



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 PM UTC

PDB ID : 5BMU / pdb_00005bmu
Title : The crystal structure of the GST-like domains complex of AIMP3-EPRS mutant C92SC105SC123S
Authors : Cho, H.J.; Kang, B.S.
Deposited on : 2015-05-23
Resolution : 2.60 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
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

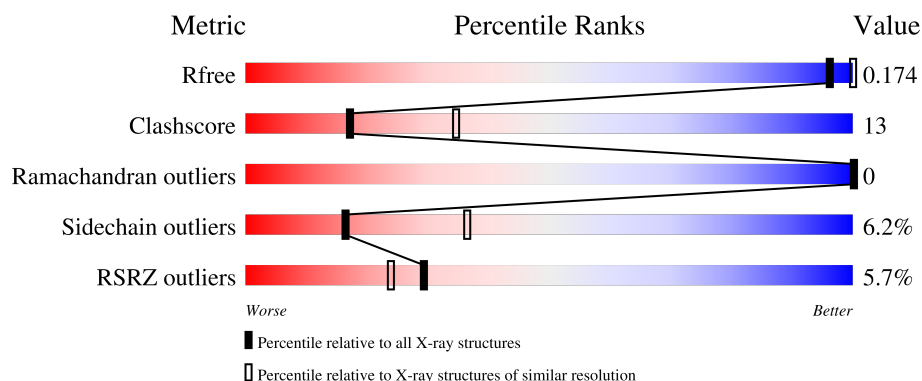
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	171	3% 59% 32% 5% .
1	C	171	% 70% 23% 6% .
1	E	171	% 71% 23%
1	G	171	4% 77% 20% . ..
2	B	175	7% 62% 25% 8% 5%

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Mol	Chain	Length	Quality of chain
2	D	175	7% 60% 24% 8% 6%
2	F	175	10% 63% 25% 5% 5%
2	H	175	10% 69% 23% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10463 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 Eukaryotic translation elongation factor 1 epsilon-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1328	852	227	247	2			
1	C	168	Total	C	N	O	S	0	0	0
			1348	863	232	251	2			
1	E	168	Total	C	N	O	S	0	0	0
			1348	863	232	251	2			
1	G	168	Total	C	N	O	S	0	0	0
			1344	860	231	251	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O43324
A	0	HIS	-	expression tag	UNP O43324
C	-1	GLY	-	expression tag	UNP O43324
C	0	HIS	-	expression tag	UNP O43324
E	-1	GLY	-	expression tag	UNP O43324
E	0	HIS	-	expression tag	UNP O43324
G	-1	GLY	-	expression tag	UNP O43324
G	0	HIS	-	expression tag	UNP O43324

- Molecule 2 is a protein called Glutamate-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1278	812	214	251	1			
2	D	164	Total	C	N	O	S	0	0	0
			1266	804	212	249	1			
2	F	166	Total	C	N	O	S	0	0	0
			1284	814	216	253	1			
2	H	165	Total	C	N	O	S	0	0	0
			1261	798	212	250	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	SER	CYS	engineered mutation	UNP P07814
B	105	SER	CYS	engineered mutation	UNP P07814
B	123	SER	CYS	engineered mutation	UNP P07814
D	92	SER	CYS	engineered mutation	UNP P07814
D	105	SER	CYS	engineered mutation	UNP P07814
D	123	SER	CYS	engineered mutation	UNP P07814
F	92	SER	CYS	engineered mutation	UNP P07814
F	105	SER	CYS	engineered mutation	UNP P07814
F	123	SER	CYS	engineered mutation	UNP P07814
H	92	SER	CYS	engineered mutation	UNP P07814
H	105	SER	CYS	engineered mutation	UNP P07814
H	123	SER	CYS	engineered mutation	UNP P07814

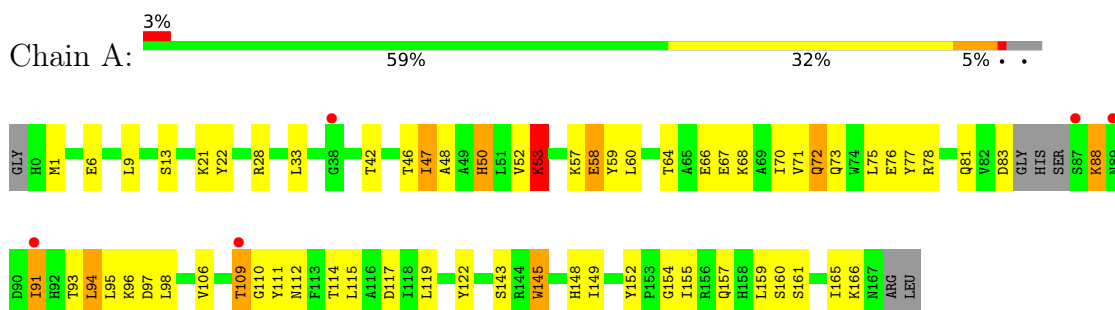
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

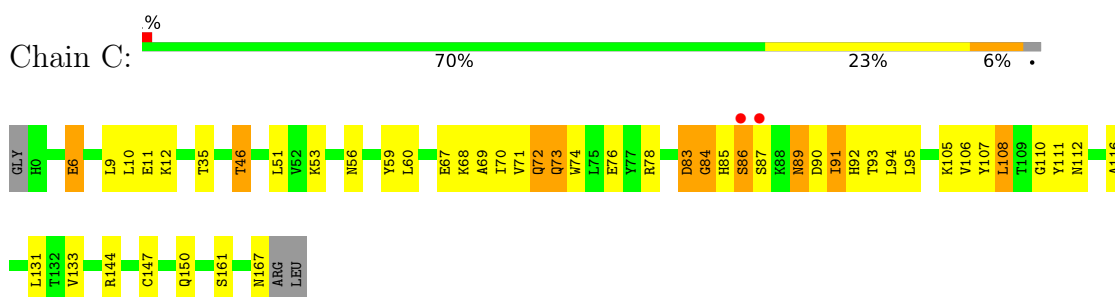
3 Residue-property plots

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.

