



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:55 AM UTC

PDB ID : 8US2 / pdb_00008us2
Title : P22121 Crystal structure of TamA from Pseudomonas aeruginosa at 3.95 Ang
Authors : Mellouk, A.; Moraes, T.F.; Calmettes, C.
Deposited on : 2023-10-27
Resolution : 3.96 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
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

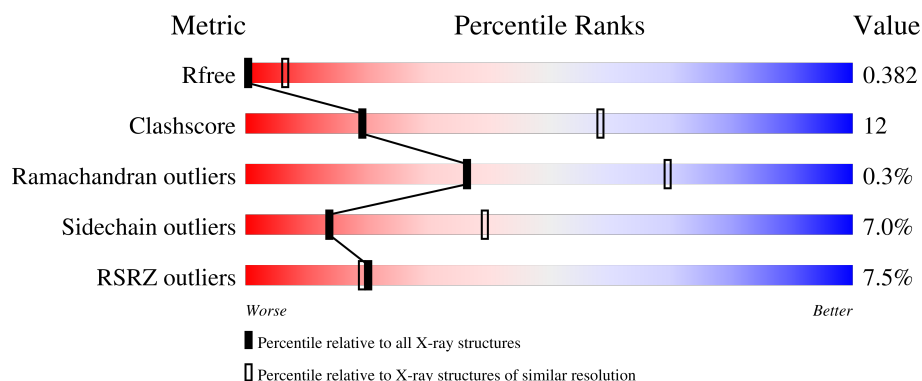
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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.

Mol	Chain	Length	Quality of chain
1	A	559	7% 63% 29% 6%
1	B	559	7% 60% 21% 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8016 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 Translocation and assembly module subunit TamA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4292	2707	767	811	7			
1	B	475	Total	C	N	O	S	0	1	0
			3724	2354	663	700	7			

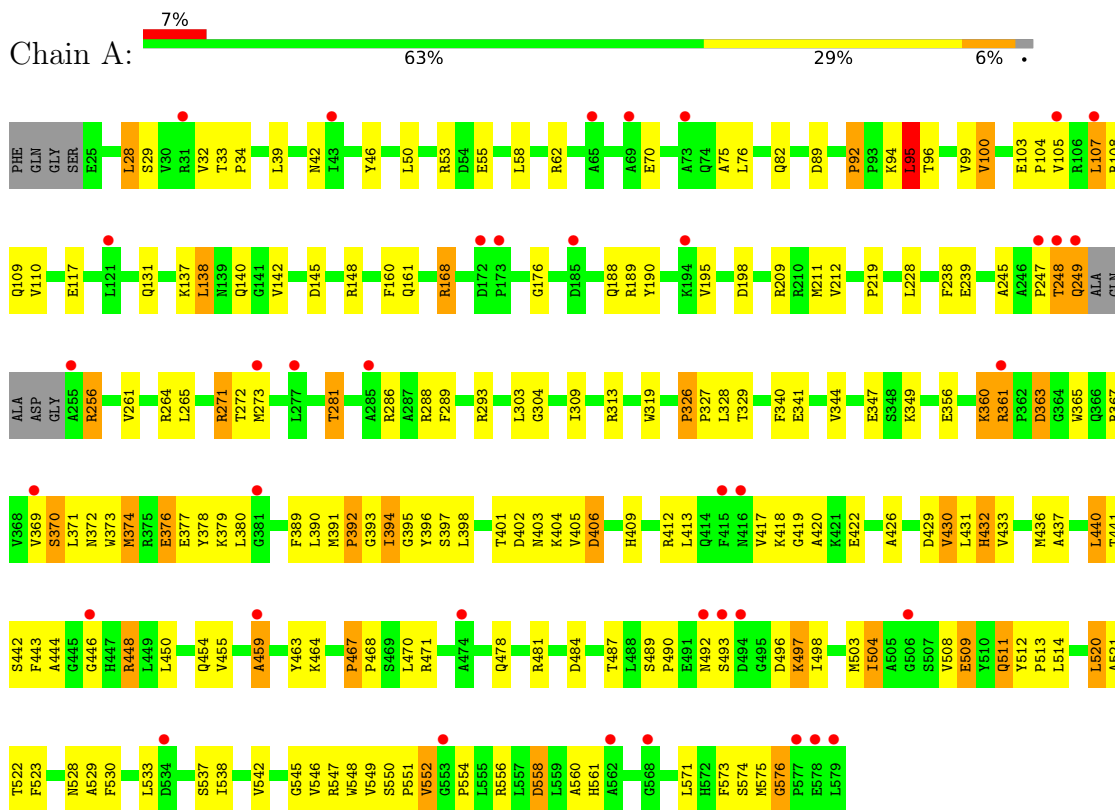
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	-	expression tag	UNP Q9I0U1
A	22	GLN	-	expression tag	UNP Q9I0U1
A	23	GLY	-	expression tag	UNP Q9I0U1
A	24	SER	-	expression tag	UNP Q9I0U1
B	21	PHE	-	expression tag	UNP Q9I0U1
B	22	GLN	-	expression tag	UNP Q9I0U1
B	23	GLY	-	expression tag	UNP Q9I0U1
B	24	SER	-	expression tag	UNP Q9I0U1

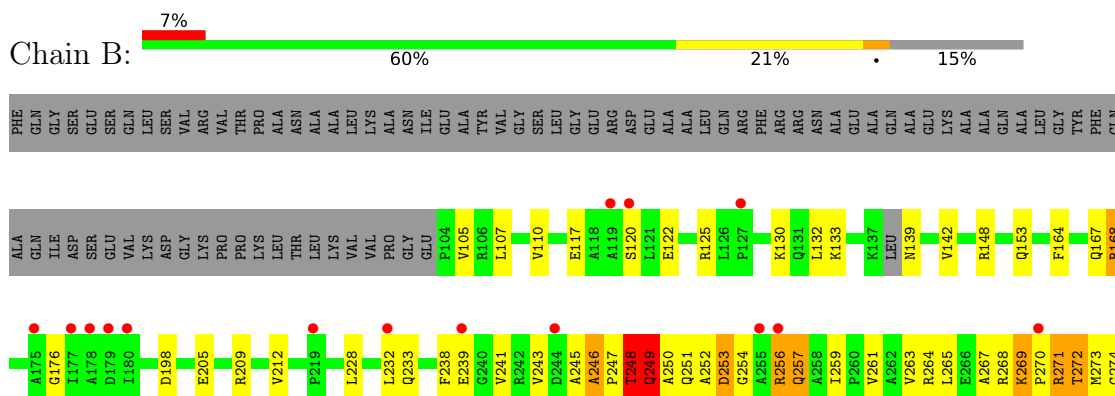
3 Residue-property plots

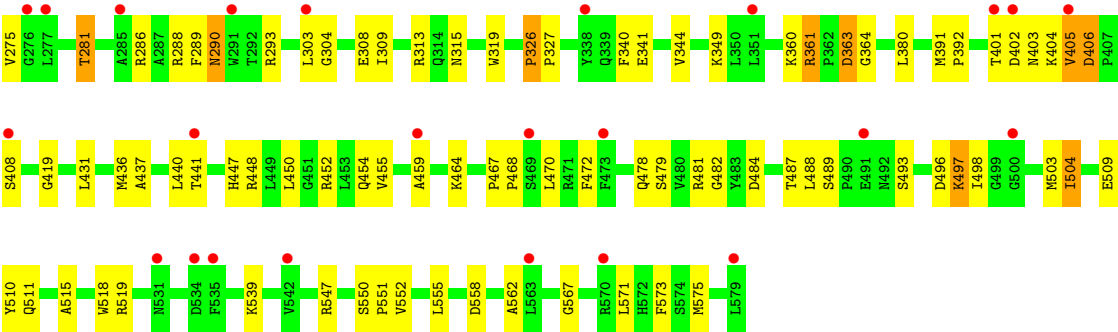
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Translocation and assembly module subunit TamA



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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.05Å 155.50Å 157.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.26 – 3.96 39.26 – 3.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.26-3.96) 88.2 (39.26-3.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.19	Depositor
R, R_{free}	0.302 , 0.381 0.312 , 0.382	Depositor DCC
R_{free} test set	807 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	109.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 171.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.37	0/4387	1.21	66/5932 (1.1%)
