



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:42 PM UTC

PDB ID : 6ZTA / pdb_00006zta
Title : X-ray structure of mutated arabinofuranosidase
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Deposited on : 2020-07-17
Resolution : 3.10 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

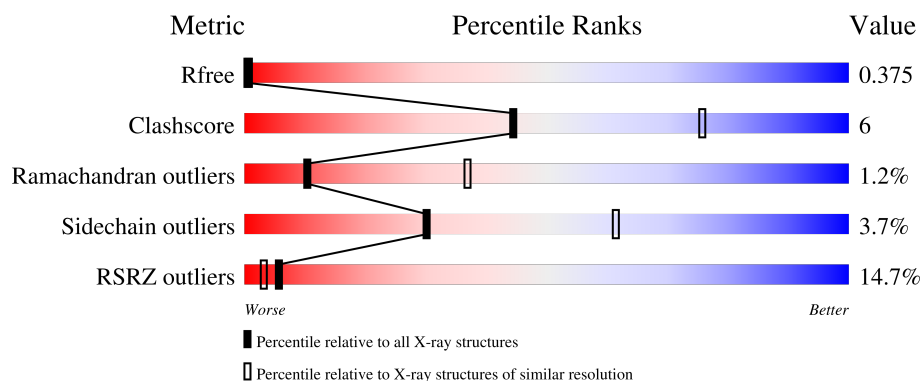
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	496	13% 81% 18% .
1	B	496	15% 80% 18% ..
1	C	496	16% 81% 17% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11833 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 Alpha-L-arabinofuranosidase.

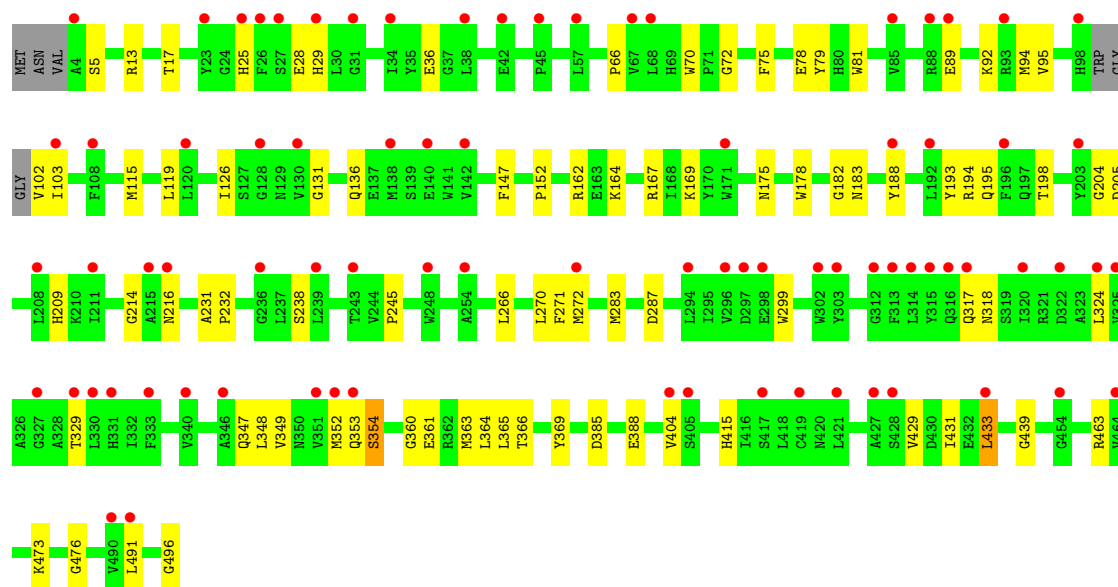
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	4	0
			3944	2496	696	728	24			
1	B	490	Total	C	N	O	S	0	5	0
			3947	2499	694	730	24			
1	C	490	Total	C	N	O	S	0	4	0
			3942	2497	693	727	25			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	HIS	ARG	conflict	UNP O69262
A	179	PHE	GLY	conflict	UNP O69262
A	352	MET	LEU	conflict	UNP O69262
B	69	HIS	ARG	conflict	UNP O69262
B	179	PHE	GLY	conflict	UNP O69262
B	352	MET	LEU	conflict	UNP O69262
C	69	HIS	ARG	conflict	UNP O69262
C	179	PHE	GLY	conflict	UNP O69262
C	352	MET	LEU	conflict	UNP O69262

