



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 02:19 PM EDT

PDB ID : 1I5P
Title : INSECTICIDAL CRYSTAL PROTEIN CRY2AA
Authors : Morse, R.J.; Stroud, R.M.; Yamamoto, T.
Deposited on : 2001-02-28
Resolution : 2.20 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

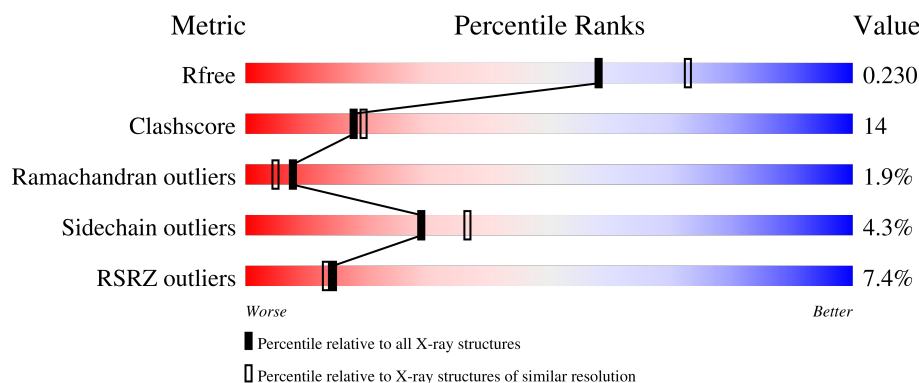
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	633	<div> <div>7%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5378 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 PESTICIDIAL CRYSTAL PROTEIN CRY2AA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			5001	3148	877	961	15			

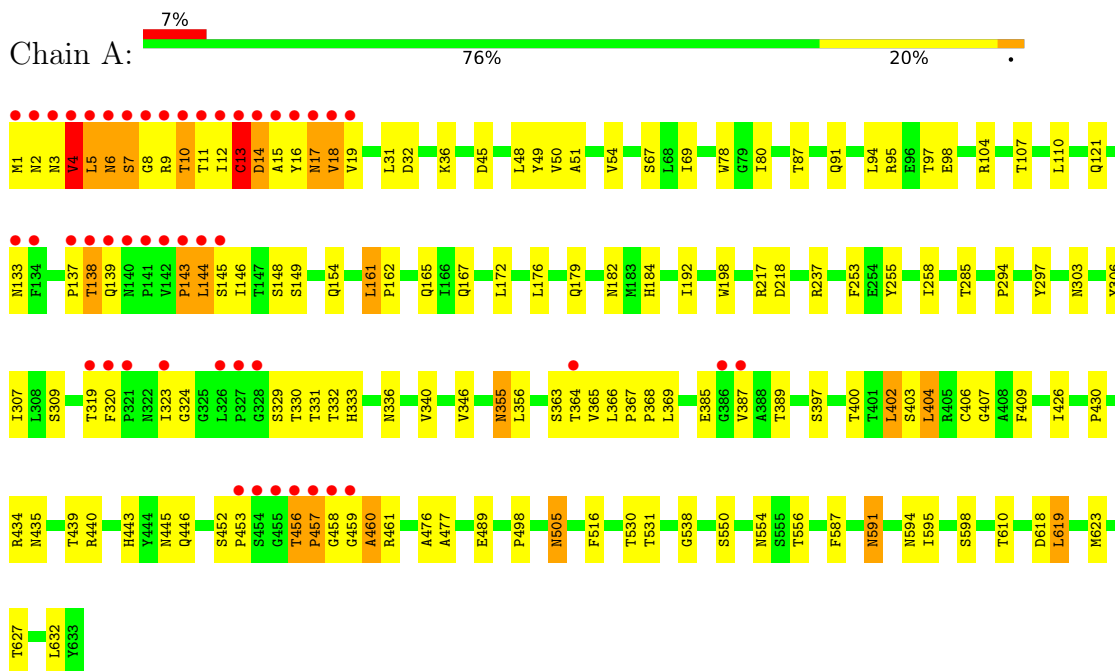
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	377	Total	O	0	0
			377	377		

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: PESTICIDIAL CRYSTAL PROTEIN CRY2AA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.60Å 85.60Å 163.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.97 – 2.20 27.97 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (27.97-2.20) 99.4 (27.97-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.11 (at 2.20Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.183 , 0.231 0.183 , 0.230	Depositor DCC
R_{free} test set	1566 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5378	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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 [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	0.33	0/5113	0.60	0/6967

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5001	0	4863	134	1
2	A	377	0	0	5	0
All	All	5378	0	4863	134	1

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 14.