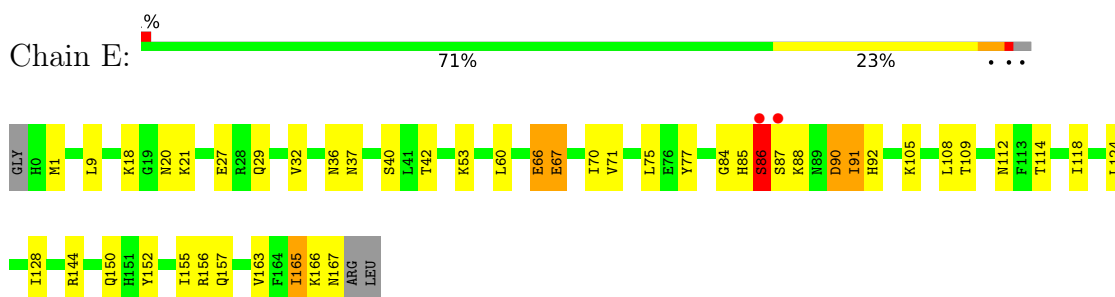
- Molecule 1: Eukaryotic translation elongation factor 1 epsilon-1



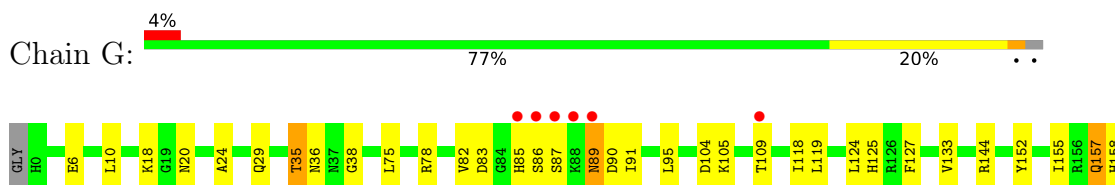
- Molecule 1: Eukaryotic translation elongation factor 1 epsilon-1

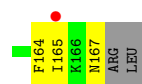


- Molecule 1: Eukaryotic translation elongation factor 1 epsilon-1

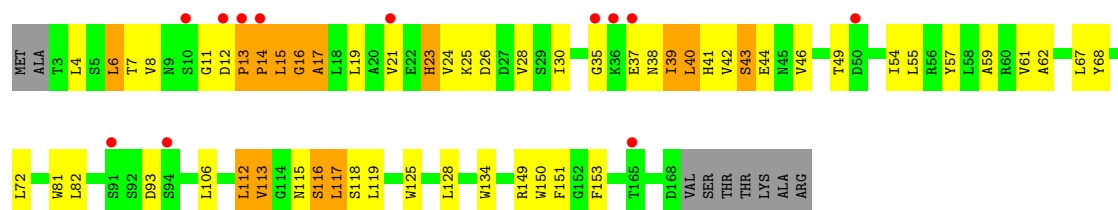


- Molecule 1: Eukaryotic translation elongation factor 1 epsilon-1

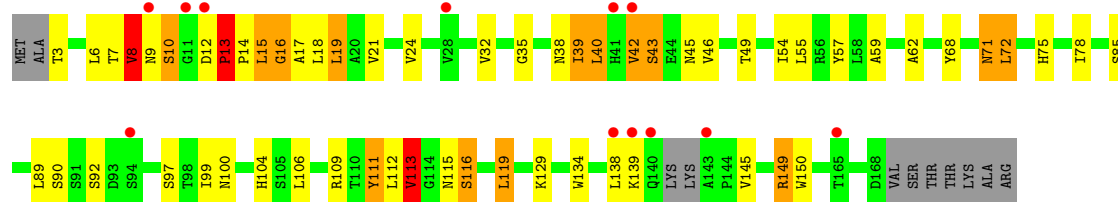




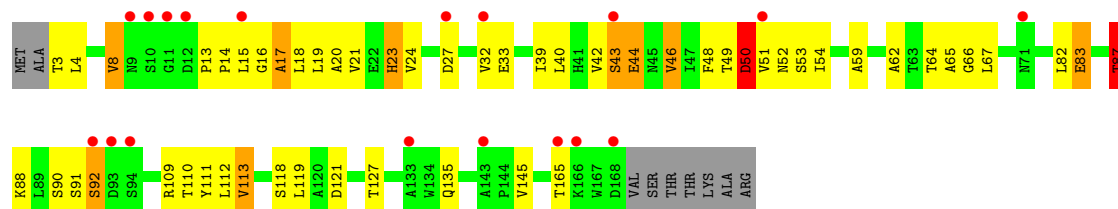
• Molecule 2: Glutamate-tRNA ligase



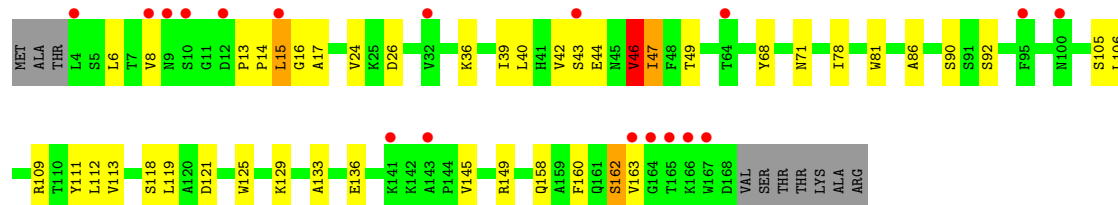
• Molecule 2: Glutamate-tRNA ligase



• Molecule 2: Glutamate-tRNA ligase



• Molecule 2: Glutamate-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	92.06Å 92.06Å 185.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.93 – 2.60 48.93 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.93-2.60) 99.7 (48.93-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.26 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.138 , 0.170 0.146 , 0.174	Depositor DCC
R_{free} test set	1980 reflections (3.67%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l 0.227 for h,-h-k,-l 0.041 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10463	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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 [i](#)

