Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:06 pm BST

PDB ID	:	2CY9
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 following versions of software and data (see references ⓘ) were used in the production of this report:

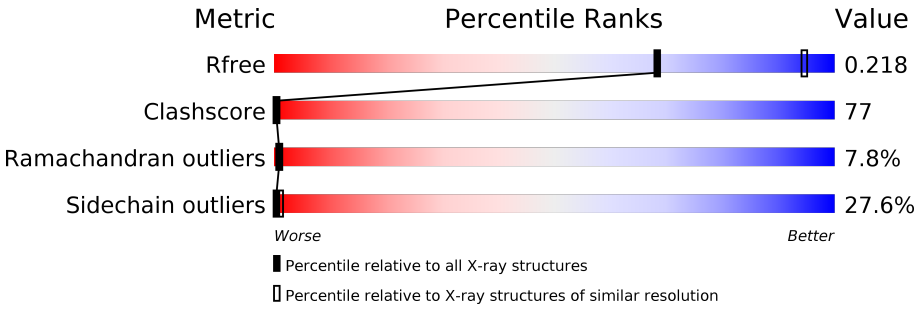
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	140	7% 27% 35% 18% 13%
1	B	140	12% 30% 38% 15% 5%

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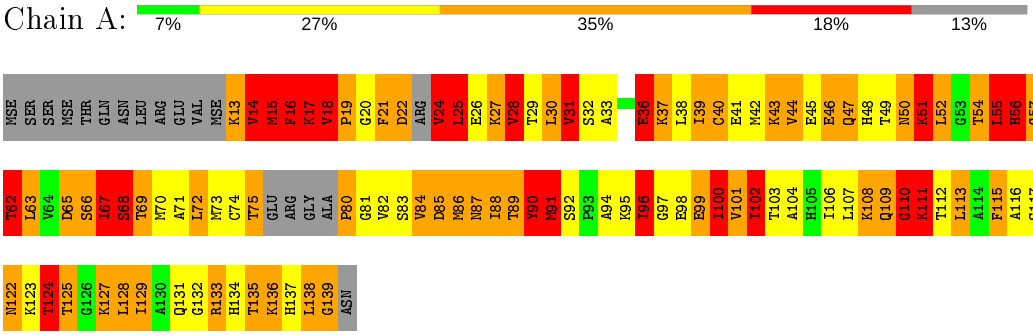
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	19	Total O 19 19	0	0

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.

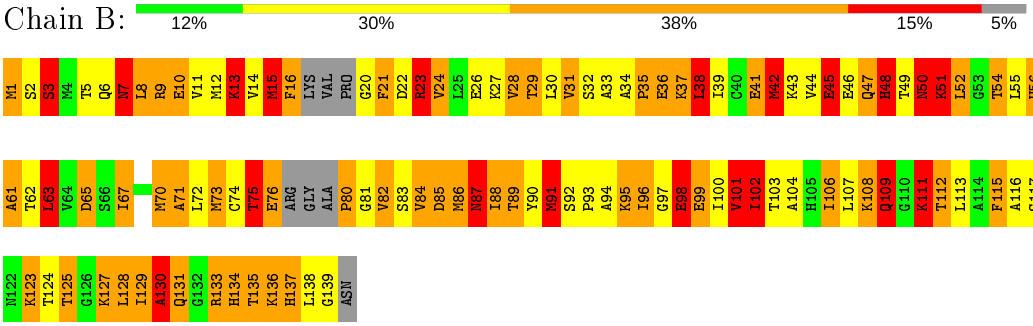
- Molecule 1: Thioesterase superfamily member 2

Chain A:



- Molecule 1: Thioesterase superfamily member 2

Chain B:



4 Data and refinement statistics (i)

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 49.12 – 2.72	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.10-2.72) 95.4 (49.12-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.191 , 0.262 0.216 , 0.218	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)	0.34 , 109.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	3.43	128/916 (14.0%)	2.36	53/1222 (4.3%)
1	B	3.42	136/1005 (13.5%)	2.34	56/1335 (4.2%)
All	All	3.42	264/1921 (13.7%)	2.35	109/2557 (4.3%)

