



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:46 AM UTC

PDB ID : 2CY9 / pdb_00002cy9
Title : Crystal structure of thioesterase superfamily member2 from Mus musculus
Authors : Hosaka, T.; Murayama, K.; Kishishita, S.; Shirouzu, M.; Yokoyama, S.;
RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-06
Resolution : 2.72 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

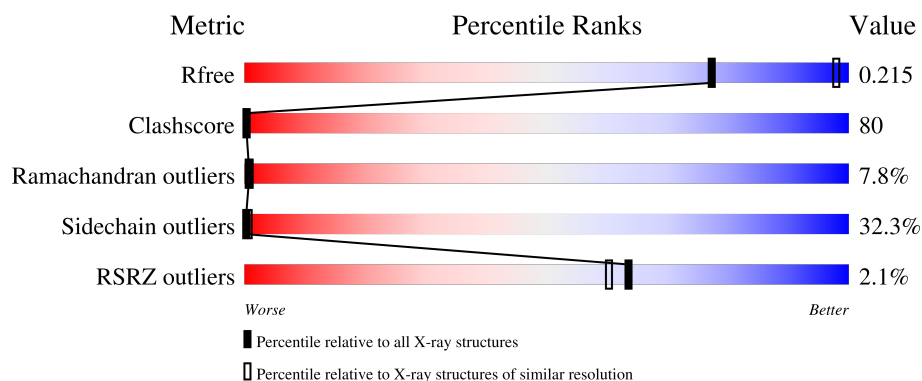
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	140	
1	B	140	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1959 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 Thioesterase superfamily member 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	Se	0	0	0
			912	580	153	171	2	6			
1	B	133	Total	C	N	O	S	Se	0	0	0
			1004	631	171	191	2	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q9CQR4
A	4	MSE	MET	modified residue	UNP Q9CQR4
A	12	MSE	MET	modified residue	UNP Q9CQR4
A	15	MSE	MET	modified residue	UNP Q9CQR4
A	42	MSE	MET	modified residue	UNP Q9CQR4
A	70	MSE	MET	modified residue	UNP Q9CQR4
A	73	MSE	MET	modified residue	UNP Q9CQR4
A	86	MSE	MET	modified residue	UNP Q9CQR4
A	91	MSE	MET	modified residue	UNP Q9CQR4
B	1	MSE	MET	modified residue	UNP Q9CQR4
B	4	MSE	MET	modified residue	UNP Q9CQR4
B	12	MSE	MET	modified residue	UNP Q9CQR4
B	15	MSE	MET	modified residue	UNP Q9CQR4
B	42	MSE	MET	modified residue	UNP Q9CQR4
B	70	MSE	MET	modified residue	UNP Q9CQR4
B	73	MSE	MET	modified residue	UNP Q9CQR4
B	86	MSE	MET	modified residue	UNP Q9CQR4
B	91	MSE	MET	modified residue	UNP Q9CQR4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	24	Total	O	0	0
			24	24		

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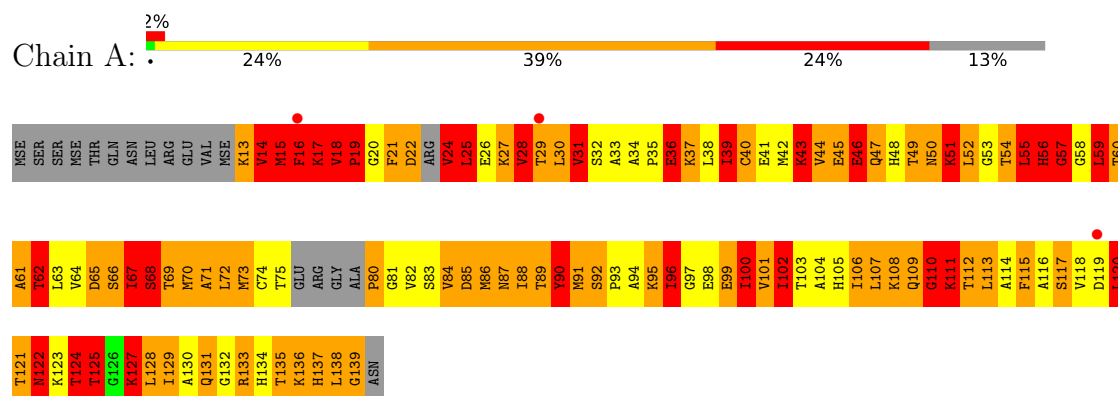
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	19	Total	O	0	0
			19	19		

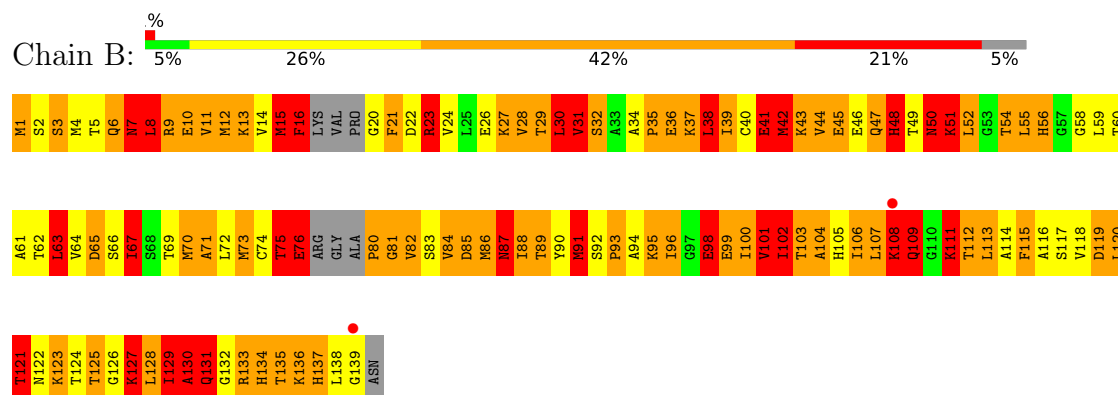
3 Residue-property plots [i](#)

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: Thioesterase superfamily member 2



• Molecule 1: Thioesterase superfamily member 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.52Å 90.19Å 61.21Å 90.00° 118.32° 90.00°	Depositor
Resolution (Å)	49.10 – 2.72 49.10 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.10-2.72) 95.4 (49.10-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.262 0.214 , 0.215	Depositor DCC
R_{free} test set	768 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 120.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1959	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	4.29	199/916 (21.7%)	2.87	95/1222 (7.8%)
1	B	4.27	221/1005 (22.0%)	3.00	128/1335 (9.6%)
All	All	4.28	420/1921 (21.9%)	2.94	223/2557 (8.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