5.1 Standard geometry [i](#)

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	1.49	20/1354 (1.5%)	1.26	5/1833 (0.3%)
1	C	1.44	23/1376 (1.7%)	1.25	10/1864 (0.5%)
1	E	0.89	1/1376 (0.1%)	1.13	4/1864 (0.2%)
1	G	0.95	1/1372 (0.1%)	1.17	7/1860 (0.4%)
2	B	1.16	7/1305 (0.5%)	1.31	15/1780 (0.8%)
2	D	1.27	10/1291 (0.8%)	1.25	16/1759 (0.9%)
2	F	1.27	12/1311 (0.9%)	1.23	12/1788 (0.7%)
2	H	0.95	6/1286 (0.5%)	1.12	10/1754 (0.6%)
All	All	1.20	80/10671 (0.7%)	1.22	79/14502 (0.5%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	C-N	15.72	1.55	1.33
1	A	110	GLY	C-N	-10.10	1.19	1.33
2	B	13	PRO	CA-C	-9.63	1.46	1.51
2	F	66	GLY	C-O	-8.62	1.18	1.24
1	C	68	LYS	C-O	-8.33	1.14	1.24
2	H	13	PRO	CA-C	-8.28	1.46	1.52
1	A	57	LYS	C-O	-8.20	1.14	1.23
1	A	50	HIS	C-O	-8.09	1.14	1.24
1	C	67	GLU	C-O	-7.95	1.14	1.24
2	D	109	ARG	C-O	-7.57	1.14	1.23
1	C	106	VAL	C-O	-7.36	1.17	1.24
1	C	94	LEU	C-O	-7.20	1.15	1.24
1	A	59	TYR	C-N	7.04	1.43	1.34
1	A	53	LYS	C-O	-6.89	1.15	1.24
1	C	70	ILE	C-O	-6.78	1.16	1.24
2	F	83	GLU	C-O	-6.63	1.16	1.24
2	F	15	LEU	CA-C	-6.55	1.44	1.52
1	C	93	THR	C-O	-6.51	1.16	1.24
1	C	69	ALA	C-O	-6.47	1.16	1.24
1	A	93	THR	C-O	-6.39	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	LEU	C-O	-6.39	1.16	1.24
1	C	73	GLN	C-O	-6.37	1.16	1.24
2	D	71	ASN	C-O	-6.34	1.15	1.23
1	C	12	LYS	C-O	-6.28	1.16	1.24
2	D	71	ASN	CA-C	-6.20	1.45	1.52
2	H	15	LEU	CA-C	-6.13	1.44	1.53
1	A	111	TYR	C-O	-6.12	1.15	1.24
1	C	10	LEU	C-O	-6.04	1.16	1.24
2	D	13	PRO	CA-C	-5.99	1.46	1.52
1	C	107	TYR	C-O	-5.86	1.16	1.23
2	D	150	TRP	C-O	-5.85	1.17	1.24
2	F	87	THR	C-O	-5.85	1.16	1.24
2	F	53	SER	C-O	-5.83	1.17	1.24
1	E	108	LEU	C-O	-5.82	1.17	1.24
2	B	12	ASP	C-N	5.80	1.38	1.33
1	C	9	LEU	C-O	-5.75	1.17	1.24
1	A	94	LEU	C-O	-5.74	1.17	1.24
2	B	117	LEU	C-O	-5.67	1.17	1.23
1	C	95	LEU	C-O	-5.67	1.17	1.24
1	C	111	TYR	C-O	-5.66	1.16	1.24
1	A	52	VAL	C-O	-5.66	1.17	1.24
2	H	46	VAL	C-O	-5.65	1.18	1.24
1	A	97	ASP	C-O	-5.62	1.17	1.24
1	A	91	ILE	C-O	-5.61	1.18	1.24
2	F	44	GLU	CA-C	-5.61	1.46	1.52
1	A	47	ILE	C-O	-5.60	1.17	1.24
1	C	108	LEU	C-O	-5.59	1.17	1.24
1	C	91	ILE	C-O	-5.52	1.18	1.24
2	D	111	TYR	CA-C	-5.52	1.45	1.52
1	C	72	GLN	C-O	-5.50	1.17	1.24
1	A	98	LEU	C-O	-5.49	1.17	1.24
1	A	148	HIS	C-O	-5.47	1.17	1.24
2	D	111	TYR	C-O	-5.44	1.17	1.23
1	C	74	TRP	C-O	-5.43	1.17	1.24
2	F	48	PHE	C-O	-5.41	1.17	1.24
2	B	115	ASN	C-O	-5.40	1.17	1.23
2	D	19	LEU	C-O	-5.40	1.17	1.24
2	B	17	ALA	C-O	-5.39	1.17	1.24
1	C	6	GLU	C-O	-5.35	1.17	1.24
1	C	112	ASN	C-O	-5.34	1.17	1.23
1	C	71	VAL	C-O	-5.34	1.18	1.24
2	F	113	VAL	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	44	GLU	CA-C	-5.30	1.49	1.52
1	A	145	TRP	C-O	-5.29	1.18	1.24
2	D	115	ASN	C-O	-5.29	1.17	1.23
2	F	17	ALA	C-O	-5.27	1.18	1.24
1	C	84	GLY	CA-C	-5.27	1.46	1.52
1	C	110	GLY	C-O	-5.21	1.16	1.23
2	F	65	ALA	C-O	-5.21	1.18	1.23
1	A	143	SER	N-CA	-5.19	1.40	1.46
2	H	47	ILE	C-O	-5.19	1.18	1.24
1	A	58	GLU	C-O	-5.16	1.17	1.24
1	A	95	LEU	C-O	-5.15	1.18	1.24
2	F	52	ASN	C-O	-5.14	1.17	1.24
1	G	164	PHE	C-O	-5.13	1.18	1.24
2	F	20	ALA	C-O	-5.13	1.18	1.24
1	A	48	ALA	C-O	-5.12	1.18	1.24
2	D	72	LEU	C-O	-5.03	1.17	1.24
2	B	67	LEU	C-O	-5.02	1.17	1.24
2	H	16	GLY	C-O	-5.01	1.19	1.23