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 (264) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	GLU	CD-OE1	14.22	1.41	1.25
1	B	117	SER	CB-OG	13.96	1.60	1.42
1	A	135	THR	CA-CB	13.47	1.88	1.53
1	B	41	GLU	CD-OE2	13.44	1.40	1.25
1	A	90	TYR	CE1-CZ	13.34	1.55	1.38
1	A	80	PRO	N-CA	13.03	1.69	1.47
1	B	139	GLY	C-O	13.01	1.44	1.23
1	A	36	GLU	CG-CD	12.26	1.70	1.51
1	B	46	GLU	CD-OE2	11.93	1.38	1.25
1	B	102	ILE	CB-CG2	11.35	1.88	1.52
1	B	2	SER	CB-OG	-11.33	1.27	1.42
1	A	111	LYS	CB-CG	11.23	1.82	1.52
1	A	31	VAL	CA-CB	11.14	1.78	1.54
1	A	100	ILE	CB-CG2	11.11	1.87	1.52
1	A	24	VAL	N-CA	10.80	1.68	1.46
1	B	94	ALA	CA-CB	-10.78	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	VAL	CB-CG1	10.40	1.74	1.52
1	A	129	ILE	CA-CB	10.40	1.78	1.54
1	A	31	VAL	CB-CG2	10.21	1.74	1.52
1	B	13	LYS	CD-CE	10.19	1.76	1.51
1	A	99	GLU	CD-OE2	10.12	1.36	1.25
1	A	51	LYS	CE-NZ	9.99	1.74	1.49
1	B	46	GLU	CD-OE1	9.95	1.36	1.25
1	B	87	ASN	CA-CB	9.92	1.78	1.53
1	A	101	VAL	CA-CB	-9.71	1.34	1.54
1	A	36	GLU	CB-CG	9.68	1.70	1.52
1	A	45	GLU	CD-OE2	9.50	1.36	1.25
1	B	3	SER	CB-OG	9.48	1.54	1.42
1	A	16	PHE	CD2-CE2	9.41	1.58	1.39
1	B	14	VAL	CB-CG1	9.40	1.72	1.52
1	B	136	LYS	CE-NZ	9.39	1.72	1.49
1	A	14	VAL	CB-CG1	9.36	1.72	1.52
1	B	62	THR	N-CA	9.32	1.65	1.46
1	A	21	PHE	CE1-CZ	9.23	1.54	1.37
1	B	108	LYS	CB-CG	9.15	1.77	1.52
1	A	24	VAL	CB-CG2	-9.12	1.33	1.52
1	B	61	ALA	CA-C	-9.12	1.29	1.52
1	A	84	VAL	CB-CG2	9.06	1.71	1.52
1	B	76	GLU	CD-OE2	9.01	1.35	1.25
1	B	36	GLU	CG-CD	9.00	1.65	1.51
1	B	47	GLN	CG-CD	8.97	1.71	1.51
1	B	71	ALA	CA-CB	-8.95	1.33	1.52
1	B	133	ARG	CG-CD	8.95	1.74	1.51
1	A	95	LYS	CD-CE	8.81	1.73	1.51
1	B	85	ASP	CG-OD2	8.79	1.45	1.25
1	A	25	LEU	C-O	8.69	1.39	1.23
1	A	116	ALA	CA-CB	-8.69	1.34	1.52
1	B	46	GLU	CG-CD	8.66	1.65	1.51
1	B	51	LYS	CD-CE	8.62	1.72	1.51
1	A	82	VAL	CA-CB	-8.61	1.36	1.54
1	B	10	GLU	CD-OE1	8.60	1.35	1.25
1	B	75	THR	CB-CG2	8.60	1.80	1.52
1	B	36	GLU	CD-OE2	8.56	1.35	1.25
1	B	16	PHE	C-O	8.54	1.39	1.23
1	A	15	MSE	C-O	8.45	1.39	1.23
1	B	84	VAL	C-O	8.46	1.39	1.23
1	A	90	TYR	CB-CG	-8.42	1.39	1.51
1	A	97	GLY	C-O	-8.41	1.10	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	16	PHE	CD1-CE1	8.23	1.55	1.39
1	B	1	MSE	SE-CE	-8.11	1.47	1.95
1	A	41	GLU	CG-CD	8.09	1.64	1.51
1	B	76	GLU	CD-OE1	7.99	1.34	1.25
1	B	133	ARG	NE-CZ	-7.94	1.22	1.33
1	B	130	ALA	CA-CB	-7.94	1.35	1.52
1	A	48	HIS	C-O	-7.89	1.08	1.23
1	A	33	ALA	CA-CB	7.88	1.69	1.52
1	B	48	HIS	C-O	-7.80	1.08	1.23
1	B	31	VAL	CB-CG1	-7.79	1.36	1.52
1	B	88	ILE	CB-CG2	7.78	1.76	1.52
1	B	85	ASP	CG-OD1	7.77	1.43	1.25
1	A	41	GLU	CD-OE1	7.72	1.34	1.25
1	B	60	THR	CA-CB	-7.72	1.33	1.53
1	A	96	ILE	CA-CB	7.62	1.72	1.54
1	B	22	ASP	CB-CG	7.53	1.67	1.51
1	A	16	PHE	CB-CG	7.49	1.64	1.51
1	B	130	ALA	N-CA	-7.47	1.31	1.46
1	A	39	ILE	C-O	-7.46	1.09	1.23
1	B	117	SER	CA-CB	7.38	1.64	1.52
1	B	90	TYR	CE1-CZ	7.31	1.48	1.38
1	B	70	MSE	N-CA	7.31	1.60	1.46
1	B	52	LEU	CG-CD1	7.26	1.78	1.51
1	A	85	ASP	CG-OD2	7.24	1.42	1.25
1	A	14	VAL	CB-CG2	7.23	1.68	1.52
1	B	65	ASP	N-CA	7.22	1.60	1.46
1	B	7	ASN	CB-CG	7.20	1.67	1.51
