



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:50 PM UTC

PDB ID : 4HQ6 / pdb_00004hq6
Title : BC domain in the presence of citrate
Authors : Heo, Y.S.
Deposited on : 2012-10-25
Resolution : 2.70 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

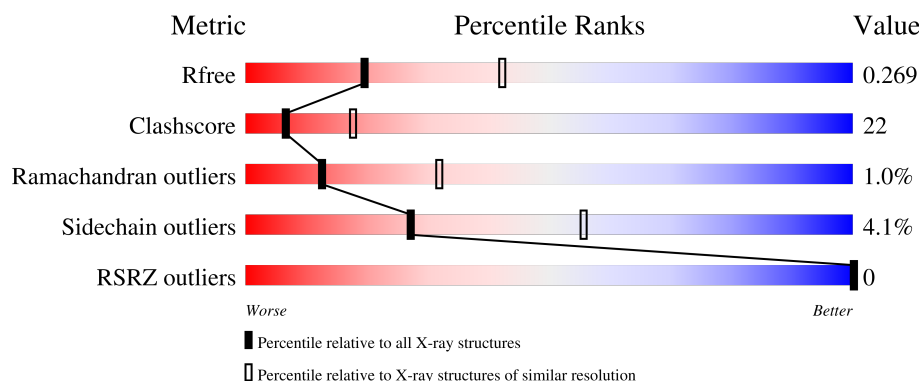
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	573	51% 32% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3915 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 Acetyl-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3871	2468	671	714	18			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	MET	-	expression tag	UNP O00763
A	212	ARG	-	expression tag	UNP O00763
A	213	GLY	-	expression tag	UNP O00763
A	214	SER	-	expression tag	UNP O00763
A	215	GLY	-	expression tag	UNP O00763
A	216	SER	-	expression tag	UNP O00763
A	236	ILE	LEU	engineered mutation	UNP O00763
A	776	LEU	VAL	engineered mutation	UNP O00763
A	777	GLU	-	expression tag	UNP O00763
A	778	HIS	-	expression tag	UNP O00763
A	779	HIS	-	expression tag	UNP O00763
A	780	HIS	-	expression tag	UNP O00763
A	781	HIS	-	expression tag	UNP O00763
A	782	HIS	-	expression tag	UNP O00763
A	783	HIS	-	expression tag	UNP O00763

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.59Å 75.59Å 188.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	86.4 (19.98-2.70) 86.2 (19.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.273 0.219 , 0.269	Depositor DCC
R_{free} test set	760 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3915	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 4.45% 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	0.49	0/3961	0.94	16/5376 (0.3%)

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 (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	353	HIS	CB-CA-C	-6.38	109.21	116.54
1	A	341	ARG	N-CA-C	6.34	118.19	111.28
1	A	637	THR	CA-C-N	6.25	126.21	119.78
1	A	637	THR	C-N-CA	6.25	126.21	119.78
1	A	247	PRO	N-CA-C	-6.19	105.29	113.65
1	A	394	THR	N-CA-C	-5.82	104.93	111.28
1	A	390	VAL	N-CA-C	-5.73	104.92	110.42
1	A	602	ALA	N-CA-C	-5.70	105.07	111.28
1	A	626	SER	CA-C-N	5.61	125.08	119.24
1	A	626	SER	C-N-CA	5.61	125.08	119.24
1	A	325	ASN	N-CA-C	5.45	119.43	112.34
1	A	487	SER	N-CA-C	5.33	117.16	109.48
1	A	557	THR	N-CA-C	5.25	117.00	111.28
1	A	548	GLU	N-CA-C	-5.22	105.50	111.14
1	A	585	LEU	N-CA-C	-5.11	102.92	110.48
1	A	278	SER	N-CA-C	5.07	116.50	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	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	3871	0	3826	166	0
2	A	44	0	0	5	0
All	All	3915	0	3826	166	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 22.