All (420) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	ALA	CA-C	-18.11	1.29	1.52
1	B	94	ALA	CA-CB	-17.97	1.29	1.53
1	A	129	ILE	CA-CB	17.88	1.78	1.54
1	A	31	VAL	CA-CB	17.42	1.78	1.54
1	B	1	MSE	SE-CE	-15.95	1.47	1.95
1	A	135	THR	CA-CB	15.12	1.88	1.53
1	B	62	THR	N-CA	14.94	1.65	1.46
1	A	80	PRO	N-CA	14.90	1.69	1.47
1	A	31	VAL	CA-C	14.19	1.70	1.52
1	A	82	VAL	CA-CB	-14.10	1.36	1.54
1	B	91	MSE	SE-CE	-14.01	1.53	1.95
1	A	101	VAL	CA-CB	-13.64	1.34	1.55
1	B	84	VAL	C-O	13.56	1.39	1.23
1	B	47	GLN	CA-C	13.00	1.70	1.52
1	B	60	THR	CA-CB	-12.83	1.33	1.53
1	A	96	ILE	CA-CB	12.72	1.72	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ALA	CA-CB	-12.67	1.33	1.53
1	A	25	LEU	C-O	12.60	1.39	1.24
1	A	48	HIS	C-O	-12.48	1.08	1.24
1	B	48	HIS	C-O	-12.46	1.08	1.24
1	A	39	ILE	C-O	-12.43	1.09	1.24
1	A	132	GLY	CA-C	12.36	1.62	1.51
1	B	135	THR	CA-CB	12.32	1.72	1.53
1	A	15	MSE	C-O	12.25	1.39	1.24
1	B	70	MSE	N-CA	12.17	1.60	1.46
1	B	87	ASN	CA-CB	11.95	1.78	1.54
1	A	136	LYS	CA-C	-11.85	1.38	1.52
1	B	65	ASP	N-CA	11.78	1.60	1.46
1	A	116	ALA	CA-CB	-11.78	1.34	1.53
1	B	130	ALA	N-CA	-11.45	1.31	1.46
1	A	103	THR	CA-CB	-11.44	1.37	1.53
1	B	86	MSE	SE-CE	-11.42	1.61	1.95
1	A	24	VAL	N-CA	11.42	1.68	1.46
1	A	33	ALA	CA-CB	11.33	1.69	1.53
1	B	22	ASP	CA-C	11.33	1.68	1.52
1	A	98	GLU	N-CA	11.15	1.59	1.46
1	B	29	THR	C-O	-11.07	1.10	1.23
1	B	5	THR	N-CA	-11.02	1.33	1.46
1	B	37	LYS	CA-C	10.81	1.66	1.52
1	A	102	ILE	CA-CB	-10.76	1.39	1.54
1	B	102	ILE	CB-CG2	10.76	1.88	1.52
1	B	82	VAL	C-O	-10.74	1.12	1.23
1	B	85	ASP	CG-OD2	10.64	1.45	1.25
1	A	100	ILE	CB-CG2	10.52	1.87	1.52
1	B	130	ALA	CA-CB	-10.47	1.35	1.53
1	B	139	GLY	C-O	10.46	1.44	1.23
1	A	91	MSE	N-CA	-10.44	1.32	1.46
1	A	36	GLU	CA-CB	10.43	1.68	1.53
1	B	28	VAL	C-O	-10.42	1.12	1.24
1	B	87	ASN	N-CA	10.42	1.59	1.45
1	A	44	VAL	CA-CB	10.40	1.67	1.54
1	A	97	GLY	C-O	-10.30	1.10	1.24
1	A	14	VAL	CA-CB	10.29	1.67	1.54
1	A	116	ALA	CA-C	-10.23	1.39	1.52
1	A	111	LYS	CB-CG	10.14	1.82	1.52
1	A	129	ILE	C-O	-10.09	1.12	1.24
1	A	26	GLU	C-O	-9.98	1.10	1.23
1	B	72	LEU	CA-C	-9.90	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ILE	CA-CB	-9.79	1.43	1.54
1	A	89	THR	N-CA	-9.75	1.34	1.46
1	B	39	ILE	CA-CB	-9.65	1.42	1.54
1	B	50	ASN	CA-C	-9.64	1.39	1.52
1	B	123	LYS	C-O	-9.64	1.12	1.24
1	A	83	SER	C-O	9.64	1.36	1.24
1	A	41	GLU	C-O	-9.61	1.11	1.23
1	A	48	HIS	CA-C	-9.57	1.39	1.52
1	B	95	LYS	CA-C	9.54	1.66	1.53
1	B	64	VAL	CA-C	-9.51	1.41	1.52
1	A	86	MSE	SE-CE	-9.48	1.67	1.95
1	B	85	ASP	CG-OD1	9.41	1.43	1.25
1	A	41	GLU	N-CA	9.40	1.58	1.46
1	B	61	ALA	CA-CB	-9.40	1.38	1.53
1	A	28	VAL	CA-CB	9.38	1.67	1.54
1	B	133	ARG	NE-CZ	-9.38	1.22	1.33
1	B	5	THR	C-O	9.32	1.34	1.24
1	B	129	ILE	C-O	-9.31	1.12	1.24
1	A	35	PRO	CA-C	9.19	1.61	1.52
1	A	106	ILE	C-O	-9.18	1.15	1.24
1	B	130	ALA	C-O	9.18	1.35	1.24
1	B	117	SER	CB-OG	9.12	1.60	1.42
1	A	54	THR	CA-C	-9.09	1.41	1.52
1	B	74	CYS	C-O	9.07	1.34	1.24
1	A	85	ASP	N-CA	-9.05	1.34	1.45
1	B	85	ASP	CA-C	-9.03	1.41	1.52
1	B	92	SER	CA-C	8.83	1.64	1.52
1	A	14	VAL	CA-C	8.81	1.62	1.52
1	B	135	THR	N-CA	-8.79	1.35	1.46
1	A	42	MSE	N-CA	-8.78	1.35	1.46
1	A	85	ASP	CG-OD2	8.76	1.42	1.25
1	A	88	ILE	CG1-CD1	8.74	1.85	1.51
1	B	70	MSE	SE-CE	-8.63	1.69	1.95
1	B	69	THR	CA-C	-8.60	1.41	1.52
1	B	88	ILE	CG1-CD1	8.60	1.85	1.51
1	B	14	VAL	CA-CB	-8.58	1.44	1.54
1	B	75	THR	CB-CG2	8.54	1.80	1.52
1	B	116	ALA	CA-C	-8.46	1.42	1.52
1	A	52	LEU	C-N	-8.46	1.20	1.33
1	A	128	LEU	N-CA	-8.44	1.35	1.46
1	A	27	LYS	CA-C	8.39	1.64	1.52
1	B	36	GLU	CD-OE1	8.39	1.41	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	LEU	C-O	-8.33	1.13	1.24
1	B	108	LYS	CB-CG	8.27	1.77	1.52
1	B	42	MSE	SE-CE	-8.26	1.70	1.95
1	A	42	MSE	CA-C	8.24	1.63	1.52
1	B	80	PRO	N-CA	8.23	1.59	1.47
1	A	47	GLN	CD-OE1	8.22	1.39	1.23
1	A	51	LYS	CE-NZ	8.22	1.74	1.49
1	A	33	ALA	N-CA	8.21	1.56	1.46
1	A	131	GLN	CA-C	-8.20	1.41	1.52
1	A	51	LYS	CA-CB	8.17	1.67	1.53
1	B	75	THR	CB-OG1	8.17	1.56	1.43
1	B	41	GLU	N-CA	8.10	1.56	1.45
1	A	102	ILE	N-CA	-8.10	1.35	1.46
1	B	13	LYS	CD-CE	8.09	1.76	1.52
1	B	54	THR	CA-C	-8.09	1.41	1.53
1	A	87	ASN	CA-CB	8.09	1.68	1.53
1	A	25	LEU	CA-C	8.08	1.63	1.52
1	A	103	THR	C-O	-8.05	1.14	1.24
1	A	88	ILE	C-O	-8.03	1.15	1.24
1	B	129	ILE	CA-C	-8.02	1.45	1.52
1	B	16	PHE	C-O	8.01	1.39	1.23
1	A	122	ASN	C-O	-8.01	1.14	1.24
1	A	70	MSE	C-O	-7.99	1.14	1.24
1	B	119	ASP	CA-CB	7.99	1.68	1.53
1	A	26	GLU	N-CA	-7.95	1.36	1.46
1	B	41	GLU	CD-OE2	7.94	1.40	1.25
1	B	102	ILE	C-O	-7.93	1.15	1.24
1	B	52	LEU	CG-CD1	7.93	1.78	1.52
1	B	69	THR	CA-CB	-7.92	1.40	1.53
1	A	37	LYS	C-O	-7.90	1.13	1.23
1	B	47	GLN	CG-CD	7.86	1.71	1.52
1	B	22	ASP	CG-OD1	7.84	1.40	1.25
1	A	47	GLN	CA-C	7.82	1.62	1.52
1	B	92	SER	C-O	7.79	1.34	1.24
1	B	4	MSE	SE-CE	-7.78	1.72	1.95
1	B	136	LYS	CE-NZ	7.73	1.72	1.49
1	B	120	LEU	CA-C	-7.67	1.43	1.52
1	B	103	THR	CA-C	7.66	1.61	1.52
