



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:04 PM UTC

PDB ID : 1Y8T / pdb_00001y8t
Title : Crystal Structure of RV0983 from Mycobacterium tuberculosis- Proteolytically active form
Authors : Palaninathan, S.K.; MohamedMohaideen, N.N.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2004-12-13
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

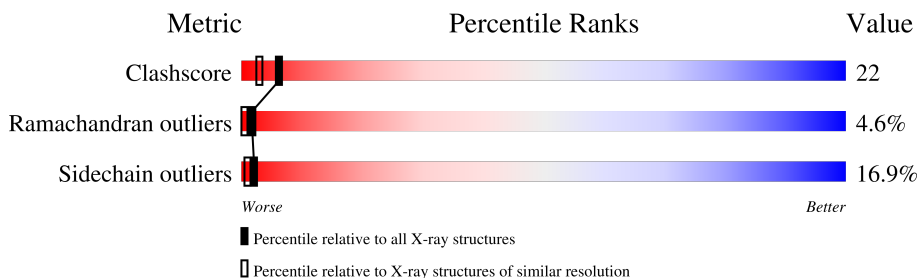
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	
1	B	324	
1	C	324	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5749 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 hypothetical protein Rv0983.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	Se	0	0	0
			1911	1186	331	392	2			
1	B	272	Total	C	N	O	Se	0	0	0
			1817	1131	314	370	2			
1	C	255	Total	C	N	O	Se	0	0	0
			1703	1059	295	347	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	MET	modified residue	UNP O53896
A	176	MSE	MET	modified residue	UNP O53896
A	317	LEU	-	expression tag	UNP O53896
A	318	GLU	-	expression tag	UNP O53896
A	319	HIS	-	expression tag	UNP O53896
A	320	HIS	-	expression tag	UNP O53896
A	321	HIS	-	expression tag	UNP O53896
A	322	HIS	-	expression tag	UNP O53896
A	323	HIS	-	expression tag	UNP O53896
A	324	HIS	-	expression tag	UNP O53896
B	21	MSE	MET	modified residue	UNP O53896
B	176	MSE	MET	modified residue	UNP O53896
B	317	LEU	-	expression tag	UNP O53896
B	318	GLU	-	expression tag	UNP O53896
B	319	HIS	-	expression tag	UNP O53896
B	320	HIS	-	expression tag	UNP O53896
B	321	HIS	-	expression tag	UNP O53896
B	322	HIS	-	expression tag	UNP O53896
B	323	HIS	-	expression tag	UNP O53896
B	324	HIS	-	expression tag	UNP O53896
C	21	MSE	MET	modified residue	UNP O53896
C	176	MSE	MET	modified residue	UNP O53896
C	317	LEU	-	expression tag	UNP O53896

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Chain	Residue	Modelled	Actual	Comment	Reference
C	318	GLU	-	expression tag	UNP O53896
C	319	HIS	-	expression tag	UNP O53896
C	320	HIS	-	expression tag	UNP O53896
C	321	HIS	-	expression tag	UNP O53896
C	322	HIS	-	expression tag	UNP O53896
C	323	HIS	-	expression tag	UNP O53896
C	324	HIS	-	expression tag	UNP O53896

- Molecule 2 is water.

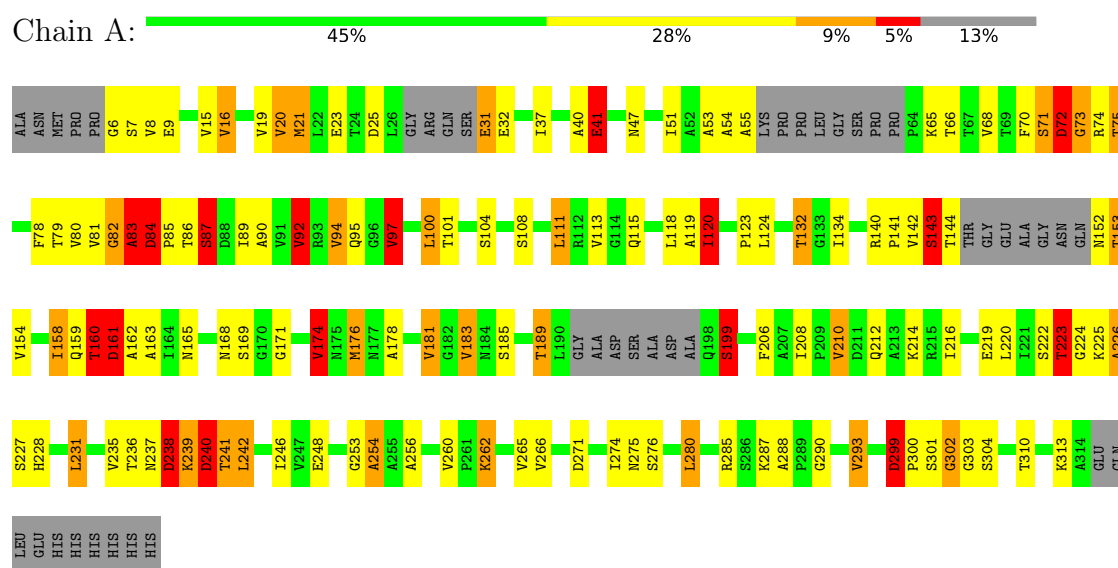
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	116	Total 116	O 116	0	0
2	B	119	Total 119	O 119	0	0
2	C	83	Total 83	O 83	0	0

3 Residue-property plots

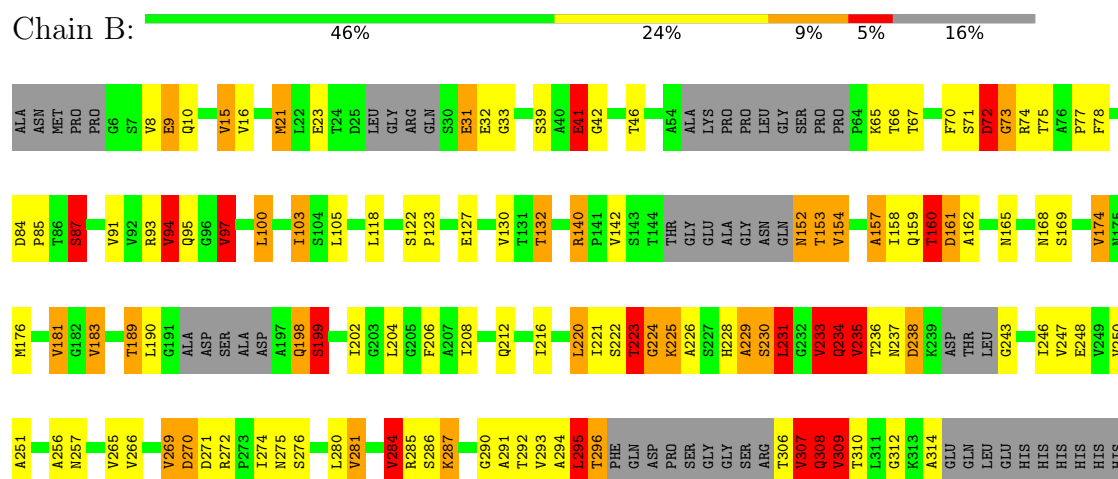
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

Note EDS was not executed.