1	B	135	THR	CA-CB	7.16	1.72	1.53
1	B	80	PRO	N-CA	7.14	1.59	1.47
1	A	115	PHE	CB-CG	7.14	1.63	1.51
1	B	16	PHE	CD2-CE2	7.13	1.53	1.39
1	B	91	MSE	SE-CE	-7.12	1.53	1.95
1	B	101	VAL	CB-CG2	7.11	1.67	1.52
1	A	66	SER	CB-OG	7.07	1.51	1.42
1	B	36	GLU	CB-CG	7.03	1.65	1.52
1	B	16	PHE	CE2-CZ	7.02	1.50	1.37
1	A	52	LEU	C-N	-7.01	1.20	1.33
1	A	27	LYS	CD-CE	7.00	1.68	1.51
1	A	13	LYS	N-CA	6.96	1.60	1.46
1	B	111	LYS	CD-CE	6.95	1.68	1.51
1	B	26	GLU	CD-OE2	6.95	1.33	1.25
1	A	16	PHE	CE1-CZ	6.93	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	GLN	CD-OE1	6.92	1.39	1.24
1	A	98	GLU	CD-OE1	6.92	1.33	1.25
1	B	85	ASP	CB-CG	6.92	1.66	1.51
1	B	29	THR	C-O	-6.90	1.10	1.23
1	B	47	GLN	CA-C	6.90	1.70	1.52
1	A	21	PHE	CG-CD2	6.90	1.49	1.38
1	B	45	GLU	CD-OE1	6.89	1.33	1.25
1	A	50	ASN	CB-CG	6.88	1.66	1.51
1	B	89	THR	CA-CB	6.88	1.71	1.53
1	A	69	THR	CB-CG2	-6.87	1.29	1.52
1	A	31	VAL	CA-C	6.85	1.70	1.52
1	A	133	ARG	CZ-NH2	-6.83	1.24	1.33
1	A	91	MSE	N-CA	-6.83	1.32	1.46
1	A	37	LYS	CE-NZ	6.82	1.66	1.49
1	A	28	VAL	CB-CG2	6.81	1.67	1.52
1	A	17	LYS	CD-CE	6.80	1.68	1.51
1	A	16	PHE	CD1-CE1	6.79	1.52	1.39
1	A	132	GLY	CA-C	6.79	1.62	1.51
1	B	75	THR	CB-OG1	6.78	1.56	1.43
1	B	28	VAL	CB-CG1	6.77	1.67	1.52
1	B	37	LYS	CE-NZ	6.76	1.66	1.49
1	A	36	GLU	CA-CB	6.75	1.68	1.53
1	A	102	ILE	CA-CB	-6.75	1.39	1.54
1	A	83	SER	C-O	6.73	1.36	1.23
1	B	111	LYS	CG-CD	6.70	1.75	1.52
1	A	124	THR	CB-CG2	6.64	1.74	1.52
1	A	98	GLU	N-CA	6.63	1.59	1.46
1	A	32	SER	CB-OG	6.63	1.50	1.42
1	A	26	GLU	C-O	-6.60	1.10	1.23
1	B	5	THR	N-CA	-6.60	1.33	1.46
1	B	16	PHE	CG-CD1	6.58	1.48	1.38
1	B	47	GLN	CB-CG	6.58	1.70	1.52
1	B	61	ALA	CA-CB	-6.58	1.38	1.52
1	A	21	PHE	CG-CD1	6.57	1.48	1.38
1	B	76	GLU	CG-CD	6.56	1.61	1.51
1	B	47	GLN	CD-NE2	6.55	1.49	1.32
1	A	36	GLU	CD-OE1	6.54	1.32	1.25
1	B	22	ASP	CG-OD1	6.48	1.40	1.25
1	B	67	ILE	CB-CG2	6.47	1.73	1.52
1	B	119	ASP	CA-CB	6.46	1.68	1.53
1	A	44	VAL	CB-CG1	6.45	1.66	1.52
1	A	16	PHE	CG-CD1	6.43	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	130	ALA	C-O	6.42	1.35	1.23
1	B	136	LYS	CB-CG	6.39	1.69	1.52
1	B	87	ASN	N-CA	6.34	1.59	1.46
1	A	90	TYR	CD2-CE2	6.34	1.48	1.39
1	A	27	LYS	CB-CG	6.30	1.69	1.52
1	A	44	VAL	CB-CG2	-6.29	1.39	1.52
1	A	30	LEU	CG-CD1	6.27	1.75	1.51
1	A	115	PHE	CE1-CZ	-6.27	1.25	1.37
1	A	103	THR	CA-CB	-6.26	1.37	1.53
1	A	108	LYS	CB-CG	6.26	1.69	1.52
1	B	112	THR	CB-CG2	6.24	1.73	1.52
1	A	101	VAL	CB-CG1	6.24	1.66	1.52
1	A	41	GLU	C-O	-6.24	1.11	1.23
1	A	68	SER	CB-OG	6.22	1.50	1.42
1	A	80	PRO	C-O	6.20	1.35	1.23
1	B	65	ASP	CG-OD2	6.18	1.39	1.25
1	B	90	TYR	CD1-CE1	6.17	1.48	1.39
1	A	89	THR	N-CA	-6.17	1.34	1.46
1	A	16	PHE	CE2-CZ	6.15	1.49	1.37
1	A	14	VAL	CA-CB	6.12	1.67	1.54
1	B	22	ASP	CA-C	6.11	1.68	1.52
1	B	5	THR	C-O	6.09	1.34	1.23
1	B	10	GLU	CD-OE2	6.09	1.32	1.25
1	A	90	TYR	CZ-OH	6.08	1.48	1.37
1	B	95	LYS	CE-NZ	6.08	1.64	1.49
1	B	70	MSE	CG-SE	6.06	2.16	1.95
1	A	51	LYS	CA-CB	6.06	1.67	1.53
1	B	5	THR	CB-CG2	-6.05	1.32	1.52
1	B	76	GLU	CB-CG	6.05	1.63	1.52
1	B	13	LYS	CE-NZ	6.04	1.64	1.49
1	B	24	VAL	CB-CG2	6.04	1.65	1.52
1	A	16	PHE	CG-CD2	6.03	1.47	1.38
