



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:16 PM UTC

PDB ID : 2Z9I / pdb_00002z9i
Title : Crystal structure of RV0983 from Mycobacterium tuberculosis- Proteolytically active form
Authors : Palaninathan, S.K.; Mohamedmohaideen, N.N.; Sacchettini, J.C.
Deposited on : 2007-09-20
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

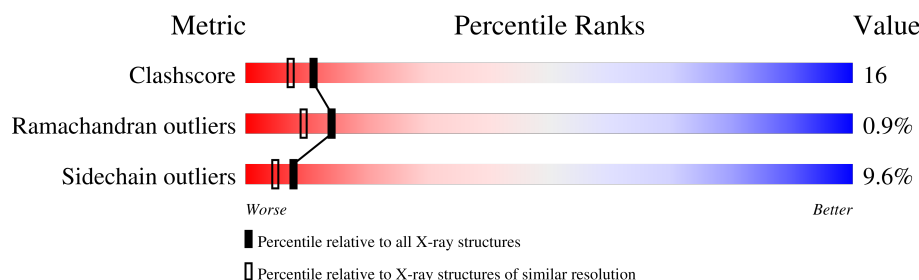
1 Overall quality at a glance

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	61% 20% 6% • 12%
1	B	324	58% 21% • 17%
1	C	324	60% 17% • 20%
2	D	5	60% 20% 20%
2	E	5	60% 20% 20%
2	F	5	40% 40% 20%
3	G	4	25% 50% 25%
3	H	4	25% 25% 50%

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Mol	Chain	Length	Quality of chain
3	I	4	 A horizontal bar chart showing the quality of chain I. The bar is divided into three segments: a yellow segment on the left labeled '50%', an orange segment in the middle labeled '25%', and a grey segment on the right labeled '25%'. The segments are separated by thin black lines.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5920 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 PROBABLE SERINE PROTEASE PEPD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	Se	0	0	0
			1929	1197	338	392	2			
1	B	269	Total	C	N	O	Se	0	0	0
			1788	1107	314	365	2			
1	C	260	Total	C	N	O	Se	0	0	0
			1726	1070	301	353	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	317	LEU	-	expression tag	UNP O53896
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	324	HIS	-	expression tag	UNP O53896

- Molecule 2 is a protein called SVEQV.

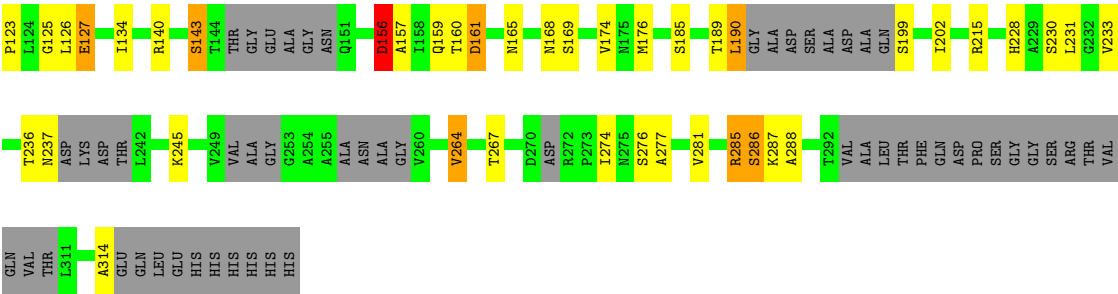
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			32	20	5	7			
2	E	4	Total	C	N	O	0	0	0
			32	20	5	7			
2	F	5	Total	C	N	O	0	0	0
			38	23	6	9			

- Molecule 3 is a protein called GATV.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	4	Total	C	N	O	0	0	0
			24	14	4	6			
3	H	2	Total	C	N	O	0	0	0
			8	4	2	2			
3	I	3	Total	C	N	O	0	0	0
			16	10	3	3			

- Molecule 4 is water.