- Molecule 1: hypothetical protein Rv0983

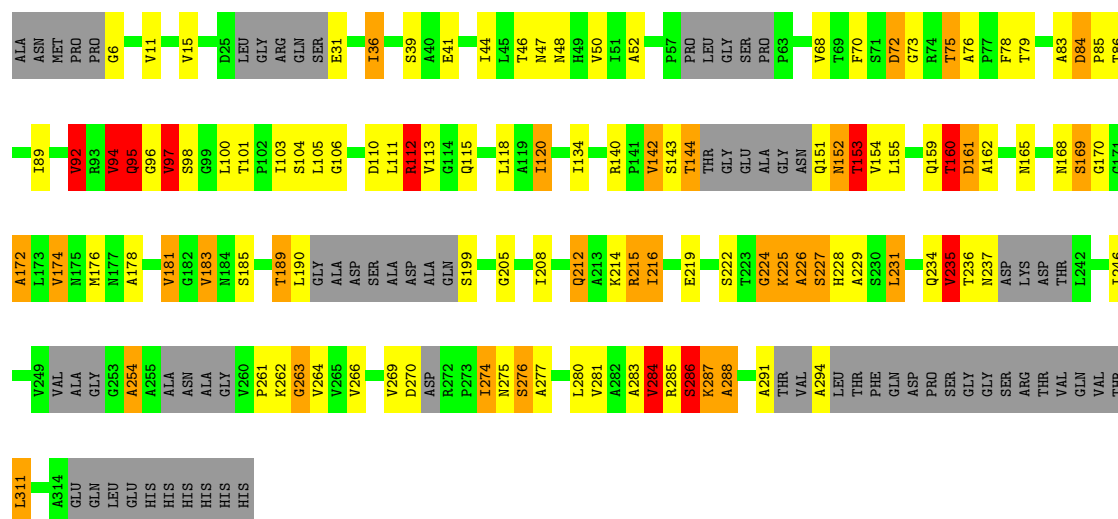


- Molecule 1: hypothetical protein Rv0983



- Molecule 1: hypothetical protein Rv0983

Chain C:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.58 Å 89.07 Å 69.41 Å 90.00° 97.55° 90.00°	Depositor
Resolution (Å)	76.70 – 2.00	Depositor
% Data completeness (in resolution range)	98.8 (76.70-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5749	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

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	2.02	57/1924 (3.0%)	1.88	70/2630 (2.7%)
1	B	2.16	55/1826 (3.0%)	1.98	60/2494 (2.4%)
1	C	1.82	22/1710 (1.3%)	1.89	57/2332 (2.4%)
All	All	2.01	134/5460 (2.5%)	1.92	187/7456 (2.5%)

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	9
1	B	0	8
1	C	1	6
All	All	1	23

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	CD-OE2	-17.45	0.92	1.25
1	C	183	VAL	CA-CB	13.43	1.70	1.54
1	B	21	MSE	SE-CE	13.14	2.34	1.95
1	B	41	GLU	CD-OE1	-12.88	1.00	1.25
1	A	161	ASP	CA-CB	11.42	1.71	1.53
1	A	223	THR	CA-CB	11.19	1.72	1.53
1	C	161	ASP	CA-CB	10.99	1.70	1.53
1	B	183	VAL	CA-CB	10.92	1.67	1.54
1	A	183	VAL	CA-CB	10.72	1.67	1.54
1	B	16	VAL	CA-C	9.81	1.63	1.52
1	B	41	GLU	CA-CB	9.61	1.70	1.53
1	B	309	VAL	N-CA	9.22	1.57	1.46
1	B	41	GLU	CB-CG	9.20	1.80	1.52
1	A	274	ILE	CA-CB	9.10	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	MSE	SE-CE	9.08	2.22	1.95
1	B	41	GLU	CA-C	8.84	1.64	1.52
1	A	253	GLY	C-O	8.74	1.35	1.23
1	B	72	ASP	CB-CG	-8.43	1.30	1.52
1	B	161	ASP	CA-CB	8.36	1.67	1.53
1	A	161	ASP	CB-CG	-8.32	1.31	1.52
1	B	174	VAL	CA-CB	8.11	1.67	1.55
1	B	42	GLY	N-CA	8.00	1.56	1.45
1	C	142	VAL	CA-CB	7.90	1.64	1.54
1	C	246	ILE	CA-CB	7.67	1.62	1.53
1	B	265	VAL	CA-CB	7.63	1.63	1.53
1	C	172	ALA	CA-CB	-7.56	1.41	1.53
1	B	296	THR	C-O	7.44	1.38	1.23
1	B	238	ASP	N-CA	7.44	1.55	1.46
1	B	154	VAL	CA-CB	7.44	1.61	1.53
1	B	309	VAL	CA-C	7.37	1.61	1.52
1	C	112	ARG	CG-CD	7.34	1.74	1.52
1	A	31	GLU	CG-CD	7.33	1.70	1.52
1	B	161	ASP	CB-CG	-7.28	1.33	1.52
1	A	132	THR	CB-CG2	7.25	1.76	1.52
1	A	83	ALA	CA-C	-7.25	1.43	1.52
1	A	310	THR	CA-CB	7.21	1.62	1.53
1	B	247	VAL	CA-CB	7.09	1.63	1.54
1	B	247	VAL	CA-C	7.08	1.60	1.52
1	B	132	THR	CB-CG2	7.03	1.75	1.52
1	A	119	ALA	N-CA	-7.01	1.37	1.46
1	A	142	VAL	CA-CB	6.98	1.62	1.54
1	C	120	ILE	CA-CB	6.90	1.63	1.54
1	B	46	THR	CA-CB	6.86	1.63	1.53
1	B	251	ALA	C-O	6.84	1.33	1.23
1	A	141	PRO	CA-C	6.82	1.59	1.52
1	A	189	THR	CB-CG2	6.82	1.75	1.52
1	A	304	SER	CA-C	6.72	1.60	1.52
1	A	226	ALA	N-CA	6.70	1.54	1.46
1	A	212	GLN	N-CA	6.68	1.54	1.46
1	A	16	VAL	CA-CB	6.65	1.62	1.54
1	B	33	GLY	C-O	6.64	1.28	1.23
1	B	31	GLU	CB-CG	6.60	1.72	1.52
1	A	174	VAL	CA-CB	6.60	1.65	1.55
1	B	208	ILE	CA-C	6.58	1.59	1.52
1	A	31	GLU	CB-CG	6.55	1.72	1.52
1	C	178	ALA	CA-CB	6.54	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	ASP	CB-CG	-6.46	1.35	1.52
1	A	219	GLU	CA-C	6.45	1.61	1.52
1	B	132	THR	CA-C	6.43	1.60	1.52
1	A	176	MSE	SE-CE	6.42	2.14	1.95
1	B	293	VAL	CA-C	6.40	1.60	1.52
1	A	265	VAL	C-O	-6.39	1.16	1.24
1	A	41	GLU	CG-CD	6.39	1.68	1.52
1	A	299	ASP	CA-C	6.37	1.60	1.52
1	A	143	SER	C-O	6.36	1.32	1.24
1	B	15	VAL	N-CA	-6.31	1.38	1.46
1	B	198	GLN	N-CA	6.28	1.54	1.46
1	A	208	ILE	CA-CB	6.27	1.62	1.53
1	B	284	VAL	CA-C	6.21	1.60	1.52
1	B	10	GLN	N-CA	6.16	1.53	1.46
1	C	89	ILE	CA-CB	6.16	1.62	1.54
1	C	275	ASN	CB-CG	6.09	1.67	1.52
1	B	198	GLN	CA-C	6.07	1.60	1.52
1	B	91	VAL	C-O	6.04	1.30	1.24
1	A	55	ALA	C-O	6.04	1.35	1.23
1	A	208	ILE	CA-C	6.04	1.57	1.53
1	A	20	VAL	CA-C	6.01	1.59	1.52
1	A	97	VAL	CA-CB	6.01	1.61	1.54
1	A	55	ALA	CA-CB	5.99	1.72	1.52
1	A	80	VAL	CA-C	5.95	1.59	1.52
1	A	266	VAL	CA-CB	5.92	1.60	1.54
1	B	73	GLY	N-CA	-5.92	1.36	1.45
1	B	309	VAL	CA-CB	5.89	1.62	1.54
1	C	52	ALA	N-CA	5.88	1.53	1.46
1	A	37	ILE	CA-CB	5.73	1.62	1.53
1	B	189	THR	CB-CG2	5.71	1.71	1.52
1	C	44	ILE	CA-CB	5.68	1.61	1.54
1	A	158	ILE	CA-CB	5.62	1.61	1.54
1	C	11	VAL	CA-C	5.59	1.59	1.52
1	A	40	ALA	CA-CB	5.57	1.62	1.53
1	C	174	VAL	CA-CB	5.57	1.63	1.55
1	B	130	VAL	CA-CB	5.54	1.60	1.54
1	A	240	ASP	CA-C	5.52	1.64	1.52
1	B	9	GLU	CB-CG	5.51	1.69	1.52
1	A	240	ASP	N-CA	5.48	1.56	1.46
1	B	208	ILE	CA-CB	5.48	1.61	1.54
1	C	46	THR	N-CA	-5.48	1.38	1.46
1	B	169	SER	N-CA	5.46	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ASP	CA-C	5.43	1.60	1.52
1	B	236	THR	CA-CB	5.40	1.61	1.53
1	A	256	ALA	N-CA	5.39	1.52	1.46
1	A	120	ILE	CB-CG2	5.39	1.70	1.52
1	A	153	THR	CA-CB	5.39	1.62	1.53
1	B	248	GLU	CA-C	5.36	1.59	1.52
1	A	262	LYS	CE-NZ	5.34	1.65	1.49
1	A	6	GLY	N-CA	5.34	1.54	1.45
1	B	181	VAL	CA-C	5.34	1.58	1.52
1	A	199	SER	N-CA	5.33	1.53	1.46
1	A	178	ALA	CA-CB	5.33	1.61	1.53
1	B	202	ILE	CA-CB	5.31	1.60	1.54
1	A	90	ALA	CA-CB	5.31	1.63	1.53
1	A	113	VAL	CA-C	5.26	1.58	1.52
1	C	6	GLY	N-CA	5.25	1.53	1.45
1	C	284	VAL	CA-CB	5.24	1.61	1.54
1	A	176	MSE	CG-SE	5.22	2.11	1.95
1	B	103	ILE	CA-CB	5.21	1.61	1.54
1	A	171	GLY	C-O	5.20	1.28	1.23
1	C	153	THR	CA-CB	5.19	1.62	1.53
1	A	293	VAL	CA-CB	5.18	1.62	1.54
1	B	236	THR	N-CA	5.17	1.53	1.46
1	A	265	VAL	CA-CB	5.17	1.60	1.53
1	C	31	GLU	CB-CG	5.16	1.68	1.52
1	B	234	GLN	N-CA	5.16	1.52	1.46
1	B	122	SER	C-O	-5.16	1.18	1.24
1	A	68	VAL	C-O	-5.15	1.18	1.24
1	A	163	ALA	CA-CB	5.15	1.61	1.53
1	A	238	ASP	CA-C	5.11	1.59	1.52
1	C	50	VAL	C-O	5.10	1.30	1.24
1	B	294	ALA	CA-CB	5.08	1.59	1.53
1	C	101	THR	CA-CB	5.07	1.60	1.53
1	B	140	ARG	C-N	5.01	1.39	1.33
1	B	226	ALA	CA-C	5.01	1.58	1.52
1	B	238	ASP	CA-C	5.00	1.59	1.52
1	B	271	ASP	CA-C	5.00	1.59	1.52