1	B	22	ASP	CA-CB	6.01	1.67	1.53
1	A	51	LYS	CB-CG	5.98	1.68	1.52
1	A	129	ILE	C-O	-5.94	1.12	1.23
1	A	139	GLY	CA-C	5.94	1.61	1.51
1	A	28	VAL	CA-CB	5.94	1.67	1.54
1	A	85	ASP	N-CA	-5.92	1.34	1.46
1	B	91	MSE	CG-SE	-5.92	1.75	1.95
1	A	44	VAL	CA-CB	5.91	1.67	1.54
1	B	74	CYS	C-O	5.90	1.34	1.23
1	B	82	VAL	C-O	-5.90	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	ASN	CG-ND2	5.88	1.47	1.32
1	B	99	GLU	CD-OE1	5.83	1.32	1.25
1	A	41	GLU	N-CA	5.83	1.58	1.46
1	B	86	MSE	SE-CE	-5.81	1.61	1.95
1	A	87	ASN	CA-CB	5.79	1.68	1.53
1	B	23	ARG	CG-CD	5.79	1.66	1.51
1	A	136	LYS	CA-C	-5.78	1.38	1.52
1	B	127	LYS	CB-CG	5.75	1.68	1.52
1	A	66	SER	CA-CB	-5.74	1.44	1.52
1	B	92	SER	C-O	5.71	1.34	1.23
1	B	21	PHE	CD1-CE1	5.70	1.50	1.39
1	A	80	PRO	CG-CD	5.70	1.69	1.50
1	B	92	SER	CA-CB	-5.68	1.44	1.52
1	A	51	LYS	CG-CD	5.67	1.71	1.52
1	B	119	ASP	CB-CG	5.65	1.63	1.51
1	B	129	ILE	C-O	-5.64	1.12	1.23
1	A	95	LYS	CG-CD	5.64	1.71	1.52
1	B	58	GLY	CA-C	-5.63	1.42	1.51
1	B	82	VAL	CB-CG1	-5.63	1.41	1.52
1	B	80	PRO	CA-C	5.62	1.64	1.52
1	A	21	PHE	CE2-CZ	5.62	1.48	1.37
1	A	67	ILE	CB-CG2	5.61	1.70	1.52
1	A	28	VAL	CB-CG1	5.59	1.64	1.52
1	A	22	ASP	CA-C	5.58	1.67	1.52
1	A	31	VAL	CB-CG1	-5.58	1.41	1.52
1	A	42	MSE	N-CA	-5.58	1.35	1.46
1	B	2	SER	CA-CB	-5.57	1.44	1.52
1	B	134	HIS	CB-CG	5.57	1.60	1.50
1	B	52	LEU	CB-CG	5.57	1.68	1.52
1	B	39	ILE	CA-CB	-5.56	1.42	1.54
1	B	28	VAL	C-O	-5.53	1.12	1.23
1	B	123	LYS	C-O	-5.53	1.12	1.23
1	A	46	GLU	CB-CG	5.52	1.62	1.52
1	A	27	LYS	CE-NZ	5.49	1.62	1.49
1	A	115	PHE	CD1-CE1	-5.49	1.28	1.39
1	B	51	LYS	CB-CG	5.45	1.67	1.52
1	A	109	GLN	C-N	-5.44	1.23	1.33
1	B	82	VAL	CB-CG2	5.42	1.64	1.52
1	B	98	GLU	CB-CG	5.41	1.62	1.52
1	A	97	GLY	CA-C	-5.40	1.43	1.51
1	A	102	ILE	N-CA	-5.40	1.35	1.46
1	B	24	VAL	CB-CG1	5.38	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	GLU	CD-OE1	5.34	1.31	1.25
1	A	45	GLU	CG-CD	5.30	1.59	1.51
1	A	42	MSE	CG-SE	-5.30	1.77	1.95
1	A	83	SER	CA-CB	-5.28	1.45	1.52
1	B	63	LEU	C-O	-5.28	1.13	1.23
1	B	135	THR	N-CA	-5.28	1.35	1.46
1	A	128	LEU	N-CA	-5.28	1.35	1.46
1	A	39	ILE	CB-CG2	5.26	1.69	1.52
1	B	42	MSE	CB-CG	5.25	1.68	1.52
1	A	109	GLN	CD-NE2	5.25	1.46	1.32
1	A	18	VAL	C-O	5.25	1.33	1.23
1	B	115	PHE	CB-CG	5.25	1.60	1.51
1	A	25	LEU	CG-CD2	5.23	1.71	1.51
1	A	138	LEU	C-O	5.22	1.33	1.23
1	B	38	LEU	CG-CD2	5.22	1.71	1.51
1	A	115	PHE	CG-CD1	-5.21	1.30	1.38
1	B	1	MSE	CG-SE	-5.20	1.77	1.95
1	A	116	ALA	CA-C	-5.19	1.39	1.52
1	B	83	SER	N-CA	-5.18	1.35	1.46
1	B	124	THR	CB-CG2	5.18	1.69	1.52
1	B	72	LEU	CA-C	-5.17	1.39	1.52
1	B	95	LYS	CB-CG	5.15	1.66	1.52
1	A	88	ILE	CG1-CD1	5.13	1.85	1.50
1	B	95	LYS	CA-C	5.13	1.66	1.52
1	B	123	LYS	CD-CE	5.13	1.64	1.51
1	B	49	THR	CB-OG1	-5.12	1.33	1.43
1	B	26	GLU	CD-OE1	5.10	1.31	1.25
1	A	36	GLU	CD-OE2	5.08	1.31	1.25
1	B	56	HIS	C-O	5.07	1.32	1.23
1	A	37	LYS	C-O	-5.07	1.13	1.23
1	B	37	LYS	CA-C	5.07	1.66	1.52
1	A	52	LEU	CG-CD2	5.07	1.70	1.51
1	A	39	ILE	CA-CB	-5.05	1.43	1.54
1	A	48	HIS	CA-C	-5.05	1.39	1.52
1	B	88	ILE	CG1-CD1	5.05	1.85	1.50
1	B	50	ASN	CA-C	-5.04	1.39	1.52
1	A	75	THR	CB-CG2	5.03	1.69	1.52
1	B	73	MSE	CG-SE	5.03	2.12	1.95