1	B	52	LEU	CB-CG	7.62	1.68	1.53
1	B	61	ALA	N-CA	7.62	1.55	1.46
1	A	25	LEU	N-CA	7.62	1.56	1.46
1	B	47	GLN	CD-NE2	7.61	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	LYS	CG-CD	7.60	1.75	1.52
1	B	88	ILE	N-CA	7.59	1.55	1.46
1	B	102	ILE	CA-CB	7.58	1.63	1.54
1	A	138	LEU	C-O	7.57	1.33	1.24
1	A	95	LYS	CA-C	7.56	1.63	1.53
1	B	13	LYS	CA-C	7.55	1.62	1.52
1	B	83	SER	N-CA	-7.54	1.35	1.45
1	B	61	ALA	C-N	7.50	1.44	1.34
1	B	73	MSE	SE-CE	-7.49	1.73	1.95
1	B	65	ASP	CG-OD2	7.49	1.39	1.25
1	B	56	HIS	C-O	7.48	1.32	1.23
1	A	15	MSE	CA-C	7.43	1.62	1.52
1	A	138	LEU	CA-CB	-7.43	1.43	1.53
1	B	88	ILE	CB-CG2	7.40	1.76	1.52
1	B	61	ALA	C-O	-7.39	1.15	1.24
1	A	13	LYS	N-CA	7.38	1.60	1.46
1	B	22	ASP	CA-CB	7.36	1.67	1.53
1	A	90	TYR	CE1-CZ	7.35	1.55	1.38
1	A	73	MSE	CA-C	7.35	1.63	1.52
1	B	131	GLN	N-CA	7.32	1.55	1.46
1	A	36	GLU	CG-CD	7.32	1.70	1.52
1	A	68	SER	CA-C	-7.31	1.43	1.52
1	B	2	SER	CB-OG	-7.31	1.27	1.42
1	A	118	VAL	CA-CB	7.29	1.63	1.54
1	B	133	ARG	CG-CD	7.29	1.74	1.52
1	A	18	VAL	CA-C	7.28	1.60	1.52
1	A	113	LEU	C-O	7.26	1.32	1.23
1	A	117	SER	CA-C	7.20	1.60	1.52
1	B	67	ILE	CA-CB	7.19	1.63	1.54
1	B	90	TYR	N-CA	7.16	1.54	1.46
1	A	133	ARG	CZ-NH2	-7.14	1.24	1.33
1	B	101	VAL	N-CA	7.13	1.54	1.46
1	B	134	HIS	CB-CG	7.09	1.60	1.50
1	B	46	GLU	CD-OE2	7.06	1.38	1.25
1	A	18	VAL	C-O	7.06	1.33	1.24
1	B	8	LEU	C-O	-7.05	1.15	1.24
1	B	73	MSE	N-CA	7.04	1.55	1.46
1	B	86	MSE	C-O	7.04	1.32	1.23
1	A	55	LEU	C-O	-7.03	1.15	1.23
1	B	11	VAL	CA-C	7.02	1.61	1.52
1	B	89	THR	CA-CB	7.02	1.71	1.53
1	A	109	GLN	C-N	-7.01	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	VAL	N-CA	-6.99	1.37	1.46
1	B	115	PHE	CA-C	-6.98	1.44	1.52
1	A	95	LYS	CD-CE	6.94	1.73	1.52
1	B	35	PRO	C-O	-6.94	1.15	1.24
1	A	69	THR	CB-CG2	-6.93	1.29	1.52
1	B	58	GLY	C-N	-6.93	1.23	1.33
1	A	22	ASP	CA-C	6.91	1.67	1.52
1	A	52	LEU	CA-C	-6.88	1.42	1.52
1	B	70	MSE	CG-SE	6.87	2.16	1.95
1	A	127	LYS	C-O	-6.83	1.15	1.23
1	A	30	LEU	CG-CD1	6.82	1.75	1.52
1	B	50	ASN	CG-ND2	6.81	1.47	1.33
1	B	125	THR	C-O	-6.78	1.16	1.24
1	B	51	LYS	CD-CE	6.78	1.72	1.52
1	B	55	LEU	C-N	-6.77	1.24	1.33
1	B	22	ASP	N-CA	6.76	1.55	1.46
1	B	63	LEU	CA-C	6.73	1.61	1.52
1	A	44	VAL	CA-C	6.73	1.60	1.52
1	A	37	LYS	CA-C	6.72	1.61	1.52
1	B	49	THR	CB-OG1	-6.72	1.33	1.43
1	B	108	LYS	N-CA	-6.72	1.38	1.46
1	A	24	VAL	CB-CG1	6.71	1.74	1.52
1	A	98	GLU	CA-C	-6.71	1.44	1.52
1	B	67	ILE	CB-CG1	6.71	1.66	1.53
1	B	91	MSE	CG-SE	-6.71	1.75	1.95
1	A	107	LEU	CA-C	6.70	1.61	1.52
1	A	46	GLU	CA-C	6.68	1.61	1.52
1	A	69	THR	N-CA	-6.68	1.38	1.46
1	A	97	GLY	CA-C	-6.63	1.43	1.52
1	A	50	ASN	CA-C	6.63	1.62	1.53
1	B	60	THR	N-CA	-6.62	1.38	1.46
1	A	31	VAL	CB-CG2	6.59	1.74	1.52
1	A	124	THR	CB-CG2	6.58	1.74	1.52
1	B	118	VAL	CA-CB	6.57	1.64	1.54
1	B	3	SER	CA-C	-6.55	1.46	1.53
1	B	87	ASN	C-O	6.50	1.31	1.23
1	B	93	PRO	CA-C	-6.50	1.45	1.52
1	B	98	GLU	CA-C	-6.49	1.44	1.52
1	A	16	PHE	CD2-CE2	6.47	1.58	1.38
1	A	17	LYS	CA-CB	6.46	1.64	1.53
1	B	66	SER	C-N	-6.44	1.25	1.33
1	A	51	LYS	CG-CD	6.43	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	LEU	C-O	-6.41	1.16	1.23
1	B	2	SER	CA-C	-6.41	1.44	1.52
1	A	95	LYS	CG-CD	6.39	1.71	1.52
1	A	102	ILE	C-O	-6.36	1.17	1.24
1	B	58	GLY	CA-C	-6.36	1.42	1.51
1	A	96	ILE	C-O	-6.35	1.18	1.24
1	A	30	LEU	C-O	6.34	1.31	1.24
1	B	23	ARG	C-O	-6.32	1.15	1.24
1	B	100	ILE	CA-CB	-6.31	1.46	1.54
1	A	116	ALA	C-N	-6.30	1.25	1.33
1	A	113	LEU	C-N	6.29	1.42	1.33
1	A	29	THR	CA-C	6.28	1.60	1.52
1	B	32	SER	C-O	-6.27	1.15	1.23
1	B	62	THR	C-O	-6.25	1.16	1.24
1	B	72	LEU	N-CA	-6.25	1.38	1.46
1	A	106	ILE	CA-CB	-6.25	1.44	1.53
1	A	34	ALA	CA-C	6.24	1.60	1.52
1	B	2	SER	C-N	-6.24	1.26	1.33
1	B	7	ASN	CB-CG	6.22	1.67	1.52
1	B	52	LEU	N-CA	-6.21	1.38	1.46
1	A	96	ILE	N-CA	-6.21	1.38	1.46
1	B	3	SER	CB-OG	6.21	1.54	1.42
1	B	22	ASP	CB-CG	6.21	1.67	1.52
1	A	137	HIS	CA-CB	6.19	1.61	1.53
1	A	130	ALA	CA-CB	-6.19	1.43	1.53
1	B	112	THR	CB-CG2	6.18	1.73	1.52
1	B	67	ILE	CB-CG2	6.17	1.73	1.52
1	A	107	LEU	C-O	6.17	1.31	1.24
1	A	118	VAL	C-O	-6.16	1.17	1.24
1	A	90	TYR	C-O	-6.14	1.16	1.24
1	A	34	ALA	CA-CB	-6.13	1.43	1.53
1	B	5	THR	CB-CG2	-6.11	1.32	1.52
1	A	89	THR	CA-CB	6.11	1.65	1.53
1	B	62	THR	CA-C	-6.09	1.44	1.52
1	B	14	VAL	CB-CG1	6.08	1.72	1.52
1	A	109	GLN	CD-NE2	6.06	1.46	1.33
1	A	80	PRO	C-O	6.05	1.35	1.23
1	B	28	VAL	N-CA	-6.05	1.38	1.46
1	A	14	VAL	CB-CG1	6.05	1.72	1.52
1	A	60	THR	C-O	-6.04	1.16	1.24
1	A	36	GLU	CB-CG	6.03	1.70	1.52
1	A	110	GLY	C-O	-6.03	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE2	6.01	1.36	1.25
1	A	42	MSE	CG-SE	-6.00	1.77	1.95
1	A	39	ILE	C-N	-5.98	1.26	1.33
1	B	52	LEU	C-O	-5.96	1.15	1.24
1	B	47	GLN	CB-CG	5.95	1.70	1.52
1	B	117	SER	CA-CB	5.95	1.64	1.53
1	A	135	THR	CA-C	-5.94	1.45	1.52
1	B	11	VAL	C-O	-5.94	1.17	1.24
1	A	50	ASN	CB-CG	5.93	1.66	1.52
1	B	35	PRO	CA-C	-5.92	1.43	1.52
1	B	132	GLY	N-CA	-5.92	1.39	1.45
