



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:24 PM UTC

PDB ID : 9H9B / pdb_00009h9b
Title : native structure of the full-length pesticidal protein Cry8Ba2, from crystals formed in vivo (form 2)
Authors : Williamson, L.J.; Best, H.L.; Oberthur, D.; Rizkallah, P.J.; Berry, C.
Deposited on : 2024-10-30
Resolution : 2.27 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

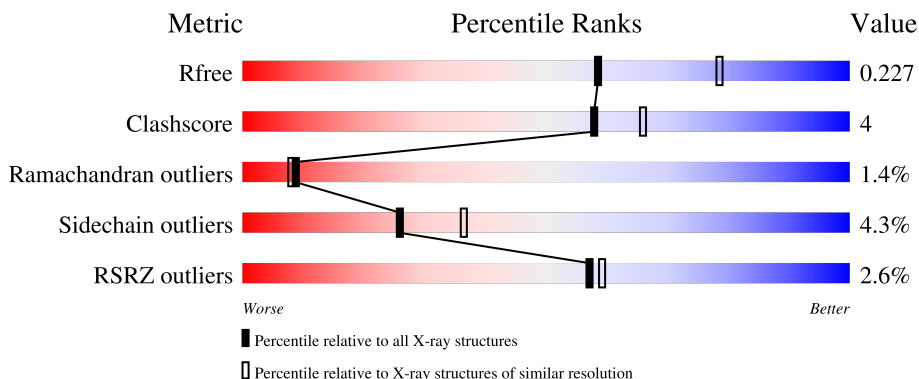
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	1169	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9360 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 Cry8Ba2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1135	Total	C	N	O	S	0	1	0
			9185	5800	1540	1823	22			

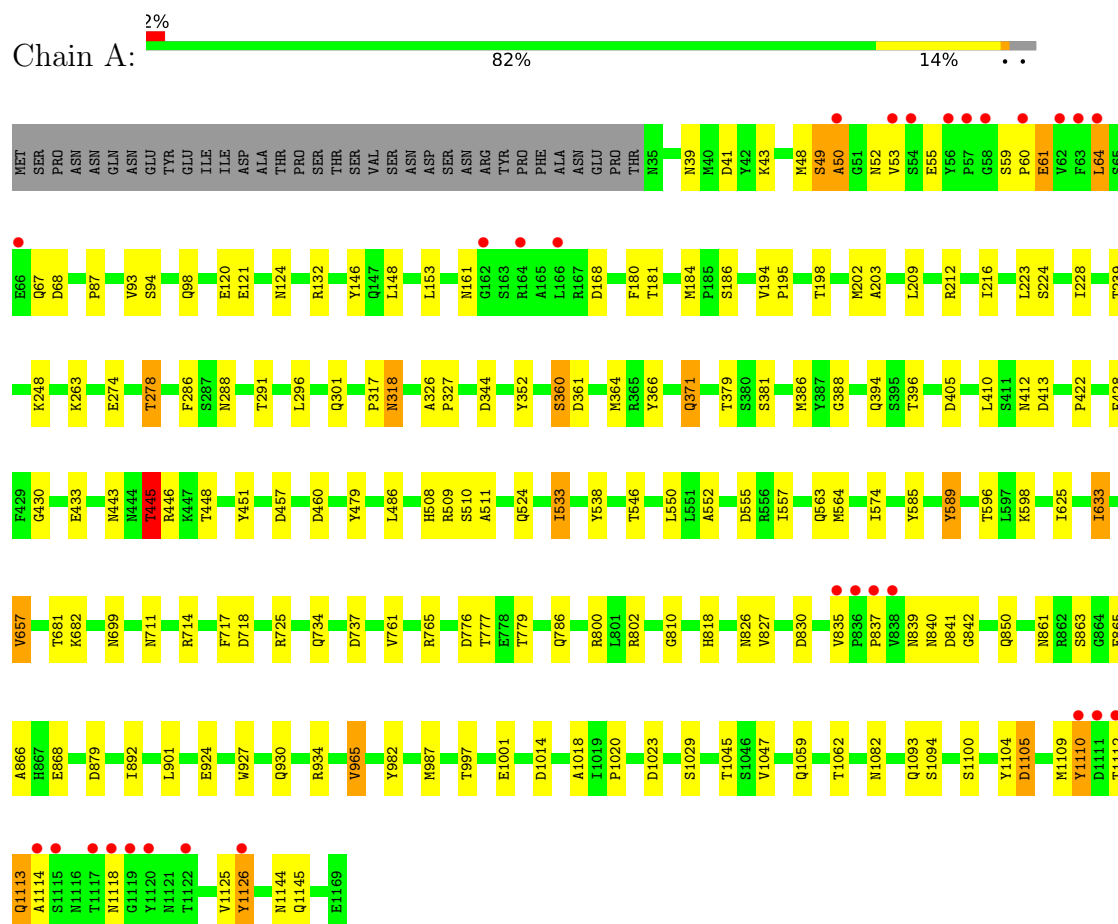
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	175	Total	O	0	0
			175	175		