All (134) 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:7:SER:HB3	1:A:368:PRO:HD3	1.45	0.96
1:A:456:THR:H	1:A:457:PRO:HD3	1.33	0.93
1:A:402:LEU:HD22	1:A:404:LEU:HD23	1.60	0.84
1:A:456:THR:H	1:A:457:PRO:CD	1.91	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HG21	1:A:402:LEU:HD12	1.60	0.82
1:A:434:ARG:HG2	1:A:453:PRO:HG3	1.64	0.79
1:A:505:ASN:HD21	1:A:531:THR:H	1.33	0.75
1:A:7:SER:CB	1:A:368:PRO:HD3	2.14	0.75
1:A:78:TRP:HZ2	1:A:121:GLN:HE21	1.34	0.73
1:A:6:ASN:HA	1:A:367:PRO:HA	1.70	0.73
1:A:5:LEU:O	1:A:368:PRO:HD2	1.87	0.73
1:A:9:ARG:HG2	1:A:10:THR:N	2.03	0.72
1:A:162:PRO:HA	1:A:165:GLN:HE21	1.55	0.71
1:A:7:SER:HB3	1:A:368:PRO:CD	2.19	0.71
1:A:67:SER:OG	1:A:69:ILE:HG22	1.89	0.71
1:A:143:PRO:C	1:A:145:SER:H	1.94	0.70
1:A:323:ILE:HG13	1:A:324:GLY:H	1.58	0.69
1:A:453:PRO:O	1:A:457:PRO:HD3	1.92	0.68
1:A:307:ILE:HD12	1:A:477:ALA:HB2	1.76	0.68
1:A:18:VAL:HG11	1:A:402:LEU:HG	1.76	0.67
1:A:146:ILE:HG21	1:A:198:TRP:HB3	1.78	0.65
1:A:5:LEU:HD23	1:A:476:ALA:HB1	1.79	0.65
1:A:9:ARG:HD3	1:A:363:SER:O	1.97	0.64
1:A:303:ASN:H	1:A:445:ASN:ND2	1.95	0.64
1:A:323:ILE:HG13	1:A:324:GLY:N	2.13	0.64
1:A:456:THR:N	1:A:457:PRO:CD	2.61	0.64
1:A:5:LEU:CD2	1:A:477:ALA:H	2.10	0.64
1:A:365:VAL:HG13	1:A:366:LEU:HG	1.80	0.63
1:A:18:VAL:HG21	1:A:402:LEU:CD1	2.28	0.63
1:A:5:LEU:HB2	1:A:369:LEU:HD12	1.80	0.62
1:A:355:ASN:H	1:A:355:ASN:HD22	1.45	0.62
1:A:9:ARG:O	1:A:10:THR:HB	2.00	0.62
1:A:505:ASN:ND2	1:A:531:THR:H	1.98	0.61
1:A:5:LEU:C	1:A:367:PRO:HB3	2.20	0.61
1:A:5:LEU:O	1:A:367:PRO:HB3	2.02	0.60
1:A:6:ASN:ND2	1:A:6:ASN:H	1.98	0.59
1:A:13:CYS:HB3	1:A:402:LEU:HD11	1.85	0.59
1:A:402:LEU:O	1:A:404:LEU:N	2.36	0.58
1:A:48:LEU:O	1:A:49:TYR:HB2	2.05	0.57
1:A:5:LEU:O	1:A:368:PRO:CD	2.53	0.56
1:A:336:ASN:HB3	1:A:459:GLY:O	2.04	0.56
1:A:5:LEU:HG	1:A:477:ALA:CB	2.34	0.56
1:A:309:SER:O	1:A:363:SER:HB2	2.05	0.56
1:A:365:VAL:HG13	1:A:366:LEU:N	2.20	0.56
1:A:95:ARG:HH21	1:A:110:LEU:HD11	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:THR:HB	1:A:610:THR:HB	1.89	0.54
1:A:5:LEU:HG	1:A:477:ALA:HB2	1.88	0.54
1:A:3:ASN:O	1:A:369:LEU:HB2	2.08	0.53
1:A:402:LEU:C	1:A:404:LEU:H	2.11	0.53
1:A:505:ASN:HD21	1:A:531:THR:N	2.04	0.53
1:A:9:ARG:HG2	1:A:10:THR:H	1.74	0.53
1:A:8:GLY:HA2	1:A:364:THR:O	2.08	0.53
1:A:51:ALA:O	1:A:54:VAL:HG22	2.08	0.52
1:A:10:THR:HG23	1:A:11:THR:N	2.24	0.52
1:A:237:ARG:HD3	1:A:285:THR:HA	1.93	0.51
1:A:356:LEU:HD11	1:A:459:GLY:HA2	1.93	0.51
1:A:87:THR:O	1:A:91:GLN:HG3	2.11	0.51
1:A:143:PRO:C	1:A:145:SER:N	2.63	0.51
1:A:107:THR:HG22	2:A:981:HOH:O	2.10	0.51
1:A:11:THR:O	1:A:365:VAL:HG21	2.10	0.51
1:A:143:PRO:O	1:A:145:SER:N	2.43	0.50
1:A:439:THR:HG23	1:A:440:ARG:HG3	1.94	0.49
1:A:31:LEU:HD21	1:A:80:ILE:HD11	1.94	0.49
1:A:133:ASN:HD21	1:A:139:GLN:N	2.11	0.49
1:A:434:ARG:HG3	2:A:646:HOH:O	2.12	0.49
1:A:6:ASN:C	1:A:368:PRO:HD2	2.33	0.48
1:A:340:VAL:HG21	1:A:426:ILE:O	2.13	0.48
1:A:32:ASP:OD2	1:A:36:LYS:HE2	2.13	0.48