1	B	46	GLU	CD-OE1	5.92	1.36	1.25
1	B	62	THR	CB-OG1	5.92	1.53	1.43
1	B	27	LYS	C-O	5.92	1.31	1.24
1	B	36	GLU	N-CA	5.90	1.53	1.45
1	B	1	MSE	CG-SE	-5.90	1.77	1.95
1	B	105	HIS	C-N	-5.90	1.28	1.33
1	A	114	ALA	N-CA	-5.88	1.38	1.45
1	A	129	ILE	C-N	-5.88	1.25	1.33
1	A	86	MSE	CA-C	-5.86	1.45	1.52
1	A	84	VAL	CB-CG2	5.85	1.71	1.52
1	A	133	ARG	CA-C	-5.85	1.45	1.52
1	B	131	GLN	C-N	-5.85	1.25	1.33
1	B	27	LYS	CA-C	5.85	1.60	1.52
1	A	40	CYS	CA-C	5.85	1.60	1.53
1	A	16	PHE	CB-CG	5.84	1.64	1.50
1	B	119	ASP	CA-C	5.84	1.59	1.52
1	A	54	THR	C-O	5.83	1.30	1.24
1	B	84	VAL	CA-CB	5.82	1.60	1.55
1	A	72	LEU	CA-C	-5.79	1.45	1.52
1	B	136	LYS	CB-CG	5.79	1.69	1.52
1	B	44	VAL	C-O	5.78	1.29	1.24
1	A	19	PRO	CA-C	5.77	1.60	1.52
1	A	105	HIS	N-CA	5.75	1.53	1.46
1	B	5	THR	CB-OG1	5.75	1.52	1.43
1	A	90	TYR	CB-CG	-5.74	1.39	1.51
1	A	87	ASN	CA-C	-5.74	1.45	1.52
1	A	84	VAL	CA-C	5.72	1.60	1.52
1	A	24	VAL	CB-CG2	-5.71	1.33	1.52
1	A	19	PRO	CA-CB	5.71	1.61	1.53
1	A	118	VAL	N-CA	-5.71	1.39	1.46
1	A	27	LYS	CB-CG	5.70	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	MSE	CG-SE	5.70	2.12	1.95
1	B	85	ASP	CB-CG	5.70	1.66	1.52
1	B	92	SER	CA-CB	-5.69	1.44	1.53
1	B	16	PHE	CD1-CE1	5.69	1.55	1.38
1	B	124	THR	C-O	-5.69	1.17	1.24
1	A	67	ILE	CA-C	-5.69	1.45	1.52
1	A	108	LYS	CB-CG	5.67	1.69	1.52
1	A	111	LYS	CG-CD	5.67	1.69	1.52
1	B	70	MSE	CA-CB	5.66	1.62	1.53
1	A	45	GLU	CD-OE2	5.66	1.36	1.25
1	A	25	LEU	CG-CD2	5.66	1.71	1.52
1	B	38	LEU	CG-CD2	5.64	1.71	1.52
1	A	36	GLU	C-O	5.64	1.31	1.23
1	B	21	PHE	CA-C	-5.63	1.45	1.52
1	A	15	MSE	CG-SE	-5.63	1.78	1.95
1	B	12	MSE	SE-CE	-5.63	1.78	1.95
1	A	43	LYS	N-CA	5.62	1.52	1.46
1	B	12	MSE	CG-SE	-5.61	1.78	1.95
1	A	37	LYS	CE-NZ	5.58	1.66	1.49
1	A	115	PHE	CB-CG	5.58	1.63	1.50
1	A	35	PRO	C-O	5.56	1.30	1.23
1	B	22	ASP	CG-OD2	5.54	1.35	1.25
1	B	122	ASN	CA-CB	-5.54	1.44	1.53
1	A	30	LEU	CA-C	5.54	1.60	1.52
1	A	66	SER	N-CA	-5.54	1.38	1.45
1	B	37	LYS	CE-NZ	5.54	1.66	1.49
1	B	134	HIS	CA-CB	5.54	1.62	1.53
1	B	101	VAL	C-N	-5.53	1.26	1.33
1	B	112	THR	CA-CB	-5.50	1.45	1.53
1	B	9	ARG	N-CA	-5.50	1.39	1.46
1	B	40	CYS	N-CA	-5.50	1.39	1.45
1	A	80	PRO	CG-CD	5.50	1.69	1.50
1	A	122	ASN	CA-C	-5.50	1.46	1.52
1	B	8	LEU	CA-C	-5.49	1.45	1.52
1	A	121	THR	C-O	-5.49	1.16	1.23
1	A	96	ILE	CG1-CD1	5.48	1.73	1.51
1	A	52	LEU	CG-CD2	5.47	1.70	1.52
1	B	135	THR	C-N	-5.47	1.25	1.33
1	B	102	ILE	CG1-CD1	-5.47	1.30	1.51
1	A	44	VAL	C-O	5.46	1.30	1.24
1	A	71	ALA	CA-CB	-5.46	1.44	1.53
1	B	102	ILE	CB-CG1	-5.46	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	122	ASN	CA-C	-5.45	1.45	1.52
1	B	3	SER	C-O	5.44	1.32	1.23
1	A	27	LYS	CD-CE	5.44	1.68	1.52
1	B	14	VAL	N-CA	-5.42	1.40	1.46
1	A	51	LYS	CB-CG	5.42	1.68	1.52
1	A	66	SER	CA-CB	-5.41	1.44	1.53
1	A	21	PHE	CE1-CZ	5.41	1.54	1.38
1	A	30	LEU	CB-CG	5.40	1.64	1.53
1	B	111	LYS	CD-CE	5.39	1.68	1.52
1	B	43	LYS	N-CA	5.39	1.53	1.46
1	B	105	HIS	CA-C	-5.38	1.46	1.52
1	B	114	ALA	N-CA	5.38	1.52	1.46
1	B	76	GLU	CD-OE2	5.37	1.35	1.25
1	A	108	LYS	CA-C	-5.37	1.46	1.52
1	B	36	GLU	CG-CD	5.36	1.65	1.52
1	A	135	THR	N-CA	-5.36	1.39	1.46
1	A	67	ILE	CB-CG2	5.36	1.70	1.52
1	B	50	ASN	N-CA	-5.35	1.39	1.46
1	A	48	HIS	C-N	-5.34	1.25	1.33
1	B	48	HIS	CA-CB	-5.32	1.44	1.53
1	B	72	LEU	CB-CG	5.31	1.64	1.53
1	B	80	PRO	CA-C	5.30	1.64	1.52
1	A	45	GLU	C-N	-5.30	1.26	1.33
1	B	14	VAL	CA-C	-5.29	1.46	1.52
1	B	38	LEU	CB-CG	-5.29	1.42	1.53
1	B	51	LYS	CG-CD	5.29	1.68	1.52
1	B	44	VAL	CA-C	5.28	1.58	1.52
1	A	83	SER	N-CA	-5.28	1.39	1.46
1	B	72	LEU	CG-CD2	-5.28	1.35	1.52
1	A	98	GLU	C-N	-5.27	1.26	1.33
1	A	17	LYS	CD-CE	5.27	1.68	1.52
1	B	42	MSE	N-CA	-5.27	1.40	1.46
1	A	92	SER	CA-CB	-5.27	1.45	1.53
1	B	42	MSE	CB-CG	5.25	1.68	1.52
1	B	46	GLU	C-O	-5.25	1.17	1.24
1	B	67	ILE	CA-C	-5.25	1.46	1.52
1	B	36	GLU	C-O	-5.25	1.17	1.24
1	B	99	GLU	N-CA	-5.25	1.39	1.46
1	A	90	TYR	CA-C	5.24	1.58	1.52
1	A	102	ILE	CB-CG1	-5.23	1.43	1.53
1	B	52	LEU	CA-C	-5.22	1.46	1.52
1	A	37	LYS	N-CA	5.22	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	SER	C-O	-5.21	1.17	1.24
1	B	127	LYS	CB-CG	5.21	1.68	1.52
1	B	1	MSE	CA-C	-5.20	1.42	1.52
1	A	82	VAL	C-O	-5.19	1.17	1.24
1	A	109	GLN	N-CA	5.19	1.52	1.46
1	B	108	LYS	CA-C	5.18	1.58	1.52
1	A	108	LYS	CG-CD	5.18	1.68	1.52
1	A	139	GLY	CA-C	5.17	1.61	1.52
1	B	122	ASN	C-O	-5.16	1.17	1.24
1	B	46	GLU	CG-CD	5.16	1.65	1.52
1	B	21	PHE	C-O	5.14	1.30	1.24
1	B	10	GLU	CD-OE1	5.14	1.35	1.25
1	B	51	LYS	C-N	-5.12	1.26	1.33
1	B	124	THR	CB-CG2	5.12	1.69	1.52
1	B	36	GLU	CD-OE2	5.11	1.35	1.25
1	A	118	VAL	CA-C	-5.10	1.46	1.52
1	B	40	CYS	C-O	-5.10	1.17	1.23
1	A	82	VAL	CA-C	-5.09	1.46	1.52
1	A	137	HIS	C-O	5.06	1.30	1.24
1	B	69	THR	C-O	-5.05	1.18	1.24
1	A	39	ILE	CB-CG2	5.04	1.69	1.52
1	B	55	LEU	CA-C	5.04	1.59	1.52
1	A	112	THR	N-CA	5.03	1.52	1.46
1	A	105	HIS	C-O	5.02	1.30	1.23
1	A	59	LEU	C-O	5.02	1.29	1.24
1	B	121	THR	CA-C	5.00	1.58	1.52

