



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:22 AM UTC

PDB ID : 1AW7 / pdb_00001aw7
Title : Q136A MUTANT OF TOXIC SHOCK SYNDROME TOXIN-1 FROM S. AU-REUS
Authors : Earhart, C.A.; Mitchell, D.T.; Murray, D.L.; Pinheiro, D.M.; Matsumura, M.; Schlievert, P.M.; Ohlendorf, D.H.
Deposited on : 1997-10-11
Resolution : 1.95 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

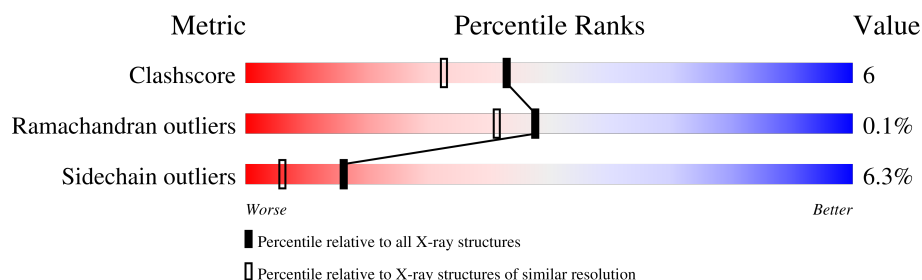
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	194	
1	B	194	
1	C	194	
1	D	194	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6539 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 TOXIC SHOCK SYNDROME TOXIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	B	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	C	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			
1	D	194	Total	C	N	O	S	0	1	0
			1562	994	256	310	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	TRP	GLY	SEE REMARK 999	UNP P06886
A	136	ALA	GLN	engineered mutation	UNP P06886
B	316	TRP	GLY	SEE REMARK 999	UNP P06886
B	336	ALA	GLN	engineered mutation	UNP P06886
C	516	TRP	GLY	SEE REMARK 999	UNP P06886
C	536	ALA	GLN	engineered mutation	UNP P06886
D	716	TRP	GLY	SEE REMARK 999	UNP P06886
D	736	ALA	GLN	engineered mutation	UNP P06886

- Molecule 2 is water.

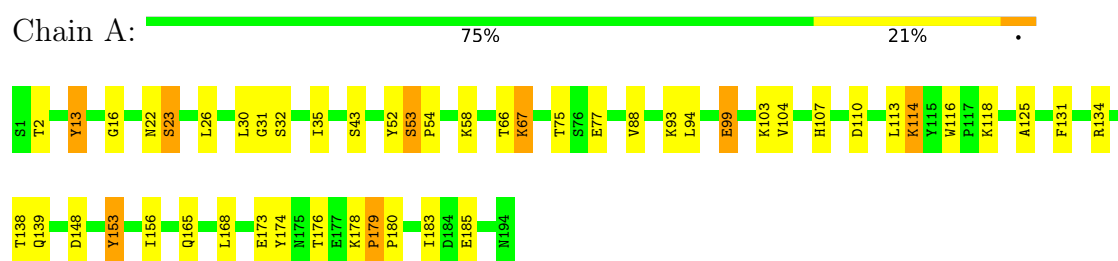
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	79	Total	O	0	0
			79	79		
2	C	64	Total	O	0	0
			64	64		
2	D	70	Total	O	0	0
			70	70		

3 Residue-property plots

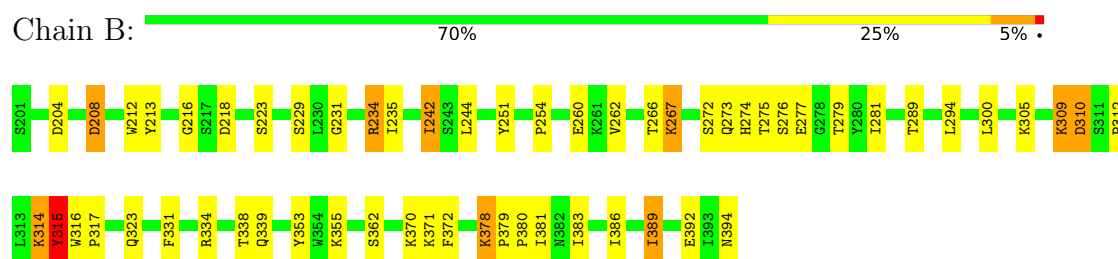
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