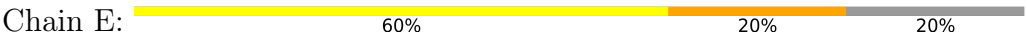
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		
4	B	127	Total	O	0	0
			127	127		
4	C	84	Total	O	0	0
			84	84		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		
4	G	2	Total	O	0	0
			2	2		



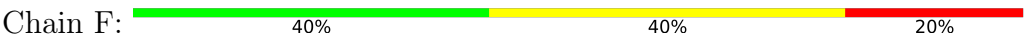
• Molecule 2: SVEQV



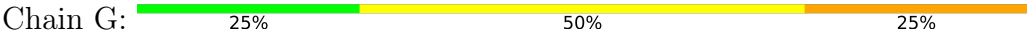
• Molecule 2: SVEQV



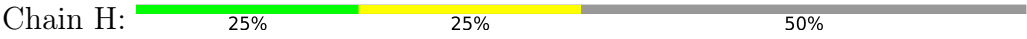
• Molecule 2: SVEQV



• Molecule 3: GATV



• Molecule 3: GATV



• Molecule 3: GATV



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)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	98.8 (50.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5920	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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	0.97	0/1942	1.36	28/2647 (1.1%)
1	B	0.97	0/1796	1.36	28/2445 (1.1%)
1	C	0.92	3/1734 (0.2%)	1.25	19/2361 (0.8%)
2	D	0.89	0/31	1.57	0/41
2	E	1.28	0/31	2.35	2/41 (4.9%)
2	F	1.10	0/37	2.45	2/49 (4.1%)
3	G	2.34	2/23 (8.7%)	2.48	0/29
3	H	2.26	0/7	3.22	0/7
3	I	1.84	1/15 (6.7%)	2.45	2/19 (10.5%)
All	All	0.97	6/5616 (0.1%)	1.36	81/7639 (1.1%)

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	1	2
1	B	0	1
1	C	0	2
2	F	0	1
3	G	0	1
3	H	0	1
3	I	0	1
All	All	1	9

