



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:22 PM UTC

PDB ID : 4MOA / pdb_00004moa
Title : Crystal structure of CRY4BA-R203Q TOXIN
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Deposited on : 2013-09-11
Resolution : 2.00 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
Xtrriage (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

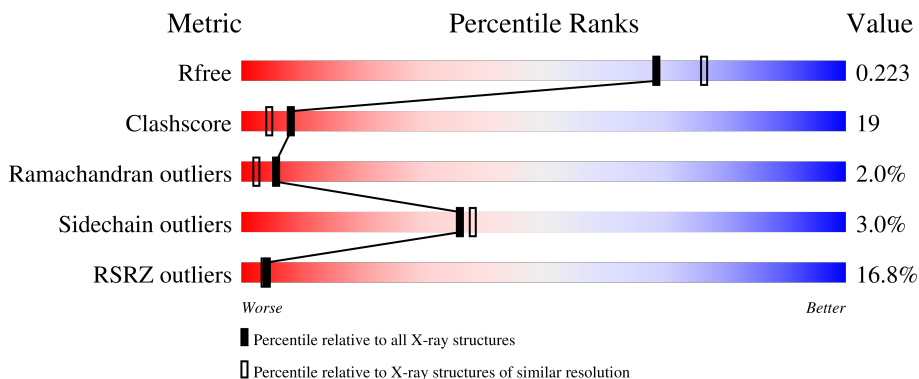
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	602	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5056 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 Pesticidal crystal protein cry4Ba.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	602	4774	3034	803	927	10	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLN	ARG	engineered mutation	UNP P05519

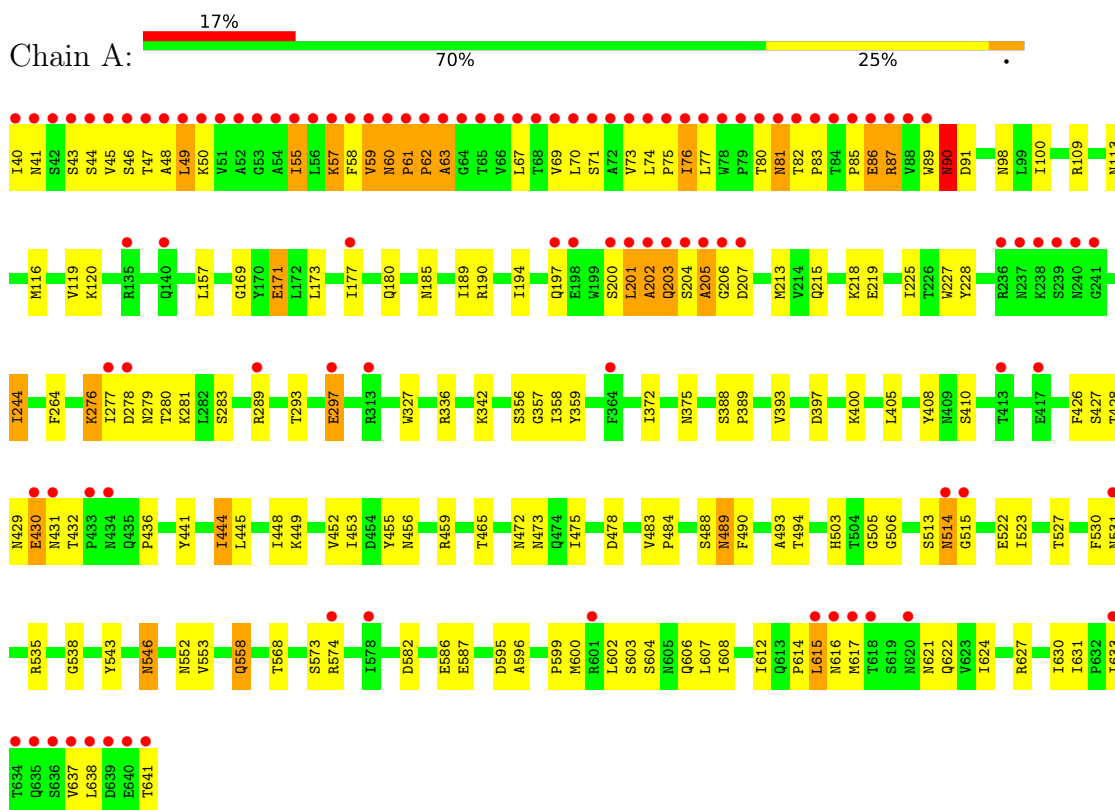
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	282	282	282	0	0

