Full wwPDB X-ray Structure Validation Report (i)

Mar 1, 2026 – 11:58 PM UTC

PDB ID	:	5UWV / pdb_00005uwv
Title	:	Crystal structure of Mycobacterium abscessus L,D-transpeptidase 2
Authors	:	Kumar, P.; Ginell, S.L.; Lamichhane, G.
Deposited on	:	2017-02-21
Resolution	:	2.98 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 (i) 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 (1)) were used in the production of this report:

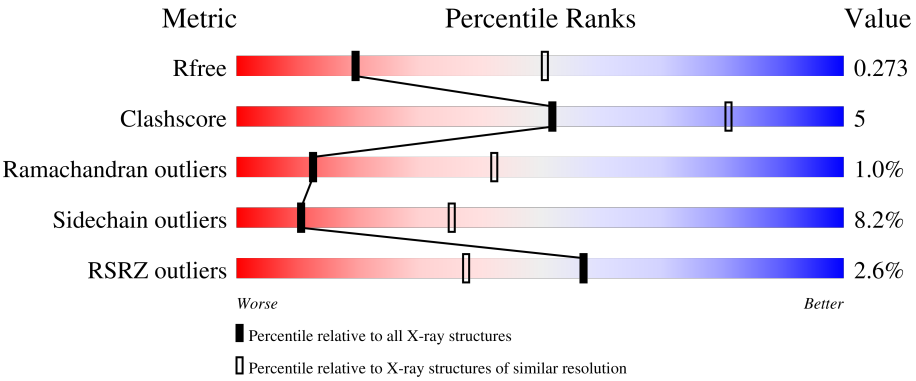
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 <=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	368	75% 14% • 10%
1	B	368	76% 14% • 9%
1	C	368	73% 16% • 8%
1	D	368	5% 70% 19% • 9%
1	E	368	2% 74% 17% • 9%

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Mol	Chain	Length	Quality of chain
1	F	368	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15188 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 L,D-TRANSPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	334	Total	C	N	O	S	0	0	0
			2517	1576	436	495	10			
1	A	333	Total	C	N	O	S	0	0	0
			2529	1582	441	496	10			
1	D	334	Total	C	N	O	S	0	0	0
			2506	1566	437	493	10			
1	E	335	Total	C	N	O	S	0	0	0
			2523	1577	439	497	10			
1	C	338	Total	C	N	O	S	0	0	0
			2533	1583	439	501	10			
1	F	337	Total	C	N	O	S	0	0	0
			2520	1577	435	498	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	39	GLY	-	expression tag	UNP B1MMQ4
B	40	HIS	-	expression tag	UNP B1MMQ4
B	41	MET	-	expression tag	UNP B1MMQ4
A	39	GLY	-	expression tag	UNP B1MMQ4
A	40	HIS	-	expression tag	UNP B1MMQ4
A	41	MET	-	expression tag	UNP B1MMQ4
D	39	GLY	-	expression tag	UNP B1MMQ4
D	40	HIS	-	expression tag	UNP B1MMQ4
D	41	MET	-	expression tag	UNP B1MMQ4
E	39	GLY	-	expression tag	UNP B1MMQ4
E	40	HIS	-	expression tag	UNP B1MMQ4
E	41	MET	-	expression tag	UNP B1MMQ4
C	39	GLY	-	expression tag	UNP B1MMQ4
C	40	HIS	-	expression tag	UNP B1MMQ4
C	41	MET	-	expression tag	UNP B1MMQ4
F	39	GLY	-	expression tag	UNP B1MMQ4
F	40	HIS	-	expression tag	UNP B1MMQ4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	41	MET	-	expression tag	UNP B1MMQ4

- Molecule 2 is water.

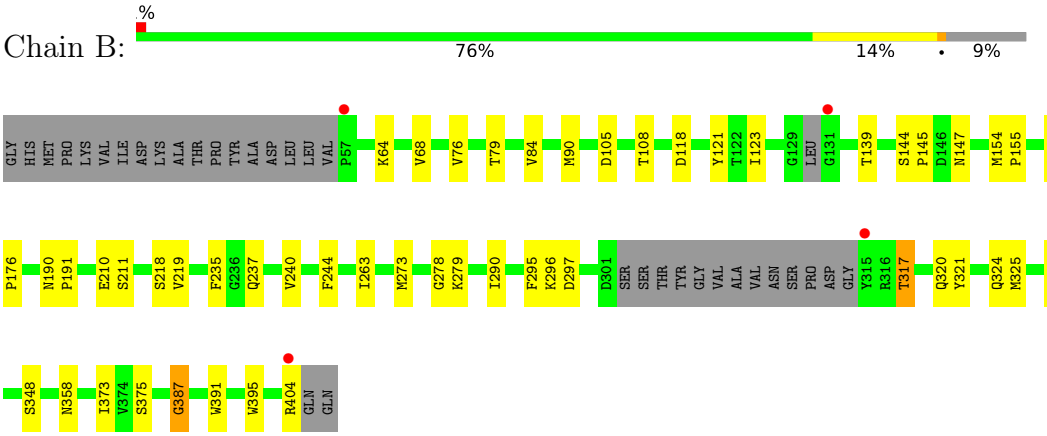
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	14	Total O 14 14	0	0
2	A	10	Total O 10 10	0	0
2	D	12	Total O 12 12	0	0
2	E	6	Total O 6 6	0	0
2	C	12	Total O 12 12	0	0
2	F	6	Total O 6 6	0	0

3 Residue-property plots (i)

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.