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	51	VAL	N-CA-C	11.72	121.54	110.53
1	A	109	THR	N-CA-C	-11.59	92.46	110.42
2	B	13	PRO	O-C-N	11.35	126.53	121.31
1	C	89	ASN	N-CA-C	11.24	123.28	111.14
2	F	92	SER	N-CA-C	10.18	122.37	111.28
2	F	67	LEU	N-CA-C	10.13	124.72	111.75
1	G	109	THR	N-CA-C	-10.06	96.97	110.55
2	D	145	VAL	N-CA-C	9.71	120.52	110.62
2	H	13	PRO	O-C-N	9.40	125.57	121.15
2	B	113	VAL	N-CA-C	8.40	119.21	110.72
1	G	90	ASP	N-CA-C	7.94	121.42	107.61
2	B	112	LEU	CA-C-N	7.79	131.48	120.42
2	B	112	LEU	C-N-CA	7.79	131.48	120.42
2	B	15	LEU	N-CA-C	-7.70	99.64	110.50
2	F	50	ASP	N-CA-C	-7.69	100.35	110.43
2	H	15	LEU	N-CA-C	-7.59	101.08	110.41
1	C	92	HIS	N-CA-C	7.39	119.34	111.28
2	D	113	VAL	CB-CA-C	-7.11	99.63	111.29
1	A	110	GLY	O-C-N	-6.84	113.81	122.70
2	F	43	SER	N-CA-C	6.74	118.62	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	12	ASP	CA-C-N	-6.70	114.77	119.66
2	B	12	ASP	C-N-CA	-6.70	114.77	119.66
2	B	113	VAL	CB-CA-C	-6.69	102.99	112.22
1	G	36	ASN	N-CA-C	6.54	118.07	111.07
2	F	44	GLU	N-CA-C	-6.54	99.52	109.85
2	D	8	VAL	CB-CA-C	-6.51	100.65	110.55
2	B	14	PRO	N-CA-C	-6.40	99.29	112.47
1	A	112	ASN	N-CA-C	6.39	120.12	109.95
2	F	145	VAL	N-CA-C	6.38	117.17	110.72
2	H	68	TYR	N-CA-C	6.37	120.36	112.59
2	F	13	PRO	N-CA-C	6.36	118.45	110.70
1	G	165	ILE	N-CA-C	6.33	118.56	109.51
2	D	15	LEU	N-CA-C	-6.27	102.09	110.55
2	D	45	ASN	N-CA-C	6.23	118.50	110.65
1	G	119	LEU	N-CA-C	6.22	118.07	111.28
1	C	83	ASP	CA-C-N	6.05	127.03	120.44
1	C	83	ASP	C-N-CA	6.05	127.03	120.44
2	F	65	ALA	N-CA-C	-6.02	100.40	109.79
1	C	86	SER	N-CA-C	-6.00	103.64	111.74
1	E	109	THR	N-CA-C	6.00	120.60	113.16
2	F	113	VAL	N-CA-CB	-5.97	101.39	111.23
2	H	44	GLU	N-CA-C	-5.95	101.97	111.02
2	B	35	GLY	N-CA-C	-5.95	105.97	112.04
1	A	93	THR	CB-CA-C	5.94	120.66	110.79
1	C	131	LEU	N-CA-C	5.94	118.67	110.35
2	D	90	SER	O-C-N	5.91	128.16	122.07
1	E	91	ILE	N-CA-C	-5.85	104.44	113.16
2	B	116	SER	N-CA-C	5.83	117.83	109.14
2	D	111	TYR	N-CA-C	-5.80	100.48	109.24
1	A	166	LYS	N-CA-C	5.76	117.64	111.36
2	H	145	VAL	N-CA-C	5.76	116.54	110.72
2	B	13	PRO	CA-C-N	-5.75	112.65	119.84
2	B	13	PRO	C-N-CA	-5.75	112.65	119.84
1	G	85	HIS	N-CA-C	5.64	117.43	111.28
1	G	89	ASN	N-CA-C	5.54	117.39	111.36
2	H	46	VAL	N-CA-C	-5.47	100.32	108.46
2	D	10	SER	N-CA-C	-5.44	105.45	111.71
2	D	42	VAL	N-CA-C	5.41	120.58	109.34
2	D	8	VAL	N-CA-C	5.37	117.81	108.95
2	H	47	ILE	N-CA-C	5.36	116.38	108.45
2	B	16	GLY	N-CA-C	-5.34	107.31	114.25
2	D	12	ASP	CA-C-N	-5.32	114.90	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	ASP	C-N-CA	-5.32	114.90	120.38
1	C	111	TYR	N-CA-C	5.26	119.01	112.59
2	B	11	GLY	N-CA-C	5.25	119.48	112.77
2	F	110	THR	N-CA-C	-5.22	105.20	112.45
2	H	92	SER	N-CA-C	5.21	117.38	111.02
1	E	118	ILE	CB-CA-C	-5.21	105.22	111.88
2	D	92	SER	N-CA-C	5.19	119.61	113.12
1	C	86	SER	CA-C-N	5.18	131.43	121.54
1	C	86	SER	C-N-CA	5.18	131.43	121.54
2	H	112	LEU	CA-C-N	5.17	128.01	121.85
2	H	112	LEU	C-N-CA	5.17	128.01	121.85
2	F	64	THR	N-CA-C	5.11	119.14	113.01
1	C	89	ASN	CB-CA-C	-5.10	102.84	110.90
2	D	16	GLY	N-CA-C	-5.10	101.74	115.86
1	E	86	SER	N-CA-C	-5.09	104.62	111.54
2	D	10	SER	CA-C-N	5.04	125.57	119.98
2	D	10	SER	C-N-CA	5.04	125.57	119.98

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1328	0	1339	50	0
1	C	1348	0	1355	22	0
1	E	1348	0	1355	26	0
1	G	1344	0	1344	21	0
2	B	1278	0	1235	41	0
2	D	1266	0	1231	48	0
2	F	1284	0	1243	42	0
2	H	1261	0	1213	26	0
3	A	4	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	10463	0	10315	261	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 13.

