Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:03 AM GMT

PDB ID	:	2Z9I
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

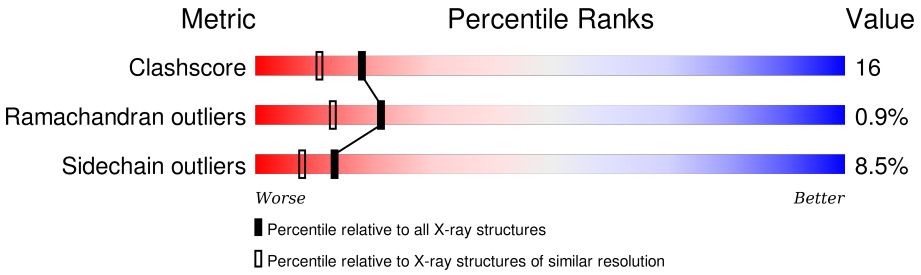
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	324	63% 19% 5% 12%
1	B	324	60% 20% • 17%
1	C	324	62% 15% • 20%
2	D	5	60% 20% 20%
2	E	5	20% 60% 20%
2	F	5	40% 40% 20%
3	G	4	25% 50% 25%

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Mol	Chain	Length	Quality of chain
3	H	4	25% 25% 50%
3	I	4	25% 50% 25%

2 Entry composition (i)

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 32 20 5 7	0	0	0
2	E	4	Total C N O 32 20 5 7	0	0	0
2	F	5	Total C N O 38 23 6 9	0	0	0

- Molecule 3 is a protein called GATV.

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

- Molecule 4 is water.

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

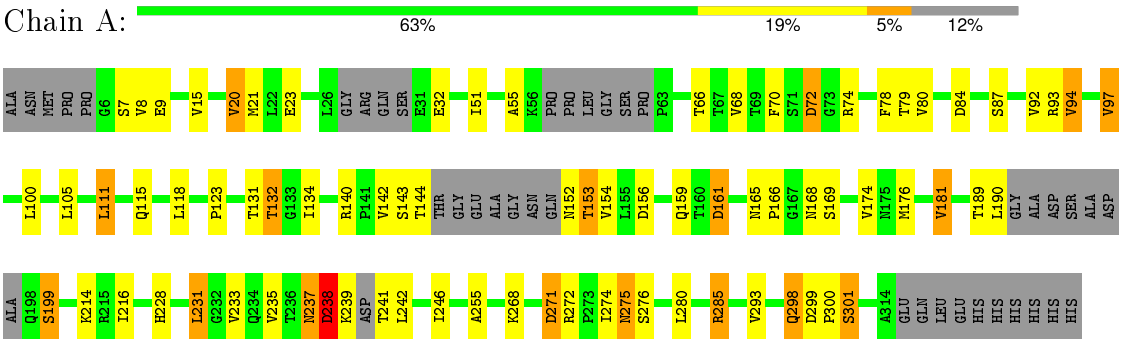
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

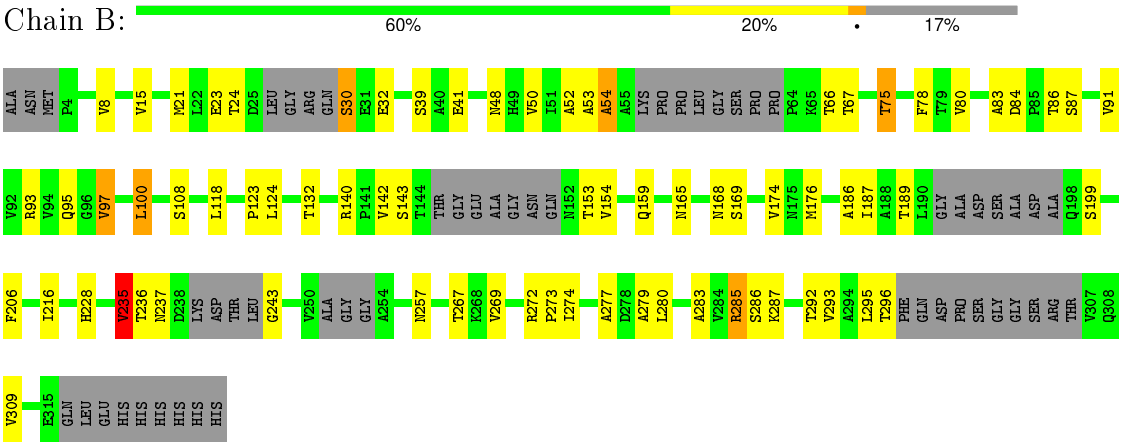
• Molecule 1: PROBABLE SERINE PROTEASE PEPD

Chain A:



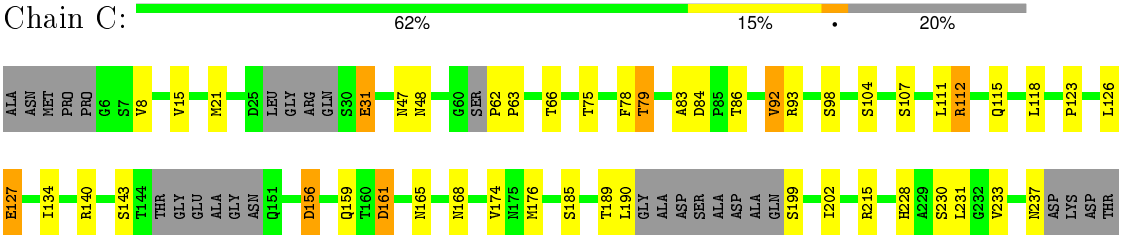
• Molecule 1: PROBABLE SERINE PROTEASE PEPD

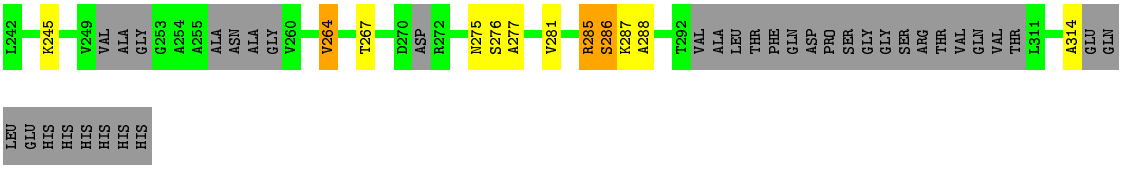
Chain B:



• Molecule 1: PROBABLE SERINE PROTEASE PEPD

Chain C:



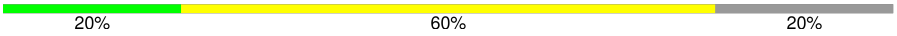


- Molecule 2: SVEQV

Chain D:

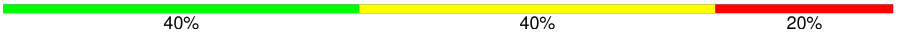
- Molecule 2: SVEQV

Chain E:



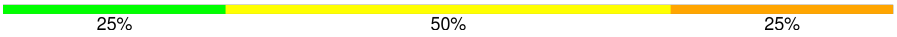
- Molecule 2: SVEQV

Chain F:



- Molecule 3: GATV

Chain G:

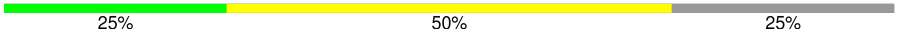


- Molecule 3: GATV

Chain H:

- Molecule 3: GATV

Chain I:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.58Å 89.07Å 69.41Å 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	0.71	0/1942	0.92	3/2647 (0.1%)
1	B	0.68	0/1796	0.95	7/2445 (0.3%)
1	C	0.65	0/1734	0.83	2/2361 (0.1%)
2	D	0.76	0/31	1.32	0/41
2	E	1.09	0/31	1.89	0/41
2	F	0.90	0/37	1.85	1/49 (2.0%)
3	G	2.12	2/23 (8.7%)	2.37	1/29 (3.4%)
3	H	1.75	0/7	2.77	0/7
3	I	1.28	0/15	1.90	0/19
All	All	0.70	2/5616 (0.0%)	0.94	14/7639 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3	THR	CB-OG1	5.50	1.54	1.43
3	G	1	GLY	N-CA	5.23	1.53	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	53	ALA	C-N-CA	6.09	136.94	121.70
3	G	1	GLY	CA-C-N	-5.95	104.11	117.20
1	B	235	VAL	N-CA-C	5.61	126.15	111.00
1	B	54	ALA	CB-CA-C	5.47	118.31	110.10
1	B	93	ARG	O-C-N	5.37	131.29	122.70
1	B	91	VAL	O-C-N	5.37	131.28	122.70
1	A	238	ASP	CB-CG-OD1	5.25	123.03	118.30
1	C	126	LEU	O-C-N	-5.23	114.33	122.70
1	A	161	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	A	298	GLN	CA-CB-CG	5.19	124.83	113.40
2	F	407	SER	C-N-CA	5.15	134.57	121.70
1	B	53	ALA	N-CA-CB	5.11	117.26	110.10
1	C	161	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	53	ALA	CB-CA-C	5.03	117.64	110.10