All (109) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	133	ARG	NE-CZ-NH1	-15.97	112.32	120.30
1	B	65	ASP	CB-CG-OD2	11.32	128.49	118.30
1	A	121	THR	CA-CB-CG2	-10.27	98.03	112.40
1	A	66	SER	CA-CB-OG	-9.71	84.99	111.20
1	B	119	ASP	CB-CG-OD1	9.71	127.03	118.30
1	A	52	LEU	C-N-CA	-9.12	103.15	122.30
1	B	138	LEU	CB-CG-CD2	8.82	125.99	111.00
1	A	22	ASP	N-CA-C	8.69	134.45	111.00
1	B	138	LEU	CB-CG-CD1	-8.63	96.32	111.00
1	A	30	LEU	CB-CG-CD1	8.42	125.31	111.00
1	B	136	LYS	CD-CE-NZ	7.93	129.94	111.70
1	A	68	SER	N-CA-C	-7.92	89.63	111.00
1	B	91	MSE	CA-CB-CG	7.79	126.55	113.30
1	B	133	ARG	NH1-CZ-NH2	7.72	127.89	119.40
1	B	139	GLY	CA-C-O	-7.67	106.79	120.60
1	B	2	SER	C-N-CA	-7.63	102.63	121.70
1	B	128	LEU	CB-CG-CD2	-7.58	98.11	111.00
1	B	16	PHE	CA-C-O	7.52	135.90	120.10
1	A	27	LYS	CD-CE-NZ	7.47	128.88	111.70
1	A	103	THR	CA-CB-CG2	-7.34	102.12	112.40
1	B	76	GLU	CA-C-O	7.30	135.44	120.10
1	B	123	LYS	CD-CE-NZ	-7.29	94.92	111.70
1	A	63	LEU	CB-CG-CD2	-7.27	98.65	111.00
1	A	24	VAL	CA-CB-CG1	7.14	121.61	110.90
1	A	110	GLY	N-CA-C	7.14	130.96	113.10
1	A	56	HIS	N-CA-CB	7.08	123.35	110.60
1	A	31	VAL	N-CA-C	7.07	130.10	111.00
1	A	17	LYS	CB-CA-C	7.05	124.50	110.40
1	A	15	MSE	CA-C-N	-6.99	101.83	117.20
1	A	100	ILE	CG1-CB-CG2	6.91	126.59	111.40
1	B	125	THR	OG1-CB-CG2	-6.75	94.47	110.00
1	B	86	MSE	CG-SE-CE	-6.73	84.10	98.90
1	A	41	GLU	CG-CD-OE1	6.66	131.61	118.30
1	B	50	ASN	CB-CA-C	-6.53	97.35	110.40
1	A	52	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	A	91	MSE	CA-CB-CG	6.48	124.32	113.30
1	A	128	LEU	CB-CG-CD2	-6.35	100.20	111.00
1	A	72	LEU	CB-CG-CD1	6.32	121.74	111.00
1	A	120	LEU	CB-CG-CD2	-6.31	100.27	111.00
1	B	28	VAL	CG1-CB-CG2	-6.24	100.91	110.90
1	A	86	MSE	CG-SE-CE	-6.22	85.21	98.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	23	ARG	CA-CB-CG	-6.14	99.90	113.40
1	A	128	LEU	CB-CG-CD1	6.13	121.42	111.00
1	A	91	MSE	CB-CA-C	6.13	122.66	110.40
1	B	92	SER	N-CA-CB	-6.05	101.42	110.50
1	B	67	ILE	CG1-CB-CG2	6.05	124.70	111.40
1	A	54	THR	OG1-CB-CG2	-6.04	96.11	110.00
1	A	26	GLU	OE1-CD-OE2	-6.02	116.07	123.30
1	B	108	LYS	C-N-CA	5.95	136.58	121.70
1	B	22	ASP	CA-C-O	5.94	132.57	120.10
1	A	17	LYS	CA-CB-CG	5.91	126.41	113.40
1	A	26	GLU	CB-CA-C	5.87	122.14	110.40
1	B	75	THR	OG1-CB-CG2	5.87	123.49	110.00
1	A	60	THR	OG1-CB-CG2	-5.85	96.54	110.00
1	A	25	LEU	CA-C-N	-5.76	104.52	117.20
1	A	80	PRO	C-N-CA	-5.75	110.22	122.30
1	B	120	LEU	CB-CG-CD1	5.75	120.78	111.00
1	B	109	GLN	CA-C-N	5.73	127.65	116.20
1	A	41	GLU	CB-CA-C	-5.70	98.99	110.40
1	A	22	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	40	CYS	CA-CB-SG	-5.65	103.84	114.00
1	B	1	MSE	N-CA-CB	5.65	120.76	110.60
1	B	128	LEU	CB-CG-CD1	-5.63	101.44	111.00
1	B	82	VAL	CG1-CB-CG2	-5.58	101.96	110.90
1	A	15	MSE	CA-C-O	5.58	131.81	120.10
1	A	22	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	85	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	B	52	LEU	CB-CG-CD1	5.51	120.37	111.00
1	B	49	THR	N-CA-C	5.51	125.88	111.00
1	B	116	ALA	N-CA-CB	-5.48	102.42	110.10
1	A	113	LEU	O-C-N	5.47	131.46	122.70
1	B	129	ILE	CG1-CB-CG2	-5.47	99.36	111.40
1	A	28	VAL	N-CA-C	-5.47	96.23	111.00
1	B	135	THR	OG1-CB-CG2	-5.45	97.46	110.00
1	B	75	THR	CA-CB-CG2	-5.44	104.79	112.40
1	B	33	ALA	N-CA-CB	5.42	117.69	110.10
1	A	36	GLU	CA-CB-CG	5.42	125.33	113.40
1	B	35	PRO	CA-C-O	-5.41	107.21	120.20
1	B	23	ARG	CG-CD-NE	5.35	123.03	111.80
1	B	65	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	B	85	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	A	63	LEU	CB-CG-CD1	5.27	119.96	111.00
1	A	41	GLU	OE1-CD-OE2	-5.27	116.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	THR	N-CA-C	-5.26	96.79	111.00
1	B	137	HIS	CB-CA-C	-5.25	99.89	110.40
1	A	30	LEU	CB-CA-C	5.23	120.13	110.20
1	A	26	GLU	CG-CD-OE1	5.21	128.73	118.30
1	A	115	PHE	CD1-CE1-CZ	5.21	126.36	120.10
1	A	25	LEU	CB-CG-CD2	5.20	119.85	111.00
1	A	52	LEU	O-C-N	-5.20	114.37	123.20
1	B	9	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	41	GLU	CG-CD-OE1	-5.19	107.92	118.30
1	B	135	THR	CA-CB-OG1	5.17	119.87	109.00
1	B	54	THR	OG1-CB-CG2	-5.17	98.11	110.00
1	A	42	MSE	CB-CA-C	5.17	120.73	110.40
1	A	135	THR	CA-CB-CG2	5.15	119.61	112.40
1	B	51	LYS	O-C-N	-5.13	114.49	122.70
1	B	38	LEU	CB-CG-CD2	-5.13	102.27	111.00
1	B	74	CYS	CA-CB-SG	-5.11	104.81	114.00
1	B	102	ILE	CG1-CB-CG2	-5.09	100.21	111.40
1	B	106	ILE	CA-CB-CG1	-5.08	101.35	111.00
1	A	55	LEU	CB-CG-CD1	-5.08	102.37	111.00
1	B	120	LEU	CA-CB-CG	-5.07	103.63	115.30
1	B	36	GLU	N-CA-C	5.07	124.68	111.00
1	B	41	GLU	OE1-CD-OE2	5.06	129.37	123.30
1	B	63	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	A	36	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	B	89	THR	CA-CB-CG2	-5.05	105.33	112.40
1	B	15	MSE	CG-SE-CE	-5.02	87.86	98.90