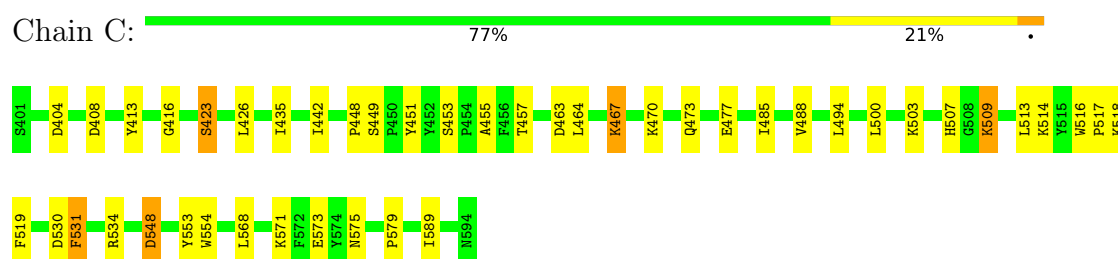
• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



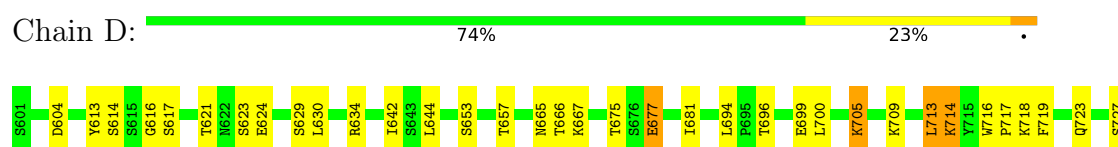
• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1



• Molecule 1: TOXIC SHOCK SYNDROME TOXIN-1





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	49.63Å 99.28Å 41.33Å 88.50° 93.30° 91.10°	Depositor
Resolution (Å)	20.00 – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	1.51	9/1603 (0.6%)	1.41	19/2168 (0.9%)
1	B	1.52	11/1603 (0.7%)	1.40	16/2168 (0.7%)
1	C	1.47	7/1603 (0.4%)	1.39	15/2168 (0.7%)
1	D	1.44	11/1603 (0.7%)	1.38	11/2168 (0.5%)
All	All	1.48	38/6412 (0.6%)	1.39	61/8672 (0.7%)