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 (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	1929	0	1950	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1788	0	1763	63	0
1	C	1726	0	1696	42	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
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	5545	175	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 (175) 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:299:ASP:OD2	1:A:301:SER:HB2	1.46	1.15
1:A:239:LYS:C	1:A:241:THR:HG22	1.65	1.15
1:B:285:ARG:HG2	1:B:285:ARG:HH11	1.12	1.14
1:A:132:THR:HG22	4:C:455:HOH:O	1.52	1.09
1:A:285:ARG:HH11	1:A:285:ARG:HG2	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:NH1	1:A:285:ARG:HG2	1.74	0.97
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:239:LYS:C	1:A:241:THR:CG2	2.38	0.92
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:CG	1:A:285:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:206:PHE:CE2	2:E:408:VAL:HG11	2.21	0.75
1:A:142:VAL:HG13	2:D:408:VAL:HG11	1.68	0.75
1:A:237:ASN:HD21	1:A:276:SER:HA	1.49	0.75
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:CG	1:B:285:ARG:HH11	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:B:186:ALA:HB1	2:E:408:VAL:HG21	1.70	0.70
1:A:237:ASN:HD21	1:A:276:SER:CB	2.03	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:165:ASN:H	1:B:168:ASN:ND2	1.93	0.66
1:B:87:SER:OG	1:B:216:ILE:HD13	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:THR:HG1	2:F:407:SER:N	1.99	0.60
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
1:B:123:PRO:HB3	1:B:168:ASN:ND2	2.19	0.57
1:A:94:VAL:CG1	1:A:97:VAL:HG13	2.35	0.57
1:A:87:SER:CB	1:A:216:ILE:HD13	2.34	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: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:A:118:LEU:HG	1:A:176:MSE:HE1	1.87	0.56
1:C:285:ARG:C	1:C:287:LYS:H	2.09	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:111:LEU:HA	1:C:115:GLN:HE22	1.76	0.50
1:B:97:VAL:HG22	1:B:100:LEU:HD13	1.92	0.50
1:C:140:ARG:HE	1:C:159:GLN:HE21	1.60	0.50
1:A:15:VAL:HG11	1:A:174:VAL:HG11	1.92	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
1:B:8:VAL:HG13	1:B:118:LEU:HD21	1.95	0.49
1:A:66:THR:HB	1:A:78:PHE:CE2	2.47	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:A:21:MSE:HE2	1:A:23:GLU:CD	2.34	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:HB3	1:A:74:ARG:H	1.77	0.48
1:A:72:ASP:OD2	1:A:74:ARG:NE	2.46	0.48
1:A:93:ARG:HG2	1:A:94:VAL:N	2.29	0.48
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:CG	1:A:285:ARG:NH1	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:277:ALA:O	1:C:281:VAL:HG23	2.16	0.45
1:C:230:SER:HB3	1:C:314:ALA:HA	1.97	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:B:84:ASP:OD1	1:B:228:HIS:HE1	2.00	0.44
1:A:105:LEU:CD1	1:A:214:LYS:HD2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:75:THR:HG22	4:B:378:HOH:O	2.18	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:21:MSE:HE2	1:B:23:GLU:CD	2.39	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: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:97:VAL:HG22	1:A:100:LEU:HD13	2.02	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:A:21:MSE:HE1	4:A:405:HOH:O	2.21	0.41
1:C:134:ILE:H	1:C:161:ASP:HB2	1.86	0.41
1:B:50:VAL:HG21	1:B:169:SER:O	2.21	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:B:143:SER:O	2:E:408:VAL:N	2.53	0.40
1:A:153:THR:HG21	4:A:426:HOH:O	2.21	0.40
1:A:70:PHE:C	1:A:72:ASP:N	2.74	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%)	26	19
1	B	253/324 (78%)	245 (97%)	6 (2%)	2 (1%)	24	15
1	C	240/324 (74%)	226 (94%)	12 (5%)	2 (1%)	24	15
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%)	21	13

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%)	181 (89%)	22 (11%)	8 4
1	B	180/242 (74%)	167 (93%)	13 (7%)	18 12
1	C	176/242 (73%)	163 (93%)	13 (7%)	17 11
2	D	4/5 (80%)	4 (100%)	0	100 100
2	E	4/5 (80%)	4 (100%)	0	100 100
2	F	5/5 (100%)	4 (80%)	1 (20%)	1 0
3	G	2/2 (100%)	2 (100%)	0	100 100
3	I	1/2 (50%)	1 (100%)	0	100 100
All	All	575/745 (77%)	526 (92%)	49 (8%)	13 8

All (49) 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	94	VAL
1	A	97	VAL
1	A	111	LEU
1	A	132	THR
1	A	153	THR
1	A	161	ASP
1	A	169	SER
1	A	181	VAL
1	A	199	SER
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	B	30	SER
1	B	75	THR
1	B	95	GLN
1	B	97	VAL
1	B	100	LEU

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Mol	Chain	Res	Type
1	B	199	SER
1	B	237	ASN
1	B	257	ASN
1	B	280	LEU
1	B	285	ARG
1	B	286	SER
1	B	295	LEU
1	B	309	VAL
1	C	31	GLU
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	231	LEU
1	C	275	ASN
1	C	285	ARG
2	F	407	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
1	C	168	ASN
1	C	228	HIS
1	C	237	ASN
1	C	275	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.