



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:18 AM UTC

PDB ID : 3MQ7 / pdb_00003mq7
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

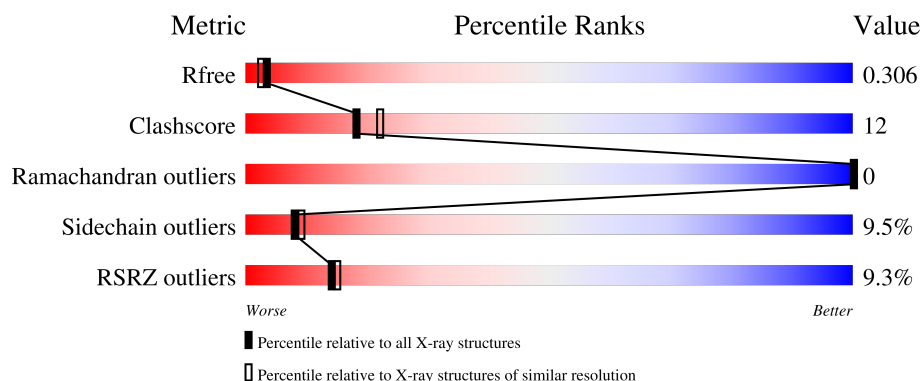
1 Overall quality at a glance

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.



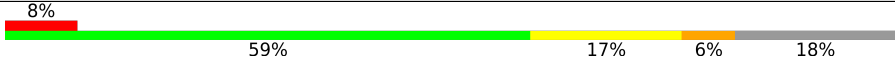
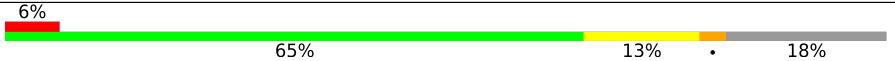
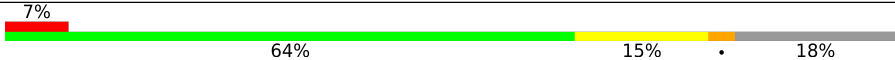
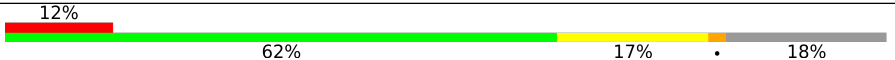
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	121	 6% 64% 17% 18%
1	B	121	 12% 59% 21% 18%
1	C	121	 7% 64% 15% 18%
1	D	121	 9% 64% 17% 18%
1	E	121	 8% 64% 14% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	121	
1	G	121	
1	H	121	
1	I	121	
1	J	121	
1	K	121	
1	L	121	

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (CCD ID: CA) (formula: Ca).

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

Continued on next page...

Continued from previous page...

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

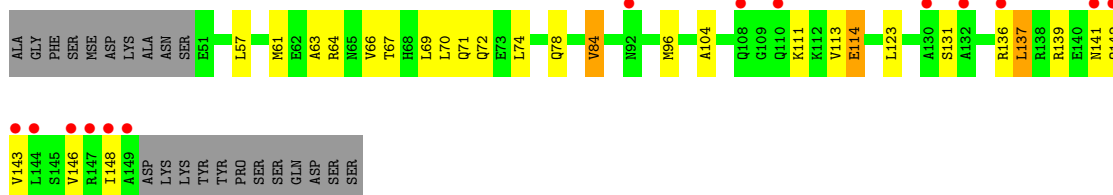
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

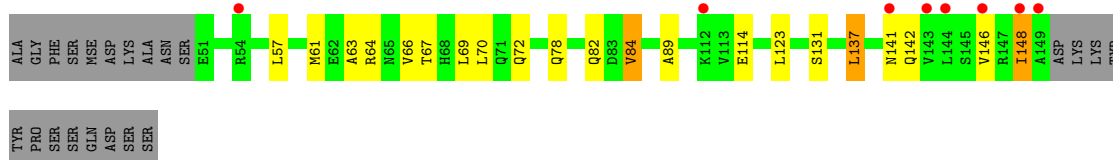
• Molecule 1: Bone marrow stromal antigen 2