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: Cry8Ba2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.32Å 93.32Å 275.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.11 – 2.27 28.11 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.11-2.27) 99.9 (28.11-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.180 , 0.226 0.185 , 0.227	Depositor DCC
R_{free} test set	2896 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9360	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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	0.55	0/9389	1.10	26/12763 (0.2%)

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	3

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	ASP	CB-CA-C	-7.37	97.91	110.22
1	A	997	THR	CA-CB-OG1	-7.19	98.81	109.60
1	A	827	VAL	N-CA-CB	-6.39	104.77	111.61
1	A	965	VAL	N-CA-CB	6.30	119.95	110.13
1	A	181	THR	CA-CB-OG1	-6.23	100.25	109.60
1	A	87	PRO	N-CA-CB	-5.87	97.08	103.25
1	A	405	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	830	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	776	ASP	CB-CA-C	-5.70	109.48	117.23
1	A	657	VAL	N-CA-CB	-5.60	100.32	111.91
1	A	837	PRO	N-CA-CB	-5.59	97.38	103.25
1	A	879	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	901	LEU	N-CA-CB	-5.50	101.57	110.81
1	A	394	GLN	CB-CA-C	-5.43	100.77	110.70
1	A	555	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	371	GLN	CB-CA-C	-5.35	100.47	109.72
1	A	445	THR	CA-CB-OG1	-5.34	101.59	109.60
1	A	460	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ASN	CB-CA-C	5.25	118.88	110.16
1	A	121	GLU	N-CA-CB	-5.17	102.38	110.44
1	A	717	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	589	TYR	N-CA-CB	5.11	120.27	111.13
1	A	1001	GLU	N-CA-CB	-5.09	102.36	109.94
1	A	718	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	344	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	168	ASP	CA-CB-CG	5.04	117.64	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	725	ARG	Sidechain
1	A	800	ARG	Sidechain
1	A	802	ARG	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	9185	0	8844	81	0
2	A	175	0	0	4	0
All	All	9360	0	8844	81	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 (81) 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:734:GLN:H	1:A:786:GLN:HE22	1.26	0.81
1:A:202:MET:HA	1:A:202:MET:HE3	1.71	0.73
1:A:184:MET:HE1	1:A:203:ALA:HB1	1.70	0.72
1:A:364:MET:HE3	1:A:366:TYR:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ASN:HD22	1:A:714:ARG:HH21	1.38	0.70
1:A:699:ASN:HD22	1:A:850:GLN:HE21	1.43	0.67
1:A:288:ASN:HD21	1:A:524:GLN:HE22	1.42	0.66
1:A:94:SER:O	1:A:98:GLN:NE2	2.31	0.62
1:A:734:GLN:N	1:A:786:GLN:HE22	1.96	0.62
1:A:737:ASP:O	1:A:765:ARG:HD3	2.03	0.59
1:A:198:THR:HG23	1:A:278:THR:HG23	1.85	0.57
1:A:288:ASN:ND2	1:A:524:GLN:HE22	2.01	0.57
1:A:861:ASN:HB2	1:A:866:ALA:HB2	1.86	0.57
1:A:364:MET:HE1	1:A:430:GLY:HA3	1.88	0.55
1:A:301:GLN:HE21	1:A:511:ALA:HA	1.71	0.55
1:A:274:GLU:O	1:A:278:THR:HB	2.05	0.55
1:A:1125:VAL:O	1:A:1126:TYR:C	2.50	0.54
1:A:202:MET:CE	2:A:1349:HOH:O	2.55	0.54
1:A:818:HIS:HD2	1:A:924:GLU:OE2	1.91	0.54