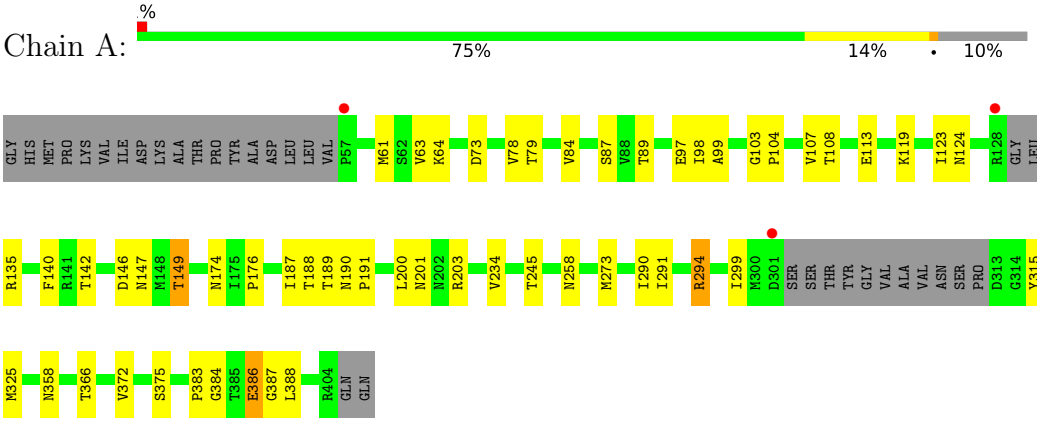
• Molecule 1: L,D-TRANSPEPTIDASE 2

Chain B:



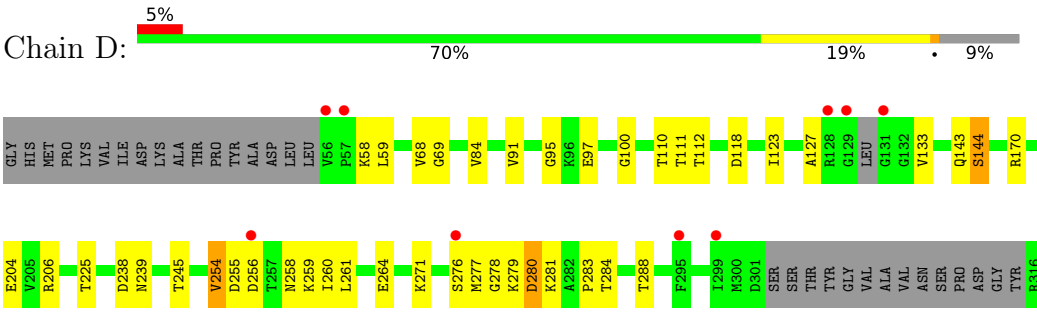
• Molecule 1: L,D-TRANSPEPTIDASE 2

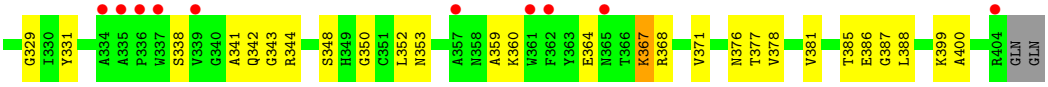
Chain A:



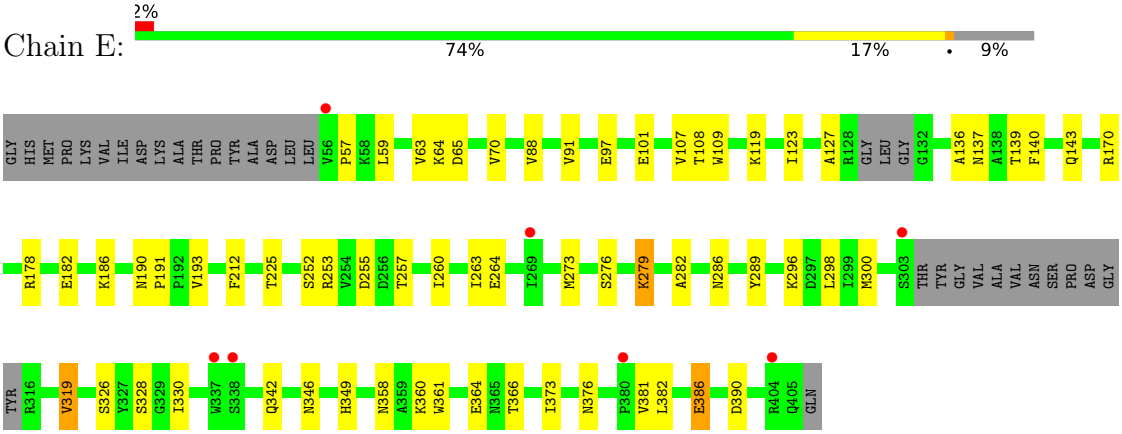
• Molecule 1: L,D-TRANSPEPTIDASE 2

Chain D:

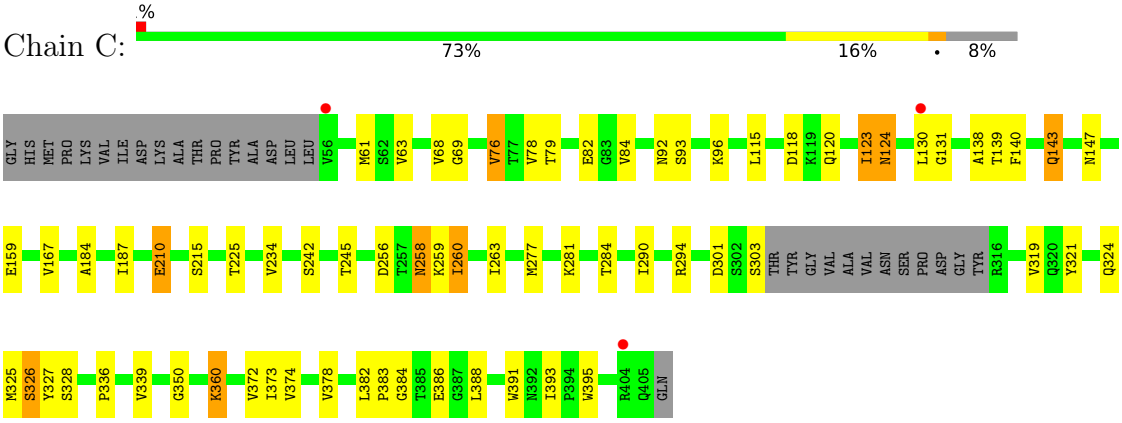




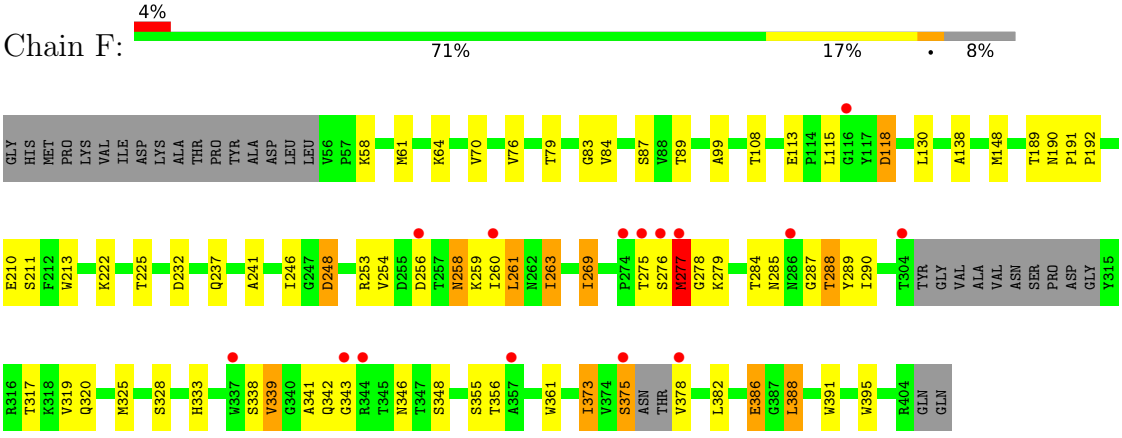
• Molecule 1: L,D-TRANSPEPTIDASE 2



• Molecule 1: L,D-TRANSPEPTIDASE 2



• Molecule 1: L,D-TRANSPEPTIDASE 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.24Å 130.94Å 135.66Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	135.53 – 2.98 135.53 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (135.53-2.98) 97.9 (135.53-2.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.197 , 0.273 0.202 , 0.273	Depositor DCC
R_{free} test set	3083 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å^2)	56.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 33.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -h,l,k 0.016 for -h,-l,-k 0.027 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15188	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (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	0.90	0/2583	1.06	6/3518 (0.2%)
1	B	0.90	0/2571	1.01	6/3503 (0.2%)
1	C	0.89	0/2587	1.03	6/3530 (0.2%)
1	D	0.96	1/2559 (0.0%)	1.07	3/3489 (0.1%)
1	E	0.84	0/2576	0.99	3/3512 (0.1%)
1	F	0.89	0/2574	1.07	5/3511 (0.1%)
All	All	0.90	1/15450 (0.0%)	1.04	29/21063 (0.1%)