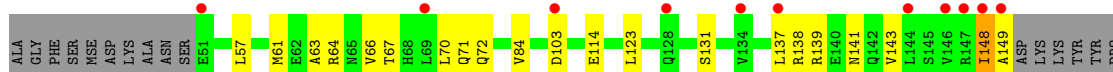
• Molecule 1: Bone marrow stromal antigen 2



• Molecule 1: Bone marrow stromal antigen 2



• Molecule 1: Bone marrow stromal antigen 2



SER
SER
GLN
ASP
SER
SER

• Molecule 1: Bone marrow stromal antigen 2



ALA GLY PHE MSE ASP LYS ALA ASN SER E51 E52 A53 G56 L57 E62 A63 R64 T67 H68 L69 L70 Q71 Q72 Q78 F81 V84 L102 K111 T121 T122 L123 V134 E135 R136 L137 R138 N141 Q142 V143 L144 S145 V146 R147 T148 A149 ASP LYS LYS

TYR
TYR
PRO
SER
SER
GLN
ASP
SER
SER

• Molecule 1: Bone marrow stromal antigen 2



ALA GLY PHE MSE ASP LYS ALA ASN SER E51 E52 A53 L57 R58 A59 A63 R64 R65 V66 T67 H68 L69 L70 Q71 Q75 T78 Q78 F81 V84 A89 H93 T94 V95 M96 L102 G109 V113 L123 V134 E135 R136 L137 N141 V146

A149 ASP LYS TYR TYR PRO SER SER GLN SER SER

• Molecule 1: Bone marrow stromal antigen 2



ALA GLY PHE MSE ASP LYS ALA ASN SER E51 M61 E62 A63 R64 R65 V66 T67 H68 L69 L70 Q71 Q72 E73 L74 T75 E76 A77 F81 Q82 D83 V84 E85 E114 L123 Q128 L137 N141 L144 S145 V146 R147 I148 A149 ASP LYS LYS TYR TYR PRO SER

GLN
ASP
SER
SER

• Molecule 1: Bone marrow stromal antigen 2

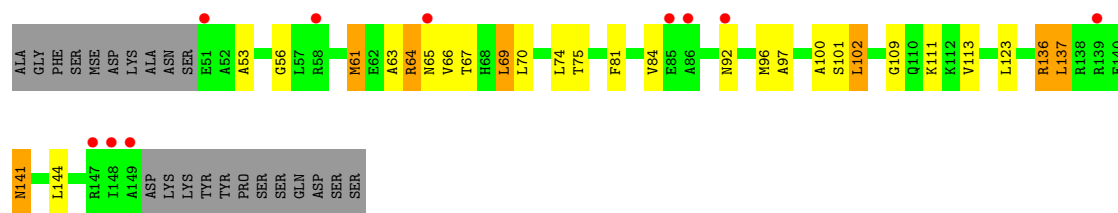


ALA GLY PHE MSE ASP LYS ALA ASN SER E51 G56 L57 R58 A59 V60 M61 R64 L69 L70 Q71 Q72 T75 E76 A77 Q78 F81 V84 E85 A86 Q87 A88 A89 T90 H93 E115 L123 Q128 A132 E135 R136 L137 R138 R139 E140 N141 R147

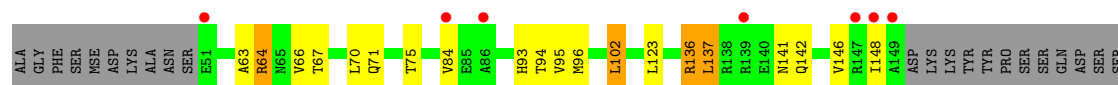
I148 A149 ASP LYS TYR TYR PRO SER SER GLN ASP SER SER