All (166) 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:464:ILE:O	1:A:465:ARG:HD3	1.78	0.84
1:A:594:MET:HE1	1:A:704:PHE:HB3	1.57	0.84
1:A:739:ASN:O	1:A:743:THR:HG23	1.78	0.83
1:A:753:THR:O	1:A:756:LEU:HD13	1.82	0.79
1:A:478:ARG:HA	1:A:481:GLN:HE21	1.48	0.79
1:A:709:ASN:ND2	1:A:712:GLU:H	1.82	0.78
1:A:267:ASN:ND2	1:A:268:ASN:H	1.83	0.76
1:A:254:PHE:HA	1:A:615:ARG:HH12	1.50	0.76
1:A:267:ASN:HD22	1:A:268:ASN:H	1.29	0.76
1:A:594:MET:HE1	1:A:704:PHE:CB	2.16	0.76
1:A:525:ARG:HB3	2:A:827:HOH:O	1.88	0.72
1:A:286:MET:HA	1:A:286:MET:HE2	1.71	0.71
1:A:391:VAL:HG13	1:A:422:ILE:HD13	1.69	0.71
1:A:436:ASP:OD1	1:A:438:ASP:HB2	1.91	0.70
1:A:708:GLU:H	1:A:708:GLU:CD	1.99	0.70
1:A:538:ILE:HD11	1:A:751:ILE:HA	1.73	0.70
1:A:296:VAL:HG21	1:A:342:ILE:HD13	1.74	0.69
1:A:655:SER:O	1:A:733:THR:HG21	1.93	0.69
1:A:594:MET:HE2	1:A:681:TRP:HE1	1.56	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:HA	1:A:615:ARG:NH1	2.10	0.66
1:A:709:ASN:C	1:A:709:ASN:HD22	2.03	0.66
1:A:745:SER:HG	1:A:755:TRP:CD1	2.13	0.66
1:A:621:LEU:HD21	1:A:627:PRO:HG3	1.78	0.65
1:A:276:MET:HE1	1:A:314:ALA:CB	2.25	0.65
1:A:385:LYS:HG2	1:A:490:PHE:CZ	2.32	0.65
1:A:276:MET:HE1	1:A:314:ALA:HA	1.77	0.65
1:A:273:VAL:HG21	1:A:669:VAL:HG11	1.78	0.65
1:A:435:LYS:HE3	1:A:439:GLU:OE2	1.96	0.65
1:A:552:ILE:HG22	1:A:556:LYS:HD2	1.77	0.65
1:A:267:ASN:HD22	1:A:268:ASN:N	1.96	0.62
1:A:276:MET:HE1	1:A:314:ALA:HB2	1.81	0.62
1:A:378:ALA:N	1:A:421:ARG:NH1	2.47	0.62
1:A:364:LEU:HD22	1:A:369:VAL:HG11	1.81	0.62
1:A:276:MET:HE1	1:A:314:ALA:CA	2.29	0.62
1:A:280:ARG:HB3	1:A:290:GLU:HG2	1.81	0.61
1:A:318:VAL:HG21	1:A:338:ILE:HD13	1.82	0.61
1:A:544:PHE:HA	1:A:547:MET:HE3	1.81	0.61
1:A:325:ASN:HA	1:A:328:ASN:OD1	2.01	0.60
1:A:435:LYS:HG2	1:A:439:GLU:OE2	2.01	0.59
1:A:403:SER:OG	1:A:432:GLY:O	2.18	0.59
1:A:473:PHE:HB3	1:A:474:PRO:HD3	1.85	0.58
1:A:378:ALA:N	1:A:421:ARG:HH11	2.02	0.58
1:A:594:MET:CE	1:A:681:TRP:HE1	2.18	0.57
1:A:289:ASN:ND2	1:A:291:ARG:H	2.03	0.57
1:A:291:ARG:HD2	2:A:808:HOH:O	2.05	0.57
1:A:351:TRP:HA	1:A:584:ARG:HD2	1.86	0.57
1:A:419:GLY:O	1:A:420:LYS:HB3	2.03	0.57