1	B	0.35	1/3815 (0.0%)	0.91	19/5158 (0.4%)
All	All	0.36	1/8202 (0.0%)	1.08	85/11090 (0.8%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	ALA	C-N	5.45	1.41	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	ILE	CA-C-N	13.30	130.69	121.65
1	A	394	ILE	C-N-CA	13.30	130.69	121.65
1	A	391	MET	N-CA-C	11.81	128.87	109.15
1	A	376	GLU	N-CA-C	10.84	126.40	108.73
1	B	250	ALA	N-CA-C	10.07	122.90	108.00
1	A	377	GLU	N-CA-C	-9.71	91.59	108.20
1	A	395	GLY	N-CA-C	9.61	128.28	111.46
1	A	100	VAL	CA-C-N	9.38	128.73	118.97
1	A	100	VAL	C-N-CA	9.38	128.73	118.97
1	A	392	PRO	N-CA-C	-8.91	97.35	110.80
1	A	378	TYR	N-CA-C	8.87	123.81	108.02
1	A	443	PHE	N-CA-C	8.69	123.58	109.59
1	A	370	SER	N-CA-C	8.21	122.25	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ASN	N-CA-C	8.12	122.67	109.59
1	A	441	THR	CA-C-N	-7.86	110.00	122.73
1	A	441	THR	C-N-CA	-7.86	110.00	122.73
1	A	374	MET	N-CA-C	7.61	121.62	108.76
1	A	432	HIS	N-CA-C	7.61	121.38	107.99
1	A	520	LEU	N-CA-C	-7.57	97.92	109.95
1	A	402	ASP	N-CA-C	-7.53	102.74	112.23
1	A	548	TRP	CA-C-N	-7.39	113.13	122.37
1	A	548	TRP	C-N-CA	-7.39	113.13	122.37
1	A	92	PRO	CA-C-N	-7.38	110.61	119.84
1	A	92	PRO	C-N-CA	-7.38	110.61	119.84
1	A	549	VAL	N-CA-C	-7.31	97.04	108.23
1	A	523	PHE	N-CA-C	7.26	120.77	109.52
1	A	522	THR	N-CA-C	-7.17	96.36	108.26
1	A	509	GLU	N-CA-C	7.10	120.75	108.76
1	B	249	GLN	N-CA-C	7.06	119.89	107.61
1	A	448	ARG	N-CA-C	7.00	120.30	108.90
1	A	521	ALA	N-CA-C	6.83	120.30	109.50
1	A	467	PRO	CA-C-N	6.77	126.28	119.24
1	A	467	PRO	C-N-CA	6.77	126.28	119.24
1	A	95	LEU	N-CA-C	-6.73	97.09	108.26
1	A	393	GLY	N-CA-C	6.71	120.95	110.96
1	A	560	ALA	N-CA-C	6.68	119.41	108.52
1	A	369	VAL	N-CA-C	-6.59	96.16	107.24
1	A	373	TRP	N-CA-C	-6.49	98.82	109.40
1	B	269	LYS	CA-C-N	6.37	126.29	119.28
1	B	269	LYS	C-N-CA	6.37	126.29	119.28
1	A	390	LEU	N-CA-C	-6.28	95.31	107.44
1	B	250	ALA	CB-CA-C	-6.09	107.81	116.34
1	A	138	LEU	N-CA-C	6.06	118.50	109.59
1	A	374	MET	CA-C-N	-6.04	114.25	122.77
1	A	374	MET	C-N-CA	-6.04	114.25	122.77
1	A	558	ASP	N-CA-C	5.98	119.29	109.72
1	A	529	ALA	N-CA-C	-5.96	101.17	110.42
1	B	259	ILE	N-CA-C	5.94	113.43	107.55
1	A	96	THR	N-CA-C	5.92	118.32	108.20