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: Pesticidal crystal protein cry4Ba



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	184.62Å 184.62Å 187.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.00-2.00) 99.8 (30.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.99Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.237 0.222 , 0.223	Depositor DCC
R_{free} test set	4126 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5056	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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	0.39	0/4878	0.94	23/6656 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ALA	N-CA-C	-10.68	99.92	113.16
1	A	515	GLY	N-CA-C	-8.27	104.46	115.21
1	A	61	PRO	N-CA-C	7.81	120.22	110.70
1	A	631	ILE	N-CA-C	7.37	115.49	107.60
1	A	459	ARG	N-CA-C	-6.43	99.21	109.76
1	A	393	VAL	N-CA-C	6.35	117.94	108.54
1	A	604	SER	N-CA-C	6.07	119.06	109.96
1	A	408	TYR	N-CA-C	-5.94	100.01	109.76
1	A	600	MET	N-CA-C	-5.84	100.97	110.20
1	A	538	GLY	N-CA-C	-5.60	104.12	113.02
1	A	478	ASP	N-CA-C	5.57	119.64	112.41
1	A	357	GLY	N-CA-C	-5.53	103.70	112.66
1	A	283	SER	N-CA-C	-5.50	101.77	109.96
1	A	293	THR	N-CA-C	-5.48	100.84	109.50
1	A	493	ALA	N-CA-C	5.47	118.75	111.75
1	A	264	PHE	N-CA-C	5.36	117.82	111.33
1	A	432	THR	CA-C-N	5.28	126.43	119.84
1	A	432	THR	C-N-CA	5.28	126.43	119.84
1	A	514	ASN	N-CA-C	-5.27	106.85	113.28
1	A	228	TYR	N-CA-C	-5.18	105.53	111.07
1	A	49	LEU	N-CA-C	-5.10	106.08	113.21
1	A	372	ILE	N-CA-C	5.07	115.40	107.99
1	A	531	ASN	N-CA-C	5.01	118.55	112.23

There are no chirality outliers.

There are no planarity outliers.

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	4774	0	4737	184	0
2	A	282	0	0	2	0
All	All	5056	0	4737	184	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 19.