All (261) 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)
2:D:8:VAL:HG11	2:D:14:PRO:HD3	1.15	1.07
1:A:46:THR:HG23	1:C:76:GLU:OE2	1.53	1.05
2:D:8:VAL:HG11	2:D:14:PRO:CD	1.87	1.04
1:G:87:SER:O	1:G:91:ILE:HG23	1.66	0.94
2:D:113:VAL:HG21	2:D:116:SER:O	1.69	0.93
1:A:67:GLU:OE2	1:A:109:THR:HG21	1.72	0.89
1:A:67:GLU:CG	1:A:109:THR:CG2	2.50	0.89
2:F:83:GLU:O	2:F:87:THR:HB	1.75	0.87
2:F:8:VAL:CG2	2:F:14:PRO:HD3	2.05	0.86
2:D:8:VAL:CG1	2:D:14:PRO:HD3	2.04	0.86
1:A:67:GLU:HG3	1:A:109:THR:CG2	2.06	0.85
2:F:8:VAL:HG21	2:F:14:PRO:HD3	1.59	0.82
2:D:78:ILE:HD11	2:D:119:LEU:HB2	1.60	0.82
1:A:67:GLU:CG	1:A:109:THR:HG21	2.09	0.81
1:A:67:GLU:CD	1:A:109:THR:HG21	2.05	0.81
1:A:76:GLU:OE1	1:C:46:THR:HG23	1.79	0.81
1:A:67:GLU:HG3	1:A:109:THR:HG23	1.62	0.81
2:F:42:VAL:HG12	2:F:46:VAL:O	1.79	0.81
2:H:43:SER:HB3	2:H:46:VAL:HG23	1.64	0.79
2:D:10:SER:O	2:D:13:PRO:HD3	1.84	0.78
2:F:8:VAL:HG21	2:F:14:PRO:CD	2.14	0.78
2:D:16:GLY:HA2	2:D:19:LEU:HD12	1.68	0.76
2:B:16:GLY:HA2	2:B:19:LEU:HD12	1.66	0.76
1:A:77:TYR:OH	1:A:94:LEU:HD22	1.86	0.75
1:G:35:THR:HG22	1:G:38:GLY:O	1.87	0.75
2:B:8:VAL:HG13	2:B:14:PRO:HD3	1.68	0.74
1:A:67:GLU:CG	1:A:109:THR:HG23	2.17	0.74
2:D:113:VAL:CG2	2:D:116:SER:O	2.37	0.72
2:B:113:VAL:HG22	2:B:118:SER:OG	1.90	0.72
2:D:8:VAL:HG12	2:D:38:ASN:OD1	1.88	0.72
2:D:8:VAL:CG1	2:D:38:ASN:OD1	2.37	0.72
2:B:4:LEU:HD13	2:B:40:LEU:HD11	1.72	0.71
2:D:78:ILE:HD11	2:D:119:LEU:CB	2.20	0.71
2:H:43:SER:HB3	2:H:46:VAL:CG2	2.20	0.70
2:F:87:THR:HG22	2:F:88:LYS:N	2.07	0.70
2:B:113:VAL:HG21	2:B:116:SER:O	1.91	0.70
2:D:42:VAL:HG11	2:D:57:TYR:CE2	2.27	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:TYR:HB3	2:D:113:VAL:HG23	1.73	0.70
1:G:86:SER:HA	1:G:89:ASN:HB3	1.73	0.70
1:A:13:SER:OG	1:A:122:TYR:OH	2.09	0.69
2:D:8:VAL:HG11	2:D:14:PRO:CG	2.21	0.69
2:D:15:LEU:HD23	2:D:18:LEU:HD12	1.74	0.69
2:D:106:LEU:O	2:D:149:ARG:NH2	2.25	0.69
1:A:53:LYS:HD3	1:A:58:GLU:HG3	1.75	0.68
2:D:16:GLY:CA	2:D:19:LEU:HD12	2.24	0.66
1:C:6:GLU:OE2	1:C:78:ARG:NH2	2.29	0.66
1:C:84:GLY:O	1:C:87:SER:HB2	1.96	0.66
1:A:73:GLN:HA	1:C:46:THR:HG21	1.77	0.66
2:F:42:VAL:HG22	2:F:43:SER:H	1.61	0.65
2:B:14:PRO:HG2	2:B:17:ALA:HB3	1.77	0.65
2:H:39:ILE:HG23	2:H:47:ILE:HG23	1.79	0.65
2:F:19:LEU:O	2:F:23:HIS:HB2	1.97	0.65
2:F:42:VAL:CG1	2:F:46:VAL:O	2.45	0.64
2:F:91:SER:OG	2:F:92:SER:N	2.22	0.64
2:F:8:VAL:HG23	2:F:14:PRO:HD3	1.78	0.64
2:H:15:LEU:CD2	2:H:129:LYS:HD2	2.27	0.64
1:G:118:ILE:HG12	1:G:155:ILE:HD12	1.78	0.64
1:A:71:VAL:O	1:A:75:LEU:HG	1.98	0.64
2:D:24:VAL:HG21	2:D:62:ALA:CB	2.28	0.63
2:D:14:PRO:O	2:D:17:ALA:HB3	1.98	0.63
2:B:39:ILE:HG22	2:B:49:THR:HA	1.80	0.62
2:D:8:VAL:HG12	2:D:9:ASN:N	2.15	0.61
1:E:71:VAL:O	1:E:75:LEU:HG	2.01	0.61
1:A:68:LYS:O	1:A:72:GLN:HG2	2.01	0.61
2:D:8:VAL:HG11	2:D:14:PRO:HG3	1.82	0.60
1:A:67:GLU:OE2	1:A:109:THR:CG2	2.47	0.60
2:F:24:VAL:HG11	2:F:62:ALA:CB	2.30	0.60
1:E:124:LEU:O	1:E:128:ILE:HG12	2.02	0.60
2:F:87:THR:O	2:F:90:SER:HB3	2.02	0.60
1:E:88:LYS:HA	1:E:91:ILE:HD11	1.84	0.59
2:F:109:ARG:HD3	2:F:112:LEU:HA	1.84	0.59
1:G:152:TYR:HB3	1:G:155:ILE:HG13	1.85	0.59
2:F:39:ILE:HG22	2:F:49:THR:HG22	1.84	0.58
2:B:23:HIS:CE1	2:B:117:LEU:HD23	2.38	0.58
2:F:113:VAL:HG22	2:F:113:VAL:O	2.02	0.58
2:H:15:LEU:HD22	2:H:129:LYS:CD	2.34	0.57
2:F:40:LEU:HD22	2:F:54:ILE:HG23	1.86	0.57
1:C:11:GLU:HG3	1:C:51:LEU:HD13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:39:ILE:HG13	2:H:49:THR:HG22	1.87	0.56
2:H:24:VAL:HG12	2:H:24:VAL:O	2.05	0.56
2:B:8:VAL:HG13	2:B:14:PRO:CD	2.36	0.56
1:G:82:VAL:O	1:G:87:SER:HB3	2.05	0.56
2:D:72:LEU:HA	2:D:75:HIS:CD2	2.41	0.56
2:F:24:VAL:HG11	2:F:62:ALA:HB2	1.87	0.56
2:H:160:PHE:O	2:H:163:VAL:HG12	2.05	0.56
1:E:150:GLN:O	1:E:156:ARG:HB2	2.06	0.55
2:D:8:VAL:HG12	2:D:9:ASN:H	1.69	0.55
1:A:9:LEU:HD21	1:A:159:LEU:HD11	1.88	0.55
2:D:15:LEU:C	2:D:17:ALA:H	2.15	0.55
1:E:84:GLY:O	1:E:87:SER:HB2	2.06	0.55
1:A:106:VAL:HG21	2:B:153:PHE:CG	2.42	0.54
2:F:14:PRO:HB2	2:F:17:ALA:HB3	1.89	0.54
2:D:16:GLY:N	2:D:19:LEU:HD12	2.22	0.54
2:F:59:ALA:HB2	2:F:119:LEU:HD11	1.90	0.54
1:A:53:LYS:HD3	1:A:58:GLU:CG	2.36	0.54
1:G:24:ALA:HB1	1:G:29:GLN:HG2	1.90	0.54
2:H:14:PRO:HG2	2:H:17:ALA:HB3	1.90	0.54
1:E:88:LYS:O	1:E:88:LYS:HG2	2.07	0.54
2:F:87:THR:CG2	2:F:88:LYS:N	2.69	0.54
1:A:106:VAL:HG21	2:B:153:PHE:CD1	2.43	0.53
2:F:87:THR:HG22	2:F:88:LYS:HG3	1.90	0.53
2:D:43:SER:O	2:D:46:VAL:HG22	2.08	0.53
1:G:35:THR:HG22	1:G:38:GLY:C	2.34	0.53
2:H:6:LEU:HD12	2:H:40:LEU:HD13	1.91	0.53
2:D:55:LEU:C	2:D:119:LEU:HD21	2.34	0.53
2:F:113:VAL:HG21	2:F:118:SER:OG	2.10	0.52
1:A:78:ARG:HH12	1:A:83:ASP:CG	2.16	0.52
2:B:42:VAL:HG23	2:B:46:VAL:HG13	1.91	0.52
2:F:42:VAL:HG22	2:F:43:SER:N	2.25	0.52
1:A:67:GLU:HG2	1:A:109:THR:CG2	2.36	0.52
2:B:81:TRP:CZ2	2:B:112:LEU:HD22	2.44	0.52
2:D:43:SER:H	2:D:46:VAL:CG2	2.23	0.52
1:A:72:GLN:HE22	1:C:72:GLN:NE2	2.08	0.51
2:B:37:GLU:HG3	2:B:39:ILE:HD13	1.90	0.51
1:E:85:HIS:O	1:E:86:SER:C	2.53	0.51
2:B:39:ILE:HG22	2:B:49:THR:CA	2.40	0.51
1:E:60:LEU:O	1:E:114:THR:HB	2.10	0.51
1:E:105:LYS:O	1:E:144:ARG:NH2	2.43	0.51
1:C:167:ASN:HD21	2:D:104:HIS:CE1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:24:VAL:CG1	2:F:27:ASP:HB2	2.41	0.51
1:G:78:ARG:NH1	1:G:83:ASP:OD1	2.43	0.51
2:B:24:VAL:HG12	2:B:24:VAL:O	2.10	0.51
1:G:87:SER:O	1:G:91:ILE:CG2	2.51	0.51
2:H:15:LEU:CD2	2:H:129:LYS:CD	2.89	0.51
2:H:78:ILE:HD11	2:H:119:LEU:HB2	1.93	0.50
2:D:134:TRP:CZ2	2:D:138:LEU:HD11	2.47	0.50
1:C:53:LYS:O	1:C:56:ASN:N	2.41	0.50
2:F:87:THR:HG22	2:F:88:LYS:H	1.73	0.50
1:C:89:ASN:N	1:C:89:ASN:OD1	2.40	0.50
2:D:42:VAL:CG1	2:D:57:TYR:CE2	2.94	0.50
1:G:82:VAL:O	1:G:87:SER:CB	2.60	0.50
1:A:1:MET:HE1	1:A:9:LEU:HD22	1.93	0.49
2:H:109:ARG:HB3	2:H:111:TYR:O	2.13	0.49
1:A:160:SER:HB2	1:E:29:GLN:HE22	1.76	0.49
2:D:6:LEU:HD13	2:D:21:VAL:HG21	1.93	0.49
1:G:91:ILE:HG21	1:G:127:PHE:CD1	2.47	0.49
1:C:85:HIS:O	1:C:86:SER:HB2	2.10	0.49
2:B:106:LEU:O	2:B:149:ARG:NH2	2.35	0.49
1:A:152:TYR:HB3	1:A:155:ILE:HG13	1.94	0.49
2:B:39:ILE:HG22	2:B:49:THR:HB	1.95	0.48
1:G:6:GLU:OE2	1:G:78:ARG:NH2	2.47	0.48
2:H:158:GLN:O	2:H:162:SER:OG	2.29	0.48