1	B	364	GLY	N-CA-C	-5.87	106.67	114.95
1	A	372	ASN	CA-C-N	-5.80	114.23	122.94
1	A	372	ASN	C-N-CA	-5.80	114.23	122.94
1	A	371	LEU	N-CA-C	-5.78	99.49	108.90
1	A	444	ALA	CB-CA-C	-5.75	109.96	116.63
1	B	272	THR	N-CA-C	5.68	118.46	108.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ALA	N-CA-C	5.61	118.48	110.24
1	A	32	VAL	N-CA-C	5.59	115.65	107.37
1	A	511	GLN	N-CA-C	5.54	117.99	109.07
1	A	397	SER	N-CA-C	5.50	118.43	109.24
1	A	508	VAL	N-CA-C	-5.49	101.11	108.35
1	A	514	LEU	N-CA-C	-5.48	106.27	113.12
1	A	396	TYR	N-CA-C	-5.43	100.92	109.50
1	A	326	PRO	CA-C-N	5.42	125.76	119.47
1	A	326	PRO	C-N-CA	5.42	125.76	119.47
1	A	430	VAL	N-CA-C	5.40	114.97	108.06
1	A	552	VAL	N-CA-C	-5.37	108.04	113.20
1	B	326	PRO	CA-C-N	5.37	125.70	119.47
1	B	326	PRO	C-N-CA	5.37	125.70	119.47
1	A	444	ALA	N-CA-C	5.36	117.13	108.08
1	A	489	SER	CA-C-N	-5.34	114.28	119.78
1	A	489	SER	C-N-CA	-5.34	114.28	119.78
1	B	315	ASN	N-CA-C	5.31	117.25	109.24
1	A	538	ILE	N-CA-C	5.27	115.18	108.12
1	B	248	THR	N-CA-C	5.27	116.31	108.31
1	B	246	ALA	CA-C-N	-5.26	113.50	118.97
1	B	246	ALA	C-N-CA	-5.26	113.50	118.97
1	B	552	VAL	N-CA-C	-5.24	108.17	113.20
1	A	576	GLY	CA-C-N	5.24	125.17	119.78
1	A	576	GLY	C-N-CA	5.24	125.17	119.78
1	B	467	PRO	CA-C-N	5.24	124.69	119.24
1	B	467	PRO	C-N-CA	5.24	124.69	119.24
1	A	395	GLY	CA-C-N	-5.22	114.48	122.62
1	A	395	GLY	C-N-CA	-5.22	114.48	122.62
1	B	482	GLY	N-CA-C	-5.12	108.60	114.69
1	A	459	ALA	N-CA-C	-5.01	102.38	110.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	249	GLN	Peptide

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	4292	0	4203	109	0
1	B	3724	0	3622	79	0
All	All	8016	0	7825	185	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 12.

All (185) 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:107:LEU:HD11	1:A:138:LEU:HD13	1.57	0.86
1:A:455:VAL:HG12	1:A:504:ILE:HG23	1.62	0.81
1:B:168:ARG:HH11	1:B:168:ARG:HG3	1.49	0.78
1:A:168:ARG:HH11	1:A:168:ARG:HG3	1.48	0.77
1:B:246:ALA:HB1	1:B:247:PRO:HD2	1.68	0.76
1:A:108:ARG:HG2	1:A:109:GLN:HG2	1.69	0.74
1:B:248:THR:OG1	1:B:249:GLN:N	2.12	0.74
1:A:431:LEU:HB3	1:A:459:ALA:HB3	1.69	0.74
1:B:274:GLY:O	1:B:290:ASN:N	2.25	0.70
1:B:361:ARG:NH2	1:B:363:ASP:OD2	2.27	0.68
