAL:HG12	1.99	0.63
1:H:56:GLY:O	1:H:59:ALA:HB3	1.99	0.63
1:B:70:LEU:HD23	1:D:67:THR:HG22	1.80	0.63
1:F:71:GLN:HE22	1:H:64:ARG:HG2	1.63	0.62
1:A:78:GLN:HG3	1:C:57:LEU:HD11	1.82	0.62
1:J:63:ALA:O	1:J:67:THR:HG23	2.00	0.62
1:E:64:ARG:NE	3:E:32:HOH:O	2.30	0.61
1:K:84:VAL:HG11	1:L:84:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:LYS:HE3	1:I:100:ALA:C	2.20	0.61
1:E:121:THR:OG1	1:I:111:LYS:HD2	2.00	0.61
1:H:72:GLN:NE2	3:H:166:HOH:O	2.32	0.61
1:G:81:PHE:CE2	1:H:81:PHE:CE2	2.88	0.61
1:B:70:LEU:HD23	1:D:67:THR:CG2	2.30	0.60
1:E:70:LEU:HD21	1:F:70:LEU:HD21	1.85	0.59
1:J:142:GLN:HG2	3:J:164:HOH:O	2.02	0.58
1:A:66:VAL:CG1	1:D:66:VAL:CG1	2.79	0.58
1:F:136:ARG:HD2	1:F:137:LEU:HD13	1.86	0.58
1:F:75:THR:OG1	1:H:64:ARG:NH2	2.37	0.57
1:E:71:GLN:NE2	1:G:67:THR:OG1	2.38	0.57
1:F:66:VAL:HG13	1:G:66:VAL:HG13	1.87	0.57
1:G:84:VAL:CG1	1:H:84:VAL:CG1	2.79	0.57
1:B:104:ALA:HB2	1:L:65:ASN:CG	2.24	0.57
1:F:67:THR:HG1	1:H:71:GLN:HE21	1.48	0.56
1:B:78:GLN:OE1	1:D:64:ARG:NH1	2.39	0.56
1:B:57:LEU:HD11	1:B:61:MSE:HE3	1.88	0.56
1:H:84:VAL:CG1	1:H:85:GLU:N	2.69	0.56
1:K:71:GLN:NE2	3:K:164:HOH:O	2.35	0.56
1:B:111:LYS:NZ	1:L:73:GLU:OE2	2.29	0.56
1:G:71:GLN:CG	3:G:162:HOH:O	2.53	0.56
1:H:139:ARG:HE	1:L:147:ARG:HG2	1.70	0.55
1:G:84:VAL:HG12	1:G:85:GLU:N	2.21	0.55
1:C:84:VAL:CG1	1:D:84:VAL:CG1	2.80	0.55
3:F:163:HOH:O	1:H:71:GLN:HG3	2.05	0.55
1:I:141:ASN:ND2	1:J:141:ASN:HD22	2.01	0.55
1:K:109:GLY:O	1:K:113:VAL:HG23	2.08	0.54
1:B:142:GLN:O	1:B:146:VAL:HG23	2.08	0.54
1:C:148:ILE:HD12	1:D:148:ILE:HD12	1.90	0.54
1:F:57:LEU:HD11	1:H:78:GLN:HG3	1.89	0.53
1:I:66:VAL:CG1	1:L:66:VAL:HG13	2.39	0.53
1:F:64:ARG:HD3	3:F:165:HOH:O	2.08	0.53
1:K:70:LEU:HD21	1:L:70:LEU:CD2	2.15	0.52
1:A:67:THR:HG22	1:C:70:LEU:HD23	1.90	0.52
1:A:63:ALA:O	1:A:67:THR:HG23	2.10	0.52
1:B:96:MSE:HE1	1:L:57:LEU:HD23	1.90	0.51
1:B:71:GLN:NE2	1:D:64:ARG:HG3	2.26	0.51
1:J:142:GLN:O	1:J:146:VAL:HG23	2.10	0.51
1:K:134:VAL:HG23	1:L:134:VAL:HG23	1.92	0.51
1:A:71:GLN:HE22	1:C:64:ARG:CG	2.23	0.51
1:J:136:ARG:HD2	1:J:137:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD21	1:D:70:LEU:CD2	2.20	0.51
1:G:63:ALA:O	1:G:67:THR:HG23	2.11	0.50
1:E:81:PHE:CD1	1:F:81:PHE:CE1	3.00	0.50
1:F:109:GLY:O	1:F:113:VAL:HG23	2.11	0.50
