



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:04 PM UTC

PDB ID : 1CIY / pdb_00001ciy
Title : INSECTICIDAL TOXIN: STRUCTURE AND CHANNEL FORMATION
Authors : Grochulski, P.; Cygler, M.
Deposited on : 1995-06-01
Resolution : 2.25 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

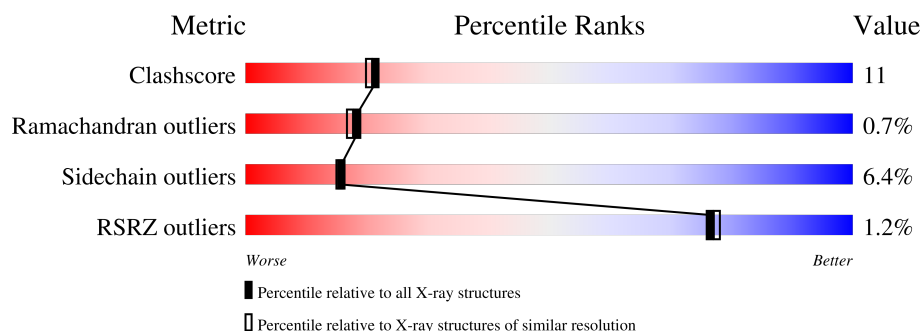
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	590	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4693 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 CRYIA(A).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	11	0	0
			4571	2908	802	855	6			

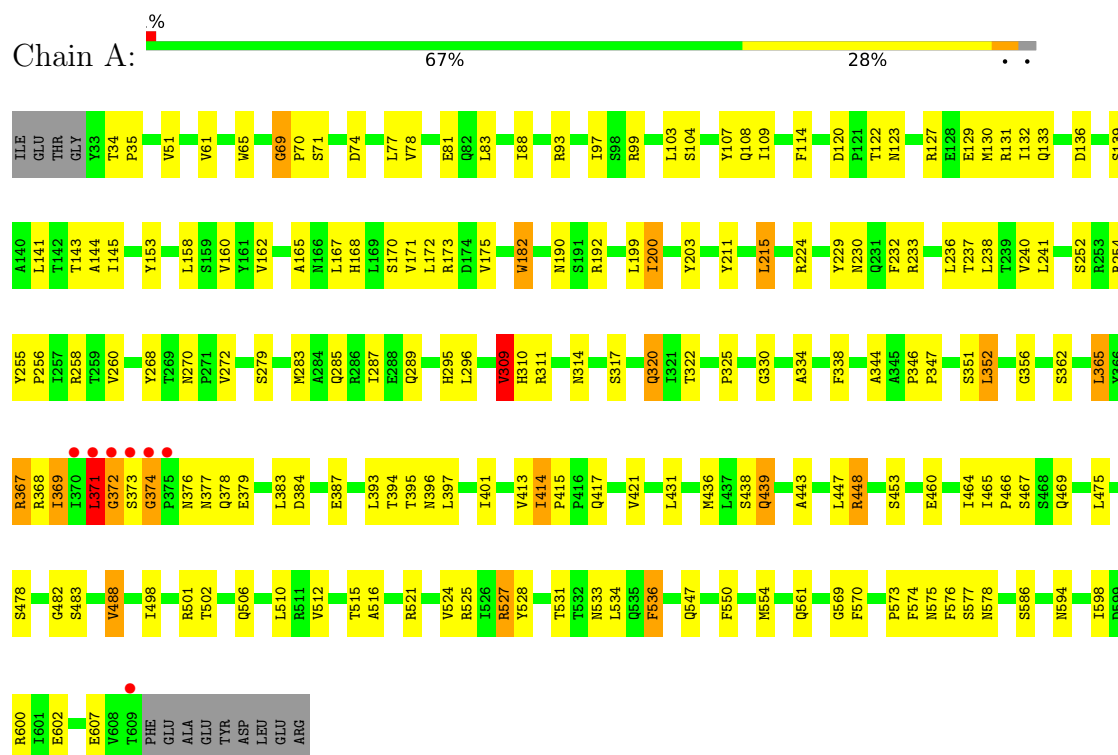
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		

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: CRYIA(A)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.00Å 111.50Å 154.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.25 8.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	73.0 (8.00-2.25) 70.8 (8.00-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.24Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.163 , 0.248 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.755	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4693	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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	0.68	0/4686	1.14	44/6390 (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	1