1:A:550:SER:OG	1:A:551:PRO:HD2	1.95	0.66
1:A:361:ARG:NH2	1:A:363:ASP:OD2	2.29	0.66
1:B:271:ARG:HG3	1:B:293:ARG:HG3	1.78	0.65
1:B:455:VAL:HG12	1:B:504:ILE:HG23	1.79	0.65
1:A:271:ARG:HG3	1:A:293:ARG:HG3	1.77	0.65
1:B:246:ALA:HB1	1:B:247:PRO:CD	2.28	0.64
1:A:392:PRO:HD2	1:A:419:GLY:O	1.98	0.64
1:A:108:ARG:NE	1:A:109:GLN:HE21	1.96	0.63
1:A:492:ASN:HB3	1:A:498:ILE:HG13	1.81	0.63
1:A:454:GLN:HG2	1:A:503:MET:HE1	1.81	0.63
1:A:168:ARG:HG3	1:A:168:ARG:NH1	2.15	0.62
1:A:380:LEU:HD21	1:A:468:PRO:HG3	1.82	0.62
1:B:117:GLU:OE2	1:B:256:ARG:NH2	2.33	0.62
1:A:289:PHE:HE2	1:A:309:ILE:HD13	1.65	0.61
1:B:454:GLN:HG2	1:B:503:MET:HE1	1.83	0.61
1:A:108:ARG:HE	1:A:109:GLN:HG2	1.66	0.60
1:A:420:ALA:HB3	1:A:430:VAL:HB	1.83	0.60
1:A:94:LYS:HG2	1:A:95:LEU:N	2.16	0.60
1:B:243:VAL:HG13	1:B:263:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ARG:NH1	1:B:558:ASP:OD2	2.33	0.59
1:B:168:ARG:HG3	1:B:168:ARG:NH1	2.16	0.59
1:B:286:ARG:HH21	1:B:288:ARG:HH12	1.50	0.58
1:B:247:PRO:HG2	1:B:248:THR:H	1.69	0.57
1:A:511:GLN:HA	1:A:520:LEU:O	2.04	0.57
1:B:245:ALA:HB2	1:B:261:VAL:HA	1.85	0.57
1:A:448:ARG:HB2	1:A:511:GLN:HB2	1.85	0.57
1:A:304:GLY:HA3	1:A:319:TRP:CE2	2.39	0.56
1:B:405:VAL:HG23	1:B:406:ASP:OD1	2.05	0.56
1:B:573:PHE:HE2	1:B:575:MET:HE3	1.68	0.56
1:A:374:MET:HG3	1:A:389:PHE:HB2	1.86	0.56
1:B:105:VAL:HG22	1:B:176:GLY:HA2	1.87	0.56
1:A:117:GLU:HG2	1:B:117:GLU:HG2	1.88	0.56
1:B:440:LEU:HD12	1:B:450:LEU:HG	1.88	0.56
1:A:340:PHE:HD2	1:A:349:LYS:HG2	1.71	0.56
1:A:547:ARG:NH1	1:A:558:ASP:OD1	2.31	0.55
1:A:556:ARG:NH2	1:A:576:GLY:O	2.39	0.55
1:B:380:LEU:HD21	1:B:468:PRO:HG3	1.89	0.55
1:B:304:GLY:HA3	1:B:319:TRP:CE2	2.42	0.54
1:B:273:MET:HG2	1:B:275:VAL:HG23	1.90	0.54
1:A:82:GLN:HB2	1:A:100:VAL:HB	1.90	0.54
1:A:550:SER:OG	1:A:552:VAL:HG22	2.08	0.54
1:B:246:ALA:O	1:B:248:THR:HG23	2.08	0.53
1:A:160:PHE:CG	1:A:247:PRO:HB3	2.43	0.53
1:B:252:ALA:HB2	1:B:257:GLN:H	1.72	0.53
1:B:515:ALA:HB3	1:B:518:TRP:HB2	1.90	0.53
1:A:248:THR:HG22	1:A:249:GLN:H	1.73	0.53
1:B:448:ARG:HB2	1:B:511:GLN:HB2	1.91	0.53
1:A:75:ALA:HA	1:A:140:GLN:HB2	1.90	0.53
1:A:440:LEU:HD12	1:A:450:LEU:HG	1.91	0.52
1:A:108:ARG:HG2	1:A:109:GLN:N	2.25	0.52