1:A:6:GLU:OE1	1:A:78:ARG:NH2	2.47	0.48
1:A:78:ARG:NH1	1:A:83:ASP:CG	2.72	0.48
2:D:85:SER:HA	2:D:89:LEU:HB2	1.94	0.48
1:G:105:LYS:O	1:G:144:ARG:NH2	2.47	0.48
1:A:117:ASP:HB3	1:A:149:ILE:HD12	1.96	0.48
2:B:6:LEU:CD2	2:B:21:VAL:HG21	2.44	0.48
1:C:105:LYS:O	1:C:144:ARG:NH2	2.46	0.48
1:C:147:CYS:HA	1:C:150:GLN:HG2	1.95	0.48
2:B:24:VAL:HG13	2:B:62:ALA:CB	2.43	0.48
2:D:8:VAL:CG1	2:D:14:PRO:HG3	2.44	0.48
2:B:40:LEU:HD22	2:B:54:ILE:HG23	1.95	0.48
1:E:1:MET:HE1	1:E:9:LEU:HD22	1.96	0.48
1:E:91:ILE:HD12	1:E:91:ILE:H	1.79	0.48
2:F:127:THR:O	2:F:127:THR:HG22	2.14	0.47
1:E:66:GLU:N	1:E:66:GLU:OE1	2.46	0.47
1:A:78:ARG:NH1	1:A:83:ASP:OD1	2.47	0.47
2:B:57:TYR:CE2	2:B:61:VAL:HG21	2.49	0.47
1:C:91:ILE:H	1:C:91:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:LEU:HD22	2:D:54:ILE:HG23	1.95	0.47
2:D:68:TYR:CD1	2:D:78:ILE:HD13	2.50	0.47
1:E:152:TYR:HB3	1:E:155:ILE:HG13	1.95	0.47
1:E:85:HIS:CD2	1:E:86:SER:H	2.33	0.47
2:F:112:LEU:HG	2:F:121:ASP:OD1	2.15	0.47
1:A:67:GLU:HG2	1:A:109:THR:HG23	1.97	0.46
2:B:39:ILE:CG2	2:B:49:THR:HB	2.46	0.46
1:G:167:ASN:HB2	2:H:105:SER:HA	1.97	0.46
1:A:22:TYR:CE1	1:A:33:LEU:HD13	2.50	0.46
1:C:78:ARG:NH1	1:C:83:ASP:OD1	2.49	0.46
1:E:70:ILE:O	1:E:71:VAL:C	2.57	0.46
2:B:38:ASN:O	2:B:39:ILE:HG23	2.16	0.46
2:B:38:ASN:C	2:B:39:ILE:HG23	2.41	0.46
1:A:47:ILE:O	1:A:50:HIS:HB3	2.16	0.45
2:F:8:VAL:HG21	2:F:14:PRO:HD2	1.93	0.45
1:G:75:LEU:O	1:G:78:ARG:HB3	2.16	0.45
1:G:157:GLN:HB3	1:G:158:HIS:H	1.57	0.45
2:B:43:SER:HB2	2:B:46:VAL:HG12	1.99	0.45
2:B:28:VAL:HG23	2:B:30:ILE:HG13	1.98	0.45
2:B:4:LEU:CD1	2:B:40:LEU:HD11	2.45	0.45
2:B:41:HIS:HB3	2:B:44:GLU:HG3	1.99	0.45
2:D:15:LEU:C	2:D:17:ALA:N	2.72	0.45
1:A:46:THR:HG21	1:C:73:GLN:HA	1.98	0.45
1:A:28:ARG:HG3	1:C:86:SER:HB2	1.99	0.44
2:D:6:LEU:O	2:D:32:VAL:HA	2.17	0.44
2:H:15:LEU:HD22	2:H:129:LYS:HD3	1.99	0.44
2:H:42:VAL:HB	2:H:46:VAL:HB	1.99	0.44
2:H:86:ALA:O	2:H:90:SER:HB2	2.17	0.44
1:E:67:GLU:OE2	1:E:112:ASN:HB2	2.17	0.44
2:F:3:THR:C	2:F:4:LEU:HD12	2.42	0.44
1:A:53:LYS:HA	1:A:53:LYS:HD2	1.56	0.44
2:D:24:VAL:CG2	2:D:62:ALA:HB1	2.48	0.44
2:F:42:VAL:HG11	2:F:46:VAL:HG12	1.99	0.44
2:D:7:THR:HG22	2:D:35:GLY:HA3	2.00	0.44
2:F:18:LEU:HD23	2:F:18:LEU:HA	1.85	0.44
2:B:14:PRO:HG2	2:B:17:ALA:CB	2.46	0.44
2:D:8:VAL:HG13	2:D:38:ASN:OD1	2.13	0.44
2:D:39:ILE:HG22	2:D:49:THR:HG22	2.00	0.44
2:B:49:THR:O	2:B:49:THR:OG1	2.27	0.43
1:E:32:VAL:HG13	1:E:42:THR:HG22	2.00	0.43
2:H:133:ALA:O	2:H:136:GLU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:NH1	1:A:83:ASP:OD2	2.50	0.43
1:E:90:ASP:OD1	1:E:92:HIS:HB2	2.18	0.43
1:A:88:LYS:HE2	1:A:88:LYS:HB3	1.61	0.43
1:C:89:ASN:CG	1:C:90:ASP:N	2.73	0.43
2:F:87:THR:CG2	2:F:88:LYS:HG3	2.48	0.43
2:F:17:ALA:O	2:F:21:VAL:HG23	2.19	0.43
2:F:49:THR:OG1	2:F:50:ASP:N	2.52	0.43
1:A:115:LEU:HD11	1:A:119:LEU:HD13	2.01	0.43
2:B:42:VAL:CG2	2:B:46:VAL:HG13	2.49	0.43
2:H:36:LYS:HD3	2:H:39:ILE:HD13	2.01	0.43
2:H:81:TRP:HH2	2:H:105:SER:HG	1.67	0.43
2:B:24:VAL:O	2:B:24:VAL:CG1	2.67	0.43
2:B:59:ALA:CB	2:B:119:LEU:HD11	2.49	0.43
2:D:42:VAL:HG11	2:D:57:TYR:CZ	2.53	0.43
1:G:124:LEU:O	1:G:125:HIS:C	2.62	0.43
2:B:134:TRP:HH2	2:B:151:PHE:CE2	2.37	0.42
1:G:18:LYS:HE3	1:G:20:ASN:HA	2.01	0.42
2:H:106:LEU:O	2:H:149:ARG:NH2	2.47	0.42
1:A:145:TRP:O	1:A:149:ILE:HG12	2.19	0.42
2:F:113:VAL:HG11	2:F:118:SER:OG	2.19	0.42
1:G:91:ILE:O	1:G:95:LEU:HG	2.19	0.42
1:A:91:ILE:O	1:A:91:ILE:HG22	2.19	0.42
2:D:97:SER:HA	2:D:100:ASN:HB3	2.01	0.42
2:B:39:ILE:HG22	2:B:49:THR:CB	2.50	0.42
2:D:59:ALA:HB2	2:D:119:LEU:HD13	2.02	0.42
2:F:16:GLY:HA2	2:F:19:LEU:HD12	2.01	0.42
1:E:18:LYS:HE3	1:E:20:ASN:HA	2.01	0.42
1:A:77:TYR:CE2	1:A:81:GLN:NE2	2.88	0.42
2:B:7:THR:HG23	2:B:37:GLU:O	2.20	0.42
2:D:112:LEU:HD23	2:D:112:LEU:HA	1.92	0.42
1:A:64:THR:HB	1:A:66:GLU:OE2	2.19	0.41
1:A:60:LEU:O	1:A:114:THR:HB	2.20	0.41
1:A:160:SER:HB2	1:E:29:GLN:NE2	2.35	0.41
1:C:59:TYR:CE1	1:C:60:LEU:HG	2.55	0.41
2:B:7:THR:O	2:B:38:ASN:HA	2.20	0.41
1:A:42:THR:O	1:A:46:THR:OG1	2.34	0.41
1:E:166:LYS:HE2	2:F:109:ARG:HG2	2.03	0.41
1:A:157:GLN:HE22	1:E:21:LYS:HD2	1.85	0.41
1:C:59:TYR:CD1	1:C:59:TYR:C	2.98	0.41
2:F:59:ALA:CB	2:F:119:LEU:HD11	2.49	0.41
1:A:21:LYS:HE3	1:E:157:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:78:ILE:HD11	2:D:119:LEU:HB3	2.02	0.41
1:A:13:SER:HA	1:A:154:GLY:O	2.21	0.41
1:A:70:ILE:HG21	1:A:109:THR:HA	2.02	0.41
2:H:113:VAL:HG22	2:H:118:SER:OG	2.20	0.41
1:G:6:GLU:O	1:G:10:LEU:N	2.52	0.40
2:H:36:LYS:CD	2:H:39:ILE:HD13	2.52	0.40
1:C:108:LEU:HD12	1:C:116:ALA:HB1	2.04	0.40
2:F:111:TYR:C	2:F:113:VAL:H	2.29	0.40
2:D:7:THR:CG2	2:D:35:GLY:HA3	2.51	0.40
1:E:87:SER:O	1:E:91:ILE:HG13	2.21	0.40
2:F:49:THR:C	2:F:50:ASP:O	2.58	0.40
2:H:14:PRO:O	2:H:14:PRO:CG	2.69	0.40
2:B:128:LEU:HD12	2:B:150:TRP:HZ3	1.87	0.40
1:E:165:ILE:H	1:E:165:ILE:HG12	1.62	0.40
2:F:16:GLY:O	2:F:19:LEU:HB2	2.22	0.40
2:B:6:LEU:HD22	2:B:21:VAL:HG21	2.04	0.40
2:B:125:TRP:NE1	2:B:151:PHE:CD1	2.89	0.40
1:C:89:ASN:CG	1:C:90:ASP:H	2.29	0.40
2:H:121:ASP:O	2:H:125:TRP:HB2	2.22	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	161/171 (94%)	147 (91%)	14 (9%)	0	100	100
1	C	166/171 (97%)	149 (90%)	17 (10%)	0	100	100
1	E	166/171 (97%)	158 (95%)	8 (5%)	0	100	100
1	G	166/171 (97%)	157 (95%)	9 (5%)	0	100	100
2	B	164/175 (94%)	154 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	160/175 (91%)	147 (92%)	13 (8%)	0	100	100
2	F	164/175 (94%)	153 (93%)	11 (7%)	0	100	100
2	H	163/175 (93%)	151 (93%)	12 (7%)	0	100	100
All	All	1310/1384 (95%)	1216 (93%)	94 (7%)	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	145/149 (97%)	139 (96%)	6 (4%)	27	54
1	C	147/149 (99%)	143 (97%)	4 (3%)	39	67
1	E	147/149 (99%)	134 (91%)	13 (9%)	9	21
1	G	146/149 (98%)	142 (97%)	4 (3%)	39	67
2	B	139/151 (92%)	125 (90%)	14 (10%)	7	15
2	D	139/151 (92%)	125 (90%)	14 (10%)	7	15
2	F	141/151 (93%)	130 (92%)	11 (8%)	11	26
2	H	137/151 (91%)	132 (96%)	5 (4%)	31	58
All	All	1141/1200 (95%)	1070 (94%)	71 (6%)	16	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LYS
1	A	72	GLN
1	A	88	LYS
1	A	96	LYS
1	A	161	SER
1	A	165	ILE
2	B	6	LEU
2	B	13	PRO