1:A:452:MET:SD	1:A:494:LEU:HD13	2.45	0.57
1:A:523:ILE:HD12	1:A:523:ILE:N	2.20	0.57
1:A:655:SER:HB2	1:A:684:PHE:CZ	2.40	0.57
1:A:584:ARG:HH11	1:A:584:ARG:HG3	1.70	0.56
1:A:276:MET:CE	1:A:314:ALA:HA	2.35	0.56
1:A:462:LYS:HE2	1:A:483:GLU:HG2	1.88	0.56
1:A:756:LEU:H	1:A:756:LEU:HD12	1.70	0.55
1:A:262:LYS:HG3	1:A:344:VAL:HG12	1.88	0.55
1:A:377:GLU:C	1:A:421:ARG:HH11	2.14	0.55
1:A:534:ALA:HB2	1:A:591:CYS:HB3	1.87	0.55
1:A:737:LEU:O	1:A:741:LEU:HG	2.05	0.55
1:A:756:LEU:HD12	1:A:756:LEU:N	2.21	0.55
1:A:530:ILE:HG22	1:A:531:VAL:HG23	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:ARG:HB3	1:A:729:ASP:OD1	2.07	0.54
1:A:572:GLN:H	1:A:572:GLN:CD	2.15	0.53
1:A:364:LEU:HD22	1:A:369:VAL:CG1	2.38	0.53
1:A:305:LYS:HA	1:A:305:LYS:HE3	1.90	0.53
1:A:561:VAL:O	1:A:562:SER:HB3	2.09	0.53
1:A:504:GLN:HG2	1:A:592:THR:HG21	1.92	0.53
1:A:709:ASN:HD21	1:A:712:GLU:H	1.54	0.53
1:A:724:LEU:HD22	1:A:730:PHE:CG	2.44	0.52
1:A:436:ASP:HB2	2:A:803:HOH:O	2.10	0.51
1:A:605:LEU:HG	1:A:609:MET:HE2	1.92	0.51
1:A:296:VAL:HG11	1:A:342:ILE:HD11	1.91	0.51
1:A:385:LYS:HD2	1:A:389:THR:OG1	2.10	0.51
1:A:534:ALA:HB3	1:A:648:VAL:HB	1.93	0.51
1:A:325:ASN:HD22	1:A:325:ASN:N	2.07	0.50
1:A:450:PRO:HB3	2:A:812:HOH:O	2.11	0.50
1:A:569:LEU:O	1:A:576:PHE:HA	2.12	0.49
1:A:289:ASN:HD22	1:A:290:GLU:N	2.09	0.49
1:A:340:LYS:O	1:A:343:PRO:HB3	2.12	0.49
1:A:287:PHE:C	1:A:289:ASN:N	2.67	0.49
1:A:301:PRO:HD3	1:A:320:VAL:O	2.13	0.49
1:A:584:ARG:HH12	1:A:586:GLN:HG2	1.77	0.49
1:A:496:GLN:O	1:A:497:HIS:C	2.56	0.48
1:A:247:PRO:O	1:A:251:VAL:HG23	2.14	0.48
1:A:262:LYS:HG2	1:A:344:VAL:HA	1.95	0.48
1:A:708:GLU:OE1	1:A:712:GLU:HG3	2.14	0.48
1:A:296:VAL:HA	1:A:316:HIS:O	2.14	0.48
1:A:299:VAL:HG12	1:A:304:LEU:HB2	1.95	0.47
1:A:676:SER:HB3	1:A:719:VAL:HG12	1.95	0.47
1:A:397:VAL:HG22	1:A:550:CYS:HB3	1.96	0.47
1:A:669:VAL:HG13	1:A:669:VAL:O	2.14	0.47
1:A:465:ARG:HG3	1:A:476:LEU:HD22	1.96	0.47
1:A:589:HIS:ND1	1:A:590:PRO:HD3	2.30	0.47
1:A:710:ARG:O	1:A:714:ILE:HG13	2.15	0.47
1:A:728:GLY:O	1:A:731:ARG:HG2	2.14	0.47
1:A:709:ASN:ND2	1:A:709:ASN:C	2.73	0.47