1:A:367:ARG:HD2	1:A:394:ILE:HD11	1.92	0.52
1:A:573:PHE:HE2	1:A:575:MET:HE3	1.73	0.52
1:A:329:THR:HB	1:A:360:LYS:HB3	1.92	0.52
1:B:281:THR:HG21	1:B:571:LEU:O	2.10	0.52
1:A:481:ARG:NH1	1:A:558:ASP:OD2	2.43	0.52
1:A:450:LEU:HB2	1:A:509:GLU:HB3	1.92	0.51
1:A:422:GLU:HA	1:A:426:ALA:HB3	1.92	0.51
1:A:103:GLU:HG3	1:A:104:PRO:HD2	1.93	0.51
1:A:161:GLN:HG3	1:A:190:TYR:HE2	1.74	0.51
1:A:490:PRO:HG3	1:A:530:PHE:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ARG:HH21	1:A:288:ARG:HH12	1.58	0.51
1:A:131:GLN:CG	1:A:142:VAL:HG11	2.41	0.51
1:A:545:GLY:HA3	1:A:558:ASP:OD1	2.11	0.50
1:B:288:ARG:HA	1:B:308:GLU:HG2	1.93	0.50
1:B:313:ARG:HD3	1:B:341:GLU:HG3	1.93	0.50
1:B:392:PRO:HD2	1:B:419:GLY:O	2.12	0.49
1:A:401:THR:OG1	1:A:403:ASN:HB3	2.11	0.49
1:A:420:ALA:O	1:A:429:ASP:HA	2.13	0.49
1:B:450:LEU:HB2	1:B:509:GLU:HB3	1.94	0.49
1:A:108:ARG:HG2	1:A:109:GLN:CG	2.41	0.49
1:B:256:ARG:HH11	1:B:256:ARG:HA	1.77	0.49
1:A:409:HIS:HA	1:A:440:LEU:HD23	1.95	0.49
1:A:131:GLN:OE1	1:A:131:GLN:N	2.40	0.49
1:A:406:ASP:N	1:A:406:ASP:OD1	2.46	0.49
1:B:212:VAL:HA	1:B:228:LEU:HD13	1.95	0.49
1:A:496:ASP:O	1:A:498:ILE:HG12	2.13	0.48
1:A:347:GLU:OE2	1:A:379:LYS:NZ	2.40	0.48
1:B:452:ARG:NH2	1:B:479:SER:O	2.47	0.48
1:A:264:ARG:HG3	1:A:265:LEU:N	2.29	0.48
1:A:50:LEU:O	1:A:53:ARG:NH1	2.46	0.47
1:A:497:LYS:N	1:A:497:LYS:HD3	2.30	0.47
1:B:497:LYS:N	1:B:497:LYS:HD3	2.30	0.47
1:A:198:ASP:O	1:A:264:ARG:HA	2.14	0.47
1:A:376:GLU:OE2	1:A:467:PRO:HB2	2.15	0.47
1:A:417:VAL:HG13	1:A:433:VAL:HG22	1.96	0.47
1:A:105:VAL:HG22	1:A:176:GLY:HA2	1.97	0.47
1:A:418:LYS:HE2	1:A:432:HIS:ND1	2.30	0.47
1:B:472:PHE:HB3	1:B:503:MET:HG2	1.97	0.47
1:A:550:SER:C	1:A:552:VAL:H	2.24	0.46
1:B:273:MET:HG3	1:B:274:GLY:HA3	1.96	0.46
1:A:212:VAL:HA	1:A:228:LEU:HD13	1.96	0.46
1:A:356:GLU:HG2	1:A:370:SER:HB3	1.97	0.46
1:B:401:THR:OG1	1:B:403:ASN:HB3	2.15	0.46
1:B:431:LEU:HB3	1:B:459:ALA:HB3	1.97	0.46
1:A:520:LEU:HD12	1:A:546:VAL:HG22	1.97	0.46
1:B:205:GLU:O	1:B:209:ARG:HG3	2.16	0.46
1:A:326:PRO:HA	1:A:327:PRO:HD3	1.83	0.46
1:A:376:GLU:CD	1:A:467:PRO:HB2	2.41	0.45
1:A:412:ARG:O	1:A:413:LEU:HD23	2.16	0.45
1:A:108:ARG:HE	1:A:109:GLN:CG	2.30	0.45