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 (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	912	0	963	181	0
1	B	1004	0	1053	137	0
2	A	24	0	0	2	0
2	B	19	0	0	0	0
All	All	1959	0	2016	303	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 77.

All (303) 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:CG	1:B:111:LYS:CD	1.75	1.65
1:A:24:VAL:CG1	1:A:24:VAL:CB	1.74	1.65
1:B:88:ILE:CB	1:B:88:ILE:CG2	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
1:B:52:LEU:CD1	1:B:52:LEU:CG	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:CE	1:B:13:LYS:CD	1.76	1.55
1:A:31:VAL:CA	1:A:31:VAL:CB	1.78	1.55
1:A:129:ILE:CA	1:A:129:ILE:CB	1.78	1.55
1:A:88:ILE:CG1	1:A:88:ILE:CD1	1.85	1.54
1:B:88:ILE:CG1	1:B:88:ILE:CD1	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:NZ	1:B:136:LYS:CE	1.72	1.49
1:A:100:ILE:CG2	1:A:100:ILE:CB	1.87	1.49
1:A:135:THR:CB	1:A:135:THR:CA	1.88	1.48
1:B:70:MSE:CG	1:B:70:MSE:SE	2.16	1.44
1:A:80:PRO:CA	1:A:80:PRO:N	1.69	1.39
1:A:16:PHE:O	1:A:18:VAL:CG2	1.78	1.32