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	65	TRP	N-CA-C	8.46	123.16	113.01
1	A	371	LEU	N-CA-C	8.00	127.84	110.80
1	A	237	THR	N-CA-C	-7.15	102.89	111.69
1	A	270	ASN	CA-C-N	7.01	126.53	119.24
1	A	270	ASN	C-N-CA	7.01	126.53	119.24
1	A	374	GLY	N-CA-C	-6.95	98.17	112.34
1	A	120	ASP	CA-C-N	6.94	128.51	119.84
1	A	120	ASP	C-N-CA	6.94	128.51	119.84
1	A	268	TYR	N-CA-C	6.65	120.37	109.72
1	A	69	GLY	CA-C-N	6.61	126.55	119.28
1	A	69	GLY	C-N-CA	6.61	126.55	119.28
1	A	576	PHE	N-CA-C	-6.58	98.96	109.76
1	A	417	GLN	N-CA-C	-6.53	105.14	113.23
1	A	373	SER	N-CA-C	6.51	120.78	107.69
1	A	123	ASN	CA-C-N	6.31	126.79	119.47
1	A	123	ASN	C-N-CA	6.31	126.79	119.47
1	A	255	TYR	CA-C-N	6.10	125.99	119.28
1	A	255	TYR	C-N-CA	6.10	125.99	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	533	ASN	N-CA-C	-6.00	100.78	110.32
1	A	372	GLY	N-CA-C	-5.94	99.11	113.18
1	A	414	ILE	CA-C-N	5.92	126.48	120.38
1	A	414	ILE	C-N-CA	5.92	126.48	120.38
1	A	570	PHE	N-CA-C	-5.83	100.68	109.95
1	A	211	TYR	N-CA-C	-5.82	104.84	111.07
1	A	182	TRP	N-CA-C	-5.81	106.36	113.50
1	A	241	LEU	N-CA-C	5.73	118.27	111.33
1	A	309	VAL	CB-CA-C	-5.69	100.24	110.48
1	A	415	PRO	N-CA-C	5.66	117.61	110.70
1	A	482	GLY	N-CA-C	-5.65	104.04	113.02
1	A	395	THR	N-CA-C	5.64	118.81	110.46
1	A	393	LEU	N-CA-C	-5.61	106.57	113.41
1	A	109	ILE	N-CA-C	-5.56	105.30	110.53
1	A	443	ALA	N-CA-C	-5.53	102.30	110.48
1	A	158	LEU	N-CA-C	5.48	122.47	110.80
1	A	421	VAL	N-CA-C	-5.39	104.77	109.19
1	A	536	PHE	N-CA-C	-5.37	100.15	108.90
1	A	252	SER	N-CA-C	5.32	117.83	111.71
1	A	369	ILE	N-CA-C	5.32	115.37	108.35
1	A	561	GLN	N-CA-C	-5.21	101.19	108.96
1	A	374	GLY	CA-C-N	-5.07	113.50	119.84
1	A	374	GLY	C-N-CA	-5.07	113.50	119.84
1	A	145	ILE	N-CA-C	5.01	119.70	108.88
1	A	260	VAL	N-CA-C	5.01	115.65	107.24
1	A	362	SER	N-CA-C	5.00	117.88	110.48

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	528	TYR	Sidechain

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	4571	0	4471	98	0
2	A	122	0	0	2	0
All	All	4693	0	4471	98	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 11.