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	PRO	CA-C	8.45	1.56	1.51
3	G	3	THR	CB-OG1	6.56	1.54	1.43
1	C	16	VAL	CA-CB	5.90	1.57	1.54
1	C	157	ALA	N-CA	5.30	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	GLY	N-CA	5.22	1.53	1.45
3	I	2	ALA	C-N	5.12	1.42	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	300	PRO	CA-C-N	10.28	133.80	120.44
1	A	300	PRO	C-N-CA	10.28	133.80	120.44
1	A	272	ARG	CA-C-O	-9.73	112.97	119.29
1	A	271	ASP	CA-C-N	9.13	133.79	121.74
1	A	271	ASP	C-N-CA	9.13	133.79	121.74
1	B	53	ALA	CA-C-N	8.78	136.94	122.62
1	B	53	ALA	C-N-CA	8.78	136.94	122.62
1	C	62	PRO	CA-C-N	8.51	125.87	119.66
1	C	62	PRO	C-N-CA	8.51	125.87	119.66
1	B	235	VAL	N-CA-C	8.08	126.15	109.34
1	A	302	GLY	CA-C-N	8.06	131.39	122.69
1	A	302	GLY	C-N-CA	8.06	131.39	122.69
1	A	270	ASP	CA-CB-CG	8.02	120.62	112.60
1	A	160	THR	CA-C-N	7.97	131.76	120.28
1	A	160	THR	C-N-CA	7.97	131.76	120.28
1	A	161	ASP	N-CA-C	7.94	120.84	111.71
1	A	299	ASP	CA-C-N	7.93	129.76	119.84
1	A	299	ASP	C-N-CA	7.93	129.76	119.84
1	A	272	ARG	O-C-N	-7.88	114.85	121.23
1	B	91	VAL	O-C-N	7.65	131.28	123.10
1	C	160	THR	CA-C-N	7.63	131.91	120.31
1	C	160	THR	C-N-CA	7.63	131.91	120.31
1	B	270	ASP	CA-CB-CG	7.56	120.16	112.60
1	A	238	ASP	N-CA-C	7.29	117.63	108.45
1	A	237	ASN	CA-C-O	-7.18	112.58	120.33
2	F	407	SER	CA-C-N	7.00	134.57	121.97
2	F	407	SER	C-N-CA	7.00	134.57	121.97
1	C	126	LEU	O-C-N	-6.83	114.33	122.46
1	A	237	ASN	CA-C-N	6.77	133.84	122.20
1	A	237	ASN	C-N-CA	6.77	133.84	122.20
1	B	54	ALA	CA-C-N	6.75	133.85	121.70
1	B	54	ALA	C-N-CA	6.75	133.85	121.70
1	B	93	ARG	O-C-N	6.74	131.29	123.41
1	B	40	ALA	CA-C-N	6.71	133.47	121.66
1	B	40	ALA	C-N-CA	6.71	133.47	121.66
1	B	88	ASP	CA-C-O	6.60	129.13	121.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	ARG	O-C-N	6.55	128.63	121.36
1	C	161	ASP	N-CA-C	6.42	119.26	111.82
1	C	156	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	57	PRO	CA-C-N	6.31	126.68	119.93
1	C	57	PRO	C-N-CA	6.31	126.68	119.93
1	B	91	VAL	CA-C-N	6.30	131.53	122.77
1	B	91	VAL	C-N-CA	6.30	131.53	122.77
2	E	408	VAL	CA-C-N	6.13	132.02	123.07
2	E	408	VAL	C-N-CA	6.13	132.02	123.07
1	B	88	ASP	CA-CB-CG	6.13	118.73	112.60
1	C	156	ASP	CB-CA-C	6.04	120.01	111.74
1	C	236	THR	CA-C-N	5.98	132.47	121.70
1	C	236	THR	C-N-CA	5.98	132.47	121.70
1	B	270	ASP	CA-C-O	5.98	129.21	122.27
1	A	238	ASP	O-C-N	-5.97	115.03	122.73
1	B	185	SER	CA-C-N	-5.97	112.81	122.36
1	B	185	SER	C-N-CA	-5.97	112.81	122.36
3	I	3	THR	N-CA-C	5.91	118.44	107.99
1	A	272	ARG	CA-C-N	5.88	125.82	119.76
1	A	272	ARG	C-N-CA	5.88	125.82	119.76
1	B	51	ILE	CA-C-O	5.87	125.31	119.97
1	B	270	ASP	CA-C-N	5.80	132.15	123.05
1	B	270	ASP	C-N-CA	5.80	132.15	123.05
1	C	63	PRO	CA-C-N	5.78	125.71	119.76
1	C	63	PRO	C-N-CA	5.78	125.71	119.76
1	B	54	ALA	N-CA-C	5.70	118.21	110.06
1	A	238	ASP	CA-C-O	-5.69	115.28	121.14
1	C	63	PRO	N-CA-C	5.68	115.92	110.47
1	A	271	ASP	CA-CB-CG	5.57	118.17	112.60
1	C	125	GLY	N-CA-C	-5.55	107.59	115.30
1	B	157	ALA	N-CA-C	5.52	118.92	110.20
1	B	237	ASN	N-CA-C	5.44	118.80	110.20
1	A	71	SER	CA-C-N	5.42	128.09	120.28
1	A	71	SER	C-N-CA	5.42	128.09	120.28
1	A	298	GLN	CA-CB-CG	5.36	124.83	114.10
1	A	72	ASP	N-CA-C	5.34	117.85	111.71
1	A	299	ASP	CA-CB-CG	5.25	117.86	112.60
3	I	2	ALA	O-C-N	-5.08	114.88	123.00
1	B	50	VAL	CA-C-N	5.04	131.75	122.88
1	B	50	VAL	C-N-CA	5.04	131.75	122.88
1	C	169	SER	CA-C-O	5.02	126.22	120.80
1	B	4	PRO	CA-C-N	5.02	125.25	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	PRO	C-N-CA	5.02	125.25	119.83
1	C	143	SER	CA-C-N	5.01	130.72	121.70
1	C	143	SER	C-N-CA	5.01	130.72	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	238	ASP	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ASN	Mainchain
1	A	238	ASP	Mainchain
1	B	235	VAL	Mainchain
1	C	156	ASP	Mainchain
1	C	267	THR	Mainchain
2	F	409	GLU	Mainchain
3	G	1	GLY	Mainchain
3	H	3	THR	Mainchain
3	I	2	ALA	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1929	0	1950	76	0
1	B	1788	0	1764	65	0
1	C	1726	0	1696	43	0
2	D	32	0	31	2	0
2	E	32	0	31	13	0
2	F	38	0	36	1	0
3	G	24	0	26	1	0
3	H	8	0	1	0	0
3	I	16	0	11	5	0
4	A	111	0	0	3	0
4	B	127	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	84	0	0	3	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
All	All	5920	0	5546	181	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 16.