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	0	2
1	B	0	2
All	All	0	4

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	642	ILE	CA-CB	8.10	1.64	1.54
1	B	242	ILE	CA-CB	7.69	1.65	1.54
1	C	548	ASP	CA-C	6.91	1.62	1.52
1	D	666	THR	CA-CB	6.84	1.64	1.53
1	A	43	SER	C-O	6.79	1.32	1.24
1	C	571	LYS	CA-C	6.29	1.60	1.52
1	A	2	THR	CA-CB	6.27	1.63	1.53
1	A	66	THR	CA-C	6.17	1.60	1.52
1	D	621	THR	CA-C	6.09	1.60	1.52
1	A	176	THR	CA-CB	6.08	1.62	1.53
1	B	260	GLU	CA-C	6.00	1.61	1.53
1	C	554	TRP	CA-C	5.87	1.59	1.52
1	C	442	ILE	CA-CB	5.85	1.62	1.54
1	B	266	THR	CA-CB	5.83	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	681	ILE	CA-CB	5.83	1.61	1.54
1	B	281	ILE	CA-CB	5.81	1.61	1.54
1	D	623	SER	CA-C	5.79	1.61	1.53
1	C	463	ASP	CA-C	5.76	1.59	1.52
1	A	88	VAL	N-CA	5.64	1.53	1.46
1	C	457	THR	CA-CB	5.57	1.62	1.53
1	D	614	SER	CA-C	5.51	1.59	1.52
1	B	254	PRO	CA-C	5.50	1.59	1.52
1	A	185	GLU	CA-C	5.47	1.60	1.52
1	C	470	LYS	CA-C	-5.42	1.46	1.52
1	A	52	TYR	CA-C	-5.42	1.48	1.53
1	A	156	ILE	CA-C	5.39	1.59	1.52
1	D	780	PRO	CA-C	-5.39	1.45	1.52
1	B	386	ILE	CA-C	5.34	1.58	1.52
1	D	617	SER	C-O	5.32	1.30	1.23
1	B	218	ASP	CA-C	-5.29	1.46	1.52
1	D	727	SER	CA-C	5.27	1.59	1.52
1	B	262	VAL	CA-C	5.26	1.58	1.52
1	A	125	ALA	C-O	5.25	1.30	1.23
1	D	657	THR	CA-CB	5.15	1.63	1.53
1	D	624	GLU	CA-C	-5.08	1.46	1.52
1	B	208	ASP	CB-CG	-5.06	1.39	1.52
1	B	289	THR	CA-CB	5.02	1.61	1.53
1	B	372	PHE	CA-C	5.02	1.58	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	404	ASP	N-CA-C	7.47	120.30	111.71
1	A	31	GLY	N-CA-C	7.44	125.70	114.61
1	A	114	LYS	N-CA-C	7.34	120.48	108.52
1	C	531[A]	PHE	N-CA-C	7.34	120.15	111.71
1	C	531[B]	PHE	N-CA-C	7.34	120.15	111.71
1	A	53	SER	CA-C-N	6.94	126.98	119.90
1	A	53	SER	C-N-CA	6.94	126.98	119.90
1	A	178	LYS	CA-C-N	-6.62	113.56	120.38
1	A	178	LYS	C-N-CA	-6.62	113.56	120.38
1	B	234	ARG	N-CA-C	-6.50	97.81	108.41
1	D	694	LEU	N-CA-C	-6.48	101.97	110.39
1	B	315	TYR	N-CA-C	-6.47	98.65	109.07
1	A	26	LEU	N-CA-C	-6.39	106.02	113.88
1	A	23	SER	N-CA-C	-6.39	102.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ILE	N-CA-C	-6.28	99.44	108.48
1	C	423	SER	N-CA-C	-6.21	102.52	110.53
1	D	779	PRO	CA-C-N	6.20	126.17	119.78
1	D	779	PRO	C-N-CA	6.20	126.17	119.78
1	C	516	TRP	CA-C-N	6.19	126.55	119.93
1	C	516	TRP	C-N-CA	6.19	126.55	119.93
1	B	204	ASP	N-CA-C	6.12	118.75	111.71
1	A	66	THR	N-CA-C	6.10	117.46	108.86
1	A	30	LEU	N-CA-C	-6.05	100.44	109.15
1	B	379	PRO	N-CA-C	6.05	118.08	110.70
1	D	714	LYS	N-CA-C	6.02	119.48	107.62
1	B	276	SER	N-CA-C	5.96	119.64	112.38
1	D	623	SER	N-CA-C	-5.95	102.85	110.53
1	C	426	LEU	N-CA-C	-5.94	106.57	113.88
1	B	266	THR	N-CA-C	5.92	117.20	108.86
1	A	104	VAL	N-CA-C	5.90	117.09	108.53
1	A	75	THR	N-CA-C	-5.88	102.61	110.55
1	C	455	ALA	N-CA-C	5.86	120.55	113.17
1	A	94	LEU	CA-C-N	5.84	125.31	119.24
1	A	94	LEU	C-N-CA	5.84	125.31	119.24
1	A	22	ASN	CB-CA-C	-5.82	104.07	111.86
1	D	604	ASP	N-CA-C	5.80	119.17	111.75
1	C	494	LEU	CA-C-N	5.74	125.21	119.24
1	C	494	LEU	C-N-CA	5.74	125.21	119.24
1	B	339	GLN	N-CA-C	5.74	117.34	111.14
1	B	275	THR	N-CA-C	-5.74	103.13	110.53
1	A	179	PRO	N-CA-C	5.72	117.68	110.70
1	C	530	ASP	N-CA-C	-5.53	105.16	111.07
1	D	665	ASN	N-CA-C	-5.51	95.96	107.37
1	C	519	PHE	N-CA-C	5.43	118.40	109.72
1	A	179	PRO	CA-C-N	5.40	125.34	119.78
1	A	179	PRO	C-N-CA	5.40	125.34	119.78
1	C	449	SER	N-CA-C	5.40	116.62	109.93
1	B	231	GLY	N-CA-C	5.28	122.23	115.32
1	C	589	ILE	N-CA-C	-5.28	100.72	108.11
1	C	514	LYS	N-CA-C	5.24	116.95	108.41
1	D	723	GLN	N-CA-C	5.22	118.08	109.72
1	A	13	TYR	N-CA-C	5.20	119.50	113.20
1	B	294	LEU	CA-C-N	5.16	125.20	119.32
1	B	294	LEU	C-N-CA	5.16	125.20	119.32
1	B	229	SER	CA-C-N	-5.12	112.58	120.88
1	B	229	SER	C-N-CA	-5.12	112.58	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	ASP	N-CA-C	-5.08	103.77	110.43
1	D	705	LYS	N-CA-C	-5.07	100.03	108.34
1	D	681	ILE	CB-CA-C	-5.07	103.11	110.81
1	B	242	ILE	CB-CA-C	-5.04	103.11	110.62
1	D	675	THR	N-CA-C	-5.02	103.31	110.59