1:A:352:TYR:OH	1:A:371:GLN:HG3	2.08	0.54
1:A:61:GLU:HA	1:A:68:ASP:HB2	1.90	0.53
1:A:734:GLN:H	1:A:786:GLN:NE2	2.00	0.53
1:A:1093:GLN:NE2	2:A:1206:HOH:O	2.42	0.52
1:A:184:MET:HE1	1:A:203:ALA:CB	2.41	0.51
1:A:317:PRO:O	1:A:318:ASN:HB2	2.11	0.51
1:A:1018:ALA:O	1:A:1020:PRO:HD3	2.11	0.51
1:A:1062:THR:HG22	1:A:1145:GLN:OE1	2.10	0.51
1:A:1082:ASN:HD22	1:A:1100:SER:HB3	1.75	0.50
1:A:364:MET:CE	1:A:428:PHE:HE2	2.25	0.49
1:A:934:ARG:HG2	1:A:982:TYR:CZ	2.48	0.49
1:A:364:MET:HE3	1:A:366:TYR:CB	2.42	0.48
1:A:433:GLU:HA	1:A:451:TYR:O	2.14	0.48
1:A:364:MET:CE	1:A:428:PHE:CE2	2.97	0.48
1:A:212:ARG:HG3	1:A:291:THR:HG23	1.96	0.47
1:A:557:ILE:O	1:A:557:ILE:HG23	2.14	0.47
1:A:538:TYR:CD2	1:A:552:ALA:HB3	2.50	0.47
1:A:49:SER:O	1:A:50:ALA:C	2.57	0.47
1:A:60:PRO:O	1:A:61:GLU:HB2	2.14	0.46
1:A:120:GLU:OE1	1:A:132:ARG:NH2	2.48	0.46
1:A:508:HIS:CD2	1:A:510:SER:H	2.33	0.46
1:A:446:ARG:HD3	1:A:479:TYR:CD2	2.50	0.46
1:A:777:THR:HG22	1:A:777:THR:O	2.16	0.46
1:A:194:VAL:HB	1:A:195:PRO:HD3	1.98	0.45
1:A:1112:THR:O	1:A:1113:GLN:C	2.59	0.45
1:A:508:HIS:HD2	1:A:510:SER:OG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:GLY:H	1:A:826:ASN:ND2	2.15	0.45
1:A:296:LEU:N	1:A:296:LEU:HD23	2.32	0.45
1:A:386:MET:HE1	1:A:388:GLY:O	2.17	0.44
1:A:563:GLN:HB3	1:A:633:ILE:HG21	1.99	0.44
1:A:326:ALA:HB1	1:A:327:PRO:HD2	1.99	0.44
1:A:360:SER:O	1:A:361:ASP:HB2	2.16	0.44
1:A:59:SER:O	1:A:67:GLN:NE2	2.52	0.43
1:A:509:ARG:HH11	1:A:509:ARG:HG2	1.83	0.43
1:A:1104:TYR:O	1:A:1105:ASP:C	2.61	0.43
1:A:840:ASN:O	1:A:842:GLY:N	2.51	0.43
1:A:64:LEU:O	1:A:67:GLN:HG2	2.18	0.43
1:A:574:ILE:HD12	1:A:625:ILE:CD1	2.49	0.43
1:A:443:ASN:OD1	1:A:445:THR:HB	2.18	0.43
1:A:681:THR:O	1:A:682:LYS:HB2	2.19	0.43
1:A:546:THR:HG21	1:A:550:LEU:HD21	2.00	0.42
1:A:198:THR:OG1	1:A:278:THR:CG2	2.68	0.42
1:A:934:ARG:HG2	1:A:982:TYR:CE2	2.53	0.42
1:A:184:MET:HA	1:A:184:MET:HE2	2.02	0.42
1:A:585:TYR:CE2	1:A:598:LYS:HB2	2.55	0.42
1:A:1109:MET:O	1:A:1110:TYR:HB3	2.20	0.42
1:A:223:LEU:HD23	1:A:228:ILE:HD13	2.01	0.42
1:A:818:HIS:O	1:A:927:TRP:CZ3	2.73	0.42
1:A:868[B]:GLU:CD	2:A:1267:HOH:O	2.63	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.96	0.42
1:A:224:SER:O	1:A:228:ILE:HG12	2.20	0.42
1:A:1014:ASP:OD1	1:A:1023:ASP:OD2	2.38	0.41
1:A:153:LEU:HD12	1:A:153:LEU:HA	1.97	0.41
1:A:180:PHE:HD1	1:A:184:MET:HE3	1.85	0.41
1:A:202:MET:HE2	2:A:1349:HOH:O	2.19	0.41
1:A:198:THR:CG2	1:A:278:THR:HG23	2.50	0.41
1:A:239:THR:HG23	1:A:286:PHE:HB3	2.01	0.41
1:A:1020:PRO:HB2	1:A:1059:GLN:HE22	1.86	0.41
1:A:563:GLN:C	1:A:564:MET:HG3	2.46	0.40
1:A:533:ILE:HD13	1:A:533:ILE:H	1.87	0.40
1:A:326:ALA:HB1	1:A:327:PRO:CD	2.52	0.40
1:A:508:HIS:HD2	1:A:510:SER:H	1.70	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	1134/1169 (97%)	1068 (94%)	50 (4%)	16 (1%)	9 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	THR
1	A	49	SER
1	A	50	ALA
1	A	61	GLU
1	A	1110	TYR
1	A	1114	ALA
1	A	839	ASN
1	A	1118	ASN
1	A	1126	TYR
1	A	48	MET
1	A	841	ASP
1	A	1105	ASP
1	A	1113	GLN
1	A	64	LEU
1	A	863	SER
1	A	761	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1010/1041 (97%)	967 (96%)	43 (4%)	26 36