All (181) 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:239:LYS:C	1:A:241:THR:HG22	1.65	1.20
1:A:299:ASP:OD2	1:A:301:SER:HB2	1.46	1.15
1:B:285:ARG:HH11	1:B:285:ARG:HG2	1.12	1.14
1:A:132:THR:HG22	4:C:455:HOH:O	1.52	1.09
1:A:285:ARG:HG2	1:A:285:ARG:HH11	0.95	1.09
1:A:21:MSE:HE3	1:A:32:GLU:HG3	1.26	1.08
1:B:118:LEU:CD2	1:B:132:THR:HG22	1.85	1.05
1:A:21:MSE:HE3	1:A:32:GLU:CG	1.88	1.03
1:B:21:MSE:HE3	1:B:32:GLU:HG3	1.44	0.97
1:A:285:ARG:HG2	1:A:285:ARG:NH1	1.74	0.97
1:A:239:LYS:C	1:A:241:THR:CG2	2.38	0.96
1:B:21:MSE:HE3	1:B:32:GLU:CG	1.97	0.94
1:B:186:ALA:HB1	2:E:408:VAL:CG2	1.99	0.93
1:A:237:ASN:ND2	1:A:276:SER:HA	1.86	0.90
1:B:165:ASN:H	1:B:168:ASN:HD22	1.19	0.85
1:B:186:ALA:HB1	2:E:408:VAL:HG23	1.57	0.85
1:A:285:ARG:HH11	1:A:285:ARG:CG	1.87	0.85
1:A:268:LYS:HD3	1:A:271:ASP:OD1	1.78	0.84
1:A:166:PRO:HG2	1:C:190:LEU:HD21	1.58	0.83
1:B:118:LEU:HD23	1:B:132:THR:HG22	1.58	0.83
1:B:283:ALA:O	1:B:287:LYS:HD3	1.81	0.79
1:C:165:ASN:H	1:C:168:ASN:HD22	1.27	0.79
1:B:285:ARG:HG2	1:B:285:ARG:NH1	1.81	0.78
1:C:118:LEU:HG	1:C:176:MSE:HE1	1.65	0.78
1:B:108:SER:HB2	4:B:487:HOH:O	1.85	0.76
1:B:54:ALA:HB3	1:B:80:VAL:HG21	1.68	0.75
1:A:142:VAL:HG13	2:D:408:VAL:HG11	1.68	0.75
1:B:206:PHE:CE2	2:E:408:VAL:HG11	2.21	0.75
1:A:237:ASN:HD21	1:A:276:SER:HA	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:HD21	1:A:276:SER:CA	2.00	0.75
1:B:118:LEU:HG	1:B:176:MSE:HE1	1.68	0.74
1:B:206:PHE:CD2	2:E:408:VAL:HG11	2.22	0.74
1:A:142:VAL:CG1	2:D:408:VAL:HG11	2.17	0.74
1:A:239:LYS:O	1:A:241:THR:HG22	1.88	0.73
1:B:186:ALA:CB	2:E:408:VAL:HG21	2.18	0.73
1:B:285:ARG:HH11	1:B:285:ARG:CG	1.97	0.73
1:A:21:MSE:CE	1:A:32:GLU:HG3	2.12	0.73
1:A:131:THR:HG22	1:C:161:ASP:OD2	1.89	0.73
1:A:156:ASP:OD1	1:A:272:ARG:NH1	2.21	0.73
1:A:78:PHE:HB2	1:A:92:VAL:HG13	1.70	0.72
1:A:165:ASN:H	1:A:168:ASN:HD22	1.36	0.72
1:C:233:VAL:HG23	3:I:4:VAL:CG1	2.20	0.71
1:B:189:THR:HG22	4:B:484:HOH:O	1.90	0.71
1:A:237:ASN:HD21	1:A:276:SER:CB	2.03	0.70
1:B:186:ALA:HB1	2:E:408:VAL:HG21	1.70	0.70
1:C:233:VAL:CG2	3:I:4:VAL:HG13	2.21	0.70