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	GLU	OE1-CD-OE2	-24.38	64.40	122.90
1	B	41	GLU	CG-CD-OE1	15.48	154.02	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	181	VAL	CB-CA-C	13.90	123.70	110.63
1	C	286	SER	N-CA-C	-13.50	94.82	114.39
1	A	161	ASP	N-CA-C	12.93	125.38	111.28
1	B	41	GLU	N-CA-C	-12.72	97.74	113.01
1	C	234	GLN	CA-C-N	11.64	142.65	121.70
1	C	234	GLN	C-N-CA	11.64	142.65	121.70
1	B	41	GLU	CB-CA-C	11.43	133.49	110.17
1	C	160	THR	CA-C-N	11.24	135.77	120.38
1	C	160	THR	C-N-CA	11.24	135.77	120.38
1	A	227	SER	N-CA-C	11.19	127.76	110.42
1	C	161	ASP	N-CA-C	11.17	124.84	111.33
1	B	41	GLU	CB-CG-CD	10.75	130.88	112.60
1	A	224	GLY	N-CA-C	10.67	138.46	113.18
1	B	309	VAL	N-CA-C	10.61	123.91	108.53
1	B	181	VAL	N-CA-CB	-9.81	100.65	112.33
1	B	42	GLY	N-CA-C	9.81	128.10	114.85
1	A	72	ASP	N-CA-C	9.71	131.48	110.80
1	B	41	GLU	CG-CD-OE2	9.68	140.66	118.40
1	A	160	THR	CA-C-N	9.65	133.21	120.28
1	A	160	THR	C-N-CA	9.65	133.21	120.28
1	B	160	THR	CB-CA-C	-9.59	90.12	109.79
1	B	160	THR	CA-C-N	9.16	136.26	120.68
1	B	160	THR	C-N-CA	9.16	136.26	120.68
1	C	86	THR	N-CA-C	9.00	121.17	111.36
1	A	161	ASP	CA-CB-CG	-8.97	103.62	112.60
1	A	181	VAL	CB-CA-C	8.96	119.05	110.63
1	B	236	THR	N-CA-C	8.90	122.50	109.69
1	A	160	THR	CB-CA-C	-8.78	90.07	109.56
1	B	72	ASP	N-CA-C	8.78	129.49	110.80
1	C	216	ILE	N-CA-C	8.76	118.83	110.42
1	C	224	GLY	N-CA-C	8.71	127.71	115.43
1	C	161	ASP	CB-CG-OD1	-8.61	98.60	118.40
1	C	224	GLY	CA-C-N	8.61	137.19	121.70
1	C	224	GLY	C-N-CA	8.61	137.19	121.70
1	A	143	SER	N-CA-C	8.57	123.79	113.16
1	C	72	ASP	N-CA-C	8.54	123.53	113.20
1	A	86	THR	CA-C-N	8.18	131.24	120.28
1	A	86	THR	C-N-CA	8.18	131.24	120.28
1	C	288	ALA	CA-C-N	8.09	128.58	119.93
1	C	288	ALA	C-N-CA	8.09	128.58	119.93
1	A	154	VAL	N-CA-C	7.97	119.36	107.80
1	A	101	THR	CA-C-N	7.92	127.68	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	THR	C-N-CA	7.92	127.68	119.76
1	A	241	THR	N-CA-C	7.91	119.04	107.88
1	A	82	GLY	CA-C-N	7.88	136.60	121.54
1	A	82	GLY	C-N-CA	7.88	136.60	121.54
1	B	161	ASP	CA-CB-CG	-7.73	104.87	112.60
1	A	161	ASP	CB-CG-OD1	-7.52	101.11	118.40
1	C	160	THR	CB-CA-C	-7.49	92.94	109.56
1	A	82	GLY	N-CA-C	7.34	121.84	111.19
1	B	307	VAL	CA-C-N	7.34	134.91	121.70
1	B	307	VAL	C-N-CA	7.34	134.91	121.70
1	C	162	ALA	N-CA-C	-7.29	99.10	109.96
1	A	288	ALA	CA-C-N	7.25	128.91	119.84
1	A	288	ALA	C-N-CA	7.25	128.91	119.84
1	B	284	VAL	N-CA-C	7.25	124.41	109.34
1	C	161	ASP	CA-CB-CG	-7.13	105.47	112.60
1	C	154	VAL	N-CA-C	-7.11	98.23	108.53
1	C	287	LYS	N-CA-C	7.05	119.46	108.96
1	C	181	VAL	N-CA-CB	-7.00	100.78	111.57
1	C	224	GLY	CA-C-O	-7.00	111.01	119.06
1	B	284	VAL	CA-C-N	6.95	134.80	121.54
1	B	284	VAL	C-N-CA	6.95	134.80	121.54
1	C	161	ASP	CB-CG-OD2	6.87	134.19	118.40
1	B	161	ASP	CB-CG-OD1	-6.86	102.63	118.40
1	A	65	LYS	N-CA-C	-6.79	100.23	110.28
1	C	110	ASP	N-CA-C	6.79	121.30	112.89
1	A	84	ASP	N-CA-C	6.72	124.66	109.81
1	A	6	GLY	CA-C-N	6.72	131.49	120.94
1	A	6	GLY	C-N-CA	6.72	131.49	120.94
1	C	120	ILE	CB-CA-C	6.64	119.39	110.42
1	C	234	GLN	N-CA-C	-6.64	98.90	109.59
1	A	299	ASP	N-CA-C	6.60	124.39	109.81
1	C	266	VAL	N-CA-C	-6.60	102.86	110.05
1	C	234	GLN	O-C-N	-6.58	114.85	123.21
1	A	31	GLU	CB-CG-CD	6.58	123.78	112.60
1	B	181	VAL	CG1-CB-CG2	6.55	125.21	110.80
1	A	83	ALA	N-CA-C	6.52	124.68	110.80
1	A	199	SER	N-CA-C	6.52	120.91	109.96
1	C	234	GLN	CA-C-O	-6.51	113.81	120.71
1	A	153	THR	CB-CA-C	6.41	123.17	110.42
1	A	223	THR	CB-CA-C	6.35	123.06	110.42
1	A	54	ALA	CA-C-N	6.29	133.03	121.70
1	A	54	ALA	C-N-CA	6.29	133.03	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	181	VAL	CB-CA-C	6.28	117.41	110.62
1	B	72	ASP	CB-CA-C	-6.26	97.96	110.42
1	A	285	ARG	N-CA-C	6.25	118.90	111.71
1	B	157	ALA	N-CA-C	6.24	120.24	110.32
1	C	112	ARG	CB-CA-C	6.22	121.67	109.35
1	B	224	GLY	N-CA-C	6.21	127.89	113.18