1:H:84:VAL:HG12	1:H:85:GLU:N	2.26	0.50
1:E:64:ARG:NH2	1:G:75:THR:OG1	2.45	0.50
1:E:141:ASN:HD22	1:F:141:ASN:HD22	1.58	0.50
1:H:128:GLN:HG2	1:L:139:ARG:HG3	1.92	0.50
1:I:81:PHE:CZ	1:K:56:GLY:HA3	2.47	0.49
1:B:63:ALA:O	1:B:67:THR:HG23	2.13	0.49
1:G:64:ARG:CZ	3:G:168:HOH:O	2.56	0.49
1:D:63:ALA:O	1:D:67:THR:HG23	2.12	0.49
1:G:148:ILE:CD1	1:H:148:ILE:HD13	2.43	0.48
1:C:57:LEU:HD11	1:C:61:MSE:HE3	1.95	0.48
1:E:111:LYS:CE	1:I:100:ALA:CB	2.92	0.48
1:K:137:LEU:HD21	1:L:138:ARG:HG3	1.96	0.48
1:A:70:LEU:HD23	1:C:67:THR:HG22	1.94	0.48
1:H:69:LEU:HD13	3:H:25:HOH:O	2.13	0.48
1:G:84:VAL:CG1	1:H:84:VAL:CG2	2.91	0.48
1:I:96:MSE:CE	3:I:165:HOH:O	2.61	0.48
1:K:81:PHE:CE2	1:L:81:PHE:CE2	3.02	0.48
1:E:78:GLN:CD	3:K:172:HOH:O	2.52	0.47
1:G:70:LEU:HD21	1:H:70:LEU:CD2	2.23	0.47
1:G:84:VAL:HG13	1:H:84:VAL:CG2	2.44	0.47
1:A:71:GLN:NE2	1:C:64:ARG:HG3	2.30	0.47
1:I:61:MSE:HE1	1:K:78:GLN:HG3	1.96	0.47
1:B:64:ARG:CG	1:D:71:GLN:HE22	2.28	0.47
1:H:90:THR:O	1:H:93:HIS:HB2	2.15	0.47
1:K:137:LEU:O	1:K:141:ASN:HB2	2.14	0.47
1:B:74:LEU:HA	1:B:74:LEU:HD23	1.79	0.46
1:E:84:VAL:HG13	1:F:84:VAL:CG1	2.43	0.46
1:G:64:ARG:HB3	3:G:166:HOH:O	2.14	0.46
1:I:61:MSE:HE1	1:K:78:GLN:CG	2.45	0.46
1:G:67:THR:O	1:G:70:LEU:HB3	2.14	0.46
1:H:128:GLN:CD	1:L:138:ARG:HB3	2.35	0.46
1:F:66:VAL:CG1	1:G:66:VAL:HG13	2.44	0.46
1:F:78:GLN:NE2	1:H:61:MSE:HE2	2.31	0.46
1:L:93:HIS:HA	1:L:96:MSE:HE3	1.97	0.46
1:E:84:VAL:HG13	1:F:84:VAL:HG13	1.98	0.46
1:F:64:ARG:HH22	1:H:75:THR:HG23	1.80	0.46
1:B:136:ARG:NH2	1:B:137:LEU:CD1	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:O	1:B:141:ASN:HB2	2.16	0.45
1:C:137:LEU:O	1:C:141:ASN:HB2	2.16	0.45
1:K:84:VAL:HG11	1:L:84:VAL:HG21	1.98	0.45
1:A:71:GLN:HE22	1:C:64:ARG:HG3	1.81	0.45
1:E:56:GLY:HA3	1:G:81:PHE:CE1	2.51	0.45
1:C:142:GLN:O	1:C:146:VAL:HG23	2.17	0.44
1:B:71:GLN:HE22	1:D:64:ARG:HG3	1.82	0.44
1:F:136:ARG:HD2	1:F:137:LEU:CD1	2.47	0.44
1:B:64:ARG:HG3	1:D:71:GLN:NE2	2.32	0.44
1:B:64:ARG:HG3	1:D:71:GLN:HE22	1.82	0.44
1:E:111:LYS:HZ1	1:I:100:ALA:HB3	1.83	0.44
1:K:84:VAL:CG1	1:L:84:VAL:HG11	2.47	0.44
1:D:137:LEU:O	1:D:141:ASN:HB2	2.18	0.44
1:E:81:PHE:CE1	1:F:81:PHE:CE1	3.05	0.44
1:K:69:LEU:HD13	3:K:165:HOH:O	2.18	0.44
1:B:136:ARG:NH2	1:B:137:LEU:HD13	2.32	0.44
1:D:57:LEU:HD11	1:D:61:MSE:HE3	2.00	0.44