1:A:189:THR:HG21	1:A:199:SER:HB3	1.74	0.70
1:A:111:LEU:HD21	1:A:181:VAL:HG13	1.74	0.70
1:C:189:THR:HG21	1:C:199:SER:HB3	1.77	0.67
1:B:165:ASN:N	1:B:168:ASN:HD22	1.93	0.66
1:B:87:SER:OG	1:B:216:ILE:HD13	1.96	0.66
1:B:165:ASN:H	1:B:168:ASN:ND2	1.93	0.66
1:B:21:MSE:CE	1:B:32:GLU:HG3	2.23	0.65
1:C:79:THR:HG23	1:C:93:ARG:HB3	1.78	0.65
1:B:186:ALA:CB	2:E:408:VAL:CG2	2.72	0.65
1:C:233:VAL:CG2	3:I:4:VAL:CG1	2.75	0.65
1:A:94:VAL:HG13	1:A:97:VAL:CG1	2.26	0.64
1:A:237:ASN:HD21	1:A:276:SER:HB2	1.63	0.63
1:C:78:PHE:HB2	1:C:92:VAL:HG13	1.79	0.63
1:B:54:ALA:HB3	1:B:80:VAL:CG2	2.29	0.62
1:A:268:LYS:CD	1:A:271:ASP:OD1	2.47	0.62
1:C:233:VAL:HG22	3:I:4:VAL:HG13	1.81	0.61
1:A:94:VAL:HG13	1:A:97:VAL:HG13	1.81	0.61
1:B:269:VAL:HG22	1:B:274:ILE:HD11	1.82	0.61
1:A:239:LYS:O	1:A:241:THR:CG2	2.47	0.60
1:B:187:ILE:O	2:E:408:VAL:HB	2.00	0.60
1:C:285:ARG:C	1:C:287:LYS:H	2.09	0.60
1:C:189:THR:HG1	2:F:407:SER:N	2.00	0.58
1:A:268:LYS:HE2	1:A:271:ASP:CB	2.32	0.58
1:A:299:ASP:OD2	1:A:301:SER:CB	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:SER:CB	1:A:216:ILE:HD13	2.34	0.57
1:A:94:VAL:CG1	1:A:97:VAL:HG13	2.35	0.57
1:B:123:PRO:HB3	1:B:168:ASN:ND2	2.19	0.57
1:A:268:LYS:HE2	1:A:271:ASP:HA	1.86	0.57
1:B:118:LEU:HD22	1:B:132:THR:HG22	1.80	0.57
1:A:134:ILE:HD13	1:B:132:THR:HG23	1.86	0.56
1:B:118:LEU:CD2	1:B:132:THR:CG2	2.74	0.56
1:B:140:ARG:HE	1:B:159:GLN:NE2	2.03	0.56
1:B:142:VAL:HG13	2:E:408:VAL:HG13	1.87	0.56
1:A:118:LEU:HG	1:A:176:MSE:HE1	1.87	0.56
1:A:165:ASN:H	1:A:168:ASN:ND2	2.04	0.56
1:B:86:THR:O	1:B:153:THR:HB	2.05	0.56
1:C:245:LYS:HA	1:C:264:VAL:O	2.06	0.55
1:C:140:ARG:HE	1:C:159:GLN:NE2	2.03	0.55
1:C:233:VAL:HG23	3:I:4:VAL:HG12	1.87	0.55
1:C:123:PRO:HB3	1:C:168:ASN:ND2	2.23	0.54
1:C:15:VAL:HG11	1:C:174:VAL:HG11	1.89	0.54
1:A:268:LYS:HB2	1:A:272:ARG:O	2.08	0.54
1:B:206:PHE:CE2	2:E:408:VAL:CG1	2.89	0.54
1:A:84:ASP:OD1	1:A:228:HIS:HE1	1.91	0.54
1:C:112:ARG:H	1:C:115:GLN:HE21	1.56	0.53
1:C:156:ASP:OD2	1:C:286:SER:HB2	2.09	0.53
1:C:112:ARG:H	1:C:115:GLN:NE2	2.07	0.53
1:A:21:MSE:HE2	1:A:23:GLU:CD	2.34	0.52