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	SER	CA-C-N	-15.05	102.63	122.79
1	B	2	SER	C-N-CA	-15.05	102.63	122.79
1	A	66	SER	CA-CB-OG	-13.05	84.99	111.10
1	A	112	THR	N-CA-C	-12.19	99.39	114.75
1	A	52	LEU	CA-C-N	-11.98	103.15	122.20
1	A	52	LEU	C-N-CA	-11.98	103.15	122.20
1	B	26	GLU	N-CA-C	-10.86	99.54	113.12
1	B	10	GLU	N-CA-C	10.82	122.82	111.14
1	B	22	ASP	CA-C-O	10.69	132.57	119.10
1	B	49	THR	N-CA-C	10.41	125.88	110.48
1	B	59	LEU	N-CA-C	-10.38	98.02	112.45
1	B	129	ILE	CA-C-O	-10.01	111.23	120.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	VAL	N-CA-C	9.98	130.10	109.34
1	A	68	SER	N-CA-C	-9.94	89.63	110.80
1	A	121	THR	N-CA-C	9.28	124.20	110.46
1	B	133	ARG	NE-CZ-NH1	-9.18	112.32	121.50
1	A	96	ILE	CA-C-N	-8.90	112.84	123.44
1	A	96	ILE	C-N-CA	-8.90	112.84	123.44
1	B	16	PHE	CA-C-O	8.88	135.90	120.80
1	B	89	THR	CA-C-N	-8.88	110.48	123.00
1	B	89	THR	C-N-CA	-8.88	110.48	123.00
1	B	35	PRO	CA-C-O	-8.76	107.21	118.86
1	B	108	LYS	N-CA-C	8.72	124.18	108.48
1	B	76	GLU	CA-C-O	8.61	135.44	120.80
1	A	22	ASP	N-CA-C	8.37	134.45	111.00
1	A	21	PHE	N-CA-C	8.29	121.94	108.34
1	A	39	ILE	N-CA-C	8.17	120.12	109.58
1	A	52	LEU	N-CA-C	8.17	121.34	110.88
1	B	104	ALA	CA-C-O	8.17	129.52	120.70
1	B	36	GLU	N-CA-C	8.04	124.68	114.31
1	B	81	GLY	CA-C-N	-8.04	109.98	122.68
1	B	81	GLY	C-N-CA	-8.04	109.98	122.68
1	A	91	MSE	CB-CA-C	7.99	122.66	109.80
1	A	56	HIS	N-CA-CB	7.97	123.35	110.51
1	B	124	THR	N-CA-C	7.94	121.09	111.40
1	A	15	MSE	CA-C-O	7.90	131.81	120.51
1	A	124	THR	CB-CA-C	7.90	123.12	110.96
1	B	108	LYS	CA-C-N	7.88	136.58	121.54
1	B	108	LYS	C-N-CA	7.88	136.58	121.54
1	A	55	LEU	CA-C-O	-7.81	111.83	120.81
1	A	55	LEU	N-CA-C	7.81	121.67	109.96
1	A	95	LYS	N-CA-C	7.75	121.01	110.55
1	A	109	GLN	N-CA-C	7.71	123.81	112.94
1	A	64	VAL	N-CA-C	-7.68	103.43	111.58
1	B	101	VAL	CA-C-N	-7.62	112.97	123.10
1	B	101	VAL	C-N-CA	-7.62	112.97	123.10
1	A	124	THR	N-CA-C	-7.60	102.69	110.97
1	B	58	GLY	CA-C-O	7.52	128.32	119.45
1	A	110	GLY	N-CA-C	7.50	130.96	113.18
1	B	98	GLU	CA-C-N	-7.48	112.58	123.05
1	B	98	GLU	C-N-CA	-7.48	112.58	123.05
1	B	125	THR	OG1-CB-CG2	-7.42	94.47	109.30
1	A	121	THR	CA-CB-CG2	-7.34	98.03	110.50
1	A	98	GLU	CA-C-N	-7.21	113.05	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLU	C-N-CA	-7.21	113.05	123.00
1	B	23	ARG	CA-CB-CG	-7.10	99.90	114.10
1	B	75	THR	OG1-CB-CG2	7.10	123.49	109.30
1	A	54	THR	N-CA-C	-7.08	96.79	108.76
1	A	17	LYS	CB-CA-C	7.08	124.50	110.42
1	A	113	LEU	O-C-N	7.06	131.46	123.27
1	B	26	GLU	CB-CG-CD	7.05	124.58	112.60
1	A	57	GLY	N-CA-C	-7.05	103.35	115.61
1	B	23	ARG	N-CA-C	-6.96	104.65	113.01
1	A	125	THR	N-CA-C	6.88	119.62	111.71
1	B	137	HIS	N-CA-C	6.87	120.86	109.46
1	B	135	THR	CA-CB-OG1	6.85	119.87	109.60
1	A	26	GLU	CB-CA-C	6.84	122.14	111.13
1	A	41	GLU	CB-CA-C	-6.83	98.99	109.99
1	B	64	VAL	N-CA-C	-6.81	104.02	110.42
1	B	60	THR	CA-C-N	-6.79	111.18	120.28
1	B	60	THR	C-N-CA	-6.79	111.18	120.28
1	B	88	ILE	CA-C-O	-6.79	113.64	120.90
1	A	117	SER	CA-C-O	6.78	128.47	120.20
1	B	102	ILE	N-CA-CB	6.77	120.44	111.64
1	B	86	MSE	CG-SE-CE	-6.74	84.10	98.92
1	B	84	VAL	O-C-N	6.72	126.95	121.85
1	B	47	GLN	CA-C-N	6.69	129.92	120.28
1	B	47	GLN	C-N-CA	6.69	129.92	120.28
1	B	126	GLY	N-CA-C	-6.68	105.57	114.25
1	B	139	GLY	CA-C-O	-6.67	106.79	120.80
1	B	21	PHE	N-CA-C	-6.67	103.48	111.69
1	B	119	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	133	ARG	NH1-CZ-NH2	6.61	127.89	119.30
1	A	24	VAL	CA-CB-CG1	6.60	121.61	110.40
1	A	54	THR	OG1-CB-CG2	-6.59	96.11	109.30
1	A	14	VAL	CB-CA-C	6.59	120.82	110.81
1	B	59	LEU	CA-C-N	-6.58	111.46	120.28
1	B	59	LEU	C-N-CA	-6.58	111.46	120.28
1	B	50	ASN	CB-CA-C	-6.57	97.35	110.42
1	B	70	MSE	N-CA-C	-6.54	103.27	111.11
1	B	124	THR	CA-C-O	-6.53	113.56	120.55
1	B	103	THR	N-CA-C	6.53	120.04	109.40
1	A	49	THR	N-CA-C	6.49	120.01	110.59
1	A	93	PRO	CA-C-N	-6.47	113.88	123.00
1	A	93	PRO	C-N-CA	-6.47	113.88	123.00
1	A	102	ILE	CB-CG1-CD1	-6.45	100.26	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ILE	CA-C-N	6.44	129.44	120.29
1	B	106	ILE	C-N-CA	6.44	129.44	120.29
1	B	30	LEU	CA-C-O	-6.40	113.26	120.43
1	A	36	GLU	CB-CG-CD	6.39	123.47	112.60
1	B	107	LEU	N-CA-CB	-6.39	100.69	110.16
1	B	123	LYS	CG-CD-CE	6.39	126.01	111.30
1	A	60	THR	OG1-CB-CG2	-6.38	96.54	109.30
1	B	106	ILE	N-CA-CB	-6.34	105.05	111.90
1	A	28	VAL	N-CA-C	-6.30	96.23	109.34
1	B	37	LYS	CA-C-O	6.29	127.78	120.80
1	B	95	LYS	N-CA-C	6.27	118.62	110.53
1	A	55	LEU	CA-C-N	-6.26	111.56	122.64
1	A	55	LEU	C-N-CA	-6.26	111.56	122.64
1	A	86	MSE	CG-SE-CE	-6.24	85.21	98.92
1	A	102	ILE	CB-CA-C	6.23	117.51	110.41
1	B	91	MSE	CA-CB-CG	6.22	126.55	114.10
1	B	82	VAL	CB-CA-C	6.22	120.00	110.55
1	B	51	LYS	CA-C-O	6.21	127.00	119.49
1	B	41	GLU	N-CA-C	6.18	119.10	109.52
1	A	112	THR	CB-CA-C	6.16	117.11	109.16
1	A	17	LYS	CA-CB-CG	6.16	126.41	114.10
1	A	27	LYS	CA-C-N	6.14	133.03	121.97
1	A	27	LYS	C-N-CA	6.14	133.03	121.97
1	A	43	LYS	N-CA-C	-6.12	98.44	108.41
1	A	29	THR	N-CA-C	6.11	119.49	109.72
1	B	51	LYS	O-C-N	-6.08	114.49	122.39
1	B	63	LEU	N-CA-CB	-6.08	100.94	110.30
1	A	95	LYS	CA-C-O	6.08	128.98	121.81
1	B	86	MSE	CA-C-N	-6.07	112.28	122.29
1	B	86	MSE	C-N-CA	-6.07	112.28	122.29
1	A	118	VAL	CA-C-N	6.04	131.51	122.99
1	A	118	VAL	C-N-CA	6.04	131.51	122.99
1	B	137	HIS	CB-CA-C	-6.04	99.89	109.80
1	B	1	MSE	N-CA-CB	6.04	120.76	110.50
1	A	31	VAL	CA-C-O	6.03	128.32	120.78
1	A	52	LEU	CD1-CG-CD2	6.01	124.03	110.80
1	A	97	GLY	CA-C-N	5.98	129.36	120.87
1	A	97	GLY	C-N-CA	5.98	129.36	120.87
1	A	56	HIS	N-CA-C	-5.97	101.16	110.17
1	A	96	ILE	CA-CB-CG2	5.97	120.64	110.50
1	A	45	GLU	CA-C-O	5.94	128.41	121.46
1	B	100	ILE	CA-C-O	5.94	126.92	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	THR	O-C-N	-5.93	115.96	122.07
1	B	135	THR	OG1-CB-CG2	-5.92	97.46	109.30
1	B	7	ASN	N-CA-C	5.92	119.60	112.38
1	B	66	SER	CA-C-N	-5.91	112.03	120.42
1	B	66	SER	C-N-CA	-5.91	112.03	120.42
1	B	130	ALA	N-CA-C	5.89	123.35	110.80
1	B	3	SER	N-CA-C	-5.81	100.86	109.11
1	B	69	THR	N-CA-CB	-5.81	101.56	110.16
1	B	129	ILE	N-CA-C	-5.79	107.26	112.12
1	B	138	LEU	CA-C-N	5.79	132.11	121.70
1	B	138	LEU	C-N-CA	5.79	132.11	121.70
1	A	42	MSE	CB-CA-C	5.78	120.73	110.16
1	B	130	ALA	CA-C-N	-5.78	110.51	121.54
1	B	130	ALA	C-N-CA	-5.78	110.51	121.54
1	B	74	CYS	N-CA-C	5.77	118.06	111.02
1	B	37	LYS	CG-CD-CE	5.75	124.52	111.30
1	A	41	GLU	CG-CD-OE1	5.75	131.61	118.40
1	B	125	THR	N-CA-C	-5.74	104.93	111.07
1	B	49	THR	O-C-N	5.73	129.43	122.96
1	A	55	LEU	CB-CA-C	-5.72	100.74	109.89
1	A	80	PRO	CA-C-N	-5.71	110.22	121.41
1	A	80	PRO	C-N-CA	-5.71	110.22	121.41
1	B	92	SER	CA-C-N	5.69	127.93	120.25
1	B	92	SER	C-N-CA	5.69	127.93	120.25
1	B	102	ILE	N-CA-C	-5.67	99.47	107.75
1	B	51	LYS	CA-C-N	-5.67	113.64	122.37
1	B	51	LYS	C-N-CA	-5.67	113.64	122.37
1	B	104	ALA	N-CA-C	5.67	118.64	109.40
1	B	8	LEU	N-CA-C	-5.65	104.60	112.45
1	B	136	LYS	CD-CE-NZ	5.64	129.94	111.90
1	B	67	ILE	N-CA-C	5.63	116.41	110.72
1	A	52	LEU	CB-CA-C	-5.62	101.79	111.45
1	A	36	GLU	CA-CB-CG	5.61	125.33	114.10
1	B	5	THR	CA-C-O	-5.61	114.93	120.70
1	B	54	THR	OG1-CB-CG2	-5.60	98.11	109.30
1	A	44	VAL	CA-C-O	5.54	127.17	120.85
1	A	99	GLU	CA-C-O	5.53	126.41	120.38
1	A	52	LEU	O-C-N	-5.53	114.37	121.83
1	A	70	MSE	CA-C-O	-5.52	114.56	121.02
1	A	127	LYS	CA-C-N	5.51	128.66	120.95
1	A	127	LYS	C-N-CA	5.51	128.66	120.95
1	B	39	ILE	CB-CA-C	-5.51	102.41	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	LEU	N-CA-CB	-5.49	101.18	110.46
1	B	101	VAL	N-CA-C	5.49	117.21	108.87
1	B	5	THR	N-CA-CB	5.46	117.99	110.07
1	B	52	LEU	N-CA-C	-5.46	105.23	112.94
1	A	137	HIS	N-CA-C	5.46	117.63	108.73
1	A	53	GLY	CA-C-O	-5.44	113.17	119.10
1	B	59	LEU	CD1-CG-CD2	-5.44	98.83	110.80
1	A	122	ASN	N-CA-C	-5.43	100.40	109.24
1	B	81	GLY	N-CA-C	5.42	122.75	112.62
1	A	131	GLN	N-CA-C	-5.39	99.33	110.80
1	B	23	ARG	CB-CG-CD	5.38	123.67	111.30
1	B	52	LEU	CA-C-O	-5.37	113.15	119.48
1	A	135	THR	CA-CB-CG2	5.36	119.61	110.50
1	A	57	GLY	O-C-N	5.35	129.03	122.29
1	B	73	MSE	CA-C-N	5.35	128.22	120.79
1	B	73	MSE	C-N-CA	5.35	128.22	120.79
1	A	112	THR	OG1-CB-CG2	-5.34	98.63	109.30
1	A	89	THR	CA-C-O	5.32	126.23	120.32
1	B	106	ILE	CA-CB-CG1	-5.32	101.35	110.40
1	B	111	LYS	CB-CG-CD	5.32	123.53	111.30
1	A	27	LYS	CD-CE-NZ	5.31	128.88	111.90
1	B	123	LYS	CD-CE-NZ	-5.30	94.92	111.90
1	A	100	ILE	CG1-CB-CG2	5.30	126.59	110.70
1	B	1	MSE	CA-C-N	-5.26	113.31	122.37
1	B	1	MSE	C-N-CA	-5.26	113.31	122.37
1	A	136	LYS	O-C-N	5.23	129.50	123.17
1	A	96	ILE	O-C-N	-5.23	117.07	122.66
1	B	13	LYS	CB-CG-CD	5.15	123.14	111.30
1	B	5	THR	OG1-CB-CG2	-5.14	99.02	109.30
1	A	14	VAL	N-CA-C	5.14	115.98	108.53
1	A	36	GLU	N-CA-C	-5.12	105.06	111.92
1	A	91	MSE	CA-CB-CG	5.11	124.32	114.10
1	B	71	ALA	O-C-N	5.11	127.40	122.09
1	B	138	LEU	CB-CG-CD2	5.10	125.99	110.70
1	B	36	GLU	CB-CG-CD	5.09	121.26	112.60
1	B	129	ILE	CA-C-N	-5.06	111.88	121.54
1	B	129	ILE	C-N-CA	-5.06	111.88	121.54
1	B	115	PHE	N-CA-C	-5.03	101.43	109.23
1	B	109	GLN	O-C-N	-5.03	115.90	122.59
1	B	15	MSE	CG-SE-CE	-5.03	87.86	98.92
1	B	92	SER	N-CA-CB	-5.03	101.42	110.37
1	A	26	GLU	O-C-N	-5.03	115.77	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	ARG	CG-CD-NE	5.01	123.03	112.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	THR	Peptide
1	A	14	VAL	Peptide
1	A	16	PHE	Peptide
1	A	57	GLY	Peptide
1	A	91	MSE	Mainchain
1	B	48	HIS	Mainchain
1	B	93	PRO	Mainchain