1:A:189:ARG:HB3	1:B:120:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ASP:OD1	1:B:406:ASP:N	2.49	0.45
1:B:562:ALA:O	1:B:567:GLY:HA3	2.16	0.45
1:A:108:ARG:NE	1:A:109:GLN:HG2	2.32	0.45
1:A:448:ARG:HD3	1:A:511:GLN:OE1	2.17	0.45
1:B:326:PRO:HA	1:B:327:PRO:HD3	1.82	0.45
1:B:519:ARG:HB2	1:B:547:ARG:HB2	1.98	0.45
1:A:238:PHE:CE1	1:A:265:LEU:HD13	2.52	0.45
1:B:269:LYS:HA	1:B:270:PRO:HD3	1.77	0.45
1:A:131:GLN:HG3	1:A:142:VAL:HG11	1.98	0.45
1:B:488:LEU:HD22	1:B:539:LYS:HG3	1.97	0.45
1:A:160:PHE:HD2	1:A:190:TYR:CD1	2.35	0.44
1:A:528:ASN:ND2	1:A:537:SER:O	2.50	0.44
1:A:556:ARG:CG	1:A:574:SER:HB3	2.46	0.44
1:B:198:ASP:O	1:B:264:ARG:HA	2.18	0.44
1:B:402:ASP:OD2	1:B:408:SER:OG	2.33	0.44
1:B:164:PHE:HB3	1:B:167:GLN:HG2	2.00	0.44
1:A:463:TYR:O	1:A:471:ARG:NH2	2.50	0.44
1:B:340:PHE:HD2	1:B:349:LYS:HG2	1.82	0.44
1:B:233:GLN:NE2	1:B:241:VAL:HG22	2.32	0.44
1:B:391:MET:HE1	1:B:470:LEU:HD21	1.99	0.44
1:B:139:ASN:O	1:B:139:ASN:ND2	2.51	0.44
1:B:257:GLN:HE21	1:B:257:GLN:HA	1.81	0.44
1:A:188:GLN:HB3	1:A:256:ARG:NH2	2.32	0.43
1:A:104:PRO:HG3	1:A:137:LYS:HD3	2.00	0.43
1:A:28:LEU:HD22	1:A:29:SER:H	1.82	0.43
1:A:39:LEU:HA	1:A:76:LEU:HD12	1.99	0.43
1:A:341:GLU:O	1:A:347:GLU:HA	2.18	0.43
1:B:447:HIS:ND1	1:B:510:TYR:OH	2.43	0.43
1:B:209:ARG:HA	1:B:212:VAL:HG23	2.00	0.43
1:B:496:ASP:O	1:B:498:ILE:HG12	2.19	0.43
1:A:219:PRO:HG3	1:B:122:GLU:HA	1.99	0.43
1:A:281:THR:HG21	1:A:571:LEU:O	2.19	0.43
1:A:42:ASN:O	1:A:46:TYR:HD2	2.01	0.43
1:A:55:GLU:OE1	1:A:89:ASP:HB2	2.19	0.43
1:A:374:MET:CG	1:A:389:PHE:HB2	2.49	0.43
1:A:442:SER:OG	1:A:448:ARG:HG2	2.19	0.43
1:A:512:TYR:CD1	1:A:513:PRO:HD2	2.54	0.42
1:B:484:ASP:HB3	1:B:487:THR:HG21	2.01	0.42
1:B:238:PHE:CE1	1:B:265:LEU:HD13	2.54	0.42
1:B:555:LEU:HD22	1:B:575:MET:HG2	2.00	0.42
1:B:132:LEU:HD21	1:B:142:VAL:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:PHE:CZ	1:B:265:LEU:HD13	2.54	0.42
1:A:420:ALA:CB	1:A:430:VAL:HB	2.47	0.42
1:A:195:VAL:O	1:A:209:ARG:NH1	2.51	0.42
1:B:247:PRO:HG2	1:B:248:THR:N	2.32	0.42
1:A:550:SER:OG	1:A:551:PRO:CD	2.65	0.42
1:A:542:VAL:HG23	1:A:561:HIS:HB3	2.02	0.42
1:A:33:THR:HA	1:A:34:PRO:HA	1.64	0.41
1:A:82:GLN:OE1	1:A:82:GLN:HA	2.18	0.41
1:A:484:ASP:HB3	1:A:487:THR:HG21	2.02	0.41