1:A:505:ASN:C	1:A:505:ASN:HD22	2.17	0.48
1:A:8:GLY:HA3	1:A:365:VAL:O	2.14	0.48
1:A:9:ARG:HB3	1:A:363:SER:H	1.79	0.47
1:A:217:ARG:HD2	1:A:218:ASP:OD1	2.15	0.47
1:A:15:ALA:O	1:A:19:VAL:HB	2.14	0.47
1:A:333:HIS:HB3	1:A:409:PHE:CE2	2.49	0.47
1:A:550:SER:HB3	1:A:618:ASP:HB2	1.98	0.46
1:A:133:ASN:HD21	1:A:139:GLN:H	1.64	0.46
1:A:538:GLY:HA3	1:A:598:SER:O	2.15	0.46
1:A:320:PHE:CZ	1:A:330:THR:HB	2.51	0.46
1:A:9:ARG:N	1:A:363:SER:OG	2.49	0.46
1:A:145:SER:O	1:A:149:SER:N	2.48	0.46
1:A:591:ASN:HD22	1:A:591:ASN:C	2.19	0.45
1:A:8:GLY:HA2	1:A:365:VAL:HA	1.98	0.45
1:A:253:PHE:CD2	1:A:516:PHE:HB3	2.51	0.44
1:A:294:PRO:HA	1:A:297:TYR:CE2	2.52	0.44
1:A:319:THR:HG23	1:A:331:THR:OG1	2.18	0.44
1:A:4:VAL:HG12	2:A:993:HOH:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TYR:CE2	1:A:346:VAL:HG21	2.53	0.44
1:A:430:PRO:HA	1:A:461:ARG:O	2.16	0.44
1:A:179:GLN:O	1:A:182:ASN:HB2	2.17	0.44
1:A:78:TRP:HZ2	1:A:121:GLN:NE2	2.11	0.44
1:A:457:PRO:HA	1:A:460:ALA:HB2	1.99	0.44
1:A:8:GLY:C	1:A:363:SER:OG	2.55	0.44
1:A:9:ARG:HD2	1:A:406:CYS:SG	2.58	0.44
1:A:8:GLY:CA	1:A:365:VAL:HA	2.48	0.43
1:A:146:ILE:HB	2:A:804:HOH:O	2.17	0.43
1:A:452:SER:O	1:A:457:PRO:HG3	2.18	0.43
1:A:13:CYS:SG	1:A:402:LEU:HD21	2.59	0.43
1:A:5:LEU:HD22	1:A:5:LEU:HA	1.84	0.43
1:A:329:SER:O	1:A:389:THR:HA	2.19	0.43
1:A:11:THR:HB	1:A:404:LEU:CD1	2.48	0.43
1:A:400:THR:O	1:A:402:LEU:O	2.37	0.43
1:A:594:ASN:ND2	1:A:627:THR:HG21	2.33	0.43
1:A:145:SER:HA	1:A:148:SER:HB3	2.01	0.42
1:A:307:ILE:HD12	1:A:477:ALA:CB	2.47	0.42
1:A:355:ASN:HD22	1:A:355:ASN:N	2.10	0.42
1:A:505:ASN:ND2	1:A:530:THR:HG23	2.34	0.42
1:A:11:THR:HB	1:A:404:LEU:HD13	2.01	0.42
1:A:17:ASN:O	1:A:18:VAL:HG13	2.19	0.42
1:A:45:ASP:HB3	2:A:932:HOH:O	2.20	0.42
1:A:161:LEU:HB2	1:A:162:PRO:HD3	2.02	0.42
1:A:97:THR:HG22	1:A:172:LEU:HD12	2.02	0.42
1:A:457:PRO:HB2	1:A:458:GLY:H	1.65	0.42
1:A:498:PRO:HB3	1:A:619:LEU:HD13	2.01	0.42
1:A:5:LEU:HD11	1:A:477:ALA:HB3	2.02	0.41
1:A:13:CYS:SG	1:A:404:LEU:HD21	2.60	0.41
1:A:332:THR:HG23	1:A:332:THR:O	2.19	0.41
1:A:595:ILE:HD12	1:A:595:ILE:C	2.41	0.41
1:A:443:HIS:CE1	1:A:446:GLN:HB2	2.55	0.41
1:A:94:LEU:HB2	1:A:176:LEU:HD11	2.01	0.41
1:A:192:ILE:HG21	1:A:632:LEU:HD13	2.03	0.41
1:A:365:VAL:CG1	1:A:366:LEU:N	2.84	0.41
1:A:48:LEU:HB2	1:A:50:VAL:HG23	2.03	0.41
1:A:154:GLN:NE2	1:A:184:HIS:NE2	2.68	0.41
1:A:255:TYR:O	1:A:258:ILE:HG22	2.21	0.41
1:A:137:PRO:O	1:A:138:THR:HG23	2.20	0.41
1:A:397:SER:HA	1:A:407:GLY:HA3	2.03	0.41
1:A:5:LEU:HG	1:A:477:ALA:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ASN:O	1:A:439:THR:HG22	2.20	0.41
1:A:16:TYR:O	1:A:17:ASN:HB2	2.21	0.40
1:A:366:LEU:HB3	1:A:367:PRO:CD	2.51	0.40
1:A:9:ARG:H	1:A:365:VAL:HA	1.87	0.40
1:A:98:GLU:CD	1:A:104:ARG:HE	2.25	0.40
1:A:366:LEU:HB3	1:A:367:PRO:HD2	2.04	0.40
1:A:364:THR:O	1:A:364:THR:OG1	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:ASN:ND2	1:A:554:ASN:ND2[7_556]	1.63	0.57