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Mol	Chain	Res	Type
2	B	15	LEU
2	B	23	HIS
2	B	25	LYS
2	B	26	ASP
2	B	39	ILE
2	B	40	LEU
2	B	43	SER
2	B	55	LEU
2	B	68	TYR
2	B	72	LEU
2	B	82	LEU
2	B	93	ASP
1	C	35	THR
1	C	46	THR
1	C	133	VAL
1	C	161	SER
2	D	3	THR
2	D	8	VAL
2	D	13	PRO
2	D	39	ILE
2	D	40	LEU
2	D	43	SER
2	D	71	ASN
2	D	99	ILE
2	D	113	VAL
2	D	116	SER
2	D	119	LEU
2	D	129	LYS
2	D	139	LYS
2	D	149	ARG
1	E	27	GLU
1	E	36	ASN
1	E	37	ASN
1	E	40	SER
1	E	53	LYS
1	E	66	GLU
1	E	67	GLU
1	E	77	TYR
1	E	86	SER
1	E	90	ASP
1	E	163	VAL
1	E	165	ILE

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Mol	Chain	Res	Type
1	E	167	ASN
2	F	8	VAL
2	F	23	HIS
2	F	32	VAL
2	F	33	GLU
2	F	44	GLU
2	F	46	VAL
2	F	50	ASP
2	F	82	LEU
2	F	87	THR
2	F	135	GLN
2	F	165	THR
1	G	35	THR
1	G	104	ASP
1	G	133	VAL
1	G	157	GLN
2	H	8	VAL
2	H	26	ASP
2	H	46	VAL
2	H	71	ASN
2	H	162	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	56	ASN
1	A	72	GLN
1	A	167	ASN
2	B	23	HIS
2	B	103	ASN
2	B	140	GLN
2	B	146	HIS
1	C	36	ASN
1	C	50	HIS
1	C	54	GLN
1	C	81	GLN
1	C	141	ASN
1	C	151	HIS
1	C	167	ASN
2	D	23	HIS
2	D	71	ASN