1:K:63:ALA:O	1:K:67:THR:HG23	2.18	0.43
1:F:78:GLN:HG3	1:H:57:LEU:HD11	1.99	0.43
1:I:144:LEU:HD22	1:J:148:ILE:HD12	2.00	0.43
1:A:78:GLN:HG3	1:C:57:LEU:CD1	2.49	0.43
1:A:78:GLN:O	1:A:82:GLN:HG3	2.18	0.43
1:K:54:ARG:NH1	3:K:166:HOH:O	2.52	0.43
1:G:64:ARG:HD3	3:G:166:HOH:O	2.19	0.43
1:H:123:LEU:HD12	1:H:123:LEU:HA	1.83	0.43
1:C:78:GLN:O	1:C:82:GLN:HG3	2.19	0.43
1:E:111:LYS:HE2	1:I:100:ALA:CB	2.49	0.42
1:E:111:LYS:CE	1:I:100:ALA:HB3	2.49	0.42
1:C:137:LEU:HD21	1:D:138:ARG:HG3	2.01	0.42
1:G:64:ARG:NH2	3:G:168:HOH:O	2.52	0.42
1:I:92:ASN:HB3	1:I:96:MSE:HE2	2.02	0.42
1:D:139:ARG:O	1:D:143:VAL:HG23	2.20	0.42
1:I:67:THR:OG1	1:K:71:GLN:NE2	2.52	0.42
1:E:67:THR:O	1:E:70:LEU:HB3	2.19	0.42
1:G:81:PHE:CD2	1:H:81:PHE:CZ	3.07	0.42
1:I:137:LEU:O	1:I:141:ASN:HB2	2.20	0.42
1:C:63:ALA:O	1:C:67:THR:HG23	2.20	0.42
1:I:109:GLY:O	1:I:113:VAL:HG23	2.20	0.42
1:K:57:LEU:O	1:K:58:ARG:C	2.58	0.42
1:J:75:THR:OG1	1:L:64:ARG:NH2	2.52	0.41
1:B:139:ARG:O	1:B:143:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:51:GLU:CG	1:F:52:ALA:N	2.75	0.41
1:I:74:LEU:HA	1:I:74:LEU:HD23	1.88	0.41
1:F:63:ALA:O	1:F:67:THR:HG23	2.21	0.41
1:L:63:ALA:O	1:L:67:THR:HG23	2.20	0.41
1:E:57:LEU:HD13	1:G:81:PHE:HB2	2.01	0.41
1:E:111:LYS:NZ	1:I:101:SER:N	2.69	0.41
1:A:148:ILE:CG2	1:A:149:ALA:N	2.84	0.41
1:D:148:ILE:CG2	1:D:149:ALA:N	2.83	0.41
1:K:56:GLY:O	1:K:59:ALA:HB3	2.21	0.41
1:C:148:ILE:CD1	1:D:148:ILE:HD12	2.51	0.41
1:F:51:GLU:CG	1:F:52:ALA:H	2.12	0.41
1:A:64:ARG:O	1:A:67:THR:OG1	2.39	0.40
1:I:53:ALA:HB2	1:L:84:VAL:CG2	2.52	0.40
1:A:142:GLN:O	1:A:146:VAL:HG23	2.21	0.40
1:A:71:GLN:HE22	1:C:64:ARG:HG2	1.86	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	97/121 (80%)	97 (100%)	0	0	100	100
1	B	97/121 (80%)	96 (99%)	1 (1%)	0	100	100
1	C	97/121 (80%)	97 (100%)	0	0	100	100
1	D	97/121 (80%)	97 (100%)	0	0	100	100
1	E	97/121 (80%)	97 (100%)	0	0	100	100
1	F	97/121 (80%)	96 (99%)	1 (1%)	0	100	100
1	G	97/121 (80%)	95 (98%)	2 (2%)	0	100	100
1	H	97/121 (80%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	97/121 (80%)	97 (100%)	0	0	100	100
1	J	97/121 (80%)	96 (99%)	1 (1%)	0	100	100
1	K	97/121 (80%)	96 (99%)	1 (1%)	0	100	100
1	L	97/121 (80%)	96 (99%)	1 (1%)	0	100	100