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	TYR	Sidechain
1	A	174	TYR	Sidechain
1	B	251	TYR	Sidechain
1	B	315	TYR	Sidechain

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	1562	0	1545	15	0
1	B	1562	0	1542	23	0
1	C	1562	0	1542	16	0
1	D	1562	0	1542	23	0
2	A	78	0	0	4	0
2	B	79	0	0	0	0
2	C	64	0	0	0	0
2	D	70	0	0	0	0
All	All	6539	0	6171	77	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 6.

All (77) 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:C:416:GLY:O	1:C:467:LYS:HE2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:LYS:HE3	1:C:531[A]:PHE:CE2	2.21	0.75
1:B:216:GLY:O	1:B:267:LYS:HE2	1.93	0.68
2:A:196:HOH:O	1:B:274:HIS:HE1	1.74	0.68
1:D:616:GLY:O	1:D:667:LYS:HE2	1.94	0.68
1:B:212:TRP:CD2	1:B:371:LYS:HE3	2.31	0.65
1:D:755:LYS:HE2	1:D:765:GLN:NE2	2.16	0.61
1:B:223:SER:HB3	1:B:235:ILE:CG2	2.30	0.61
1:D:753:TYR:C	1:D:753:TYR:CD1	2.80	0.59
1:C:500:LEU:O	1:C:517:PRO:HD2	2.04	0.58
1:D:713:LEU:HD11	1:D:741:HIS:CE1	2.39	0.58
1:A:16:GLY:O	1:A:67:LYS:HE2	2.05	0.57
1:A:173:GLU:HG2	2:A:250:HOH:O	2.08	0.54
1:B:315:TYR:O	1:B:316:TRP:HD1	1.91	0.54
1:A:13:TYR:CZ	1:A:134:ARG:HD2	2.43	0.53
1:D:667:LYS:CE	1:D:731[A]:PHE:CE2	2.92	0.52
1:B:272:SER:C	1:B:273:GLN:HG2	2.33	0.52
1:D:613:TYR:CZ	1:D:734:ARG:HD2	2.44	0.52
1:B:213:TYR:CZ	1:B:334:ARG:HD2	2.45	0.52
1:B:242:ILE:HG12	1:B:279:THR:HG21	1.92	0.52
1:C:467:LYS:CE	1:C:531[A]:PHE:CE2	2.93	0.51
1:C:451:TYR:O	1:C:579:PRO:HD3	2.11	0.51
1:B:267:LYS:HE3	1:B:331[A]:PHE:HE2	1.75	0.50
1:B:267:LYS:CE	1:B:331[A]:PHE:CE2	2.93	0.50
1:B:212:TRP:CE2	1:B:371:LYS:HE3	2.47	0.50
1:B:378:LYS:N	1:B:378:LYS:HD3	2.26	0.50
1:D:634:ARG:HG3	1:D:644:LEU:HD23	1.93	0.49
1:A:103:LYS:HE2	1:A:110:ASP:OD1	2.13	0.48
1:C:413:TYR:CZ	1:C:534:ARG:HD2	2.48	0.48
1:A:134:ARG:O	1:A:138:THR:HG23	2.13	0.48
1:C:507:HIS:CE1	1:C:548:ASP:O	2.67	0.48
1:C:553:TYR:HA	1:C:568:LEU:HG	1.95	0.48
2:A:196:HOH:O	1:B:274:HIS:CE1	2.59	0.47
1:B:267:LYS:HE3	1:B:331[A]:PHE:CE2	2.50	0.47
1:D:667:LYS:HE3	1:D:731[A]:PHE:CE2	2.49	0.47
1:D:778:LYS:N	1:D:778:LYS:HD3	2.29	0.47