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	912	0	963	191	0
1	B	1004	0	1053	140	0
2	A	24	0	0	2	0
2	B	19	0	0	0	0
All	All	1959	0	2016	316	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 80.

All (316) 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:111:LYS:CD	1:B:111:LYS:CG	1.75	1.65
1:A:24:VAL:CG1	1:A:24:VAL:CB	1.74	1.65
1:B:88:ILE:CG2	1:B:88:ILE:CB	1.77	1.62
1:B:75:THR:CG2	1:B:75:THR:CB	1.80	1.59
1:A:30:LEU:CG	1:A:30:LEU:CD1	1.75	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LEU:CG	1:B:52:LEU:CD1	1.78	1.58
1:B:108:LYS:CB	1:B:108:LYS:CG	1.77	1.57
1:A:111:LYS:CG	1:A:111:LYS:CB	1.82	1.57
1:B:87:ASN:CB	1:B:87:ASN:CA	1.78	1.56
1:B:13:LYS:CD	1:B:13:LYS:CE	1.76	1.55
1:A:31:VAL:CB	1:A:31:VAL:CA	1.78	1.55
1:A:129:ILE:CB	1:A:129:ILE:CA	1.78	1.55
1:A:88:ILE:CD1	1:A:88:ILE:CG1	1.85	1.54
1:B:88:ILE:CD1	1:B:88:ILE:CG1	1.85	1.54
1:A:24:VAL:N	1:A:24:VAL:CA	1.67	1.53
1:B:102:ILE:CG2	1:B:102:ILE:CB	1.88	1.50
1:A:51:LYS:NZ	1:A:51:LYS:CE	1.74	1.49
1:B:136:LYS:CE	1:B:136:LYS:NZ	1.72	1.49
1:A:100:ILE:CB	1:A:100:ILE:CG2	1.87	1.49
1:A:135:THR:CB	1:A:135:THR:CA	1.88	1.48
1:B:70:MSE:SE	1:B:70:MSE:CG	2.16	1.44
1:A:80:PRO:N	1:A:80:PRO:CA	1.69	1.39
1:A:16:PHE:O	1:A:18:VAL:CG2	1.78	1.32
1:A:30:LEU:O	1:A:31:VAL:HG12	1.15	1.29
1:A:15:MSE:CG	1:A:16:PHE:H	1.55	1.15
1:A:16:PHE:O	1:A:18:VAL:HG22	0.97	1.14
1:A:25:LEU:HG	1:A:25:LEU:O	1.40	1.13
1:A:55:LEU:HD13	1:A:55:LEU:O	1.47	1.12
1:A:15:MSE:HG2	1:A:16:PHE:H	1.03	1.11
1:A:30:LEU:O	1:A:31:VAL:CG1	1.98	1.10
1:B:112:THR:HG23	1:B:113:LEU:HD22	1.21	1.09
1:A:58:GLY:O	1:A:62:THR:HG22	1.52	1.08
1:B:86:MSE:SE	1:B:88:ILE:HD11	2.05	1.06
1:A:92:SER:HB3	1:A:129:ILE:HA	1.40	1.04
1:A:87:ASN:ND2	1:B:133:ARG:HH22	1.58	1.02
1:A:122:ASN:HD21	1:A:124:THR:HG22	1.23	1.02
1:A:70:MSE:HE1	1:A:73:MSE:HE2	1.44	0.98
1:B:31:VAL:HG11	1:B:41:GLU:OE1	1.64	0.97
1:A:13:LYS:O	1:A:15:MSE:CE	2.12	0.97
1:A:15:MSE:CG	1:A:16:PHE:N	2.20	0.96
1:A:87:ASN:HD22	1:B:133:ARG:HH22	0.97	0.95
1:A:55:LEU:HD12	1:A:55:LEU:H	1.36	0.90
1:B:45:GLU:O	1:B:96:ILE:HG23	1.71	0.90
1:A:55:LEU:HD12	1:A:55:LEU:N	1.86	0.89
1:A:24:VAL:CG1	1:A:24:VAL:CG2	2.49	0.89
1:A:122:ASN:HD21	1:A:124:THR:CG2	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:O	1:A:43:LYS:NZ	2.04	0.89
1:A:74:CYS:O	1:A:75:THR:O	1.90	0.88
1:B:112:THR:CG2	1:B:113:LEU:HD22	2.03	0.88
1:A:13:LYS:O	1:A:15:MSE:HE3	1.72	0.88
1:A:30:LEU:C	1:A:31:VAL:HG12	2.01	0.85
1:A:30:LEU:CD1	1:A:30:LEU:HG	2.04	0.85
1:A:87:ASN:ND2	1:B:133:ARG:NH2	2.25	0.84
1:B:102:ILE:CG2	1:B:102:ILE:CG1	2.55	0.84
1:A:100:ILE:CG2	1:A:100:ILE:HB	2.06	0.84
1:B:3:SER:O	1:B:7:ASN:HB2	1.76	0.84
1:B:38:LEU:C	1:B:38:LEU:HD23	2.02	0.84
1:A:57:GLY:HA2	1:A:60:THR:HB	1.61	0.83
1:A:38:LEU:HD23	1:A:38:LEU:O	1.79	0.83
1:A:54:THR:HA	1:A:94:ALA:O	1.77	0.82
1:A:70:MSE:CE	1:A:73:MSE:HE2	2.09	0.82
1:B:70:MSE:SE	1:B:73:MSE:CE	2.78	0.82
1:A:59:LEU:O	1:A:62:THR:HG23	1.79	0.81
1:B:70:MSE:SE	1:B:73:MSE:HE1	2.29	0.81
1:A:133:ARG:HD2	1:B:89:THR:HG21	1.61	0.81
1:B:50:ASN:HB3	1:B:52:LEU:H	1.47	0.80
1:A:87:ASN:HD21	1:B:133:ARG:HH12	1.29	0.80
1:B:102:ILE:C	1:B:102:ILE:HD12	2.05	0.80
1:A:21:PHE:HA	1:A:25:LEU:HD13	1.65	0.79
1:A:13:LYS:C	1:A:15:MSE:HE2	2.08	0.78
1:A:102:ILE:HG12	1:A:102:ILE:O	1.82	0.78
1:A:122:ASN:HD22	1:A:123:LYS:N	1.81	0.78
1:A:15:MSE:HG2	1:A:16:PHE:N	1.87	0.78
1:A:87:ASN:HD22	1:B:133:ARG:NH2	1.79	0.78
1:A:13:LYS:O	1:A:15:MSE:HE2	1.83	0.77
1:B:125:THR:HB	1:B:127:LYS:HB2	1.67	0.77
1:A:125:THR:HG21	1:A:127:LYS:HB2	1.67	0.76
1:B:50:ASN:HA	1:B:56:HIS:HD2	1.49	0.75
1:B:130:ALA:O	1:B:131:GLN:O	2.04	0.75
1:B:84:VAL:HG12	1:B:85:ASP:OD2	1.86	0.75
1:A:87:ASN:HD21	1:B:133:ARG:NH1	1.84	0.74
1:A:30:LEU:HD21	1:A:43:LYS:HZ3	1.53	0.73
1:B:67:ILE:HG21	1:B:102:ILE:HD11	1.70	0.73
1:A:75:THR:HB	1:A:109:GLN:HE22	1.53	0.73
1:B:100:ILE:O	1:B:100:ILE:HG13	1.88	0.73
1:B:75:THR:CG2	1:B:75:THR:CA	2.65	0.72
1:A:67:ILE:O	1:A:67:ILE:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LYS:HB3	1:B:115:PHE:HD1	1.53	0.72
1:A:27:LYS:HA	1:A:29:THR:HG22	1.70	0.72
1:A:68:SER:O	1:A:72:LEU:HB2	1.89	0.72
1:A:106:ILE:HG21	1:A:109:GLN:HG2	1.71	0.72
1:A:30:LEU:HD21	1:A:43:LYS:NZ	2.04	0.72
1:A:107:LEU:HD11	1:A:117:SER:HB2	1.71	0.71
1:A:30:LEU:O	1:A:31:VAL:CB	2.39	0.71
1:B:50:ASN:HB2	1:B:54:THR:O	1.90	0.71
1:A:31:VAL:CA	1:A:31:VAL:CG1	2.66	0.70
1:B:88:ILE:CG2	1:B:88:ILE:CA	2.66	0.70
1:B:87:ASN:CA	1:B:87:ASN:CG	2.64	0.70
1:A:58:GLY:O	1:A:62:THR:CG2	2.36	0.69
1:B:86:MSE:CG	1:B:88:ILE:HD11	2.21	0.69
1:A:66:SER:HA	1:A:69:THR:HG22	1.72	0.69
1:B:70:MSE:CG	1:B:70:MSE:CE	2.70	0.69
1:A:66:SER:HA	1:A:69:THR:CG2	2.22	0.69
1:A:51:LYS:O	1:A:52:LEU:HD23	1.93	0.68
1:A:15:MSE:HG3	1:A:16:PHE:N	2.09	0.68
1:A:50:ASN:O	1:A:51:LYS:C	2.37	0.68
1:B:36:GLU:O	1:B:106:ILE:HD12	1.93	0.67
1:B:87:ASN:CB	1:B:87:ASN:C	2.64	0.67
1:A:55:LEU:O	1:A:55:LEU:CD1	2.36	0.67
1:A:55:LEU:N	1:A:55:LEU:CD1	2.57	0.66
1:B:11:VAL:O	1:B:15:MSE:HG2	1.94	0.66
1:A:13:LYS:NZ	1:A:14:VAL:O	2.29	0.66
1:A:50:ASN:OD1	1:A:54:THR:O	2.13	0.66
1:A:122:ASN:ND2	1:A:124:THR:HG22	2.05	0.66
1:A:135:THR:CB	1:A:135:THR:C	2.67	0.65
1:B:63:LEU:HD12	1:B:67:ILE:HG13	1.79	0.65
1:A:50:ASN:O	1:A:52:LEU:N	2.30	0.65
1:A:24:VAL:CG1	1:A:24:VAL:HB	2.15	0.65
1:B:30:LEU:HD12	1:B:32:SER:H	1.61	0.65
1:B:129:ILE:O	1:B:130:ALA:HB2	1.95	0.65
1:A:60:THR:O	1:A:63:LEU:HB2	1.97	0.65
1:A:122:ASN:ND2	1:A:124:THR:CG2	2.57	0.65
1:A:125:THR:CG2	1:A:127:LYS:HB2	2.27	0.65
1:B:87:ASN:O	1:B:88:ILE:HG13	1.96	0.65
1:B:51:LYS:H	1:B:51:LYS:HD3	1.63	0.64
1:B:80:PRO:O	1:B:136:LYS:HE2	1.97	0.64
1:B:70:MSE:HA	1:B:73:MSE:HE3	1.80	0.63
1:B:108:LYS:CB	1:B:108:LYS:CD	2.71	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:VAL:HG12	1:A:49:THR:CG2	2.28	0.63
1:A:122:ASN:ND2	1:A:124:THR:H	1.97	0.63
1:A:20:GLY:O	1:A:25:LEU:HD12	1.99	0.62
1:A:84:VAL:HG21	1:A:137:HIS:HB2	1.81	0.62
1:A:133:ARG:CD	1:B:89:THR:HG21	2.29	0.62
1:B:86:MSE:HG2	1:B:88:ILE:HD11	1.81	0.62
1:A:111:LYS:H	1:A:111:LYS:HG3	1.65	0.61
1:B:71:ALA:HB1	1:B:106:ILE:HD11	1.82	0.61
1:B:101:VAL:HG13	1:B:121:THR:OG1	2.01	0.60
1:A:100:ILE:O	1:A:100:ILE:HG12	1.88	0.59
1:A:107:LEU:HD11	1:A:117:SER:CB	2.32	0.59
1:A:137:HIS:CD2	1:A:139:GLY:O	2.56	0.59
1:A:30:LEU:HD11	1:A:43:LYS:HE2	1.85	0.59
1:A:67:ILE:O	1:A:67:ILE:CG2	2.51	0.59
1:B:130:ALA:O	1:B:131:GLN:C	2.43	0.59
1:A:109:GLN:O	1:A:110:GLY:O	2.21	0.58
1:A:129:ILE:CB	1:A:129:ILE:C	2.72	0.58
1:A:81:GLY:O	1:A:136:LYS:HE2	2.02	0.58
1:A:87:ASN:ND2	1:B:133:ARG:CZ	2.67	0.58
1:B:113:LEU:HD13	1:B:137:HIS:HA	1.86	0.58
1:B:70:MSE:SE	1:B:70:MSE:HA	2.54	0.58
1:A:87:ASN:ND2	1:B:133:ARG:HH12	2.01	0.58
1:A:70:MSE:HE1	1:A:73:MSE:CE	2.27	0.58
1:B:6:GLN:O	1:B:9:ARG:HB3	2.04	0.58
1:B:70:MSE:CE	1:B:73:MSE:CE	2.82	0.58
1:B:52:LEU:CD1	1:B:52:LEU:CD2	2.79	0.57