All (184) 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:60:ASN:CG	1:A:278:ASP:HB2	1.95	0.90
1:A:55:ILE:HA	1:A:59:VAL:HG21	1.54	0.87
1:A:60:ASN:HD22	1:A:60:ASN:N	1.73	0.86
1:A:171:GLU:HG3	1:A:227:TRP:CZ2	2.11	0.85
1:A:475:ILE:HG12	1:A:630:ILE:HD13	1.60	0.83
1:A:55:ILE:HD13	1:A:55:ILE:H	1.41	0.83
1:A:81:ASN:HD21	1:A:113:ASN:HB3	1.43	0.83
1:A:80:THR:HG23	1:A:81:ASN:H	1.45	0.81
1:A:60:ASN:N	1:A:60:ASN:ND2	2.30	0.80
1:A:60:ASN:CB	1:A:278:ASP:HB2	2.14	0.77
1:A:60:ASN:HB2	1:A:278:ASP:HB2	1.66	0.76
1:A:89:TRP:O	1:A:90:ASN:ND2	2.18	0.73
1:A:171:GLU:HG3	1:A:227:TRP:CE2	2.24	0.72
1:A:617:MET:HG3	1:A:621:ASN:HB2	1.74	0.70
1:A:67:LEU:HA	1:A:71:SER:OG	1.92	0.69
1:A:444:ILE:H	1:A:444:ILE:HD13	1.58	0.69
1:A:57:LYS:HG3	1:A:58:PHE:CD2	2.28	0.69
1:A:203:GLN:HA	1:A:206:GLY:HA3	1.72	0.69
1:A:573:SER:O	1:A:574:ARG:HD3	1.93	0.69
1:A:289:ARG:CG	1:A:506:GLY:HA2	2.22	0.68
1:A:278:ASP:OD1	1:A:281:LYS:HE3	1.94	0.67
1:A:87:ARG:HB3	1:A:109:ARG:NH2	2.10	0.67
1:A:61:PRO:HB3	1:A:70:LEU:HG	1.75	0.67
1:A:40:ILE:HG21	1:A:89:TRP:HB3	1.77	0.66
1:A:62:PRO:HG2	1:A:279:ASN:H	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:TRP:CE3	1:A:90:ASN:HB3	2.31	0.66
1:A:444:ILE:HD13	1:A:465:THR:O	1.95	0.65
1:A:429:ASN:ND2	1:A:431:ASN:H	1.95	0.65
1:A:552:ASN:HB2	1:A:615:LEU:HD23	1.78	0.65
1:A:297:GLU:HG2	1:A:453:ILE:HD13	1.78	0.64
1:A:289:ARG:HG2	1:A:506:GLY:HA2	1.78	0.64
1:A:60:ASN:HB3	1:A:280:THR:HG23	1.78	0.64
1:A:375:ASN:HD21	1:A:400:LYS:NZ	1.97	0.63
1:A:81:ASN:ND2	1:A:113:ASN:HB3	2.13	0.63
1:A:55:ILE:HG12	1:A:55:ILE:O	1.99	0.62
1:A:490:PHE:HB3	1:A:522:GLU:HB2	1.81	0.62
1:A:203:GLN:C	1:A:206:GLY:H	2.07	0.62
1:A:76:ILE:HD13	1:A:76:ILE:O	1.99	0.62
1:A:638:LEU:O	1:A:638:LEU:HD13	2.00	0.61
1:A:46:SER:HB2	1:A:428:THR:C	2.26	0.61
1:A:574:ARG:NH1	1:A:582:ASP:OD1	2.34	0.61
1:A:89:TRP:C	1:A:90:ASN:HD22	2.07	0.60
1:A:475:ILE:HG12	1:A:630:ILE:CD1	2.30	0.59
1:A:483:VAL:HG12	1:A:523:ILE:HD11	1.83	0.59
1:A:297:GLU:HG2	1:A:453:ILE:CD1	2.33	0.59
1:A:80:THR:HG23	1:A:81:ASN:N	2.17	0.58
1:A:427:SER:HB2	1:A:436:PRO:HB3	1.85	0.58
1:A:244:ILE:HD13	1:A:244:ILE:O	2.04	0.58
1:A:375:ASN:H	1:A:375:ASN:HD22	1.51	0.58
1:A:494:THR:HG21	1:A:514:ASN:HB2	1.87	0.57
1:A:203:GLN:O	1:A:205:ALA:N	2.36	0.56
1:A:225:ILE:HD11	1:A:503:HIS:CD2	2.40	0.56
1:A:289:ARG:HG3	1:A:506:GLY:HA2	1.86	0.56
1:A:599:PRO:HB3	1:A:633:ILE:CD1	2.35	0.56
1:A:546:ASN:HD21	1:A:622:GLN:H	1.52	0.56
1:A:60:ASN:HD22	1:A:60:ASN:H	1.50	0.55
1:A:61:PRO:HD3	1:A:70:LEU:HD21	1.89	0.55
1:A:596:ALA:HA	1:A:633:ILE:HD13	1.89	0.55
1:A:225:ILE:CD1	1:A:503:HIS:HD2	2.20	0.55
1:A:397:ASP:HB3	1:A:405:LEU:HD11	1.88	0.55
1:A:43:SER:HB3	1:A:430:GLU:OE2	2.07	0.54