1:B:436:MET:HG3	1:B:437:ALA:N	2.35	0.41
1:A:211:MET:HB2	1:A:328:LEU:HD11	2.02	0.41
1:A:467:PRO:HD2	1:A:470:LEU:HD12	2.02	0.41
1:B:130:LYS:O	1:B:133:LYS:HG3	2.20	0.41
1:B:232:LEU:HD13	1:B:265:LEU:HD21	2.02	0.41
1:A:28:LEU:HD22	1:A:29:SER:N	2.35	0.41
1:A:313:ARG:HD3	1:A:341:GLU:OE2	2.21	0.41
1:B:243:VAL:HG22	1:B:263:VAL:HG13	2.02	0.41
1:B:289:PHE:HE2	1:B:309:ILE:HD13	1.85	0.41
1:B:509:GLU:OE1	1:B:547:ARG:NH2	2.53	0.41
1:A:142:VAL:O	1:A:145:ASP:HB2	2.20	0.41
1:A:418:LYS:HG3	1:A:432:HIS:HB3	2.03	0.41
1:A:58:LEU:O	1:A:62:ARG:HG3	2.20	0.41
1:A:446:GLY:O	1:A:513:PRO:HD3	2.21	0.41
1:B:125:ARG:HB2	1:B:153:GLN:OE1	2.21	0.41
1:A:530:PHE:HE2	1:A:533:LEU:HA	1.85	0.41
1:B:550:SER:HB2	1:B:551:PRO:HD2	2.03	0.41
1:B:253:ASP:N	1:B:254:GLY:HA3	2.36	0.41
1:A:436:MET:HG3	1:A:437:ALA:N	2.35	0.41
1:B:273:MET:HA	1:B:274:GLY:HA3	1.76	0.41
1:B:286:ARG:NH2	1:B:288:ARG:HH12	2.14	0.41
1:A:245:ALA:HB2	1:A:261:VAL:HA	2.04	0.40
1:B:268:ARG:HG2	1:B:269:LYS:N	2.36	0.40
1:A:365:TRP:CE2	1:A:398:LEU:HD22	2.56	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	546/559 (98%)	523 (96%)	22 (4%)	1 (0%)	43	75
1	B	472/559 (84%)	447 (95%)	23 (5%)	2 (0%)	30	65
All	All	1018/1118 (91%)	970 (95%)	45 (4%)	3 (0%)	36	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	ASP
1	B	344	VAL
1	A	344	VAL

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/450 (99%)	414 (93%)	31 (7%)	14	39
1	B	387/450 (86%)	360 (93%)	27 (7%)	14	39
All	All	832/900 (92%)	774 (93%)	58 (7%)	14	39

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	70	GLU
1	A	92	PRO

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Mol	Chain	Res	Type
1	A	95	LEU
1	A	99	VAL
1	A	107	LEU
1	A	110	VAL
1	A	148	ARG
1	A	168	ARG
1	A	239	GLU
1	A	248	THR
1	A	249	GLN
1	A	256	ARG
1	A	271	ARG
1	A	272	THR
1	A	273	MET
1	A	281	THR
1	A	303	LEU
1	A	360	LYS
1	A	361	ARG
1	A	363	ASP
1	A	404	LYS
1	A	405	VAL
1	A	406	ASP
1	A	440	LEU
1	A	464	LYS
1	A	478	GLN
1	A	493	SER
1	A	497	LYS
1	A	504	ILE
1	A	554	PRO
1	B	107	LEU
1	B	110	VAL
1	B	148	ARG
1	B	168	ARG
1	B	239	GLU
1	B	248	THR
1	B	251	GLN
1	B	256	ARG
1	B	257	GLN
1	B	271	ARG
1	B	272	THR
1	B	281	THR
1	B	290	ASN
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	360	LYS