1:C:467:LYS:HE3	1:C:531[A]:PHE:HE2	1.71	0.46
1:A:99:GLU:HG2	1:A:116:TRP:HB3	1.98	0.46
1:C:509:LYS:HB2	1:C:509:LYS:NZ	2.30	0.46
1:D:699:GLU:HG2	1:D:718:LYS:HG2	1.96	0.46
1:D:700:LEU:O	1:D:717:PRO:HD2	2.15	0.46
1:A:107:HIS:HE1	1:A:148:ASP:O	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:464:LEU:HD22	1:C:488:VAL:HG22	1.98	0.45
1:B:267:LYS:HE2	1:B:331[A]:PHE:CE2	2.51	0.45
1:A:58:LYS:HE3	1:A:58:LYS:HB2	1.69	0.45
1:D:667:LYS:HE2	1:D:731[A]:PHE:CE2	2.52	0.45
1:A:153:TYR:HA	1:A:168:LEU:HG	1.99	0.44
1:D:719:PHE:HZ	1:D:732:GLU:HG3	1.83	0.44
1:D:667:LYS:HE3	1:D:731[A]:PHE:HE2	1.82	0.44
1:D:716:TRP:HA	1:D:717:PRO:HD3	1.82	0.44
1:D:754:TRP:CE2	1:D:766:SER:HB3	2.53	0.44
1:D:677:GLU:H	1:D:677:GLU:HG3	1.40	0.44
1:C:448:PRO:HB2	1:C:575:ASN:ND2	2.32	0.44
1:B:305:LYS:HB3	1:B:392:GLU:HG2	2.00	0.43
1:A:53:SER:HA	1:A:54:PRO:HD3	1.86	0.43
1:A:118:LYS:HB3	1:A:118:LYS:HE3	1.71	0.43
1:B:353:TYR:CD1	1:B:353:TYR:C	2.96	0.43
1:B:334:ARG:O	1:B:338:THR:HG23	2.18	0.43
1:D:742:GLY:O	1:D:743:LEU:C	2.62	0.43
1:A:173:GLU:CG	2:A:250:HOH:O	2.66	0.43
1:D:613:TYR:CE1	1:D:734:ARG:HD2	2.53	0.43
1:D:718:LYS:HB3	1:D:718:LYS:HE3	1.64	0.43
1:A:23:SER:HB3	1:A:35:ILE:CG2	2.48	0.42
1:B:234:ARG:HG3	1:B:244:LEU:CD2	2.49	0.42
1:B:314:LYS:HG2	1:B:316:TRP:NE1	2.34	0.42
1:B:383:ILE:HG21	1:B:383:ILE:HD13	1.82	0.42
1:B:300:LEU:O	1:B:317:PRO:HD2	2.20	0.41
1:C:423:SER:HB3	1:C:435:ILE:CG2	2.50	0.41
1:A:179:PRO:HA	1:A:180:PRO:HD3	1.94	0.41
1:C:507:HIS:HE1	1:C:548:ASP:O	2.04	0.41
1:A:183:ILE:HG21	1:A:183:ILE:HD13	1.65	0.40
1:B:309:LYS:C	1:B:310:ASP:O	2.61	0.40
1:C:448:PRO:HB2	1:C:575:ASN:HD22	1.87	0.40
1:D:629:SER:HB3	1:D:630:LEU:H	1.60	0.40
1:D:630:LEU:HD12	1:D:630:LEU:HA	1.96	0.40
1:D:667:LYS:HD2	1:D:731[A]:PHE:CD2	2.57	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	193/194 (100%)	187 (97%)	6 (3%)	0	100	100
1	B	193/194 (100%)	187 (97%)	5 (3%)	1 (0%)	24	16
1	C	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
1	D	193/194 (100%)	185 (96%)	8 (4%)	0	100	100
All	All	772/776 (100%)	744 (96%)	27 (4%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	PRO