1:A:60:THR:HA	1:A:63:LEU:HD12	1.86	0.57
1:B:125:THR:CB	1:B:127:LYS:HB2	2.33	0.57
1:A:16:PHE:O	1:A:18:VAL:HG23	1.97	0.57
1:A:37:LYS:HA	1:A:104:ALA:O	2.04	0.57
1:B:50:ASN:HA	1:B:56:HIS:CD2	2.37	0.57
1:A:49:THR:HA	1:A:55:LEU:HA	1.88	0.56
1:A:31:VAL:CA	1:A:31:VAL:HB	2.18	0.56
1:B:16:PHE:N	1:B:16:PHE:CD2	2.70	0.56
1:A:134:HIS:HD2	1:A:135:THR:N	2.04	0.56
1:A:84:VAL:CG2	1:A:137:HIS:HB2	2.36	0.56
1:A:134:HIS:CD2	1:A:135:THR:N	2.74	0.56
1:B:8:LEU:HB3	1:B:30:LEU:CD2	2.35	0.56
1:B:88:ILE:CG2	1:B:88:ILE:CG1	2.79	0.56
1:A:67:ILE:HA	1:A:70:MSE:HB3	1.88	0.55
1:A:87:ASN:HD21	1:B:133:ARG:CZ	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:C	1:B:38:LEU:CD2	2.78	0.55
1:B:108:LYS:CG	1:B:108:LYS:CA	2.80	0.55
1:A:134:HIS:HD2	1:A:135:THR:H	1.55	0.54
1:B:70:MSE:CE	1:B:73:MSE:HE3	2.38	0.54
1:B:111:LYS:CD	1:B:111:LYS:H	2.20	0.54
1:A:111:LYS:HG3	2:A:145:HOH:O	2.07	0.54
1:A:80:PRO:HD3	2:A:142:HOH:O	2.08	0.54
1:A:57:GLY:CA	1:A:60:THR:HB	2.35	0.54
1:A:65:ASP:O	1:A:69:THR:HG22	2.08	0.54
1:B:8:LEU:HD21	1:B:70:MSE:HE3	1.89	0.54
1:B:31:VAL:HG11	1:B:41:GLU:CD	2.32	0.53
1:B:37:LYS:HA	1:B:104:ALA:O	2.09	0.53
1:A:120:LEU:C	1:A:120:LEU:CD2	2.81	0.53
1:A:43:LYS:H	1:A:43:LYS:HD2	1.71	0.53
1:A:74:CYS:O	1:A:75:THR:C	2.50	0.53
1:A:80:PRO:N	1:A:80:PRO:C	2.62	0.53
1:A:43:LYS:HG3	1:A:99:GLU:OE1	2.09	0.52
1:A:59:LEU:HD12	1:A:63:LEU:HD11	1.91	0.52
1:A:13:LYS:C	1:A:15:MSE:CE	2.73	0.52
1:A:87:ASN:ND2	1:B:133:ARG:NH1	2.57	0.52
1:A:135:THR:CB	1:A:135:THR:N	2.67	0.52
1:A:30:LEU:CD1	1:A:30:LEU:CD2	2.80	0.52
1:A:121:THR:HG22	1:A:128:LEU:HA	1.91	0.52
1:B:34:ALA:HB1	1:B:35:PRO:HD2	1.93	0.51
1:B:87:ASN:C	1:B:88:ILE:HG13	2.34	0.51
1:A:38:LEU:HD13	1:A:71:ALA:HA	1.92	0.51
1:A:72:LEU:HD13	1:A:106:ILE:HD12	1.91	0.51
1:B:45:GLU:HG2	1:B:48:HIS:CE1	2.45	0.51
1:B:43:LYS:HA	1:B:99:GLU:HA	1.93	0.51
1:A:36:GLU:OE1	1:A:109:GLN:HG3	2.11	0.51
1:B:111:LYS:CG	1:B:111:LYS:CE	2.83	0.51
1:A:43:LYS:HD2	1:A:43:LYS:N	2.27	0.50
1:A:69:THR:HG23	1:A:70:MSE:H	1.76	0.50
1:B:70:MSE:SE	1:B:70:MSE:CB	3.06	0.50
1:B:8:LEU:HD21	1:B:70:MSE:CE	2.42	0.50
1:B:70:MSE:CE	1:B:73:MSE:HE1	2.42	0.50
1:B:81:GLY:C	1:B:82:VAL:CG1	2.85	0.50
1:B:20:GLY:O	1:B:23:ARG:HD3	2.11	0.49
1:B:50:ASN:HB3	1:B:52:LEU:N	2.22	0.49
1:B:75:THR:CG2	1:B:75:THR:C	2.85	0.49
1:A:57:GLY:HA2	1:A:60:THR:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:THR:HG23	1:A:113:LEU:HG	1.93	0.49
1:B:13:LYS:CE	1:B:13:LYS:CG	2.82	0.49
1:A:120:LEU:C	1:A:120:LEU:HD23	2.37	0.49
1:B:10:GLU:OE2	1:B:13:LYS:HE2	2.13	0.49
1:B:15:MSE:C	1:B:16:PHE:HD2	2.19	0.49
1:B:70:MSE:SE	1:B:73:MSE:HE3	2.60	0.49
1:A:129:ILE:CA	1:A:129:ILE:CG1	2.79	0.49
1:A:38:LEU:CD2	1:A:67:ILE:HG23	2.43	0.49
1:A:122:ASN:HB3	1:A:125:THR:HB	1.93	0.49
1:A:92:SER:O	1:A:129:ILE:HG23	2.12	0.48
1:A:44:VAL:CG1	1:A:49:THR:HG22	2.42	0.48
1:A:30:LEU:CD2	1:A:43:LYS:NZ	2.75	0.48
1:A:129:ILE:CA	1:A:129:ILE:CG2	2.85	0.48
1:A:133:ARG:NH1	1:B:133:ARG:HB2	2.27	0.48
1:B:42:MSE:O	1:B:100:ILE:HG12	2.14	0.48
1:B:21:PHE:O	1:B:24:VAL:HG22	2.12	0.48
1:A:69:THR:HG23	1:A:70:MSE:N	2.28	0.48
1:A:21:PHE:HA	1:A:25:LEU:CD1	2.41	0.48
1:A:65:ASP:O	1:A:68:SER:HB3	2.14	0.48
1:B:8:LEU:CD2	1:B:70:MSE:CE	2.92	0.47
1:A:44:VAL:HG12	1:A:49:THR:HG23	1.96	0.47
1:B:28:VAL:HG13	1:B:28:VAL:O	2.14	0.47
1:B:65:ASP:OD1	1:B:65:ASP:C	2.58	0.47
1:B:86:MSE:SE	1:B:88:ILE:CD1	2.97	0.47
1:A:22:ASP:H	1:A:25:LEU:HD13	1.79	0.47
1:A:122:ASN:HD22	1:A:122:ASN:C	2.23	0.47
1:A:24:VAL:N	1:A:24:VAL:HA	2.06	0.46
1:A:111:LYS:CG	1:A:111:LYS:H	2.26	0.46
1:A:17:LYS:HE2	1:A:17:LYS:O	2.16	0.46
1:A:69:THR:HB	1:A:136:LYS:NZ	2.30	0.46
1:A:17:LYS:HE2	1:A:27:LYS:HD3	1.96	0.46
1:B:30:LEU:CD1	1:B:32:SER:H	2.26	0.46
1:A:25:LEU:O	1:A:25:LEU:CG	2.34	0.46
1:B:30:LEU:HD12	1:B:30:LEU:C	2.41	0.46
1:B:86:MSE:HG2	1:B:88:ILE:CD1	2.45	0.46
1:B:99:GLU:HG2	1:B:123:LYS:HD2	1.97	0.46
1:B:10:GLU:O	1:B:11:VAL:C	2.57	0.46
1:A:19:PRO:O	1:A:27:LYS:HD2	2.16	0.45
1:A:108:LYS:HB3	1:A:115:PHE:HD2	1.81	0.45
1:B:120:LEU:HD12	1:B:120:LEU:N	2.31	0.45
1:A:106:ILE:HG21	1:A:109:GLN:CG	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:VAL:O	1:B:28:VAL:CG1	2.64	0.45
1:A:30:LEU:C	1:A:31:VAL:CG1	2.75	0.45
1:A:72:LEU:CD1	1:A:106:ILE:HD12	2.45	0.45
1:B:51:LYS:HD3	1:B:51:LYS:N	2.31	0.45
1:B:128:LEU:HD13	1:B:128:LEU:HA	1.74	0.45
1:A:129:ILE:CA	1:A:129:ILE:HB	2.21	0.45
1:A:122:ASN:HB2	1:A:129:ILE:HD11	1.98	0.45
1:B:125:THR:HB	1:B:127:LYS:H	1.80	0.45
1:A:30:LEU:CD2	1:A:43:LYS:HZ1	2.29	0.45
1:A:125:THR:HG22	1:A:127:LYS:H	1.82	0.45
1:A:50:ASN:C	1:A:52:LEU:N	2.75	0.44
1:A:111:LYS:NZ	1:A:112:THR:HG22	2.32	0.44
1:B:16:PHE:N	1:B:16:PHE:HD2	2.14	0.44
1:A:30:LEU:C	1:A:31:VAL:CB	2.90	0.44
1:A:122:ASN:ND2	1:A:124:THR:HG23	2.33	0.44
1:B:133:ARG:HH21	1:B:133:ARG:HD2	1.61	0.44
1:A:66:SER:O	1:A:67:ILE:HB	2.17	0.44
1:A:89:THR:OG1	1:B:133:ARG:HD2	2.18	0.43
1:B:81:GLY:C	1:B:82:VAL:HG13	2.43	0.43
1:A:133:ARG:HD2	1:B:89:THR:CG2	2.40	0.43
1:A:31:VAL:CB	1:A:31:VAL:N	2.70	0.43
1:B:43:LYS:HA	1:B:98:GLU:O	2.18	0.43
1:A:24:VAL:N	1:A:24:VAL:CG2	2.82	0.43
1:A:70:MSE:C	1:A:72:LEU:H	2.27	0.43
1:A:19:PRO:HG2	1:A:73:MSE:HE1	1.99	0.43
1:B:81:GLY:O	1:B:82:VAL:HG12	2.19	0.43
1:A:39:ILE:C	1:A:40:CYS:SG	3.00	0.43
1:A:18:VAL:N	1:A:19:PRO:CD	2.81	0.43
1:B:63:LEU:CD1	1:B:67:ILE:HG13	2.48	0.43
1:A:57:GLY:HA3	1:A:90:TYR:CE2	2.53	0.43
1:A:109:GLN:O	1:A:110:GLY:C	2.60	0.43
1:B:70:MSE:HE1	1:B:73:MSE:HE1	2.01	0.43
1:A:86:MSE:HG3	1:A:87:ASN:N	2.34	0.43
1:B:30:LEU:HD12	1:B:32:SER:N	2.32	0.43
1:A:59:LEU:HA	1:A:59:LEU:HD22	1.78	0.42
1:A:122:ASN:ND2	1:A:124:THR:N	2.66	0.42
1:A:22:ASP:N	1:A:25:LEU:HD13	2.34	0.42
1:A:95:LYS:O	1:A:96:ILE:C	2.58	0.42
1:B:108:LYS:HB3	1:B:115:PHE:CD1	2.43	0.42
1:A:96:ILE:C	1:A:96:ILE:HD13	2.44	0.42
1:A:39:ILE:O	1:A:40:CYS:SG	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LYS:H	1:B:111:LYS:HD2	1.83	0.41
1:A:49:THR:HG21	1:A:96:ILE:HB	2.02	0.41
1:B:125:THR:C	1:B:127:LYS:H	2.28	0.41
1:B:11:VAL:O	1:B:12:MSE:C	2.63	0.41
1:B:44:VAL:HG13	1:B:95:LYS:O	2.19	0.41
1:B:119:ASP:C	1:B:120:LEU:HD12	2.45	0.41
1:B:12:MSE:CG	1:B:70:MSE:HE2	2.50	0.41
1:B:88:ILE:CB	1:B:88:ILE:CD1	2.86	0.41
1:B:12:MSE:HG3	1:B:70:MSE:HE2	2.03	0.41
1:A:88:ILE:CD1	1:A:88:ILE:CB	2.82	0.41
1:B:38:LEU:HD23	1:B:38:LEU:O	2.20	0.41
1:A:61:ALA:O	1:A:62:THR:C	2.62	0.41
1:B:34:ALA:HB1	1:B:35:PRO:CD	2.51	0.41
1:A:69:THR:O	1:A:72:LEU:HB3	2.21	0.41
1:B:30:LEU:HD12	1:B:31:VAL:N	2.35	0.41
1:B:43:LYS:HZ2	1:B:43:LYS:HG2	1.62	0.41
1:B:134:HIS:CD2	1:B:136:LYS:HG3	2.56	0.41
1:A:45:GLU:O	1:A:46:GLU:C	2.63	0.40
1:A:56:HIS:H	1:A:56:HIS:CD2	2.39	0.40
1:A:37:LYS:O	1:A:38:LEU:HB2	2.20	0.40
1:A:75:THR:HB	1:A:109:GLN:NE2	2.29	0.40
1:B:67:ILE:CG2	1:B:102:ILE:HD11	2.44	0.40
1:B:75:THR:O	1:B:76:GLU:C	2.65	0.40
1:B:89:THR:HG23	1:B:91:MSE:HE1	2.04	0.40