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	B	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	319	VAL	N-CA	5.55	1.53	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	386	GLU	N-CA-C	8.70	120.84	111.36
1	A	146	ASP	N-CA-C	-7.49	102.81	110.97
1	F	287	GLY	N-CA-C	7.35	120.47	110.69
1	E	386	GLU	N-CA-C	6.72	119.96	111.69
1	D	254	VAL	N-CA-C	6.41	116.26	108.06
1	A	386	GLU	N-CA-C	6.21	119.02	111.82
1	C	184	ALA	N-CA-C	6.12	119.85	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	317	THR	N-CA-C	5.96	118.14	109.07
1	B	333	HIS	N-CA-C	5.85	117.14	108.60
1	F	84	VAL	CB-CA-C	-5.59	104.03	111.80
1	A	149	THR	N-CA-C	5.53	117.78	107.99
1	A	147	ASN	N-CA-C	5.52	117.79	109.23
1	F	84	VAL	N-CA-C	5.51	115.48	107.88
1	C	301	ASP	N-CA-C	5.44	118.27	109.79
1	C	263	ILE	N-CA-C	5.43	115.45	107.15
1	F	263	ILE	N-CA-C	5.37	111.96	106.21
1	A	103	GLY	CA-C-N	5.37	126.55	119.84
1	A	103	GLY	C-N-CA	5.37	126.55	119.84
1	B	387	GLY	CA-C-N	5.26	131.16	121.70
1	B	387	GLY	C-N-CA	5.26	131.16	121.70
1	C	167	VAL	N-CA-C	-5.18	102.05	108.89
1	F	386	GLU	N-CA-C	5.16	116.72	111.14
1	D	348	SER	N-CA-C	5.09	116.54	108.96
1	C	76	VAL	CB-CA-C	-5.08	105.14	111.08
1	B	144	SER	CA-C-N	5.06	124.98	119.76
1	B	144	SER	C-N-CA	5.06	124.98	119.76
1	C	294	ARG	CG-CD-NE	-5.02	100.95	112.00
1	E	101	GLU	N-CA-C	5.02	117.59	109.06
1	E	264	GLU	N-CA-C	5.00	117.28	107.57

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	387	GLY	Peptide
1	F	83	GLY	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	2529	0	2451	18	0
1	B	2517	0	2431	20	0
1	C	2533	0	2438	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2506	0	2407	31	0
1	E	2523	0	2436	22	0
1	F	2520	0	2412	31	0
2	A	10	0	0	0	0
2	B	14	0	0	0	0
2	C	12	0	0	0	0
2	D	12	0	0	1	0
2	E	6	0	0	0	0
2	F	6	0	0	0	0
All	All	15188	0	14575	151	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 5.