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:25:LEU:HG	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:H	1:A:55:LEU:HD12	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
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:CD1	1:A:30:LEU:HG	2.04	0.85
1:B:102:ILE:CG1	1:B:102:ILE:CG2	2.55	0.84
1:A:87:ASN:ND2	1:B:133:ARG:NH2	2.25	0.84
1:A:100:ILE:HB	1:A:100:ILE:CG2	2.06	0.84
1:B:3:SER:O	1:B:7:ASN:HB2	1.76	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:A:30:LEU:C	1:A:31:VAL:HG12	2.01	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:21:PHE:HA	1:A:25:LEU:HD13	1.65	0.79
1:B:38:LEU:HD23	1:B:38:LEU:C	2.02	0.79
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:102:ILE:HD12	1:B:102:ILE:C	2.05	0.75
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:13:LYS:C	1:A:15:MSE:HE2	2.08	0.74
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:HG13	1:B:100:ILE:O	1.88	0.73
1:A:67:ILE:O	1:A:67:ILE:HG22	1.89	0.72
1:B:75:THR:CG2	1:B:75:THR:CA	2.65	0.72
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:CG1	1:A:31:VAL:CA	2.66	0.70
1:B:88:ILE:CG2	1:B:88:ILE:CA	2.66	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:B:36:GLU:O	1:B:106:ILE:HD12	1.93	0.67
1:A:55:LEU:CD1	1:A:55:LEU:O	2.36	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LEU:CD1	1:A:55:LEU:N	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: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:80:PRO:O	1:B:136:LYS:HE2	1.97	0.64
1:B:51:LYS:HD3	1:B:51:LYS:H	1.63	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
1:A:44:VAL:HG12	1:A:49:THR:CG2	2.28	0.63
1:A:50:ASN:O	1:A:51:LYS:C	2.37	0.63
1:A:122:ASN:ND2	1:A:124:THR:H	1.97	0.63
1:A:84:VAL:HG21	1:A:137:HIS:HB2	1.81	0.62
1:A:20:GLY:O	1:A:25:LEU:HD12	1.99	0.62
1:B:87:ASN:CB	1:B:87:ASN:C	2.64	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:30:LEU:HD21	1:A:43:LYS:HZ3	1.63	0.61
1:A:111:LYS:HG3	1:A:111:LYS:H	1.65	0.61
1:B:71:ALA:HB1	1:B:106:ILE:HD11	1.82	0.61
1:A:135:THR:CB	1:A:135:THR:C	2.67	0.61
1:B:101:VAL:HG13	1:B:121:THR:OG1	2.01	0.60
1:A:100:ILE:HG12	1:A:100:ILE:O	1.88	0.59
1:B:87:ASN:CA	1:B:87:ASN:CG	2.64	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:A:109:GLN:O	1:A:110:GLY:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:MSE:HA	1:B:70:MSE:SE	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:70:MSE:CE	1:B:73:MSE:CE	2.82	0.58
1:B:6:GLN:O	1:B:9:ARG:HB3	2.04	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:HB	1:A:31:VAL:CA	2.18	0.56
1:B:16:PHE:CD2	1:B:16:PHE:N	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:88:ILE:CG2	1:B:88:ILE:CG1	2.79	0.56
1:B:8:LEU:HB3	1:B:30:LEU:CD2	2.35	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
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:H	1:B:111:LYS:CD	2.20	0.54
1:A:111:LYS:HG3	2:A:145:HOH:O	2.07	0.54
1:A:30:LEU:CD2	1:A:43:LYS:HZ1	2.20	0.54
1:B:130:ALA:O	1:B:131:GLN:C	2.43	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:A:129:ILE:C	1:A:129:ILE:CB	2.72	0.54
1:B:37:LYS:HA	1:B:104:ALA:O	2.09	0.53
1:A:43:LYS:H	1:A:43:LYS:HD2	1.71	0.53
1:A:59:LEU:HD12	1:A:63:LEU:HD11	1.91	0.52
1:A:43:LYS:HG3	1:A:99:GLU:OE1	2.09	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:121:THR:HG22	1:A:128:LEU:HA	1.91	0.52
1:A:30:LEU:CD1	1:A:30:LEU:CD2	2.80	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ALA:HB1	1:B:35:PRO:HD2	1.93	0.51
1:A:72:LEU:HD13	1:A:106:ILE:HD12	1.91	0.51
1:A:38:LEU:HD13	1:A:71:ALA:HA	1.92	0.51
1:B:45:GLU:HG2	1:B:48:HIS:CE1	2.45	0.51
1:B:38:LEU:CD2	1:B:38:LEU:C	2.78	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:CE	1:B:111:LYS:CG	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:CB	1:B:70:MSE:SE	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: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:A:112:THR:HG23	1:A:113:LEU:HG	1.93	0.49