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	631/633 (100%)	591 (94%)	28 (4%)	12 (2%)	 

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	17	ASN
1	A	403	SER
1	A	10	THR
1	A	13	CYS
1	A	18	VAL
1	A	143	PRO
1	A	457	PRO
1	A	460	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	LEU
1	A	456	THR
1	A	4	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	561/561 (100%)	537 (96%)	24 (4%)	29	36

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASN
1	A	4	VAL
1	A	5	LEU
1	A	6	ASN
1	A	7	SER
1	A	12	ILE
1	A	13	CYS
1	A	14	ASP
1	A	138	THR
1	A	144	LEU
1	A	161	LEU
1	A	167	GLN
1	A	355	ASN
1	A	385	GLU
1	A	387	VAL
1	A	402	LEU
1	A	404	LEU
1	A	489	GLU
1	A	505	ASN
1	A	587	PHE
1	A	591	ASN
1	A	619	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	623	MET

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	6	ASN
1	A	103	GLN
1	A	121	GLN
1	A	133	ASN
1	A	136	ASN
1	A	154	GLN
1	A	165	GLN
1	A	291	GLN
1	A	355	ASN
1	A	392	ASN
1	A	445	ASN
1	A	505	ASN
1	A	506	ASN
1	A	519	GLN
1	A	576	ASN
1	A	591	ASN
1	A	594	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 monosaccharides 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, 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	633/633 (100%)	0.09	47 (7%)	14 13	9, 18, 49, 66	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	VAL	17.8
1	A	8	GLY	15.2
1	A	5	LEU	15.1
1	A	11	THR	11.6
1	A	459	GLY	11.4
1	A	13	CYS	11.2
1	A	7	SER	11.1
1	A	143	PRO	10.9
1	A	10	THR	10.6
1	A	141	PRO	10.4
1	A	4	VAL	9.8
1	A	17	ASN	9.0
1	A	6	ASN	8.6
1	A	14	ASP	8.1
1	A	15	ALA	8.1
1	A	140	ASN	7.6
1	A	16	TYR	7.2
1	A	12	ILE	7.0
1	A	386	GLY	6.3
1	A	145	SER	5.9
1	A	457	PRO	5.7
1	A	3	ASN	5.3
1	A	328	GLY	5.3
1	A	456	THR	5.0
1	A	458	GLY	4.9
1	A	1	MET	4.8
1	A	9	ARG	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	19	VAL	4.8
1	A	2	ASN	4.7
1	A	144	LEU	4.6
1	A	139	GLN	4.5
1	A	321	PRO	4.5
1	A	327	PRO	3.9
1	A	326	LEU	3.8
1	A	138	THR	3.7
1	A	142	VAL	3.7
1	A	387	VAL	3.3
1	A	137	PRO	3.1
1	A	364	THR	2.8
1	A	454	SER	2.8
1	A	323	ILE	2.7
1	A	320	PHE	2.7
1	A	319	THR	2.7
1	A	455	GLY	2.6
1	A	453	PRO	2.4
1	A	133	ASN	2.3
1	A	134	PHE	2.3

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.