All (151) 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:F:258:ASN:C	1:F:258:ASN:HD22	1.92	0.78
1:B:263:ILE:HD11	1:B:273:MET:HE3	1.69	0.74
1:A:294:ARG:NH1	1:A:366:THR:OG1	2.27	0.67
1:E:298:LEU:HD23	1:E:300:MET:HE2	1.77	0.65
1:A:174:ASN:OD1	1:A:203:ARG:NH2	2.31	0.64
1:D:118:ASP:OD1	1:D:144:SER:OG	2.15	0.63
1:A:63:VAL:HG21	1:A:140:PHE:CE1	2.34	0.63
1:D:280:ASP:HA	1:D:378:VAL:HG21	1.82	0.62
1:B:210:GLU:HA	1:B:395:TRP:CE3	2.35	0.61
1:F:263:ILE:HD13	1:F:361:TRP:CZ3	2.35	0.61
1:E:360:LYS:O	1:E:364:GLU:HG2	1.99	0.60
1:F:258:ASN:C	1:F:258:ASN:ND2	2.56	0.60
1:F:289:TYR:CE1	1:F:382:LEU:HD22	2.36	0.60
1:C:284:THR:OG1	1:C:350:GLY:O	2.19	0.59
1:A:290:ILE:O	1:A:388:LEU:HG	2.03	0.58
1:C:63:VAL:HG21	1:C:140:PHE:CE2	2.39	0.58
1:C:210:GLU:HG2	1:C:395:TRP:CG	2.39	0.58
1:F:99:ALA:HB3	1:F:113:GLU:HG2	1.84	0.58
1:F:338:SER:O	1:F:339:VAL:C	2.47	0.58
1:C:327:TYR:N	1:C:386:GLU:OE2	2.34	0.57
1:F:61:MET:HE1	1:F:138:ALA:HB2	1.84	0.57
1:A:200:LEU:HD13	1:A:387:GLY:HA3	1.86	0.57
1:D:387:GLY:HA2	2:D:501:HOH:O	2.04	0.56
1:E:326:SER:HB2	1:E:386:GLU:OE2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:THR:HG22	1:D:111:THR:O	2.06	0.56
1:B:324:GLN:HA	1:B:331:TYR:CD2	2.41	0.55
1:F:148:MET:HB3	1:F:237:GLN:HG2	1.88	0.55
1:A:325:MET:HE3	1:A:372:VAL:HG11	1.88	0.55
1:F:213:TRP:CG	1:F:246:ILE:HD13	2.42	0.55
1:F:76:VAL:HG23	1:F:115:LEU:HD11	1.88	0.55
1:C:382:LEU:HD12	1:C:383:PRO:HD2	1.89	0.54
1:C:277:MET:HE1	1:C:374:VAL:HG13	1.88	0.54
1:C:325:MET:HE3	1:C:372:VAL:HG11	1.89	0.54
1:A:79:THR:OG1	1:A:108:THR:HG22	2.08	0.54
1:F:213:TRP:CG	1:F:246:ILE:CD1	2.91	0.54
1:E:91:VAL:HG12	1:E:97:GLU:HA	1.90	0.54
1:C:61:MET:HE1	1:C:138:ALA:HB3	1.90	0.54
1:F:289:TYR:CD1	1:F:382:LEU:HD22	2.43	0.54
1:D:200:LEU:HD11	1:D:206:ARG:CZ	2.39	0.53
1:F:190:ASN:HA	1:F:191:PRO:C	2.33	0.53
1:C:124:ASN:OD1	1:C:124:ASN:N	2.42	0.53
1:D:360:LYS:O	1:D:364:GLU:HG3	2.09	0.52
1:C:321:TYR:CZ	1:C:360:LYS:HG3	2.44	0.52
1:C:76:VAL:HG23	1:C:115:LEU:HD11	1.92	0.51
1:B:273:MET:SD	1:B:358:ASN:HB3	2.51	0.51
1:C:325:MET:HE3	1:C:372:VAL:CG1	2.41	0.51
1:F:256:ASP:OD2	1:F:378:VAL:HG12	2.08	0.51
1:C:63:VAL:HG21	1:C:140:PHE:CD2	2.45	0.51
1:D:321:TYR:HB2	1:D:359:ALA:HB1	1.92	0.51
1:A:383:PRO:O	1:A:386:GLU:HB2	2.10	0.51
1:F:254:VAL:HA	1:F:260:ILE:O	2.10	0.51
1:E:70:VAL:HG21	1:E:140:PHE:CD1	2.46	0.50
1:F:341:ALA:C	1:F:343:GLY:HA3	2.36	0.50
1:D:254:VAL:HB	1:D:261:LEU:HD12	1.94	0.50
1:C:147:ASN:O	1:C:234:VAL:HA	2.12	0.50
1:D:254:VAL:HG23	1:D:260:ILE:C	2.37	0.50
1:E:178:ARG:O	1:E:182:GLU:HG3	2.13	0.49
1:C:61:MET:HG2	1:C:78:VAL:HG22	1.94	0.49
1:B:190:ASN:HA	1:B:191:PRO:C	2.37	0.49
1:D:170:ARG:HG3	1:D:204:GLU:HB2	1.94	0.49
1:F:253:ARG:O	1:F:261:LEU:HA	2.12	0.49
1:F:278:GLY:C	1:F:346:ASN:HB3	2.38	0.49
1:A:63:VAL:HG21	1:A:140:PHE:CD1	2.48	0.48
1:B:145:PRO:HB3	1:B:235:PHE:CD1	2.49	0.48
1:C:290:ILE:O	1:C:388:LEU:HD22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:MET:HB2	1:B:168:ALA:HB3	1.95	0.48
1:E:65:ASP:HB3	1:E:139:THR:H	1.78	0.47
1:A:149:THR:O	1:A:149:THR:HG23	2.15	0.47
1:D:288:THR:HG23	1:D:371:VAL:HG13	1.97	0.47
1:F:210:GLU:HA	1:F:395:TRP:CE3	2.49	0.47
1:E:88:VAL:HG11	1:E:109:TRP:CD2	2.51	0.46
1:B:155:PRO:HG2	1:B:244:PHE:CD2	2.50	0.46
1:D:200:LEU:HD22	1:D:385:THR:HA	1.98	0.46
1:F:288:THR:HG23	1:F:373:ILE:HG23	1.98	0.46
1:C:290:ILE:HD11	1:C:391:TRP:CD1	2.51	0.46
1:D:284:THR:OG1	1:D:350:GLY:O	2.31	0.46
1:E:273:MET:HE1	1:E:358:ASN:O	2.16	0.46
1:E:59:LEU:HD13	1:E:127:ALA:HB2	1.97	0.45
1:D:367:LYS:O	1:D:368:ARG:C	2.58	0.45
1:F:388:LEU:HD12	1:F:388:LEU:HA	1.82	0.45
1:B:76:VAL:HG11	1:B:123:ILE:HD11	1.99	0.45