1:A:268:LYS:HE2	1:A:271:ASP:HB3	1.91	0.52
1:B:66:THR:HB	1:B:78:PHE:CE2	2.44	0.52
1:A:235:VAL:HG12	1:A:246:ILE:HD13	1.91	0.52
1:C:165:ASN:H	1:C:168:ASN:ND2	2.01	0.52
1:A:55:ALA:HB2	1:A:80:VAL:HG21	1.92	0.52
1:C:48:ASN:ND2	1:C:83:ALA:HB1	2.25	0.51
2:E:409:GLU:O	2:E:411:VAL:HG13	2.10	0.51
1:B:24:THR:O	1:B:30:SER:HA	2.11	0.51
1:B:15:VAL:HG11	1:B:174:VAL:HG11	1.92	0.51
1:C:47:ASN:HD21	1:C:185:SER:HA	1.75	0.51
1:B:54:ALA:CB	1:B:80:VAL:HG21	2.40	0.50
1:B:97:VAL:HG22	1:B:100:LEU:HD13	1.92	0.50
1:C:111:LEU:HA	1:C:115:GLN:HE22	1.76	0.50
1:A:15:VAL:HG11	1:A:174:VAL:HG11	1.92	0.50
1:C:140:ARG:HE	1:C:159:GLN:HE21	1.60	0.50
1:B:67:THR:HG23	1:B:75:THR:HG23	1.92	0.50
1:B:186:ALA:HB3	2:E:408:VAL:HG21	1.91	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:HB	1:A:78:PHE:CE2	2.47	0.49
1:B:8:VAL:HG13	1:B:118:LEU:HD21	1.95	0.49
1:C:21:MSE:HE2	1:C:127:GLU:HG3	1.94	0.49
1:B:48:ASN:OD1	1:B:83:ALA:HB1	2.13	0.49
1:C:31:GLU:HG3	4:C:461:HOH:O	2.12	0.49
1:A:144:THR:O	1:A:152:ASN:HA	2.12	0.48
1:C:237:ASN:HD21	1:C:276:SER:HB2	1.78	0.48
1:A:143:SER:HB3	1:A:154:VAL:HG22	1.95	0.48
1:A:123:PRO:HB3	1:A:168:ASN:ND2	2.29	0.48
1:B:87:SER:CB	1:B:216:ILE:HD13	2.44	0.48
1:A:72:ASP:OD2	1:A:74:ARG:NE	2.46	0.48
1:A:72:ASP:HB3	1:A:74:ARG:H	1.77	0.48
1:A:93:ARG:HG2	1:A:94:VAL:N	2.29	0.48
1:B:21:MSE:HE2	1:B:23:GLU:CD	2.39	0.47
1:C:66:THR:HB	1:C:78:PHE:CE2	2.49	0.47
1:A:190:LEU:HD21	1:B:124:LEU:HD21	1.96	0.47
1:A:233:VAL:HG23	1:A:235:VAL:HG13	1.96	0.47
1:A:132:THR:HG23	4:A:334:HOH:O	2.15	0.47
1:B:54:ALA:CB	1:B:80:VAL:CG2	2.93	0.47
1:C:84:ASP:OD1	1:C:228:HIS:HE1	1.98	0.46
3:G:4:VAL:HG22	3:G:4:VAL:OXT	2.16	0.46
1:C:8:VAL:HG13	1:C:118:LEU:HD21	1.97	0.46
1:C:190:LEU:HD12	1:C:202:ILE:HD13	1.97	0.46
1:A:285:ARG:NH1	1:A:285:ARG:CG	2.57	0.46
1:A:140:ARG:HE	1:A:159:GLN:NE2	2.14	0.46
1:A:97:VAL:HG22	1:A:100:LEU:CD1	2.46	0.45
1:C:230:SER:HB3	1:C:314:ALA:HA	1.97	0.45
1:C:277:ALA:O	1:C:281:VAL:HG23	2.16	0.45
1:A:9:GLU:HG2	1:C:112:ARG:HG3	1.97	0.45
1:B:97:VAL:HG22	1:B:100:LEU:CD1	2.47	0.45
1:A:105:LEU:CD1	1:A:214:LYS:HD2	2.46	0.44
1:B:84:ASP:OD1	1:B:228:HIS:HE1	2.00	0.44