1:A:617:MET:CG	1:A:621:ASN:HB2	2.36	0.54
1:A:55:ILE:HD13	1:A:55:ILE:N	2.17	0.54
1:A:617:MET:HG3	1:A:621:ASN:CB	2.36	0.54
1:A:169:GLY:N	1:A:171:GLU:OE1	2.40	0.54
1:A:60:ASN:HB2	1:A:62:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PRO:CD	1:A:62:PRO:HD3	2.37	0.54
1:A:70:LEU:H	1:A:70:LEU:HD22	1.73	0.54
1:A:189:ILE:HG21	1:A:213:MET:HB2	1.89	0.54
1:A:76:ILE:HD13	1:A:76:ILE:C	2.33	0.54
1:A:444:ILE:HD13	1:A:444:ILE:N	2.23	0.53
1:A:624:ILE:HD12	1:A:624:ILE:N	2.23	0.53
1:A:475:ILE:CG1	1:A:630:ILE:HD13	2.35	0.52
1:A:60:ASN:ND2	1:A:278:ASP:OD1	2.43	0.52
1:A:45:VAL:HG22	1:A:45:VAL:O	2.10	0.51
1:A:116:MET:HE3	1:A:180:GLN:HE21	1.74	0.51
1:A:608:ILE:N	1:A:608:ILE:HD12	2.26	0.51
1:A:40:ILE:CG2	1:A:89:TRP:HB3	2.39	0.51
1:A:327:TRP:CH2	1:A:358:ILE:HD12	2.46	0.51
1:A:74:LEU:HD12	1:A:74:LEU:N	2.26	0.51
1:A:574:ARG:HH11	1:A:574:ARG:HG3	1.76	0.51
1:A:47:THR:HG22	1:A:50:LYS:HD3	1.91	0.51
1:A:119:VAL:HG13	1:A:157:LEU:CD2	2.41	0.51
1:A:637:VAL:O	1:A:641:THR:N	2.40	0.51
1:A:74:LEU:N	1:A:75:PRO:HD2	2.25	0.50
1:A:552:ASN:HB2	1:A:615:LEU:CD2	2.41	0.50
1:A:60:ASN:CG	1:A:278:ASP:CB	2.79	0.50
1:A:61:PRO:HD3	1:A:70:LEU:CG	2.42	0.50
1:A:77:LEU:HG	1:A:120:LYS:HD3	1.93	0.50
1:A:225:ILE:HD11	1:A:503:HIS:HD2	1.76	0.50
1:A:614:PRO:HB2	1:A:617:MET:HE2	1.94	0.50
1:A:455:TYR:O	1:A:456:ASN:HB2	2.12	0.50
1:A:553:VAL:HG13	1:A:612:ILE:CD1	2.42	0.50
1:A:276:LYS:NZ	1:A:276:LYS:H	2.10	0.49
1:A:87:ARG:HH12	1:A:177:ILE:CG1	2.25	0.49
1:A:89:TRP:CZ3	1:A:90:ASN:HB3	2.47	0.49
1:A:375:ASN:HD21	1:A:400:LYS:HZ1	1.60	0.49
1:A:203:GLN:O	1:A:204:SER:HB2	2.13	0.49
1:A:70:LEU:H	1:A:70:LEU:CD2	2.24	0.49
1:A:484:PRO:HA	1:A:627:ARG:HB3	1.95	0.49
1:A:59:VAL:HB	1:A:69:VAL:HG21	1.95	0.48
1:A:546:ASN:ND2	1:A:622:GLN:H	2.11	0.48
1:A:60:ASN:HA	1:A:70:LEU:HD21	1.96	0.48
1:A:87:ARG:HB3	1:A:109:ARG:HH21	1.74	0.48
1:A:429:ASN:C	1:A:429:ASN:HD22	2.20	0.48
1:A:119:VAL:HG13	1:A:157:LEU:HD21	1.96	0.48
1:A:215:GLN:O	1:A:219:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:VAL:CG1	1:A:523:ILE:HD11	2.43	0.48
1:A:553:VAL:HG13	1:A:612:ILE:HD13	1.96	0.48
1:A:74:LEU:HD12	1:A:74:LEU:H	1.80	0.47
1:A:43:SER:HA	1:A:430:GLU:HB3	1.96	0.47
1:A:197:GLN:HG3	1:A:202:ALA:HB2	1.97	0.47
1:A:62:PRO:HB2	1:A:277:ILE:O	2.13	0.47
1:A:70:LEU:HD22	1:A:70:LEU:N	2.29	0.47
1:A:225:ILE:HD11	1:A:503:HIS:HB3	1.97	0.47
1:A:388:SER:HA	1:A:389:PRO:C	2.39	0.47
1:A:171:GLU:HG3	1:A:227:TRP:CH2	2.49	0.47
1:A:488:SER:HB3	1:A:522:GLU:O	2.15	0.47
1:A:69:VAL:O	1:A:73:VAL:HB	2.14	0.47
1:A:603:SER:OG	1:A:606:GLN:HG3	2.15	0.47
1:A:109:ARG:HG2	1:A:173:LEU:HD11	1.97	0.46
1:A:558:GLN:HE21	1:A:558:GLN:HB2	1.45	0.46
1:A:60:ASN:HB3	1:A:280:THR:CG2	2.42	0.46