1:A:457:GLU:HB2	1:A:487:SER:HB2	1.97	0.47
1:A:325:ASN:N	1:A:325:ASN:ND2	2.64	0.46
1:A:495:ALA:HB1	1:A:569:LEU:HD21	1.98	0.46
1:A:647:HIS:CD2	1:A:710:ARG:HA	2.51	0.46
1:A:454:LYS:HG2	1:A:464:ILE:HG23	1.97	0.46
1:A:457:GLU:HB2	1:A:487:SER:CB	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ARG:CG	1:A:476:LEU:HD22	2.45	0.46
1:A:289:ASN:HD22	1:A:289:ASN:C	2.24	0.45
1:A:726:ILE:O	1:A:727:ARG:C	2.58	0.45
1:A:457:GLU:HB2	1:A:487:SER:OG	2.16	0.45
1:A:656:GLU:HA	1:A:656:GLU:OE1	2.17	0.45
1:A:380:TRP:CE3	1:A:380:TRP:HA	2.52	0.45
1:A:300:THR:HG22	1:A:320:VAL:HG23	1.99	0.44
1:A:523:ILE:N	1:A:523:ILE:CD1	2.80	0.44
1:A:439:GLU:O	1:A:442:GLU:HB2	2.17	0.44
1:A:357:ASN:O	1:A:361:PRO:HD2	2.17	0.44
1:A:589:HIS:N	1:A:590:PRO:CD	2.80	0.44
1:A:543:ILE:HG22	1:A:547:MET:HE2	2.00	0.44
1:A:581:LEU:C	1:A:581:LEU:HD23	2.42	0.44
1:A:614:HIS:HD2	2:A:830:HOH:O	2.00	0.44
1:A:267:ASN:ND2	1:A:268:ASN:N	2.59	0.44
1:A:523:ILE:CD1	1:A:523:ILE:H	2.31	0.44
1:A:268:ASN:HA	1:A:272:ALA:HB2	2.00	0.44
1:A:289:ASN:ND2	1:A:289:ASN:C	2.75	0.43
1:A:336:VAL:HG21	1:A:363:LEU:CB	2.48	0.43
1:A:545:GLU:O	1:A:548:GLU:HB2	2.18	0.43
1:A:668:THR:O	1:A:685:SER:HA	2.18	0.43
1:A:264:LEU:HB3	1:A:347:VAL:HG22	1.99	0.43
1:A:357:ASN:HD21	1:A:359:LYS:HE3	1.82	0.43
1:A:402:TRP:H	1:A:405:SER:HG	1.66	0.43
1:A:268:ASN:HB2	1:A:310:TYR:CE2	2.53	0.43
1:A:377:GLU:H	1:A:377:GLU:CD	2.26	0.43
1:A:499:ARG:HD3	1:A:751:ILE:O	2.17	0.43
1:A:756:LEU:H	1:A:756:LEU:CD1	2.31	0.43
1:A:287:PHE:C	1:A:289:ASN:H	2.25	0.43
1:A:683:TYR:HE1	1:A:702:HIS:HB2	1.84	0.43
1:A:377:GLU:HB2	1:A:421:ARG:NH1	2.34	0.43
1:A:655:SER:N	1:A:684:PHE:HZ	2.16	0.43
1:A:751:ILE:HG23	1:A:752:ASP:N	2.34	0.43
1:A:520:ASP:HB3	1:A:533:GLU:HB2	2.00	0.42
1:A:410:GLU:H	1:A:410:GLU:HG3	1.62	0.42
1:A:262:LYS:CG	1:A:344:VAL:HA	2.49	0.42
1:A:318:VAL:HA	1:A:319:PRO:HD3	1.83	0.42
1:A:409:VAL:HG11	1:A:423:SER:O	2.19	0.42
1:A:584:ARG:HG3	1:A:584:ARG:NH1	2.34	0.42
1:A:703:CYS:O	1:A:717:MET:HE1	2.19	0.42
1:A:318:VAL:O	1:A:318:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HB3	1:A:371:PHE:CD2	2.55	0.42
1:A:303:ASP:OD1	1:A:668:THR:HG21	2.20	0.42