All (98) 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:310:HIS:HE1	1:A:378:GLN:H	1.15	0.90
1:A:439:GLN:NE2	1:A:439:GLN:H	1.86	0.71
1:A:311:ARG:HG3	1:A:367:ARG:HH22	1.54	0.71
1:A:387:GLU:HG3	1:A:401:ILE:HG12	1.71	0.70
1:A:439:GLN:HE22	1:A:448:ARG:HH21	1.39	0.70
1:A:310:HIS:CE1	1:A:378:GLN:H	2.05	0.70
1:A:224:ARG:HB2	1:A:279:SER:HB2	1.77	0.66
1:A:439:GLN:H	1:A:439:GLN:HE21	1.46	0.62
1:A:439:GLN:NE2	1:A:447:LEU:H	1.99	0.60
1:A:77:LEU:O	1:A:81:GLU:HG3	2.02	0.59
1:A:192:ARG:HA	1:A:192:ARG:HE	1.67	0.59
1:A:103:LEU:HD11	1:A:144:ALA:CB	2.33	0.58
1:A:283:MET:O	1:A:287:ILE:HG13	2.04	0.58
1:A:133:GLN:NE2	1:A:133:GLN:HA	2.17	0.58
1:A:61:VAL:HG23	1:A:107:TYR:CE2	2.37	0.58
1:A:317:SER:O	1:A:448:ARG:HD2	2.04	0.57
1:A:309:VAL:HG13	1:A:314:ASN:OD1	2.05	0.57
1:A:127:ARG:O	1:A:131:ARG:HG3	2.04	0.56
1:A:83:LEU:HD21	1:A:232:PHE:HA	1.88	0.56
1:A:521:ARG:HD2	1:A:575:ASN:HD21	1.71	0.56
1:A:99:ARG:HH12	1:A:143:THR:HG22	1.71	0.55
1:A:295:HIS:HD2	1:A:296:LEU:O	1.88	0.55
1:A:283:MET:HE1	1:A:447:LEU:HD22	1.89	0.55
1:A:61:VAL:HG23	1:A:107:TYR:HE2	1.71	0.55
1:A:230:ASN:HB3	2:A:705:HOH:O	2.06	0.54
1:A:311:ARG:NH2	1:A:377:ASN:HB2	2.23	0.54
1:A:74:ASP:O	1:A:78:VAL:HG23	2.07	0.54
1:A:325:PRO:HG2	1:A:330:GLY:HA3	1.90	0.54
1:A:311:ARG:HG3	1:A:367:ARG:NH2	2.21	0.53
1:A:93:ARG:O	1:A:97:ILE:HG13	2.09	0.52
1:A:483:SER:O	1:A:501:ARG:NH2	2.42	0.52
1:A:374:GLY:O	1:A:376:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HB3	1:A:97:ILE:HG21	1.92	0.51
1:A:232:PHE:CZ	1:A:236:LEU:HD22	2.44	0.51
1:A:317:SER:HA	1:A:448:ARG:HG2	1.91	0.51
1:A:130:MET:HE2	1:A:182:TRP:CZ2	2.45	0.51
1:A:254:ARG:C	1:A:256:PRO:HD3	2.36	0.51
1:A:322:THR:HG22	1:A:334:ALA:HB2	1.91	0.51
1:A:88:ILE:HA	1:A:153:TYR:CD1	2.47	0.50
1:A:488:VAL:HG12	1:A:498:ILE:HG13	1.93	0.50
1:A:521:ARG:HD2	1:A:575:ASN:ND2	2.27	0.50
1:A:107:TYR:CD1	1:A:167:LEU:HD11	2.47	0.49
1:A:431:LEU:HD12	1:A:453:SER:O	2.12	0.49
1:A:309:VAL:HG22	1:A:344:ALA:HB2	1.94	0.49
1:A:272:VAL:HG23	1:A:383:LEU:HG	1.94	0.49
1:A:502:THR:HA	1:A:594:ASN:O	2.12	0.49
1:A:129:GLU:HA	1:A:129:GLU:OE1	2.13	0.48
1:A:521:ARG:NH2	1:A:573:PRO:HG2	2.27	0.48
1:A:295:HIS:CD2	1:A:296:LEU:O	2.67	0.47
1:A:199:LEU:O	1:A:200:ILE:C	2.58	0.47
1:A:413:VAL:HG23	1:A:414:ILE:HG13	1.96	0.47
1:A:162:VAL:HG21	1:A:240:VAL:HG13	1.97	0.47
1:A:165:ALA:HB1	1:A:203:TYR:CD2	2.48	0.47
1:A:192:ARG:HA	1:A:192:ARG:NE	2.30	0.47
1:A:254:ARG:O	1:A:525:ARG:NH2	2.48	0.47
1:A:365:LEU:HB2	1:A:384:ASP:OD2	2.15	0.47
1:A:531:THR:HA	1:A:554:MET:O	2.16	0.46
1:A:467:SER:N	1:A:516:ALA:HB2	2.30	0.46
1:A:285:GLN:O	1:A:289:GLN:HG3	2.16	0.46
1:A:464:ILE:HG23	1:A:515:THR:HG23	1.98	0.46
1:A:521:ARG:HH11	1:A:521:ARG:HG3	1.80	0.46
1:A:131:ARG:HD3	1:A:182:TRP:O	2.16	0.46
1:A:141:LEU:HD13	1:A:168:HIS:HA	1.98	0.46
1:A:107:TYR:CE1	1:A:167:LEU:HD11	2.51	0.45
1:A:607:GLU:CD	1:A:607:GLU:H	2.24	0.45
1:A:230:ASN:OD1	1:A:233:ARG:NH1	2.50	0.45
1:A:465:ILE:HG12	1:A:512:VAL:HG13	1.99	0.45
1:A:525:ARG:HA	1:A:569:GLY:HA2	1.99	0.44
1:A:69:GLY:HA2	1:A:70:PRO:HD3	1.82	0.44
1:A:99:ARG:HH12	1:A:143:THR:CG2	2.30	0.44
1:A:352:LEU:HD13	1:A:356:GLY:HA2	2.00	0.44
1:A:475:LEU:HD12	1:A:598:ILE:HG22	2.00	0.44
1:A:296:LEU:HD13	1:A:478:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:GLU:HA	1:A:132:ILE:HD12	2.00	0.44
1:A:534:LEU:C	1:A:534:LEU:HD12	2.43	0.43
1:A:368:ARG:NH1	1:A:379:GLU:OE2	2.51	0.43
1:A:320:GLN:HA	2:A:757:HOH:O	2.19	0.43
1:A:338:PHE:HB3	1:A:436:MET:HB3	2.01	0.43
1:A:506:GLN:HA	1:A:586:SER:HB3	2.00	0.43
1:A:368:ARG:NH1	1:A:368:ARG:HB3	2.35	0.42
1:A:439:GLN:HE22	1:A:448:ARG:NH2	2.11	0.42
1:A:475:LEU:HD12	1:A:598:ILE:CG2	2.49	0.42
1:A:258:ARG:NH1	1:A:469:GLN:NE2	2.68	0.42
1:A:103:LEU:HD11	1:A:144:ALA:HB1	2.02	0.42
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.74	0.42
1:A:272:VAL:CG2	1:A:383:LEU:HG	2.49	0.42
1:A:527:ARG:HH21	1:A:600:ARG:NH1	2.16	0.42
1:A:346:PRO:HA	1:A:347:PRO:HD3	1.92	0.42
1:A:525:ARG:NH1	1:A:602:GLU:OE1	2.53	0.42
1:A:215:LEU:HD22	1:A:229:TYR:CE1	2.55	0.41
1:A:438:SER:HA	1:A:447:LEU:O	2.20	0.41
1:A:104:SER:O	1:A:108:GLN:HG3	2.21	0.41
1:A:114:PHE:HA	1:A:130:MET:SD	2.61	0.41
1:A:536:PHE:HB2	1:A:550:PHE:CE1	2.55	0.41
1:A:34:THR:HB	1:A:35:PRO:HD2	2.02	0.41
1:A:467:SER:HB3	1:A:516:ALA:HB1	2.03	0.41
1:A:524:VAL:HG23	1:A:574:PHE:HE2	1.85	0.41
1:A:167:LEU:O	1:A:170:SER:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	575/590 (98%)	540 (94%)	31 (5%)	4 (1%)	18 17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	LEU
1	A	372	GLY
1	A	71	SER
1	A	466	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	502/513 (98%)	470 (94%)	32 (6%)	16	15