1	B	199	SER	N-CA-C	6.16	119.57	109.72
1	C	39	SER	CA-C-N	6.15	128.80	120.38
1	C	39	SER	C-N-CA	6.15	128.80	120.38
1	C	84	ASP	CA-C-N	6.14	125.87	119.05
1	C	84	ASP	C-N-CA	6.14	125.87	119.05
1	B	158	ILE	N-CA-C	-6.14	100.78	108.89
1	B	154	VAL	CA-C-N	6.12	129.99	120.75
1	B	154	VAL	C-N-CA	6.12	129.99	120.75
1	B	276	SER	N-CA-C	6.11	117.42	108.14
1	B	233	VAL	N-CA-C	-6.09	96.68	109.34
1	B	272	ARG	N-CA-C	6.04	118.62	110.29
1	B	233	VAL	CA-C-N	6.04	133.07	121.54
1	B	233	VAL	C-N-CA	6.04	133.07	121.54
1	A	120	ILE	CB-CA-C	6.03	119.13	110.33
1	B	71	SER	CA-C-N	6.01	133.03	121.54
1	B	71	SER	C-N-CA	6.01	133.03	121.54
1	A	253	GLY	CA-C-N	6.00	133.00	121.54
1	A	253	GLY	C-N-CA	6.00	133.00	121.54
1	B	161	ASP	N-CA-CB	-5.94	101.16	110.30
1	C	181	VAL	N-CA-C	-5.93	108.07	113.71
1	C	92	VAL	N-CA-CB	-5.87	104.31	112.52
1	C	208	ILE	CA-C-N	5.85	125.78	119.76
1	C	208	ILE	C-N-CA	5.85	125.78	119.76
1	A	143	SER	CA-C-O	-5.81	112.25	119.28
1	B	284	VAL	O-C-N	-5.79	115.33	122.57
1	A	212	GLN	N-CA-C	5.79	117.26	111.07
1	C	106	GLY	N-CA-C	-5.77	104.35	112.60
1	C	94	VAL	CB-CA-C	5.75	119.55	110.81
1	B	237	ASN	N-CA-C	5.73	119.44	110.32
1	A	81	VAL	N-CA-C	-5.70	106.91	111.81
1	A	241	THR	CA-C-N	5.70	128.97	120.87
1	A	241	THR	C-N-CA	5.70	128.97	120.87
1	C	235	VAL	N-CA-C	5.70	126.96	111.00
1	C	120	ILE	N-CA-C	5.68	116.17	107.77
1	A	161	ASP	CB-CG-OD2	5.67	131.45	118.40
1	A	240	ASP	N-CA-C	5.66	126.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	VAL	N-CA-C	-5.63	105.01	110.42
1	C	189	THR	N-CA-C	5.62	117.96	109.41
1	A	299	ASP	CA-C-N	5.62	140.49	127.00
1	A	299	ASP	C-N-CA	5.62	140.49	127.00
1	B	234	GLN	CA-C-N	5.59	131.76	121.70
1	B	234	GLN	C-N-CA	5.59	131.76	121.70
1	B	234	GLN	N-CA-C	5.59	122.71	110.80
1	B	233	VAL	CA-C-O	-5.54	113.85	120.78
1	A	20	VAL	N-CA-CB	-5.52	101.71	111.93
1	A	183	VAL	N-CA-CB	5.52	118.82	111.64
1	B	87	SER	CA-CB-OG	-5.49	100.11	111.10
1	B	140	ARG	N-CA-C	-5.49	101.61	109.24
1	B	183	VAL	N-CA-CB	5.47	118.35	111.46
1	C	181	VAL	CG1-CB-CG2	5.46	122.81	110.80
1	C	112	ARG	CA-CB-CG	5.46	125.01	114.10
1	A	253	GLY	O-C-N	5.45	129.79	122.70
1	B	230	SER	N-CA-C	-5.42	99.25	110.80
1	A	254	ALA	N-CA-C	5.41	122.33	110.80
1	A	83	ALA	O-C-N	5.41	129.78	122.59
1	A	181	VAL	CG1-CB-CG2	5.40	122.68	110.80
1	A	95	GLN	N-CA-C	5.39	118.27	109.59
1	C	284	VAL	CA-C-N	5.33	130.93	122.61
1	C	284	VAL	C-N-CA	5.33	130.93	122.61
1	C	215	ARG	CA-CB-CG	-5.32	103.45	114.10
1	A	71	SER	CA-C-N	5.32	131.69	121.54
1	A	71	SER	C-N-CA	5.32	131.69	121.54
1	B	229	ALA	O-C-N	-5.29	117.05	123.03
1	B	132	THR	CA-CB-CG2	5.28	119.48	110.50
1	B	94	VAL	N-CA-CB	-5.27	101.00	111.91
1	A	87	SER	N-CA-CB	-5.27	102.38	110.12
1	B	291	ALA	N-CA-C	5.25	117.83	110.23
1	C	170	GLY	N-CA-C	-5.24	107.88	115.27
1	A	161	ASP	CB-CA-C	-5.24	102.09	110.79
1	B	221	ILE	N-CA-C	5.24	115.45	110.42
1	A	120	ILE	CA-CB-CG2	5.21	119.36	110.50
1	B	97	VAL	CB-CA-C	5.21	117.26	110.96
1	A	189	THR	OG1-CB-CG2	5.21	119.72	109.30
1	B	295	LEU	CA-CB-CG	5.20	134.51	116.30
1	A	55	ALA	CA-C-O	-5.20	111.96	120.80
1	A	226	ALA	N-CA-C	-5.20	101.24	109.76
1	A	210	VAL	N-CA-C	5.18	115.79	110.36
1	A	239	LYS	CA-C-N	5.16	130.98	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	LYS	C-N-CA	5.16	130.98	121.70
1	B	308	GLN	N-CA-C	-5.15	96.57	111.00
1	A	41	GLU	CB-CA-C	5.14	120.65	110.17
1	B	231	LEU	N-CA-C	5.14	121.74	110.80
1	A	290	GLY	N-CA-C	5.13	122.18	115.40
1	C	285	ARG	CB-CA-C	5.13	119.63	111.48
1	C	76	ALA	CA-C-N	-5.11	114.45	119.92
1	C	76	ALA	C-N-CA	-5.11	114.45	119.92
1	C	212	GLN	N-CA-C	5.09	116.51	111.07
1	C	284	VAL	N-CA-C	5.08	119.90	109.34
1	B	189	THR	N-CA-C	5.06	116.50	108.96
1	A	92	VAL	N-CA-CB	-5.06	103.96	112.47
1	B	181	VAL	CA-C-O	5.03	123.51	118.98
1	A	231	LEU	N-CA-C	-5.02	107.28	113.41
1	C	36	ILE	N-CA-C	-5.02	100.90	108.12
1	A	299	ASP	C-N-CD	-5.01	109.58	120.60
1	C	276	SER	N-CA-C	5.00	115.64	108.74