1:A:725:SER:HA	1:A:730:PHE:O	2.20	0.42
1:A:276:MET:HE3	1:A:295:PHE:HB3	2.02	0.41
1:A:561:VAL:O	1:A:562:SER:CB	2.68	0.41
1:A:630:VAL:O	1:A:630:VAL:HG12	2.19	0.41
1:A:523:ILE:HD12	1:A:523:ILE:H	1.86	0.41
1:A:496:GLN:O	1:A:497:HIS:O	2.39	0.41
1:A:587:VAL:HG13	1:A:588:GLU:HG3	2.01	0.41
1:A:496:GLN:HE21	1:A:496:GLN:HB2	1.62	0.41
1:A:736:TYR:CE2	1:A:737:LEU:HG	2.56	0.41
1:A:299:VAL:O	1:A:319:PRO:HA	2.21	0.41
1:A:332:VAL:O	1:A:336:VAL:HG23	2.21	0.41
1:A:336:VAL:HG21	1:A:363:LEU:HB3	2.03	0.41
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.85	0.41
1:A:683:TYR:CE1	1:A:702:HIS:HB2	2.56	0.41
1:A:418:GLN:HG2	1:A:418:GLN:O	2.20	0.41
1:A:551:ALA:HB1	1:A:566:VAL:HG21	2.03	0.41
1:A:275:CYS:HB2	1:A:348:TRP:CH2	2.57	0.40
1:A:402:TRP:HB2	1:A:491:LEU:O	2.20	0.40
1:A:402:TRP:CH2	1:A:404:GLY:HA3	2.57	0.40
1:A:709:ASN:HD22	1:A:712:GLU:H	1.64	0.40
1:A:257:ASP:O	1:A:258:ARG:HB2	2.20	0.40
1:A:426:GLU:O	1:A:426:GLU:HG2	2.21	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	486/573 (85%)	448 (92%)	33 (7%)	5 (1%)	12 32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	HIS
1	A	562	SER
1	A	573	ASP
1	A	574	GLY
1	A	420	LYS

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	412/477 (86%)	395 (96%)	17 (4%)	27 56

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	281	ARG
1	A	305	LYS
1	A	325	ASN
1	A	343	PRO
1	A	410	GLU
1	A	445	GLU
1	A	465	ARG
1	A	497	HIS
1	A	528	GLN
1	A	572	GLN
1	A	573	ASP
1	A	613	LEU
1	A	615	ARG
1	A	708	GLU
1	A	709	ASN
1	A	711	GLU
1	A	729	ASP

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	239	HIS
1	A	267	ASN
1	A	289	ASN
1	A	307	ASN
1	A	325	ASN
1	A	327	ASN
1	A	353	HIS
1	A	367	ASN
1	A	481	GLN
1	A	496	GLN
1	A	512	ASN
1	A	524	GLN
1	A	528	GLN
1	A	673	ASN
1	A	699	GLN
1	A	709	ASN
1	A	716	ASN
1	A	739	ASN
1	A	747	GLN
1	A	748	ASN
1	A	749	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 [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	494/573 (86%)	-0.28	0 100 100	31, 53, 79, 103	0

There are no RSRZ outliers to report.

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.