1:A:218:LYS:HE2	1:A:586:GLU:HB3	1.97	0.46
1:A:452:VAL:HG12	2:A:852:HOH:O	2.15	0.46
1:A:55:ILE:HG22	1:A:59:VAL:CG2	2.45	0.46
1:A:173:LEU:C	1:A:173:LEU:HD13	2.41	0.46
1:A:530:PHE:CD1	1:A:535:ARG:HD3	2.51	0.46
1:A:87:ARG:O	1:A:109:ARG:CZ	2.64	0.46
1:A:61:PRO:O	1:A:63:ALA:N	2.48	0.46
1:A:87:ARG:HH12	1:A:177:ILE:HG12	1.80	0.46
1:A:426:PHE:O	1:A:441:TYR:HA	2.16	0.45
1:A:91:ASP:OD2	1:A:91:ASP:C	2.59	0.45
1:A:190:ARG:O	1:A:194:ILE:HG12	2.17	0.45
1:A:200:SER:O	1:A:202:ALA:N	2.49	0.45
1:A:60:ASN:CG	1:A:280:THR:HG1	2.24	0.45
1:A:46:SER:HB2	1:A:428:THR:HA	1.99	0.45
1:A:225:ILE:CD1	1:A:503:HIS:CD2	3.00	0.45
1:A:595:ASP:HB2	1:A:641:THR:OXT	2.17	0.44
1:A:530:PHE:CE1	1:A:535:ARG:HD3	2.52	0.44
1:A:60:ASN:CG	1:A:280:THR:OG1	2.60	0.44
1:A:289:ARG:HG3	1:A:505:GLY:O	2.18	0.44
1:A:201:LEU:O	1:A:202:ALA:C	2.61	0.44
1:A:185:ASN:O	1:A:189:ILE:HG12	2.17	0.44
1:A:46:SER:HB2	1:A:428:THR:CA	2.48	0.44
1:A:61:PRO:N	1:A:62:PRO:CD	2.81	0.44
1:A:203:GLN:NE2	1:A:206:GLY:HA3	2.33	0.44
1:A:44:SER:O	1:A:48:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:C	1:A:205:ALA:N	2.74	0.43
1:A:527:THR:HG23	1:A:608:ILE:HD13	2.01	0.43
1:A:375:ASN:H	1:A:375:ASN:ND2	2.16	0.43
1:A:513:SER:HB2	1:A:617:MET:HG2	2.01	0.43
1:A:61:PRO:HD2	1:A:62:PRO:HD3	2.00	0.43
1:A:80:THR:O	1:A:81:ASN:HB2	2.19	0.43
1:A:278:ASP:OD2	1:A:281:LYS:HD2	2.18	0.43
1:A:67:LEU:HA	1:A:71:SER:HG	1.84	0.43
1:A:98:ASN:HD21	1:A:100:ILE:HB	1.84	0.43
1:A:574:ARG:NH2	1:A:587:GLU:OE1	2.52	0.43
1:A:59:VAL:C	1:A:60:ASN:ND2	2.76	0.43
1:A:429:ASN:ND2	1:A:429:ASN:C	2.76	0.43
1:A:472:ASN:O	1:A:473:ASN:C	2.61	0.43
1:A:336:ARG:HD3	1:A:410:SER:O	2.19	0.42
1:A:82:THR:N	1:A:83:PRO:HD3	2.34	0.42
1:A:543:TYR:CE2	1:A:568:THR:HB	2.54	0.42
1:A:85:PRO:O	1:A:86:GLU:HB3	2.19	0.42
1:A:602:LEU:HD22	1:A:608:ILE:HG12	2.01	0.42
1:A:74:LEU:H	1:A:74:LEU:CD1	2.33	0.42
1:A:171:GLU:H	1:A:171:GLU:CD	2.24	0.42
1:A:489:ASN:C	1:A:489:ASN:HD22	2.28	0.42
1:A:61:PRO:HD3	1:A:70:LEU:CD2	2.49	0.42
1:A:342:LYS:HE3	1:A:356:SER:O	2.20	0.42
1:A:615:LEU:O	1:A:616:ASN:C	2.62	0.42
1:A:61:PRO:HG2	1:A:62:PRO:HD3	2.02	0.42
1:A:98:ASN:ND2	1:A:100:ILE:HB	2.35	0.41
1:A:359:TYR:CE1	1:A:449:LYS:HE3	2.56	0.41
1:A:445:LEU:HD21	1:A:448:ILE:HD11	2.03	0.41
1:A:607:LEU:C	1:A:608:ILE:HD12	2.46	0.41
1:A:289:ARG:HD2	2:A:723:HOH:O	2.19	0.41
1:A:289:ARG:HG3	1:A:505:GLY:C	2.46	0.41
1:A:513:SER:HB2	1:A:617:MET:HE3	2.03	0.40
1:A:429:ASN:HD21	1:A:431:ASN:HB2	1.85	0.40
1:A:61:PRO:CB	1:A:70:LEU:HG	2.47	0.40
1:A:475:ILE:CD1	1:A:630:ILE:HD13	2.51	0.40
1:A:203:GLN:HA	1:A:206:GLY:CA	2.46	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	600/602 (100%)	560 (93%)	28 (5%)	12 (2%)	6 2