There are no symmetry-related clashes.

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	116/140 (83%)	82 (71%)	20 (17%)	14 (12%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	127/140 (91%)	111 (87%)	11 (9%)	5 (4%)	2	5
All	All	243/280 (87%)	193 (79%)	31 (13%)	19 (8%)	1	1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	MSE
1	A	51	LYS
1	A	110	GLY
1	B	109	GLN
1	B	131	GLN
1	A	25	LEU
1	A	62	THR
1	A	67	ILE
1	A	16	PHE
1	A	31	VAL
1	A	61	ALA
1	A	68	SER
1	A	65	ASP
1	B	45	GLU
1	B	50	ASN
1	B	130	ALA
1	A	19	PRO
1	A	28	VAL
1	A	18	VAL

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	103/110 (94%)	73 (71%)	30 (29%)	0	1
1	B	114/110 (104%)	74 (65%)	40 (35%)	0	0
All	All	217/220 (99%)	147 (68%)	70 (32%)	0	1

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	17	LYS
1	A	18	VAL
1	A	24	VAL
1	A	25	LEU
1	A	31	VAL
1	A	36	GLU
1	A	39	ILE
1	A	43	LYS
1	A	46	GLU
1	A	47	GLN
1	A	51	LYS
1	A	55	LEU
1	A	56	HIS
1	A	59	LEU
1	A	62	THR
1	A	85	ASP
1	A	90	TYR
1	A	96	ILE
1	A	100	ILE
1	A	101	VAL
1	A	102	ILE
1	A	111	LYS
1	A	119	ASP
1	A	120	LEU
1	A	122	ASN
1	A	124	THR
1	A	127	LYS
1	A	131	GLN
1	A	138	LEU
1	B	1	MSE
1	B	6	GLN
1	B	7	ASN
1	B	8	LEU
1	B	15	MSE
1	B	16	PHE
1	B	23	ARG
1	B	27	LYS
1	B	29	THR
1	B	30	LEU
1	B	31	VAL
1	B	38	LEU
1	B	39	ILE

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Mol	Chain	Res	Type
1	B	41	GLU
1	B	42	MSE
1	B	47	GLN
1	B	50	ASN
1	B	51	LYS
1	B	55	LEU
1	B	63	LEU
1	B	67	ILE
1	B	75	THR
1	B	76	GLU
1	B	87	ASN
1	B	91	MSE
1	B	96	ILE
1	B	98	GLU
1	B	101	VAL
1	B	102	ILE
1	B	103	THR
1	B	107	LEU
1	B	108	LYS
1	B	109	GLN
1	B	111	LYS
1	B	113	LEU
1	B	121	THR
1	B	127	LYS
1	B	128	LEU
1	B	129	ILE
1	B	135	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	87	ASN
1	A	109	GLN
1	A	122	ASN
1	A	131	GLN
1	B	50	ASN
1	B	56	HIS
1	B	109	GLN
1	B	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	52:LEU	C	53:GLY	N	1.20

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	116/140 (82%)	0.09	3 (2%) 57 54	23, 59, 94, 110	0
1	B	124/140 (88%)	-0.23	2 (1%) 70 68	20, 51, 71, 88	0
All	All	240/280 (85%)	-0.08	5 (2%) 63 60	20, 55, 84, 110	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	139	GLY	2.7
1	A	16	PHE	2.5
1	B	108	LYS	2.4
1	A	29	THR	2.1
1	A	119	ASP	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.