



Full wwPDB X-ray Structure Validation Report i

Sep 24, 2023 – 10:02 PM EDT

PDB ID : 5UWV
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

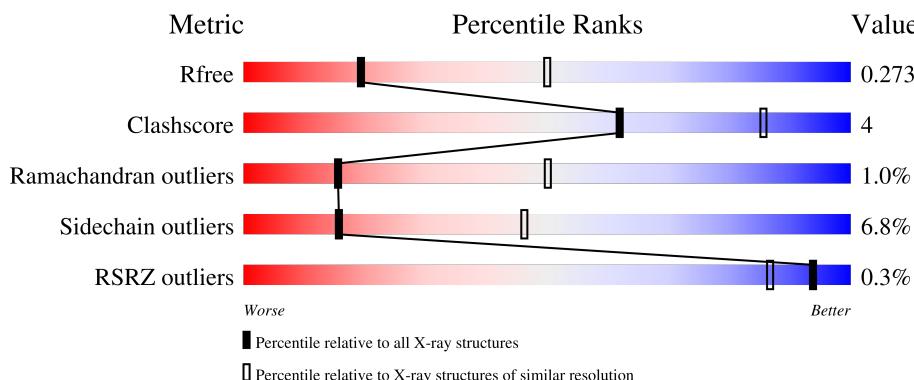
1 Overall quality at a glance (i)

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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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Mol	Chain	Length	Quality of chain
1	F	368	 72% • 17% 8%

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

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

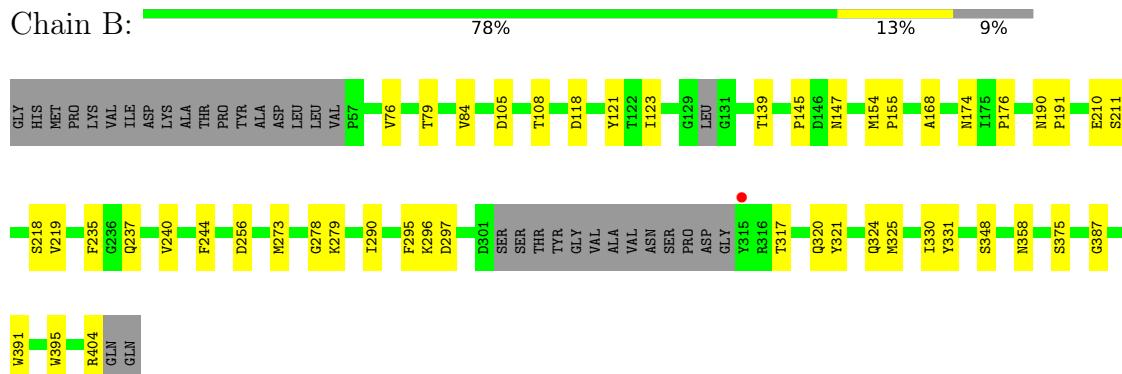
- Molecule 2 is water.

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

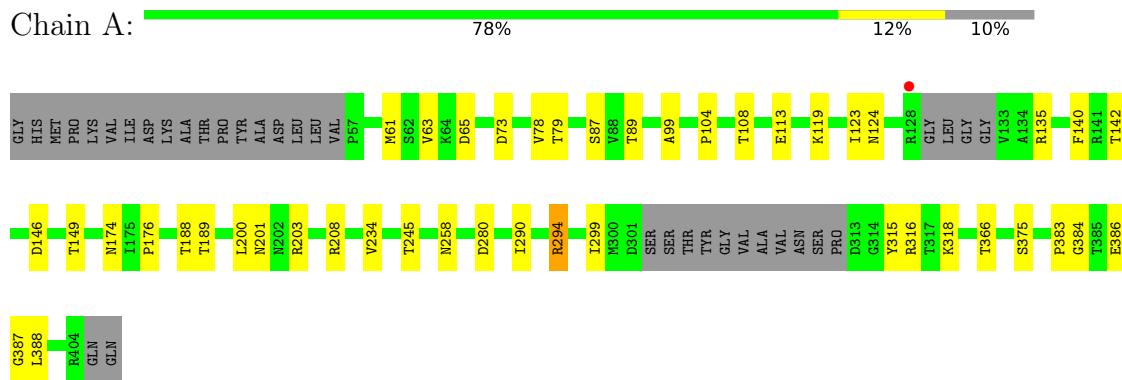
3 Residue-property plots

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.