1:A:57:GLY:HA2	1:A:60:THR:CB	2.39	0.49
1:B:13:LYS:CE	1:B:13:LYS:CG	2.82	0.49
1:B:10:GLU:OE2	1:B:13:LYS:HE2	2.13	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:122:ASN:HB3	1:A:125:THR:HB	1.93	0.49
1:A:38:LEU:CD2	1:A:67:ILE:HG23	2.43	0.49
1:B:31:VAL:HG11	1:B:41:GLU:CD	2.32	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:120:LEU:CD2	1:A:120:LEU:C	2.81	0.48
1:A:129:ILE:CG2	1:A:129:ILE:CA	2.85	0.48
1:A:133:ARG:NH1	1:B:133:ARG:HB2	2.27	0.48
1:A:74:CYS:O	1:A:75:THR:C	2.50	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:A:13:LYS:C	1:A:15:MSE:CE	2.73	0.47
1:B:28:VAL:O	1:B:28:VAL:HG13	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASN:C	1:B:88:ILE:HG13	2.34	0.47
1:A:111:LYS:CG	1:A:111:LYS:H	2.26	0.46
1:A:24:VAL:N	1:A:24:VAL:HA	2.06	0.46
1:A:17:LYS:O	1:A:17:LYS:HE2	2.16	0.46
1:A:69:THR:HB	1:A:136:LYS:NZ	2.30	0.46
1:B:100:ILE:CG1	1:B:100:ILE:O	2.61	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:CG	1:A:25:LEU:O	2.34	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:15:MSE:C	1:B:16:PHE:HD2	2.19	0.46
1:B:43:LYS:HZ3	1:B:97:GLY:HA2	1.81	0.46
1:A:108:LYS:HB3	1:A:115:PHE:HD2	1.81	0.45
1:A:19:PRO:O	1:A:27:LYS:HD2	2.16	0.45
1:A:30:LEU:HD21	1:A:43:LYS:HZ1	1.76	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
1:B:28:VAL:O	1:B:28:VAL:CG1	2.64	0.45
1:A:72:LEU:CD1	1:A:106:ILE:HD12	2.45	0.45
1:B:128:LEU:HD13	1:B:128:LEU:HA	1.74	0.45
1:B:51:LYS:HD3	1:B:51:LYS:N	2.31	0.45
1:A:129:ILE:HB	1:A:129:ILE:CA	2.21	0.45
1:A:122:ASN:HB2	1:A:129:ILE:HD11	1.98	0.45
1:B:81:GLY:C	1:B:82:VAL:CG1	2.85	0.45
1:B:75:THR:CG2	1:B:75:THR:C	2.85	0.45
1:B:125:THR:HB	1:B:127:LYS:H	1.80	0.45
1:A:125:THR:HG22	1:A:127:LYS:H	1.82	0.45
1:A:111:LYS:NZ	1:A:112:THR:HG22	2.32	0.44
1:B:16:PHE:HD2	1:B:16:PHE:N	2.14	0.44
1:A:120:LEU:HD23	1:A:120:LEU:C	2.37	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:65:ASP:OD1	1:B:65:ASP:C	2.58	0.42
1:A:122:ASN:ND2	1:A:124:THR:N	2.66	0.42
1:A:122:ASN:HD22	1:A:122:ASN:C	2.23	0.42
1:A:22:ASP:N	1:A:25:LEU:HD13	2.34	0.42
1:B:108:LYS:HB3	1:B:115:PHE:CD1	2.43	0.42
1:A:37:LYS:O	1:A:38:LEU:HB2	2.20	0.42
1:A:39:ILE:O	1:A:40:CYS:SG	2.77	0.42
1:B:111:LYS:H	1:B:111:LYS:HD2	1.83	0.41
1:A:30:LEU:C	1:A:31:VAL:CG1	2.75	0.41
1:A:49:THR:HG21	1:A:96:ILE:HB	2.02	0.41
1:B:44:VAL:HG13	1:B:95:LYS:O	2.19	0.41
1:B:12:MSE:CG	1:B:70:MSE:HE2	2.50	0.41
1:B:30:LEU:C	1:B:30:LEU:HD12	2.41	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:10:GLU:O	1:B:11:VAL:C	2.57	0.41
1:B:38:LEU:HD23	1:B:38:LEU:O	2.20	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:134:HIS:CD2	1:B:136:LYS:HG3	2.56	0.41
1:B:30:LEU:HD12	1:B:31:VAL:N	2.35	0.41
1:A:56:HIS:H	1:A:56:HIS:CD2	2.39	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:60:THR:O	1:B:61:ALA:C	2.59	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

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	116/140 (83%)	82 (71%)	20 (17%)	14 (12%)	0	0
1	B	127/140 (91%)	111 (87%)	11 (9%)	5 (4%)	3	6
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%)	84 (74%)	30 (26%)	0 1
All	All	217/220 (99%)	157 (72%)	60 (28%)	0 1

All (60) 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	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	91	MSE
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	3	SER
1	B	7	ASN

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Mol	Chain	Res	Type
1	B	8	LEU
1	B	13	LYS
1	B	15	MSE
1	B	23	ARG
1	B	27	LYS
1	B	29	THR
1	B	38	LEU
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	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	109	GLN
1	B	111	LYS
1	B	121	THR
1	B	135	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	56	HIS
1	A	87	ASN
1	A	109	GLN
1	A	122	ASN
1	A	134	HIS
1	B	6	GLN
1	B	50	ASN
1	B	56	HIS
1	B	109	GLN
1	B	134	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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