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	235	VAL	CA

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ASN	Peptide
1	A	226	ALA	Peptide
1	A	240	ASP	Peptide
1	A	25	ASP	Peptide
1	A	71	SER	Peptide
1	A	73	GLY	Peptide
1	A	82	GLY	Peptide
1	A	83	ALA	Peptide,Mainchain
1	B	152	ASN	Peptide
1	B	223	THR	Peptide
1	B	229	ALA	Peptide
1	B	233	VAL	Peptide
1	B	235	VAL	Peptide
1	B	275	ASN	Peptide
1	B	284	VAL	Peptide
1	B	72	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	C	152	ASN	Peptide
1	C	224	GLY	Peptide
1	C	284	VAL	Peptide
1	C	286	SER	Peptide
1	C	72	ASP	Peptide
1	C	95	GLN	Peptide

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	1911	0	1922	82	0
1	B	1817	0	1831	96	0
1	C	1703	0	1686	68	0
2	A	116	0	0	4	0
2	B	119	0	0	11	0
2	C	83	0	0	1	0
All	All	5749	0	5439	243	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 22.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:CG2	1:A:132:THR:CB	1.76	1.63
1:C:112:ARG:CD	1:C:112:ARG:CG	1.74	1.61
1:B:132:THR:CB	1:B:132:THR:CG2	1.75	1.59
1:A:189:THR:CG2	1:A:189:THR:CB	1.75	1.56
1:B:41:GLU:CG	1:B:41:GLU:CB	1.80	1.54
1:B:21:MSE:HE3	1:B:32:GLU:CG	1.42	1.49
1:A:176:MSE:SE	1:A:176:MSE:CE	2.14	1.44
1:A:21:MSE:CE	1:A:21:MSE:SE	2.22	1.37
1:B:21:MSE:CE	1:B:32:GLU:HG3	1.67	1.25
1:B:21:MSE:CE	1:B:21:MSE:SE	2.34	1.24
1:C:96:GLY:HA2	1:C:97:VAL:HG12	1.23	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:VAL:HG22	1:B:274:ILE:HD11	1.15	1.15
1:A:21:MSE:HE3	1:A:32:GLU:CG	1.82	1.09
1:A:21:MSE:HE3	1:A:32:GLU:HG3	1.25	1.08
1:B:269:VAL:CG2	1:B:274:ILE:HD11	1.83	1.08
1:C:96:GLY:HA2	1:C:97:VAL:CG1	1.85	1.06
1:B:233:VAL:CG1	1:B:246:ILE:HG23	1.86	1.06
1:B:21:MSE:CE	1:B:32:GLU:CG	2.29	1.06
1:B:269:VAL:HG22	1:B:274:ILE:CD1	1.88	1.03
1:B:233:VAL:HG11	1:B:246:ILE:HD12	1.41	1.02
1:B:21:MSE:HE3	1:B:32:GLU:HG3	1.05	1.02
1:B:153:THR:HG21	2:B:384:HOH:O	1.61	1.00
1:A:84:ASP:OD1	1:A:87:SER:HB2	1.62	0.99
1:C:94:VAL:HG13	1:C:97:VAL:HG21	1.45	0.99
1:B:306:THR:HB	1:B:307:VAL:HG13	1.49	0.95
1:B:233:VAL:HG13	1:B:246:ILE:HG23	1.46	0.94
1:B:41:GLU:H	1:B:41:GLU:HG2	1.37	0.90
1:B:127:GLU:OE2	2:B:365:HOH:O	1.89	0.88
1:A:118:LEU:HG	1:A:176:MSE:HE1	1.54	0.87
1:B:153:THR:HG21	2:B:367:HOH:O	1.72	0.87
1:B:72:ASP:HB3	1:B:74:ARG:H	1.38	0.86
1:B:21:MSE:HE3	1:B:32:GLU:HG2	1.52	0.86
1:B:21:MSE:HE3	1:B:32:GLU:CD	2.01	0.86
1:C:235:VAL:HG11	1:C:280:LEU:HD23	1.56	0.85
1:B:295:LEU:HD12	1:B:309:VAL:CG1	2.08	0.84
1:A:236:THR:HG22	1:A:237:ASN:H	1.44	0.83
1:C:96:GLY:HA2	1:C:97:VAL:CB	2.09	0.82
1:A:72:ASP:HB3	1:A:74:ARG:H	1.44	0.81
1:A:300:PRO:HA	1:A:301:SER:C	2.05	0.81
1:A:41:GLU:HG2	2:A:397:HOH:O	1.81	0.81
1:C:96:GLY:CA	1:C:97:VAL:HG12	2.11	0.80
1:A:21:MSE:HE2	1:A:23:GLU:OE2	1.81	0.80
1:C:94:VAL:CG1	1:C:97:VAL:HG21	2.11	0.79
1:C:15:VAL:HG11	1:C:174:VAL:HG11	1.66	0.78
1:A:70:PHE:O	1:A:73:GLY:HA2	1.84	0.77
1:A:301:SER:O	1:A:303:GLY:N	2.17	0.76
1:A:239:LYS:H	1:A:241:THR:H	1.34	0.74
1:A:21:MSE:CE	1:A:32:GLU:HG3	2.11	0.74
1:B:132:THR:CG2	1:B:132:THR:HB	2.13	0.74
1:A:189:THR:CG2	1:A:189:THR:CA	2.67	0.72
1:B:281:VAL:O	1:B:285:ARG:HB2	1.91	0.71
1:C:225:LYS:O	1:C:226:ALA:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:VAL:HG11	1:B:246:ILE:HG23	1.73	0.70
1:B:307:VAL:HA	1:B:308:GLN:HB3	1.73	0.70
1:C:261:PRO:O	1:C:263:GLY:N	2.24	0.70
1:B:41:GLU:HG2	1:B:41:GLU:N	2.07	0.69
1:A:87:SER:HB3	1:A:89:ILE:H	1.58	0.69
1:C:118:LEU:HG	1:C:176:MSE:HE1	1.73	0.69
1:C:231:LEU:O	1:C:254:ALA:HB3	1.93	0.69
1:B:269:VAL:CG2	1:B:274:ILE:CD1	2.61	0.69
1:A:222:SER:O	1:A:223:THR:HB	1.91	0.69
1:A:94:VAL:HG13	1:A:97:VAL:HG13	1.75	0.68
1:B:118:LEU:HG	1:B:176:MSE:HE1	1.75	0.68
1:C:189:THR:HG21	1:C:199:SER:HB3	1.76	0.68
1:C:78:PHE:HB2	1:C:92:VAL:HG13	1.76	0.67
1:B:41:GLU:OE1	2:B:326:HOH:O	2.10	0.67
1:C:269:VAL:O	1:C:270:ASP:HB2	1.94	0.66
1:B:314:ALA:HA	2:B:368:HOH:O	1.96	0.66
1:B:230:SER:OG	1:B:231:LEU:N	2.30	0.65
1:C:284:VAL:O	1:C:287:LYS:HB2	1.97	0.65
1:A:72:ASP:OD2	1:A:74:ARG:NE	2.29	0.64
1:B:243:GLY:HA2	1:B:274:ILE:O	1.98	0.64
1:B:84:ASP:OD1	1:B:228:HIS:HE1	1.81	0.63