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Mol	Chain	Res	Type
2	D	115	ASN
2	D	137	GLN
1	E	29	GLN
1	E	85	HIS
1	E	167	ASN
2	F	45	ASN
2	F	146	HIS
2	F	157	GLN
2	H	23	HIS
2	H	45	ASN
2	H	103	ASN
2	H	146	HIS
2	H	157	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	110:GLY	C	111:TYR	N	1.19

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	165/171 (96%)	-0.33	5 (3%) 52 47	10, 19, 47, 68	0
1	C	168/171 (98%)	-0.38	2 (1%) 76 73	9, 20, 45, 67	0
1	E	168/171 (98%)	-0.37	2 (1%) 76 73	11, 21, 40, 59	0
1	G	168/171 (98%)	-0.34	7 (4%) 40 35	8, 22, 43, 78	0
2	B	166/175 (94%)	0.29	12 (7%) 21 17	17, 35, 67, 80	0
2	D	164/175 (93%)	0.33	12 (7%) 21 17	17, 36, 68, 80	0
2	F	166/175 (94%)	0.46	18 (10%) 11 8	22, 43, 79, 96	0
2	H	165/175 (94%)	0.50	18 (10%) 10 8	17, 45, 78, 95	0
All	All	1330/1384 (96%)	0.02	76 (5%) 29 24	8, 28, 68, 96	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	86	SER	6.4
2	B	94	SER	5.1
2	D	165	THR	4.9
2	D	94	SER	4.8
1	G	87	SER	4.5
2	H	4	LEU	4.0
1	A	89	ASN	3.8
1	A	91	ILE	3.5
1	C	86	SER	3.4
2	H	166	LYS	3.4
2	D	12	ASP	3.3
2	F	32	VAL	3.3
2	D	11	GLY	3.2
1	G	89	ASN	3.2
2	D	41	HIS	3.2
1	E	87	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	88	LYS	3.2
1	A	109	THR	3.1
1	C	87	SER	3.1
2	H	32	VAL	3.1
2	H	43	SER	3.1
1	G	85	HIS	3.0
2	B	12	ASP	3.0
2	H	143	ALA	3.0
2	F	9	ASN	3.0
2	H	163	VAL	2.9
1	G	109	THR	2.9
2	F	15	LEU	2.9
2	B	10	SER	2.9
1	G	165	ILE	2.9
2	B	36	LYS	2.8
2	F	11	GLY	2.8
2	H	10	SER	2.8
2	D	139	LYS	2.8
2	B	35	GLY	2.8
2	D	9	ASN	2.7
2	B	165	THR	2.7
2	F	93	ASP	2.7
2	H	12	ASP	2.7
2	H	165	THR	2.7
2	F	92	SER	2.6
2	H	141	LYS	2.6
2	D	42	VAL	2.6
2	H	8	VAL	2.6
2	D	28	VAL	2.6
2	F	166	LYS	2.5
2	H	164	GLY	2.5
2	B	91	SER	2.5
2	H	167	TRP	2.5
2	F	71	ASN	2.5
2	D	138	LEU	2.5
2	F	27	ASP	2.4
2	F	43	SER	2.4
2	H	95	PHE	2.4
2	B	13	PRO	2.4
2	D	140	GLN	2.4
2	H	9	ASN	2.4
2	F	168	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	165	THR	2.3
2	F	51	VAL	2.3
1	A	38	GLY	2.3
2	F	133	ALA	2.2
2	B	50	ASP	2.2
2	F	12	ASP	2.2
2	H	15	LEU	2.2
2	B	14	PRO	2.2
1	G	86	SER	2.2
2	H	64	THR	2.2
2	F	10	SER	2.2
2	B	21	VAL	2.1
2	F	143	ALA	2.1
2	B	37	GLU	2.1
2	D	143	ALA	2.1
2	H	100	ASN	2.0
1	A	87	SER	2.0
2	F	94	SER	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.