• Molecule 1: Bone marrow stromal antigen 2

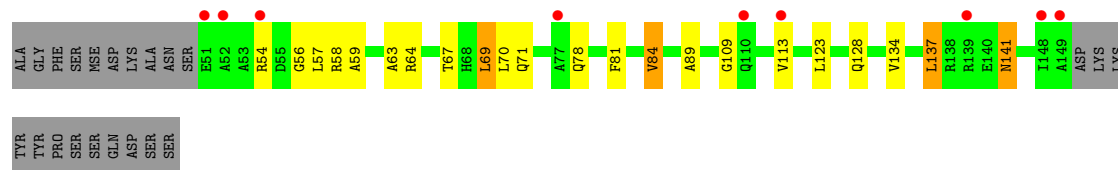




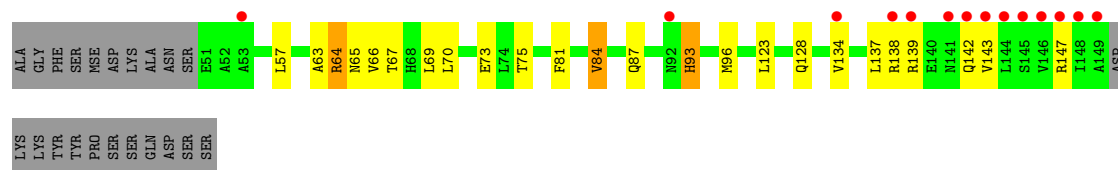
• Molecule 1: Bone marrow stromal antigen 2



• Molecule 1: Bone marrow stromal antigen 2



• Molecule 1: Bone marrow stromal antigen 2



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 38.68 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.0 (38.68-2.28) 97.5 (38.68-2.28)	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 0.280 , 0.306	Depositor DCC
R_{free} test set	3142 reflections (4.85%)	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)	0.31 , 20.4	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 [i](#)

5.1 Standard geometry [i](#)

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	0.87	1/765 (0.1%)	0.94	2/1023 (0.2%)
1	B	0.83	0/765	0.92	0/1023
1	C	0.80	1/765 (0.1%)	0.98	0/1023
1	D	0.85	0/765	0.92	0/1023
1	E	1.03	0/765	1.07	0/1023
1	F	0.89	2/765 (0.3%)	1.01	0/1023
1	G	1.05	2/765 (0.3%)	1.14	3/1023 (0.3%)
1	H	0.89	1/765 (0.1%)	1.02	4/1023 (0.4%)
1	I	0.94	0/765	1.12	1/1023 (0.1%)
1	J	0.86	1/765 (0.1%)	0.97	1/1023 (0.1%)
1	K	1.01	0/765	1.06	1/1023 (0.1%)
1	L	0.97	0/765	1.08	2/1023 (0.2%)
All	All	0.92	8/9180 (0.1%)	1.02	14/12276 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	81	PHE	CA-C	-6.29	1.44	1.52
1	G	72	GLN	CA-C	-5.63	1.45	1.52
1	F	89	ALA	CA-CB	5.49	1.62	1.53
1	H	59	ALA	CA-CB	5.36	1.62	1.53
1	A	100	ALA	CA-CB	5.23	1.61	1.53
1	J	66	VAL	CA-CB	-5.15	1.48	1.54
1	F	59	ALA	CA-CB	-5.05	1.45	1.53
1	C	89	ALA	CA-CB	5.01	1.61	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	65	ASN	N-CA-C	-7.36	103.26	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	81	PHE	N-CA-C	-6.56	104.05	111.07
1	H	93	HIS	CB-CA-C	-5.86	101.68	110.88
1	A	119	GLU	N-CA-C	-5.73	104.64	111.69
1	H	77	ALA	N-CA-C	-5.64	105.03	111.07
1	A	102	LEU	N-CA-C	-5.45	105.42	111.36
1	J	84	VAL	N-CA-C	5.27	115.90	110.36
1	G	82	GLN	N-CA-C	-5.22	105.59	111.28
1	G	74	LEU	N-CA-C	-5.21	105.72	111.71
1	H	84	VAL	CB-CA-C	-5.08	105.29	112.14
1	L	87	GLN	N-CA-C	5.07	116.81	111.28
1	K	89	ALA	N-CA-C	-5.07	105.45	111.69
1	L	93	HIS	CB-CA-C	-5.03	102.44	110.79
1	H	81	PHE	N-CA-C	-5.02	105.50	110.97