1:B:79:THR:HG22	1:B:108:THR:HG22	1.99	0.45
1:B:278:GLY:HA2	1:B:348:SER:O	2.17	0.45
1:B:90:MET:HE3	1:B:121:TYR:CG	2.52	0.45
1:E:286:ASN:O	1:E:381:VAL:HA	2.17	0.45
1:F:342:GLN:N	1:F:343:GLY:HA3	2.31	0.45
1:A:190:ASN:HA	1:A:191:PRO:C	2.42	0.45
1:D:59:LEU:HD13	1:D:127:ALA:HB2	1.99	0.45
1:B:295:PHE:HB3	1:B:297:ASP:O	2.17	0.44
1:C:256:ASP:OD1	1:C:259:LYS:NZ	2.50	0.44
1:D:100:GLY:HA2	1:D:112:THR:HG23	1.99	0.44
1:B:219:VAL:HG11	1:B:244:PHE:CZ	2.52	0.44
1:D:238:ASP:OD1	1:D:239:ASN:N	2.50	0.44
1:D:256:ASP:HB3	1:D:376:ASN:O	2.16	0.44
1:D:69:GLY:HA2	1:D:143:GLN:HA	2.00	0.44
1:C:130:LEU:HD12	1:C:131:GLY:N	2.33	0.44
1:D:259:LYS:NZ	1:D:344:ARG:O	2.31	0.44
1:D:338:SER:HB3	1:D:341:ALA:HB3	1.99	0.44
1:B:325:MET:HB2	1:B:330:ILE:HG22	1.99	0.44
1:C:325:MET:CE	1:C:372:VAL:HG11	2.47	0.44
1:C:336:PRO:O	1:C:339:VAL:HG23	2.18	0.43
1:D:256:ASP:HB2	1:D:377:THR:HG22	2.00	0.43
1:D:278:GLY:HA3	1:D:283:PRO:C	2.43	0.43
1:F:248:ASP:OD1	1:F:248:ASP:N	2.51	0.43
1:D:279:LYS:O	1:D:281:LYS:N	2.51	0.43
1:F:277:MET:HG2	1:F:284:THR:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:TYR:CE1	1:C:360:LYS:HG3	2.53	0.43
1:C:61:MET:HE3	1:C:123:ILE:HG12	1.99	0.43
1:D:91:VAL:HG12	1:D:97:GLU:HA	2.01	0.43
1:F:189:THR:OG1	1:F:192:PRO:HA	2.18	0.43
1:C:258:ASN:HB3	1:C:260:ILE:HG22	2.01	0.43
1:F:289:TYR:CD2	1:F:325:MET:HE3	2.54	0.42
1:E:107:VAL:HG23	1:E:108:THR:HG23	2.00	0.42
1:F:319:VAL:HG21	1:F:333:HIS:ND1	2.34	0.42
1:B:121:TYR:O	1:B:139:THR:HA	2.19	0.42
1:D:399:LYS:O	1:D:400:ALA:C	2.62	0.42
1:E:279:LYS:HA	1:E:346:ASN:HB3	1.99	0.42
1:C:120:GLN:HE21	1:C:139:THR:HG22	1.85	0.42
1:D:276:SER:OG	1:D:353:ASN:HB2	2.19	0.42
1:E:255:ASP:CG	1:E:376:ASN:HD22	2.28	0.42
1:E:282:ALA:HB1	1:E:349:HIS:O	2.19	0.42
1:F:256:ASP:HB2	1:F:375:SER:O	2.20	0.42
1:F:328:SER:N	1:F:386:GLU:OE2	2.45	0.42
1:E:300:MET:HE3	1:E:319:VAL:HG11	2.02	0.42
1:B:324:GLN:HB2	1:B:331:TYR:CE2	2.55	0.42
1:A:78:VAL:HG21	1:A:123:ILE:HD11	2.00	0.42
1:D:255:ASP:O	1:D:259:LYS:N	2.48	0.42
1:E:63:VAL:HG21	1:E:140:PHE:CE2	2.54	0.42
1:A:99:ALA:HB3	1:A:113:GLU:HG2	2.01	0.42
1:C:69:GLY:HA2	1:C:143:GLN:HA	2.02	0.42
1:A:273:MET:HE1	1:A:358:ASN:O	2.19	0.41
1:A:325:MET:C	1:A:388:LEU:HD23	2.45	0.41
1:D:277:MET:HG2	1:D:352:LEU:HG	2.01	0.41
1:D:329:GLY:O	1:D:331:TYR:HD1	2.03	0.41
1:C:321:TYR:CE2	1:C:360:LYS:HG3	2.55	0.41
1:A:386:GLU:N	1:A:387:GLY:HA2	2.35	0.41
1:C:384:GLY:HA3	1:C:393:ILE:HG13	2.02	0.41
1:D:342:GLN:HA	1:D:343:GLY:HA2	1.89	0.41
1:B:174:ASN:O	1:B:176:PRO:HD3	2.20	0.41
1:E:190:ASN:HA	1:E:191:PRO:C	2.46	0.41
1:E:263:ILE:HG21	1:E:361:TRP:CH2	2.56	0.41
1:B:320:GLN:HB3	1:B:321:TYR:CD2	2.56	0.41
1:F:290:ILE:HD11	1:F:391:TRP:CD1	2.56	0.41
1:B:290:ILE:HD11	1:B:391:TRP:CD1	2.55	0.41
1:A:97:GLU:C	1:A:98:ILE:HD12	2.46	0.41
1:A:61:MET:HG2	1:A:78:VAL:HG22	2.03	0.40
1:E:273:MET:SD	1:E:358:ASN:HB3	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:TYR:CE2	1:E:382:LEU:HD22	2.56	0.40
1:E:59:LEU:HD23	1:E:136:ALA:HB2	2.03	0.40
1:C:326:SER:OG	1:C:328:SER:OG	2.25	0.40
1:F:222:LYS:HE3	1:F:241:ALA:CB	2.52	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	327/368 (89%)	298 (91%)	27 (8%)	2 (1%)	21 53
1	B	328/368 (89%)	310 (94%)	17 (5%)	1 (0%)	36 67
1	C	334/368 (91%)	304 (91%)	28 (8%)	2 (1%)	21 53
1	D	328/368 (89%)	296 (90%)	29 (9%)	3 (1%)	14 45
1	E	329/368 (89%)	298 (91%)	28 (8%)	3 (1%)	14 45
1	F	331/368 (90%)	288 (87%)	34 (10%)	9 (3%)	4 20
All	All	1977/2208 (90%)	1794 (91%)	163 (8%)	20 (1%)	12 42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	LYS
1	D	319	VAL
1	F	232	ASP
1	F	279	LYS
1	D	280	ASP
1	E	212	PHE
1	F	339	VAL
1	E	328	SER