1:B:165:ASN:H	1:B:168:ASN:HD22	1.45	0.63
1:A:275:ASN:HB3	2:B:433:HOH:O	1.97	0.63
1:A:87:SER:OG	1:A:216:ILE:HD12	1.98	0.63
1:B:281:VAL:O	1:B:285:ARG:CG	2.47	0.63
1:A:189:THR:HG21	1:A:199:SER:HB3	1.81	0.63
1:B:153:THR:CG2	2:B:367:HOH:O	2.39	0.62
1:C:105:LEU:HD13	1:C:214:LYS:HD2	1.80	0.62
1:A:236:THR:HG23	2:A:407:HOH:O	1.98	0.62
1:A:87:SER:OG	1:A:216:ILE:CD1	2.48	0.61
1:A:143:SER:O	1:A:153:THR:HG22	2.00	0.61
1:C:165:ASN:H	1:C:168:ASN:HD22	1.46	0.61
1:C:236:THR:HG22	1:C:237:ASN:H	1.66	0.60
1:A:9:GLU:HB3	1:C:112:ARG:HD3	1.84	0.60
1:B:212:GLN:O	1:B:216:ILE:HD12	2.02	0.60
1:B:284:VAL:O	1:B:287:LYS:HB2	2.00	0.60
1:C:219:GLU:OE1	1:C:226:ALA:O	2.20	0.59
1:A:97:VAL:HG22	1:A:100:LEU:CD1	2.33	0.59
1:B:41:GLU:CG	1:B:41:GLU:H	2.11	0.59
1:B:281:VAL:O	1:B:285:ARG:CB	2.49	0.59
1:A:236:THR:HG22	1:A:237:ASN:N	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:CG2	1:A:132:THR:HB	2.15	0.59
1:B:94:VAL:HG13	1:B:97:VAL:HG13	1.85	0.59
1:B:97:VAL:HG22	1:B:100:LEU:CD1	2.33	0.59
1:A:189:THR:CG2	1:A:189:THR:HB	2.15	0.58
1:C:283:ALA:O	1:C:286:SER:HB3	2.04	0.58
1:A:238:ASP:HA	1:A:241:THR:O	2.04	0.58
1:B:39:SER:HB2	1:B:41:GLU:HG3	1.85	0.57
1:B:230:SER:HB3	1:B:312:GLY:O	2.04	0.57
1:A:47:ASN:HD22	1:A:169:SER:HB3	1.69	0.57
1:B:15:VAL:HG11	1:B:174:VAL:HG11	1.86	0.57
1:A:300:PRO:HA	1:A:302:GLY:N	2.21	0.56
1:C:111:LEU:HA	1:C:115:GLN:HE22	1.70	0.56
1:C:70:PHE:O	1:C:73:GLY:HA2	2.06	0.56
1:B:123:PRO:HB3	1:B:168:ASN:ND2	2.20	0.56
1:B:295:LEU:CD1	1:B:309:VAL:CG1	2.83	0.56
1:C:215:ARG:CD	1:C:288:ALA:HB2	2.36	0.56
1:A:97:VAL:HG22	1:A:100:LEU:HD11	1.88	0.56
1:B:153:THR:CB	2:B:384:HOH:O	2.53	0.56
1:B:224:GLY:HA2	1:B:225:LYS:C	2.31	0.55
1:A:47:ASN:HD21	1:A:185:SER:HA	1.70	0.55
1:A:299:ASP:HB2	1:A:301:SER:O	2.07	0.55
1:C:229:ALA:HB1	1:C:311:LEU:HD13	1.87	0.55
1:B:140:ARG:HE	1:B:159:GLN:NE2	2.04	0.55
1:C:140:ARG:HE	1:C:159:GLN:NE2	2.05	0.55
1:A:301:SER:C	1:A:303:GLY:H	2.14	0.55
1:A:165:ASN:H	1:A:168:ASN:HD22	1.54	0.54
1:C:47:ASN:HD21	1:C:185:SER:HA	1.72	0.54
1:B:160:THR:HG22	1:B:162:ALA:H	1.71	0.54
1:B:230:SER:HB3	1:B:312:GLY:C	2.32	0.54
1:A:299:ASP:HB3	1:A:300:PRO:C	2.32	0.54
1:A:72:ASP:HB3	1:A:74:ARG:N	2.20	0.54
1:A:241:THR:OG1	1:A:242:LEU:N	2.39	0.53
1:B:224:GLY:HA2	1:B:225:LYS:O	2.07	0.53
1:C:237:ASN:HD21	1:C:276:SER:HB2	1.74	0.53
1:C:291:ALA:O	2:C:399:HOH:O	2.19	0.53
1:B:21:MSE:CE	1:B:32:GLU:HG2	2.24	0.52
1:B:103:ILE:HG23	1:B:105:LEU:HD23	1.92	0.52
1:B:41:GLU:CG	1:B:41:GLU:N	2.70	0.52
1:C:277:ALA:O	1:C:281:VAL:HG23	2.10	0.52
1:A:21:MSE:HE3	1:A:32:GLU:HG2	1.84	0.51
1:A:239:LYS:CB	1:A:240:ASP:CB	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:GLY:O	1:B:310:THR:HG23	2.10	0.51
1:C:215:ARG:HD2	1:C:288:ALA:HB2	1.92	0.51
1:B:295:LEU:CD1	1:B:309:VAL:HG11	2.40	0.51
1:A:248:GLU:OE2	1:A:262:LYS:NZ	2.41	0.51
1:A:21:MSE:CE	1:A:32:GLU:CG	2.74	0.51
1:B:246:ILE:HD11	1:B:266:VAL:HG21	1.92	0.51
1:B:189:THR:HG21	1:B:199:SER:HB3	1.92	0.50
1:C:134:ILE:O	1:C:160:THR:CG2	2.60	0.50
1:C:112:ARG:H	1:C:115:GLN:HE21	1.59	0.50
1:B:72:ASP:CB	1:B:74:ARG:H	2.17	0.50
1:A:300:PRO:CA	1:A:301:SER:C	2.81	0.50
1:C:96:GLY:HA2	1:C:97:VAL:HB	1.89	0.50
1:C:140:ARG:HE	1:C:159:GLN:HE21	1.59	0.50
1:A:8:VAL:HG13	1:A:118:LEU:HD21	1.94	0.50
1:B:72:ASP:HB3	1:B:74:ARG:N	2.17	0.49
1:C:236:THR:CG2	1:C:237:ASN:H	2.26	0.49
1:C:236:THR:HG22	1:C:237:ASN:N	2.27	0.49
1:B:295:LEU:HD12	1:B:309:VAL:HG12	1.92	0.49
1:B:165:ASN:H	1:B:168:ASN:ND2	2.11	0.49
1:A:132:THR:CG2	1:A:132:THR:CA	2.82	0.49
1:C:96:GLY:CA	1:C:97:VAL:CB	2.86	0.49
1:B:142:VAL:O	1:B:154:VAL:HA	2.13	0.48
1:A:66:THR:HB	1:A:78:PHE:CE2	2.48	0.48
1:B:21:MSE:HE2	1:B:23:GLU:CD	2.38	0.48
1:C:112:ARG:H	1:C:115:GLN:NE2	2.11	0.48
1:B:41:GLU:CG	1:B:41:GLU:CA	2.86	0.48
1:C:47:ASN:HD22	1:C:169:SER:HB3	1.78	0.48
1:A:21:MSE:HE2	1:A:23:GLU:CD	2.38	0.48
1:A:158:ILE:O	1:A:206:PHE:HA	2.14	0.47
1:B:222:SER:O	1:B:223:THR:HG23	2.14	0.47
1:C:48:ASN:ND2	1:C:83:ALA:HB1	2.29	0.47
1:B:306:THR:HB	1:B:307:VAL:CG1	2.34	0.47
1:A:123:PRO:HB3	1:A:168:ASN:ND2	2.29	0.47