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	765	0	766	25	0
1	B	765	0	766	32	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	36	0
1	H	765	0	766	45	0
1	I	765	0	766	33	0
1	J	765	0	766	15	0
1	K	765	0	766	26	0
1	L	765	0	766	27	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	223	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 (223) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:78:GLN:CD	3:K:5:HOH:O	2.21	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:E:78:GLN:CD	1:G:61:MSE:HE1	2.07	0.79
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: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
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: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:I:61:MSE:HE1	1:K:78:GLN:CD	2.14	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: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:E:111:LYS:HE3	1:I:100:ALA:C	2.20	0.66
1:F:67:THR:HG1	1:H:71:GLN:NE2	1.94	0.65
1:G:84:VAL:CG1	1:H:84:VAL:HG21	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:104:ALA:HB2	1:L:65:ASN:CG	2.24	0.61
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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:78:GLN:CD	3:K:172:HOH:O	2.52	0.52
1:K:70:LEU:HD21	1:L:70:LEU:CD2	2.15	0.52
1:A:63:ALA:O	1:A:67:THR:HG23	2.10	0.52
1:A:67:THR:HG22	1:C:70:LEU:HD23	1.90	0.52
1:B:111:LYS:NZ	1:L:73:GLU:OE2	2.29	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
1:C:70:LEU:HD21	1:D:70:LEU:CD2	2.20	0.51
1:E:111:LYS:HZ1	1:I:101:SER:N	2.08	0.51
1:H:128:GLN:CD	1:L:138:ARG:HB3	2.35	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:G:84:VAL:CG1	1:H:84:VAL:CG2	2.91	0.48
1:H:69:LEU:HD13	3:H:25:HOH:O	2.13	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:B:74:LEU:HA	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:K:57:LEU:O	1:K:58:ARG:C	2.58	0.46
1:G:67:THR:O	1:G:70:LEU:HB3	2.14	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
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:B:71:GLN:HE22	1:D:64:ARG:HG3	1.82	0.44
1:C:142:GLN:O	1:C:146:VAL:HG23	2.17	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: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:G:76:GLU:O	1:G:77:ALA:C	2.58	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:H:132:ALA:HB2	1:L:142:GLN:CD	2.43	0.43
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:B:113:VAL:O	1:B:114:GLU:C	2.61	0.43
1:K:54:ARG:NH1	3:K:166:HOH:O	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:94:THR:O	1:J:95:VAL:C	2.62	0.43
1:C:78:GLN:O	1:C:82:GLN:HG3	2.19	0.43
1:E:111:LYS:CE	1:I:100:ALA:HB3	2.49	0.42
1:E:111:LYS:HE2	1:I:100:ALA:CB	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: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
1:I:74:LEU:HD23	1:I:74:LEU:HA	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:L:65:ASN:O	1:L:66:VAL:C	2.62	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:I:69:LEU:O	1:I:70:LEU:C	2.63	0.41
1:F:94:THR:O	1:F:95:VAL:C	2.62	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:H:87:GLN:O	1:H:88:ALA:C	2.65	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
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%)	12	15
1	B	79/94 (84%)	71 (90%)	8 (10%)	7	8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	79/94 (84%)	71 (90%)	8 (10%)	7	8
1	D	79/94 (84%)	73 (92%)	6 (8%)	12	15
1	E	79/94 (84%)	69 (87%)	10 (13%)	4	4
1	F	79/94 (84%)	70 (89%)	9 (11%)	5	5
1	G	79/94 (84%)	72 (91%)	7 (9%)	9	10
1	H	79/94 (84%)	72 (91%)	7 (9%)	9	10
1	I	79/94 (84%)	69 (87%)	10 (13%)	4	4
1	J	79/94 (84%)	73 (92%)	6 (8%)	12	15
1	K	79/94 (84%)	72 (91%)	7 (9%)	9	10
1	L	79/94 (84%)	73 (92%)	6 (8%)	12	15
All	All	948/1128 (84%)	858 (90%)	90 (10%)	8	9