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	41	ASP
1	A	43	LYS
1	A	52	ASN
1	A	53	VAL
1	A	55	GLU
1	A	93	VAL
1	A	124	ASN
1	A	146	TYR
1	A	148	LEU
1	A	161	ASN
1	A	186	SER
1	A	216	ILE
1	A	248	LYS
1	A	263	LYS
1	A	278	THR
1	A	318	ASN
1	A	360	SER
1	A	381	SER
1	A	396	THR
1	A	410	LEU
1	A	422	PRO
1	A	445	THR
1	A	448	THR
1	A	457	ASP
1	A	486	LEU
1	A	533	ILE
1	A	589	TYR
1	A	596	THR
1	A	633	ILE
1	A	657	VAL
1	A	779	THR
1	A	835	VAL
1	A	865	GLU
1	A	892	ILE

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Mol	Chain	Res	Type
1	A	930	GLN
1	A	965	VAL
1	A	987	MET
1	A	1029	SER
1	A	1045	THR
1	A	1047	VAL
1	A	1094	SER
1	A	1144	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	133	ASN
1	A	144	ASN
1	A	205	ASN
1	A	230	ASN
1	A	245	HIS
1	A	288	ASN
1	A	301	GLN
1	A	318	ASN
1	A	385	GLN
1	A	403	ASN
1	A	412	ASN
1	A	441	GLN
1	A	508	HIS
1	A	563	GLN
1	A	711	ASN
1	A	739	GLN
1	A	786	GLN
1	A	818	HIS
1	A	826	ASN
1	A	850	GLN
1	A	854	ASN
1	A	903	ASN
1	A	974	GLN
1	A	1032	ASN
1	A	1040	GLN
1	A	1059	GLN
1	A	1082	ASN
1	A	1144	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 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	1135/1169 (97%)	-0.27	29 (2%) 57 59	18, 45, 120, 301	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	57	PRO	4.4
1	A	1117	THR	3.7
1	A	53	VAL	3.7
1	A	56	TYR	3.7
1	A	54	SER	3.5
1	A	62	VAL	3.5
1	A	50	ALA	3.5
1	A	1118	ASN	3.3
1	A	835	VAL	3.2
1	A	1114	ALA	3.0
1	A	64	LEU	2.8
1	A	1126	TYR	2.7
1	A	836	PRO	2.7
1	A	1111	ASP	2.6
1	A	60	PRO	2.6
1	A	162	GLY	2.5
1	A	66	GLU	2.5
1	A	1112	THR	2.5
1	A	1110	TYR	2.3
1	A	837	PRO	2.3
1	A	838	VAL	2.3
1	A	1119	GLY	2.2
1	A	1115	SER	2.2
1	A	58	GLY	2.1
1	A	164	ARG	2.1
1	A	1120	TYR	2.1
1	A	63	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	LEU	2.0
1	A	1122	THR	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.