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	180/179 (101%)	169 (94%)	11 (6%)	17	7
1	B	180/179 (101%)	166 (92%)	14 (8%)	11	3
1	C	180/179 (101%)	169 (94%)	11 (6%)	17	7
1	D	180/179 (101%)	170 (94%)	10 (6%)	19	8
All	All	720/716 (101%)	674 (94%)	46 (6%)	16	6

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	SER
1	A	67	LYS
1	A	77	GLU
1	A	93	LYS
1	A	99	GLU
1	A	113	LEU
1	A	114	LYS
1	A	131[A]	PHE
1	A	131[B]	PHE
1	A	139	GLN
1	A	165	GLN
1	B	208	ASP
1	B	267	LYS
1	B	277	GLU
1	B	309	LYS
1	B	314	LYS
1	B	323	GLN
1	B	355	LYS
1	B	362	SER
1	B	370	LYS
1	B	378	LYS
1	B	380	PRO
1	B	381	ILE
1	B	389	ILE
1	B	394	ASN
1	C	408	ASP
1	C	453	SER
1	C	467	LYS
1	C	473	GLN
1	C	477	GLU
1	C	485	ILE
1	C	503	LYS
1	C	509	LYS
1	C	513	LEU
1	C	518	LYS
1	C	573	GLU
1	D	653	SER
1	D	677	GLU
1	D	696	THR
1	D	705	LYS
1	D	709	LYS
1	D	713	LEU
1	D	714	LYS

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Mol	Chain	Res	Type
1	D	778	LYS
1	D	780	PRO
1	D	789	ILE

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

Mol	Chain	Res	Type
1	A	37	ASN
1	A	65	ASN
1	A	139	GLN
1	A	141	HIS
1	A	175	ASN
1	B	265	ASN
1	B	274	HIS
1	B	307	HIS
1	B	335	HIS
1	B	375	ASN
1	C	422	ASN
1	C	473	GLN
1	C	507	HIS
1	C	539	GLN
1	C	541	HIS
1	C	575	ASN
1	D	665	ASN
1	D	723	GLN
1	D	741	HIS
1	D	765	GLN
1	D	775	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 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.