1	B	361	ARG
1	B	363	ASP
1	B	404	LYS
1	B	405	VAL
1	B	406	ASP
1	B	441	THR
1	B	464	LYS
1	B	478	GLN
1	B	489	SER
1	B	493	SER
1	B	497	LYS
1	B	504	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	109	GLN
1	A	111	ASN
1	A	139	ASN
1	A	229	ASN
1	A	372	ASN
1	A	416	ASN
1	A	478	GLN
1	A	526	GLN
1	A	528	ASN
1	B	111	ASN
1	B	257	GLN
1	B	416	ASN
1	B	478	GLN
1	B	526	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 [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

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	550/559 (98%)	0.75	38 (6%)	23 20	41, 139, 300, 537	0
1	B	475/559 (84%)	0.71	39 (8%)	17 18	29, 145, 336, 550	1 (0%)
All	All	1025/1118 (91%)	0.73	77 (7%)	20 19	29, 141, 306, 550	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	579	LEU	6.2
1	B	469	SER	4.8
1	B	535	PHE	4.5
1	A	249	GLN	4.3
1	B	120	SER	4.1
1	A	493	SER	3.9
1	A	506	GLY	3.9
1	A	247	PRO	3.8
1	B	351	LEU	3.8
1	B	127	PRO	3.4
1	A	248	THR	3.4
1	A	534	ASP	3.4
1	B	232	LEU	3.3
1	B	291	TRP	3.2
1	A	416	ASN	3.1
1	A	494	ASP	3.1
1	B	119	ALA	3.1
1	B	277	LEU	3.1
1	A	459	ALA	3.0
1	B	255	ALA	3.0
1	B	405	VAL	2.9
1	B	179	ASP	2.9
1	A	43	ILE	2.9
1	B	402	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	500	GLY	2.7
1	B	534	ASP	2.7
1	A	369	VAL	2.7
1	A	173	PRO	2.7
1	B	270	PRO	2.7
1	A	381	GLY	2.7
1	A	31	ARG	2.6
1	B	178	ALA	2.6
1	B	177	ILE	2.6
1	B	542	VAL	2.6
1	A	107	LEU	2.5
1	A	285	ALA	2.5
1	B	408	SER	2.5
1	A	579	LEU	2.5
1	A	578	GLU	2.4
1	B	401	THR	2.4
1	B	219	PRO	2.4
1	A	185	ASP	2.4
1	B	244	ASP	2.4
1	B	338	TYR	2.3
1	B	239	GLU	2.3
1	A	562	ALA	2.3
1	B	570	ARG	2.3
1	A	73	ALA	2.3
1	A	105	VAL	2.3
1	A	492	ASN	2.3
1	A	65	ALA	2.3
1	B	175	ALA	2.3
1	A	568	GLY	2.3
1	B	256	ARG	2.3
1	B	276	GLY	2.2
1	A	415	PHE	2.2
1	A	361	ARG	2.2
1	B	180	ILE	2.2
1	A	474	ALA	2.2
1	A	121	LEU	2.2
1	B	303	LEU	2.2
1	B	473	PHE	2.2
1	A	172	ASP	2.1
1	B	563	LEU	2.1
1	B	285	ALA	2.1
1	B	459	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	2.1
1	A	194	LYS	2.1
1	A	446	GLY	2.1
1	A	273	MET	2.1
1	A	69	ALA	2.1
1	A	553	GLY	2.1
1	A	277	LEU	2.1
1	B	531	ASN	2.0
1	A	577	PRO	2.0
1	B	441	THR	2.0
1	B	491	GLU	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.