1:A:275:ASN:ND2	1:A:275:ASN:C	2.75	0.44
1:A:8:VAL:HG13	1:A:118:LEU:HD21	2.00	0.44
1:C:62:PRO:HA	1:C:63:PRO:HD2	1.78	0.44
1:B:21:MSE:HE3	1:B:32:GLU:CD	2.43	0.44
1:B:274:ILE:HG23	1:B:279:ALA:HB3	1.98	0.44
1:B:39:SER:HB2	1:B:41:GLU:HG2	1.99	0.44
1:B:243:GLY:HA2	1:B:274:ILE:O	2.18	0.44
1:C:237:ASN:HD21	1:C:276:SER:CB	2.31	0.44
1:B:236:THR:HA	1:B:277:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:THR:HG22	4:B:378:HOH:O	2.18	0.43
1:A:51:ILE:HD12	1:A:51:ILE:C	2.44	0.43
1:C:140:ARG:HH21	1:C:159:GLN:HE22	1.65	0.43
1:A:20:VAL:CG1	1:A:68:VAL:HG13	2.49	0.43
1:B:272:ARG:HA	1:B:273:PRO:HD3	1.85	0.43
1:B:140:ARG:HH21	1:B:159:GLN:HE22	1.66	0.42
1:A:231:LEU:HD22	1:A:255:ALA:HB2	2.00	0.42
1:B:39:SER:C	1:B:41:GLU:H	2.26	0.42
1:A:275:ASN:HB3	4:B:457:HOH:O	2.20	0.42
1:A:21:MSE:HE3	1:A:32:GLU:HG2	1.92	0.42
1:A:268:LYS:HA	1:A:274:ILE:HG12	2.02	0.42
1:C:215:ARG:CD	1:C:288:ALA:HB2	2.49	0.42
1:A:70:PHE:C	1:A:72:ASP:N	2.74	0.42
1:A:97:VAL:HG22	1:A:100:LEU:HD13	2.02	0.42
1:A:239:LYS:C	1:A:241:THR:HG21	2.39	0.42
1:C:86:THR:HG23	4:C:444:HOH:O	2.19	0.42
1:A:51:ILE:HG21	1:A:92:VAL:HG21	2.02	0.41
1:C:285:ARG:C	1:C:287:LYS:N	2.76	0.41
1:A:21:MSE:HE1	4:A:405:HOH:O	2.21	0.41
1:B:50:VAL:HG21	1:B:169:SER:O	2.21	0.41
1:C:134:ILE:H	1:C:161:ASP:HB2	1.86	0.41
1:A:111:LEU:HA	1:A:115:GLN:HE22	1.85	0.41
1:B:165:ASN:O	1:B:168:ASN:HB2	2.21	0.40
1:A:165:ASN:O	1:A:168:ASN:HB2	2.21	0.40
1:B:267:THR:H	1:B:296:THR:HB	1.86	0.40
1:B:292:THR:HG22	1:B:293:VAL:N	2.36	0.40
1:A:153:THR:HG21	4:A:426:HOH:O	2.21	0.40
1:B:143:SER:O	2:E:408:VAL:N	2.53	0.40
1:B:142:VAL:O	1:B:154:VAL:HA	2.21	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	272/324 (84%)	266 (98%)	4 (2%)	2 (1%)	18	14
1	B	253/324 (78%)	245 (97%)	6 (2%)	2 (1%)	16	11
1	C	240/324 (74%)	226 (94%)	12 (5%)	2 (1%)	16	11
2	D	2/5 (40%)	2 (100%)	0	0	100	100
2	E	2/5 (40%)	2 (100%)	0	0	100	100
2	F	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
3	G	2/4 (50%)	2 (100%)	0	0	100	100
3	I	1/4 (25%)	1 (100%)	0	0	100	100
All	All	775/995 (78%)	746 (96%)	22 (3%)	7 (1%)	14	9