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	LEU
1	A	57	LYS
1	A	62	PRO
1	A	63	ALA
1	A	81	ASN
1	A	87	ARG
1	A	202	ALA
1	A	203	GLN
1	A	41	ASN
1	A	86	GLU
1	A	90	ASN
1	A	59	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	539/539 (100%)	523 (97%)	16 (3%)	36 38

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	55	ILE
1	A	60	ASN
1	A	76	ILE
1	A	90	ASN
1	A	171	GLU
1	A	207	ASP
1	A	244	ILE
1	A	276	LYS
1	A	297	GLU
1	A	430	GLU
1	A	444	ILE
1	A	489	ASN
1	A	546	ASN
1	A	558	GLN
1	A	615	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	98	ASN
1	A	102	GLN
1	A	180	GLN
1	A	183	ASN
1	A	185	ASN
1	A	203	GLN
1	A	215	GLN
1	A	247	ASN
1	A	349	ASN
1	A	367	ASN
1	A	375	ASN
1	A	377	ASN
1	A	429	ASN
1	A	431	ASN
1	A	434	ASN
1	A	439	ASN
1	A	474	GLN
1	A	489	ASN
1	A	524	GLN
1	A	546	ASN
1	A	558	GLN
1	A	606	GLN

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	602/602 (100%)	1.21	101 (16%) 4 4	11, 19, 136, 149	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	ILE	16.9
1	A	70	LEU	16.3
1	A	62	PRO	16.1
1	A	52	ALA	15.4
1	A	77	LEU	15.3
1	A	74	LEU	15.2
1	A	45	VAL	14.6
1	A	55	ILE	14.4
1	A	56	LEU	14.3
1	A	49	LEU	14.2
1	A	83	PRO	14.0
1	A	69	VAL	14.0
1	A	51	VAL	13.8
1	A	78	TRP	13.6
1	A	73	VAL	13.5
1	A	80	THR	12.4
1	A	47	THR	12.0
1	A	85	PRO	12.0
1	A	58	PHE	11.7
1	A	202	ALA	11.7
1	A	88	VAL	11.5
1	A	87	ARG	11.5
1	A	82	THR	11.3
1	A	76	ILE	11.2
1	A	54	ALA	11.1
1	A	66	VAL	11.0
1	A	59	VAL	10.9