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	122	THR
1	A	136	ASP
1	A	139	SER
1	A	160	VAL
1	A	171	VAL
1	A	173	ARG
1	A	175	VAL
1	A	190	ASN
1	A	200	ILE
1	A	215	LEU
1	A	238	LEU
1	A	309	VAL
1	A	320	GLN
1	A	351	SER
1	A	352	LEU
1	A	365	LEU
1	A	367	ARG
1	A	369	ILE
1	A	371	LEU
1	A	394	THR

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Mol	Chain	Res	Type
1	A	396	ASN
1	A	397	LEU
1	A	439	GLN
1	A	448	ARG
1	A	460	GLU
1	A	488	VAL
1	A	510	LEU
1	A	527	ARG
1	A	547	GLN
1	A	577	SER
1	A	578	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	72	GLN
1	A	79	GLN
1	A	133	GLN
1	A	231	GLN
1	A	249	ASN
1	A	275	ASN
1	A	290	ASN
1	A	301	ASN
1	A	310	HIS
1	A	340	ASN
1	A	417	GLN
1	A	439	GLN
1	A	455	GLN
1	A	469	GLN
1	A	513	ASN
1	A	546	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 [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 [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	577/590 (97%)	-0.81	7 (1%) 76 77	6, 24, 51, 82	8 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	8.5
1	A	375	PRO	5.9
1	A	370	ILE	5.2
1	A	372	GLY	4.4
1	A	373	SER	3.3
1	A	374	GLY	3.0
1	A	609	THR	2.7

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.