1:A:132:THR:HG22	1:C:161:ASP:OD2	2.14	0.47
1:B:281:VAL:O	1:B:285:ARG:HG3	2.14	0.47
1:C:96:GLY:CA	1:C:97:VAL:HB	2.44	0.47
1:A:165:ASN:H	1:A:168:ASN:ND2	2.12	0.47
1:A:236:THR:CG2	1:A:237:ASN:H	2.23	0.47
1:C:84:ASP:OD1	1:C:228:HIS:HE1	1.98	0.47
1:B:292:THR:HA	1:B:309:VAL:O	2.15	0.47
1:A:19:VAL:HG21	1:A:120:ILE:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:VAL:HG13	1:A:97:VAL:CG1	2.43	0.47
1:C:269:VAL:HG23	1:C:274:ILE:HD13	1.96	0.47
1:A:140:ARG:HE	1:A:159:GLN:NE2	2.13	0.46
1:A:237:ASN:HD21	1:A:276:SER:HB2	1.79	0.46
1:B:160:THR:CG2	1:B:162:ALA:H	2.28	0.46
1:C:212:GLN:O	1:C:216:ILE:HG13	2.15	0.46
1:A:51:ILE:HG21	1:A:92:VAL:HG21	1.97	0.46
1:A:235:VAL:HG12	1:A:246:ILE:HD13	1.97	0.46
1:B:97:VAL:HG22	1:B:100:LEU:HD13	1.97	0.46
1:B:234:GLN:HA	1:B:235:VAL:HG13	1.98	0.46
1:B:66:THR:HB	1:B:78:PHE:CE2	2.50	0.45
1:C:134:ILE:O	1:C:160:THR:HG23	2.17	0.45
1:A:118:LEU:HB2	1:A:174:VAL:HG22	1.97	0.45
1:B:8:VAL:HG13	1:B:118:LEU:HD21	1.97	0.45
1:C:112:ARG:NH2	1:C:113:VAL:O	2.49	0.45
1:B:21:MSE:HE2	1:B:23:GLU:OE2	2.16	0.45
1:C:134:ILE:H	1:C:161:ASP:HB2	1.80	0.45
1:A:97:VAL:HG22	1:A:100:LEU:HD13	1.99	0.45
1:A:111:LEU:HA	1:A:115:GLN:HE22	1.81	0.45
1:C:84:ASP:OD1	1:C:228:HIS:CE1	2.70	0.45
1:A:19:VAL:HG21	1:A:120:ILE:CG1	2.48	0.44
1:B:246:ILE:HD11	1:B:266:VAL:CG2	2.47	0.44
1:B:266:VAL:HA	1:B:296:THR:O	2.17	0.44
1:A:134:ILE:O	1:A:160:THR:CG2	2.65	0.44
1:A:75:THR:HG21	2:A:342:HOH:O	2.17	0.44
1:C:95:GLN:HA	1:C:95:GLN:HE21	1.82	0.44
1:A:53:ALA:HB3	2:A:357:HOH:O	2.18	0.44
1:B:284:VAL:HB	1:B:285:ARG:HG2	1.99	0.44
1:C:144:THR:HA	1:C:153:THR:O	2.18	0.44
1:B:77:PRO:HD2	2:B:366:HOH:O	2.18	0.44
1:B:97:VAL:HG22	1:B:100:LEU:HD11	1.99	0.44
1:B:270:ASP:OD2	2:B:377:HOH:O	2.21	0.43
1:A:108:SER:HB3	1:A:210:VAL:HG12	2.00	0.43
1:C:118:LEU:HB2	1:C:174:VAL:HG22	2.00	0.43
1:A:84:ASP:HA	1:A:85:PRO:HD3	1.83	0.43
1:A:161:ASP:OD2	1:B:132:THR:HG22	2.19	0.43
1:B:39:SER:HB2	1:B:41:GLU:CG	2.49	0.43
1:C:112:ARG:CD	1:C:112:ARG:CB	2.82	0.43
1:B:216:ILE:HG22	1:B:220:LEU:HD22	2.01	0.43
1:A:118:LEU:HG	1:A:176:MSE:CE	2.38	0.42
1:A:15:VAL:HG11	1:A:174:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:OD1	1:C:85:PRO:HA	2.20	0.42
1:C:270:ASP:OD1	1:C:294:ALA:CB	2.67	0.42
1:C:36:ILE:HG12	1:C:172:ALA:HB2	2.01	0.42
1:A:134:ILE:O	1:A:160:THR:HG23	2.20	0.42
1:B:266:VAL:HG12	1:B:274:ILE:HD12	2.01	0.42
1:A:94:VAL:CG1	1:A:97:VAL:HG13	2.47	0.42
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.86	0.42
1:B:220:LEU:HA	1:B:224:GLY:HA3	2.01	0.41
1:A:19:VAL:HG11	1:A:120:ILE:HG13	2.03	0.41
1:B:250:VAL:O	1:B:256:ALA:HB2	2.20	0.41
1:C:111:LEU:HA	1:C:111:LEU:HD23	1.79	0.41
1:B:85:PRO:O	1:B:152:ASN:HA	2.21	0.41
1:B:153:THR:CG2	2:B:384:HOH:O	2.34	0.41
1:C:68:VAL:O	1:C:75:THR:HA	2.19	0.41
1:C:151:GLN:HA	1:C:152:ASN:CB	2.50	0.41
1:A:83:ALA:H	1:A:220:LEU:HD22	1.86	0.41
1:B:157:ALA:HB1	1:B:206:PHE:HB3	2.03	0.41
1:C:48:ASN:HD22	1:C:83:ALA:HB1	1.85	0.41
1:B:70:PHE:O	1:B:73:GLY:HA2	2.21	0.41
1:C:237:ASN:HD21	1:C:276:SER:CB	2.34	0.41
1:B:84:ASP:OD1	1:B:87:SER:HB2	2.20	0.41
1:C:111:LEU:HA	1:C:115:GLN:NE2	2.36	0.40
1:C:159:GLN:HA	1:C:205:GLY:O	2.21	0.40
1:A:160:THR:HG22	1:A:162:ALA:H	1.87	0.40
1:B:266:VAL:HG13	1:B:295:LEU:HD23	2.04	0.40
1:A:235:VAL:HG11	1:A:280:LEU:HD12	2.04	0.40
1:C:261:PRO:C	1:C:263:GLY:N	2.79	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	273/324 (84%)	252 (92%)	11 (4%)	10 (4%)	2	1
1	B	258/324 (80%)	228 (88%)	16 (6%)	14 (5%)	1	0
1	C	234/324 (72%)	209 (89%)	14 (6%)	11 (5%)	2	0
All	All	765/972 (79%)	689 (90%)	41 (5%)	35 (5%)	2	0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	ASP
1	A	223	THR
1	A	225	LYS
1	A	240	ASP
1	A	254	ALA
1	A	299	ASP
1	A	302	GLY
1	B	198	GLN
1	B	234	GLN
1	B	238	ASP
1	B	270	ASP
1	B	284	VAL
1	B	308	GLN
1	C	97	VAL
1	C	225	LYS
1	C	226	ALA
1	C	262	LYS
1	B	72	ASP
1	B	231	LEU
1	B	235	VAL
1	C	153	THR
1	C	227	SER
1	C	254	ALA
1	C	284	VAL
1	A	83	ALA
1	B	257	ASN
1	C	235	VAL
1	C	263	GLY
1	B	223	THR
1	B	225	LYS
1	A	84	ASP
1	A	238	ASP
1	B	65	LYS
1	C	264	VAL