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Mol	Chain	Res	Type	RSRZ
1	A	641	THR	10.8
1	A	42	SER	10.7
1	A	638	LEU	10.4
1	A	68	THR	10.3
1	A	364	PHE	10.2
1	A	67	LEU	10.2
1	A	72	ALA	10.2
1	A	63	ALA	9.6
1	A	201	LEU	9.6
1	A	75	PRO	9.6
1	A	203	GLN	9.5
1	A	79	PRO	9.5
1	A	84	THR	9.5
1	A	41	ASN	9.3
1	A	60	ASN	9.3
1	A	61	PRO	9.3
1	A	64	GLY	9.3
1	A	205	ALA	9.3
1	A	48	ALA	9.2
1	A	50	LYS	9.1
1	A	65	THR	9.1
1	A	46	SER	8.7
1	A	640	GLU	8.2
1	A	81	ASN	8.2
1	A	57	LYS	8.1
1	A	43	SER	7.9
1	A	637	VAL	7.9
1	A	71	SER	7.8
1	A	53	GLY	7.1
1	A	200	SER	6.9
1	A	204	SER	6.9
1	A	639	ASP	6.6
1	A	44	SER	6.4
1	A	636	SER	6.3
1	A	86	GLU	5.6
1	A	514	ASN	5.6
1	A	417	GLU	5.0
1	A	278	ASP	5.0
1	A	206	GLY	4.5
1	A	289	ARG	4.3
1	A	89	TRP	4.1
1	A	635	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	634	THR	3.7
1	A	430	GLU	3.7
1	A	433	PRO	3.3
1	A	617	MET	3.2
1	A	313	ARG	3.1
1	A	578	ILE	3.1
1	A	236	ARG	3.0
1	A	237	ASN	3.0
1	A	198	GLU	2.9
1	A	239	SER	2.9
1	A	515	GLY	2.9
1	A	616	ASN	2.8
1	A	531	ASN	2.8
1	A	633	ILE	2.8
1	A	177	ILE	2.7
1	A	207	ASP	2.7
1	A	140	GLN	2.5
1	A	297	GLU	2.4
1	A	240	ASN	2.4
1	A	618	THR	2.4
1	A	238	LYS	2.4
1	A	277	ILE	2.2
1	A	431	ASN	2.2
1	A	434	ASN	2.2
1	A	620	ASN	2.2
1	A	601	ARG	2.2
1	A	413	THR	2.2
1	A	574	ARG	2.2
1	A	197	GLN	2.1
1	A	135	ARG	2.1
1	A	241	GLY	2.1
1	A	615	LEU	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.