All	All	1164/1452 (80%)	1155 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	79/94 (84%)	73 (92%)	6 (8%)	14	17
1	B	79/94 (84%)	73 (92%)	6 (8%)	14	17
1	C	79/94 (84%)	72 (91%)	7 (9%)	11	11
1	D	79/94 (84%)	74 (94%)	5 (6%)	20	24
1	E	79/94 (84%)	72 (91%)	7 (9%)	11	11
1	F	79/94 (84%)	70 (89%)	9 (11%)	6	6
1	G	79/94 (84%)	72 (91%)	7 (9%)	11	11
1	H	79/94 (84%)	72 (91%)	7 (9%)	11	11
1	I	79/94 (84%)	70 (89%)	9 (11%)	6	6
1	J	79/94 (84%)	72 (91%)	7 (9%)	11	11
1	K	79/94 (84%)	74 (94%)	5 (6%)	20	24
1	L	79/94 (84%)	75 (95%)	4 (5%)	26	34
All	All	948/1128 (84%)	869 (92%)	79 (8%)	12	14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	114	GLU
1	A	121	THR
1	A	131	SER
1	A	137	LEU
1	A	148	ILE
1	B	69	LEU
1	B	72	GLN
1	B	114	GLU
1	B	123	LEU
1	B	131	SER
1	B	137	LEU
1	C	72	GLN
1	C	114	GLU
1	C	123	LEU
1	C	131	SER
1	C	137	LEU
1	C	141	ASN
1	C	148	ILE
1	D	72	GLN
1	D	103	ASP
1	D	114	GLU
1	D	131	SER
1	D	148	ILE
1	E	64	ARG
1	E	69	LEU
1	E	102	LEU
1	E	123	LEU
1	E	136	ARG
1	E	137	LEU
1	E	147	ARG
1	F	64	ARG
1	F	69	LEU
1	F	71	GLN
1	F	102	LEU
1	F	123	LEU
1	F	136	ARG
1	F	137	LEU
1	F	141	ASN
1	F	147	ARG
1	G	64	ARG
1	G	69	LEU
1	G	71	GLN

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Mol	Chain	Res	Type
1	G	84	VAL
1	G	123	LEU
1	G	128	GLN
1	G	137	LEU
1	H	64	ARG
1	H	84	VAL
1	H	93	HIS
1	H	108	GLN
1	H	123	LEU
1	H	137	LEU
1	H	141	ASN
1	I	61	MSE
1	I	64	ARG
1	I	69	LEU
1	I	102	LEU
1	I	123	LEU
1	I	136	ARG
1	I	137	LEU
1	I	141	ASN
1	I	147	ARG
1	J	64	ARG
1	J	71	GLN
1	J	102	LEU
1	J	123	LEU
1	J	136	ARG
1	J	137	LEU
1	J	147	ARG
1	K	64	ARG
1	K	84	VAL
1	K	123	LEU
1	K	137	LEU
1	K	141	ASN
1	L	64	ARG
1	L	69	LEU
1	L	84	VAL
1	L	137	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	72	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	A	92	ASN
1	A	128	GLN
1	B	71	GLN
1	B	72	GLN
1	B	128	GLN
1	C	72	GLN
1	C	92	ASN
1	C	128	GLN
1	D	82	GLN
1	D	141	ASN
1	E	71	GLN
1	E	72	GLN
1	E	110	GLN
1	E	128	GLN
1	F	71	GLN
1	F	78	GLN
1	F	110	GLN
1	F	128	GLN
1	F	141	ASN
1	G	71	GLN
1	G	92	ASN
1	H	71	GLN
1	H	72	GLN
1	H	82	GLN
1	H	87	GLN
1	H	92	ASN
1	H	141	ASN
1	I	87	GLN
1	I	110	GLN
1	J	71	GLN
1	J	110	GLN
1	J	128	GLN
1	J	141	ASN
1	K	71	GLN
1	K	72	GLN
1	K	92	ASN
1	K	141	ASN
1	L	92	ASN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.