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Mol	Chain	Res	Type
1	B	233	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	200/242 (83%)	165 (82%)	35 (18%)	2	1
1	B	187/242 (77%)	156 (83%)	31 (17%)	2	1
1	C	174/242 (72%)	145 (83%)	29 (17%)	2	1
All	All	561/726 (77%)	466 (83%)	95 (17%)	2	1

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	16	VAL
1	A	20	VAL
1	A	31	GLU
1	A	41	GLU
1	A	75	THR
1	A	79	THR
1	A	87	SER
1	A	92	VAL
1	A	94	VAL
1	A	97	VAL
1	A	100	LEU
1	A	104	SER
1	A	111	LEU
1	A	120	ILE
1	A	124	LEU
1	A	143	SER
1	A	144	THR
1	A	160	THR
1	A	161	ASP
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	181	VAL
1	A	183	VAL
1	A	199	SER
1	A	214	LYS
1	A	223	THR
1	A	228	HIS
1	A	231	LEU
1	A	238	ASP
1	A	242	LEU
1	A	260	VAL
1	A	280	LEU
1	A	287	LYS
1	A	293	VAL
1	A	313	LYS
1	B	9	GLU
1	B	31	GLU
1	B	41	GLU
1	B	67	THR
1	B	75	THR
1	B	87	SER
1	B	93	ARG
1	B	94	VAL
1	B	95	GLN
1	B	97	VAL
1	B	100	LEU
1	B	153	THR
1	B	160	THR
1	B	161	ASP
1	B	181	VAL
1	B	183	VAL
1	B	190	LEU
1	B	199	SER
1	B	204	LEU
1	B	220	LEU
1	B	223	THR
1	B	231	LEU
1	B	235	VAL
1	B	269	VAL
1	B	280	LEU
1	B	286	SER
1	B	287	LYS
1	B	295	LEU

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Mol	Chain	Res	Type
1	B	307	VAL
1	B	308	GLN
1	B	309	VAL
1	C	41	GLU
1	C	75	THR
1	C	79	THR
1	C	92	VAL
1	C	94	VAL
1	C	95	GLN
1	C	97	VAL
1	C	98	SER
1	C	103	ILE
1	C	104	SER
1	C	112	ARG
1	C	120	ILE
1	C	142	VAL
1	C	143	SER
1	C	144	THR
1	C	153	THR
1	C	155	LEU
1	C	160	THR
1	C	169	SER
1	C	181	VAL
1	C	183	VAL
1	C	190	LEU
1	C	222	SER
1	C	227	SER
1	C	231	LEU
1	C	235	VAL
1	C	274	ILE
1	C	286	SER
1	C	311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	95	GLN
1	A	115	GLN
1	A	159	GLN
1	A	168	ASN
1	A	177	ASN

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Mol	Chain	Res	Type
1	A	179	GLN
1	A	237	ASN
1	A	257	ASN
1	B	95	GLN
1	B	159	GLN
1	B	168	ASN
1	B	177	ASN
1	B	228	HIS
1	C	47	ASN
1	C	95	GLN
1	C	115	GLN
1	C	159	GLN
1	C	168	ASN
1	C	228	HIS
1	C	237	ASN
1	C	275	ASN

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.