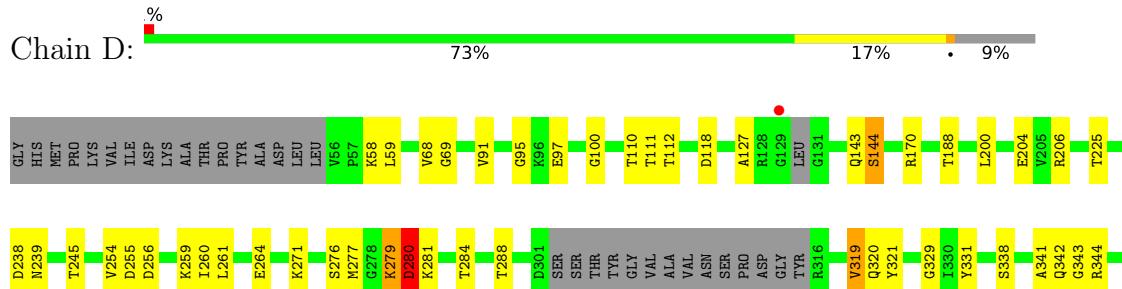
- Molecule 1: L,D-TRANSPEPTIDASE 2



- Molecule 1: L,D-TRANSPEPTIDASE 2

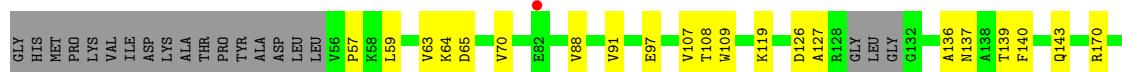
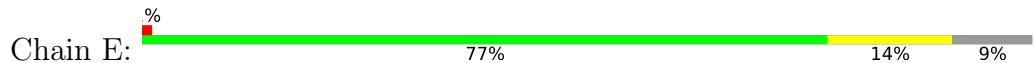


- Molecule 1: L,D-TRANSPEPTIDASE 2





- 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 49.54 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (135.53-2.98) 98.0 (49.54-2.98)	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 (4.68%)	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)	0.29 , 34.9	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	0.92	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.64	0/2583	0.87	2/3518 (0.1%)
1	B	0.65	0/2571	0.84	1/3503 (0.0%)
1	C	0.64	0/2587	0.83	5/3530 (0.1%)
1	D	0.68	0/2559	0.85	0/3489
1	E	0.59	0/2576	0.78	0/3512
1	F	0.63	0/2574	0.83	0/3511
All	All	0.64	0/15450	0.83	8/21063 (0.0%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	256	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	65	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	208	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	294	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	C	65	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	294	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	C	294	ARG	CG-CD-NE	-5.17	100.95	111.80
1	C	344	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	13	0
1	B	2517	0	2431	18	0
1	C	2533	0	2438	25	0
1	D	2506	0	2407	29	0
1	E	2523	0	2436	17	0
1	F	2520	0	2412	30	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	132	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 4.

All (132) 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	0.74
1:A:294:ARG:NH1	1:A:366:THR:OG1	2.27	0.67
1:A:174:ASN:OD1	1:A:203:ARG:NH2	2.31	0.64
1:C:277:MET:HE2	1:C:284:THR:HG21	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:327:TYR:N	1:C:386:GLU:OE2	2.34	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
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:F:258:ASN:C	1:F:258:ASN:ND2	2.56	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: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: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:338:SER:O	1:F:339:VAL:C	2.47	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: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: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: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:D:170:ARG:HG3	1:D:204:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:ARG:O	1:F:261:LEU:HA	2.12	0.49
1:F:190:ASN:HA	1:F:191:PRO:C	2.33	0.48
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
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:341:ALA:C	1:F:343:GLY:HA3	2.36	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:59:LEU:HD13	1:E:127:ALA:HB2	1.97	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:D:254:VAL:HG23	1:D:260:ILE:C	2.37	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: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:190:ASN:HA	1:B:191:PRO:C	2.37	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:F:278:GLY:C	1:F:346:ASN:HB3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:ASP:HB2	1:D:377:THR:HG22	2.00	0.43
1:F:248:ASP:N	1:F:248:ASP:OD1	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
1:C:321:TYR:CE1	1:C:360:LYS:HG3	2.53	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:F:289:TYR:CD2	1:F:325:MET:HE3	2.53	0.43
1:C:258:ASN:HB3	1:C:260:ILE:HG22	2.01	0.43
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: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: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: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: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: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:D:367:LYS:O	1:D:368:ARG:C	2.58	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	25 61
1	B	328/368 (89%)	310 (94%)	17 (5%)	1 (0%)	41 74
1	C	334/368 (91%)	304 (91%)	28 (8%)	2 (1%)	25 61
1	D	328/368 (89%)	296 (90%)	29 (9%)	3 (1%)	17 53
1	E	329/368 (89%)	298 (91%)	28 (8%)	3 (1%)	17 53
1	F	331/368 (90%)	288 (87%)	34 (10%)	9 (3%)	5 24
All	All	1977/2208 (90%)	1794 (91%)	163 (8%)	20 (1%)	15 50