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Mol	Chain	Res	Type
1	F	277	MET
1	C	159	GLU
1	F	130	LEU
1	F	269	ILE
1	A	384	GLY
1	C	143	GLN
1	F	118	ASP
1	F	356	THR
1	F	259	LYS
1	A	176	PRO
1	D	95	GLY
1	E	57	PRO

5.3.2 Protein sidechains (i)

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	268/295 (91%)	244 (91%)	24 (9%)	9 32
1	B	265/295 (90%)	250 (94%)	15 (6%)	18 50
1	C	267/295 (90%)	241 (90%)	26 (10%)	8 29
1	D	262/295 (89%)	245 (94%)	17 (6%)	15 45
1	E	267/295 (90%)	245 (92%)	22 (8%)	10 35
1	F	263/295 (89%)	237 (90%)	26 (10%)	7 28
All	All	1592/1770 (90%)	1462 (92%)	130 (8%)	10 35

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	64	LYS
1	B	68	VAL
1	B	84	VAL
1	B	105	ASP
1	B	118	ASP
1	B	147	ASN

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Mol	Chain	Res	Type
1	B	211	SER
1	B	218	SER
1	B	237	GLN
1	B	240	VAL
1	B	296	LYS
1	B	317	THR
1	B	373	ILE
1	B	375	SER
1	B	404	ARG
1	A	64	LYS
1	A	73	ASP
1	A	84	VAL
1	A	87	SER
1	A	89	THR
1	A	104	PRO
1	A	107	VAL
1	A	119	LYS
1	A	124	ASN
1	A	135	ARG
1	A	142	THR
1	A	187	ILE
1	A	188	THR
1	A	189	THR
1	A	201	ASN
1	A	234	VAL
1	A	245	THR
1	A	258	ASN
1	A	291	ILE
1	A	294	ARG
1	A	299	ILE
1	A	315	TYR
1	A	318	LYS
1	A	375	SER
1	D	58	LYS
1	D	68	VAL
1	D	84	VAL
1	D	123	ILE
1	D	133	VAL
1	D	144	SER
1	D	188	THR
1	D	225	THR
1	D	245	THR