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	ASP
1	B	235	VAL
1	C	264	VAL
1	A	300	PRO
1	B	52	ALA
2	F	408	VAL
1	C	286	SER

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	203/242 (84%)	177 (87%)	26 (13%)	4	2
1	B	180/242 (74%)	166 (92%)	14 (8%)	11	8
1	C	176/242 (73%)	163 (93%)	13 (7%)	13	9
2	D	4/5 (80%)	4 (100%)	0	100	100
2	E	4/5 (80%)	3 (75%)	1 (25%)	0	0
2	F	5/5 (100%)	4 (80%)	1 (20%)	1	0
3	G	2/2 (100%)	2 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	1/2 (50%)	1 (100%)	0	100	100
All	All	575/745 (77%)	520 (90%)	55 (10%)	8	5

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	20	VAL
1	A	72	ASP
1	A	79	THR
1	A	92	VAL
1	A	94	VAL
1	A	97	VAL
1	A	100	LEU
1	A	101	THR
1	A	111	LEU
1	A	132	THR
1	A	153	THR
1	A	169	SER
1	A	174	VAL
1	A	181	VAL
1	A	198	GLN
1	A	231	LEU
1	A	238	ASP
1	A	242	LEU
1	A	275	ASN
1	A	280	LEU
1	A	285	ARG
1	A	293	VAL
1	A	298	GLN
1	A	301	SER
1	A	313	LYS
1	B	30	SER
1	B	41	GLU
1	B	75	THR
1	B	95	GLN
1	B	97	VAL
1	B	100	LEU
1	B	199	SER
1	B	237	ASN
1	B	257	ASN
1	B	280	LEU

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Mol	Chain	Res	Type
1	B	285	ARG
1	B	286	SER
1	B	295	LEU
1	B	309	VAL
1	C	75	THR
1	C	79	THR
1	C	92	VAL
1	C	98	SER
1	C	104	SER
1	C	107	SER
1	C	112	ARG
1	C	127	GLU
1	C	143	SER
1	C	190	LEU
1	C	231	LEU
1	C	274	ILE
1	C	285	ARG
2	E	410	GLN
2	F	407	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	115	GLN
1	A	159	GLN
1	A	168	ASN
1	A	198	GLN
1	A	228	HIS
1	A	237	ASN
1	A	257	ASN
1	A	275	ASN
1	A	298	GLN
1	B	95	GLN
1	B	159	GLN
1	B	168	ASN
1	B	228	HIS
1	C	47	ASN
1	C	115	GLN
1	C	159	GLN
1	C	168	ASN
1	C	228	HIS

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Mol	Chain	Res	Type
1	C	237	ASN
2	E	410	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](#)

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.