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
1	F	277	MET
1	C	159	GLU
1	F	130	LEU

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Mol	Chain	Res	Type
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%)	246 (92%)	22 (8%)	11 37
1	B	265/295 (90%)	253 (96%)	12 (4%)	27 62
1	C	267/295 (90%)	248 (93%)	19 (7%)	14 44
1	D	262/295 (89%)	246 (94%)	16 (6%)	18 51
1	E	267/295 (90%)	250 (94%)	17 (6%)	17 49
1	F	263/295 (89%)	240 (91%)	23 (9%)	10 35
All	All	1592/1770 (90%)	1483 (93%)	109 (7%)	16 46

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	84	VAL
1	B	105	ASP
1	B	118	ASP
1	B	147	ASN
1	B	211	SER
1	B	218	SER
1	B	237	GLN
1	B	240	VAL
1	B	296	LYS

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Mol	Chain	Res	Type
1	B	317	THR
1	B	375	SER
1	B	404	ARG
1	A	73	ASP
1	A	87	SER
1	A	89	THR
1	A	104	PRO
1	A	119	LYS
1	A	124	ASN
1	A	135	ARG
1	A	142	THR
1	A	146	ASP
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	280	ASP
1	A	294	ARG
1	A	299	ILE
1	A	315	TYR
1	A	316	ARG
1	A	318	LYS
1	A	375	SER
1	D	58	LYS
1	D	68	VAL
1	D	144	SER
1	D	188	THR
1	D	225	THR
1	D	245	THR
1	D	264	GLU
1	D	271	LYS
1	D	279	LYS
1	D	280	ASP
1	D	319	VAL
1	D	320	GLN
1	D	367	LYS
1	D	381	VAL
1	D	388	LEU
1	D	390	ASP
1	E	64	LYS

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Mol	Chain	Res	Type
1	E	119	LYS
1	E	126	ASP
1	E	137	ASN
1	E	143	GLN
1	E	170	ARG
1	E	186	LYS
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	342	GLN
1	E	366	THR
1	E	390	ASP
1	C	68	VAL
1	C	79	THR
1	C	82	GLU
1	C	92	ASN
1	C	93	SER
1	C	118	ASP
1	C	123	ILE
1	C	124	ASN
1	C	210	GLU
1	C	215	SER
1	C	225	THR
1	C	242	SER
1	C	245	THR
1	C	258	ASN
1	C	281	LYS
1	C	303	SER
1	C	324	GLN
1	C	326	SER
1	C	360	LYS
1	F	58	LYS
1	F	64	LYS
1	F	87	SER
1	F	89	THR
1	F	108	THR
1	F	118	ASP
1	F	126	ASP

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Mol	Chain	Res	Type
1	F	211	SER
1	F	225	THR
1	F	232	ASP
1	F	248	ASP
1	F	258	ASN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	201	ASN
1	E	143	GLN
1	E	229	ASN
1	E	258	ASN
1	E	365	ASN
1	E	376	ASN
1	C	120	GLN
1	C	358	ASN
1	F	147	ASN
1	F	258	ASN
1	F	358	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 monosaccharides 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 [\(i\)](#)

6.1 Protein, DNA and RNA chains [\(i\)](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	333/368 (90%)	-0.30	1 (0%)	94 87	29, 51, 85, 123	0
1	B	334/368 (90%)	-0.31	1 (0%)	94 87	30, 48, 77, 108	0
1	C	338/368 (91%)	-0.11	1 (0%)	94 87	35, 58, 90, 119	0
1	D	334/368 (90%)	-0.13	2 (0%)	89 77	29, 58, 94, 117	0
1	E	335/368 (91%)	-0.14	2 (0%)	89 77	34, 64, 97, 125	0
1	F	337/368 (91%)	-0.13	0 100 100		31, 62, 94, 106	0
All	All	2011/2208 (91%)	-0.19	7 (0%)	94 87	29, 56, 93, 125	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	365	ASN	2.6
1	E	82	GLU	2.6
1	D	129	GLY	2.4
1	B	315	TYR	2.3
1	C	378	VAL	2.2
1	E	378	VAL	2.1
1	A	128	ARG	2.1

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 monosaccharides 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.