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Mol	Chain	Res	Type
1	D	258	ASN
1	D	264	GLU
1	D	271	LYS
1	D	319	VAL
1	D	320	GLN
1	D	367	LYS
1	D	381	VAL
1	D	388	LEU
1	E	64	LYS
1	E	119	LYS
1	E	123	ILE
1	E	137	ASN
1	E	143	GLN
1	E	170	ARG
1	E	186	LYS
1	E	193	VAL
1	E	225	THR
1	E	252	SER
1	E	253	ARG
1	E	257	THR
1	E	260	ILE
1	E	276	SER
1	E	279	LYS
1	E	296	LYS
1	E	319	VAL
1	E	330	ILE
1	E	342	GLN
1	E	366	THR
1	E	373	ILE
1	E	390	ASP
1	C	68	VAL
1	C	79	THR
1	C	82	GLU
1	C	84	VAL
1	C	92	ASN
1	C	93	SER
1	C	96	LYS
1	C	118	ASP
1	C	123	ILE
1	C	124	ASN
1	C	187	ILE
1	C	210	GLU

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Mol	Chain	Res	Type
1	C	215	SER
1	C	225	THR
1	C	242	SER
1	C	245	THR
1	C	258	ASN
1	C	260	ILE
1	C	281	LYS
1	C	303	SER
1	C	319	VAL
1	C	324	GLN
1	C	326	SER
1	C	360	LYS
1	C	373	ILE
1	C	378	VAL
1	F	58	LYS
1	F	64	LYS
1	F	70	VAL
1	F	79	THR
1	F	87	SER
1	F	89	THR
1	F	108	THR
1	F	118	ASP
1	F	211	SER
1	F	225	THR
1	F	248	ASP
1	F	258	ASN
1	F	261	LEU
1	F	269	ILE
1	F	275	THR
1	F	276	SER
1	F	277	MET
1	F	285	ASN
1	F	288	THR
1	F	317	THR
1	F	320	GLN
1	F	348	SER
1	F	355	SER
1	F	373	ILE
1	F	375	SER
1	F	388	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	147	ASN
1	B	229	ASN
1	A	124	ASN
1	A	201	ASN
1	A	320	GLN
1	D	165	GLN
1	D	262	ASN
1	D	266	ASN
1	D	333	HIS
1	E	143	GLN
1	E	174	ASN
1	E	258	ASN
1	E	262	ASN
1	E	353	ASN
1	E	365	ASN
1	E	376	ASN
1	C	120	GLN
1	C	147	ASN
1	C	224	ASN
1	C	320	GLN
1	C	358	ASN
1	F	124	ASN
1	F	147	ASN
1	F	258	ASN
1	F	262	ASN
1	F	358	ASN
1	F	365	ASN
1	F	397	GLN

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 oligosaccharides 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

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, 95^{th} 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	333/368 (90%)	-0.16	5 (1%)	72	53	29, 51, 85, 123	0
1	B	334/368 (90%)	-0.26	4 (1%)	76	59	30, 48, 77, 108	0
1	C	338/368 (91%)	0.12	3 (0%)	81	65	35, 58, 90, 119	0
1	D	334/368 (90%)	0.24	19 (5%)	29	17	29, 58, 94, 117	0
1	E	335/368 (91%)	0.10	7 (2%)	63	44	34, 64, 97, 125	0
1	F	337/368 (91%)	0.26	15 (4%)	38	23	31, 62, 94, 106	0
All	All	2011/2208 (91%)	0.05	53 (2%)	57	38	29, 56, 93, 125	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ASP	4.3
1	B	57	PRO	4.2
1	C	130	LEU	4.0
1	D	56	VAL	3.9
1	D	339	VAL	3.8
1	B	131	GLY	3.7
1	D	299	ILE	3.7
1	F	357	ALA	3.4
1	A	57	PRO	3.4
1	D	131	GLY	3.3
1	D	404	ARG	3.3
1	D	336	PRO	3.3
1	F	274	PRO	3.3
1	F	378	VAL	3.3
1	D	365	ASN	3.1
1	D	129	GLY	3.0
1	F	375	SER	2.8
1	F	260	ILE	2.8
1	F	337	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	256	ASP	2.7
1	E	303	SER	2.7
1	C	56	VAL	2.7
1	A	316	ARG	2.6
1	F	286	ASN	2.6
1	B	404	ARG	2.6
1	F	344	ARG	2.6
1	F	275	THR	2.6
1	D	128	ARG	2.5
1	A	133	VAL	2.5
1	D	337	TRP	2.4
1	E	404	ARG	2.4
1	D	276	SER	2.4
1	E	56	VAL	2.4
1	B	315	TYR	2.3
1	A	128	ARG	2.3
1	C	404	ARG	2.3
1	D	361	TRP	2.3
1	F	277	MET	2.2
1	E	337	TRP	2.2
1	F	304	THR	2.2
1	F	276	SER	2.2
1	E	380	PRO	2.2
1	E	338	SER	2.2
1	D	334	ALA	2.1
1	E	269	ILE	2.1
1	D	256	ASP	2.1
1	F	343	GLY	2.1
1	D	362	PHE	2.0
1	D	357	ALA	2.0
1	D	57	PRO	2.0
1	D	295	PHE	2.0
1	F	116	GLY	2.0
1	D	335	ALA	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.