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
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	84	VAL
1	B	114	GLU
1	B	123	LEU
1	B	131	SER
1	B	137	LEU
1	B	148	ILE
1	C	69	LEU
1	C	72	GLN
1	C	84	VAL
1	C	114	GLU
1	C	123	LEU
1	C	131	SER
1	C	137	LEU
1	C	148	ILE
1	D	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	103	ASP
1	D	114	GLU
1	D	123	LEU
1	D	131	SER
1	D	148	ILE
1	E	64	ARG
1	E	69	LEU
1	E	72	GLN
1	E	84	VAL
1	E	102	LEU
1	E	123	LEU
1	E	134	VAL
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	134	VAL
1	F	136	ARG
1	F	137	LEU
1	F	141	ASN
1	G	64	ARG
1	G	69	LEU
1	G	71	GLN
1	G	84	VAL
1	G	123	LEU
1	G	128	GLN
1	G	137	LEU
1	H	64	ARG
1	H	69	LEU
1	H	84	VAL
1	H	90	THR
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	75	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	84	VAL
1	I	102	LEU
1	I	123	LEU
1	I	136	ARG
1	I	137	LEU
1	I	141	ASN
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	K	64	ARG
1	K	69	LEU
1	K	84	VAL
1	K	123	LEU
1	K	128	GLN
1	K	137	LEU
1	K	141	ASN
1	L	64	ARG
1	L	69	LEU
1	L	84	VAL
1	L	123	LEU
1	L	128	GLN
1	L	137	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	72	GLN
1	A	92	ASN
1	B	71	GLN
1	B	72	GLN
1	B	128	GLN
1	C	72	GLN
1	C	92	ASN
1	C	125	HIS
1	C	128	GLN
1	D	71	GLN
1	D	82	GLN
1	D	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	141	ASN
1	G	68	HIS
1	G	71	GLN
1	G	92	ASN
1	G	125	HIS
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	68	HIS
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	71	GLN
1	L	72	GLN
1	L	92	ASN
1	L	93	HIS
1	L	142	GLN

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 [i](#)

There are no oligosaccharides 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 ⓘ

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, 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	96/121 (79%)	0.62	7 (7%) 21 22	2, 22, 58, 72	0
1	B	96/121 (79%)	0.95	14 (14%) 6 6	3, 27, 67, 84	0
1	C	96/121 (79%)	0.87	8 (8%) 17 18	2, 24, 57, 71	0
1	D	96/121 (79%)	0.82	11 (11%) 9 10	2, 24, 64, 78	0
1	E	96/121 (79%)	1.02	10 (10%) 11 12	2, 19, 52, 69	0
1	F	96/121 (79%)	0.45	4 (4%) 40 42	2, 22, 43, 59	0
1	G	96/121 (79%)	0.77	6 (6%) 26 27	2, 22, 57, 89	0
1	H	96/121 (79%)	0.67	7 (7%) 21 22	2, 23, 52, 88	0
1	I	96/121 (79%)	0.84	10 (10%) 11 12	2, 24, 46, 62	0
1	J	96/121 (79%)	0.77	7 (7%) 21 22	2, 26, 51, 59	0
1	K	96/121 (79%)	0.90	9 (9%) 14 15	2, 22, 61, 83	0
1	L	96/121 (79%)	0.83	14 (14%) 6 6	3, 22, 57, 83	0
All	All	1152/1452 (79%)	0.79	107 (9%) 14 15	2, 23, 57, 89	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	149	ALA	7.7
1	E	149	ALA	6.4
1	A	148	ILE	6.0
1	B	148	ILE	6.0
1	D	149	ALA	5.7
1	L	149	ALA	5.7
1	J	148	ILE	5.4
1	H	148	ILE	5.1
1	A	144	LEU	5.1
1	E	148	ILE	5.1
1	B	143	VAL	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	149	ALA	4.8
1	K	148	ILE	4.5
1	A	143	VAL	4.5
1	C	148	ILE	4.4
1	F	53	ALA	4.4
1	L	148	ILE	4.1
1	G	148	ILE	3.9
1	B	144	LEU	3.8
1	C	143	VAL	3.8
1	D	148	ILE	3.7
1	B	146	VAL	3.7
1	F	146	VAL	3.7
1	L	141	ASN	3.5
1	H	147	ARG	3.5
1	B	149	ALA	3.5
1	I	149	ALA	3.5
1	F	149	ALA	3.4
1	E	53	ALA	3.4
1	D	147	ARG	3.4
1	B	110	GLN	3.4
1	J	139	ARG	3.4
1	L	146	VAL	3.3
1	G	149	ALA	3.3
1	B	141	ASN	3.2
1	J	86	ALA	3.2
1	A	146	VAL	3.2
1	E	146	VAL	3.2
1	H	139	ARG	3.1
1	L	142	GLN	3.0
1	K	52	ALA	3.0
1	D	144	LEU	3.0
1	I	58	ARG	3.0
1	C	146	VAL	3.0
1	D	146	VAL	3.0
1	A	149	ALA	2.9
1	A	145	SER	2.8
1	I	85	GLU	2.8
1	C	149	ALA	2.8
1	L	144	LEU	2.8
1	C	54	ARG	2.8
1	I	148	ILE	2.7
1	L	92	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	51	GLU	2.7
1	K	110	GLN	2.7
1	L	145	SER	2.6
1	D	128	GLN	2.6
1	K	77	ALA	2.6
1	C	112	LYS	2.5
1	L	139	ARG	2.4
1	F	51	GLU	2.4
1	I	139	ARG	2.4
1	J	147	ARG	2.4
1	K	113	VAL	2.4
1	I	147	ARG	2.4
1	E	52	ALA	2.4
1	I	92	ASN	2.3
1	C	141	ASN	2.3
1	I	86	ALA	2.3
1	L	138	ARG	2.3
1	E	143	VAL	2.3
1	G	146	VAL	2.3
1	L	143	VAL	2.3
1	B	92	ASN	2.3
1	B	147	ARG	2.3
1	G	67	THR	2.3
1	A	141	ASN	2.2
1	G	114	GLU	2.2
1	K	149	ALA	2.2
1	D	134	VAL	2.2
1	L	134	VAL	2.2
1	B	108	GLN	2.2
1	L	53	ALA	2.2
1	E	144	LEU	2.2
1	G	144	LEU	2.2
1	J	84	VAL	2.2
1	E	62	GLU	2.2
1	L	147	ARG	2.2
1	D	51	GLU	2.2
1	K	51	GLU	2.2
1	B	142	GLN	2.2
1	H	84	VAL	2.1
1	E	51	GLU	2.1
1	K	54	ARG	2.1
1	D	103	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	139	ARG	2.1
1	C	144	LEU	2.1
1	D	69	LEU	2.1
1	B	130	ALA	2.0
1	I	51	GLU	2.0
1	B	136	ARG	2.0
1	H	81	PHE	2.0
1	H	115	GLU	2.0
1	B	132	ALA	2.0
1	D	137	LEU	2.0
1	I	65	ASN	2.0
1	E	138	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CA	E	1	1/1	0.68	0.13	79,79,79,79	0
2	CA	K	1	1/1	0.76	0.14	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.