● Molecule 1: Alpha-L-arabinofuranosidase

Chain C:  16% 81% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	156.49Å 156.49Å 376.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 3.10 49.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-3.10) 99.9 (49.01-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.345 , 0.375 0.347 , 0.375	Depositor DCC
R_{free} test set	499 reflections (0.27%)	wwPDB-VP
Wilson B-factor (Å ²)	57.7	Xtriage
Anisotropy	1.095	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11833	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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	0.60	0/4060	0.92	2/5508 (0.0%)
1	B	0.60	0/4066	0.91	0/5516
1	C	0.59	0/4058	0.91	0/5504
All	All	0.60	0/12184	0.91	2/16528 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	VAL	CA-C-N	5.08	125.73	119.99
1	A	130	VAL	C-N-CA	5.08	125.73	119.99

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	3944	0	3794	55	0
1	B	3947	0	3798	49	0
1	C	3942	0	3797	48	0
All	All	11833	0	11389	140	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 6.

All (140) 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:13[B]:ARG:CG	1:A:13[B]:ARG:HH11	1.59	1.15
1:A:13[B]:ARG:HH11	1:A:13[B]:ARG:HG3	1.06	1.12
1:A:13[B]:ARG:HG3	1:A:13[B]:ARG:NH1	1.85	0.84
1:A:13[B]:ARG:CG	1:A:13[B]:ARG:NH1	2.29	0.81
1:C:365:LEU:HD13	1:C:369:TYR:CE2	2.26	0.71
1:B:362:ARG:NH2	1:B:458:PHE:O	2.24	0.70
1:A:88[B]:ARG:CG	1:A:88[B]:ARG:HH21	2.05	0.70
1:A:88[B]:ARG:HH21	1:A:88[B]:ARG:HG2	1.55	0.69
1:A:13[B]:ARG:NH1	1:A:13[B]:ARG:HG2	2.09	0.66
1:A:13[B]:ARG:HH11	1:A:13[B]:ARG:HG2	1.55	0.66
1:B:299:TRP:CE3	1:B:329:THR:HG21	2.36	0.61
1:A:317:GLN:OE1	1:A:318:ASN:N	2.36	0.59
1:B:317:GLN:OE1	1:B:318:ASN:N	2.35	0.58
1:A:299:TRP:CE3	1:A:329:THR:HG21	2.38	0.58
1:A:88[B]:ARG:HG2	1:A:88[B]:ARG:NH2	2.17	0.57
1:C:299:TRP:CE3	1:C:329:THR:HG21	2.38	0.57
1:C:317:GLN:OE1	1:C:318:ASN:N	2.36	0.56
1:B:95:VAL:HG13	1:B:103:ILE:HG12	1.89	0.56
1:A:95:VAL:HB	1:B:150:GLU:HB3	1.89	0.55
1:B:92:LYS:HE2	1:C:152:PRO:HD2	1.88	0.54
1:A:388:GLU:HG3	1:A:390:VAL:HG13	1.90	0.54
1:C:365:LEU:HD13	1:C:369:TYR:CD2	2.44	0.53
1:B:70:TRP:O	1:B:126:ILE:HA	2.09	0.53
1:A:431:ILE:HG22	1:A:433:LEU:HD23	1.91	0.52
1:C:70:TRP:O	1:C:126:ILE:HA	2.09	0.52
1:A:150:GLU:HG3	1:A:155:ASN:HD21	1.75	0.52
1:A:201:ARG:NH2	1:C:78:GLU:OE1	2.42	0.52
1:C:431:ILE:HG22	1:C:433:LEU:HD23	1.92	0.52
1:A:70:TRP:O	1:A:126:ILE:HA	2.10	0.52
1:A:205:ASP:OD1	1:A:205:ASP:C	2.52	0.52
1:B:92:LYS:HE3	1:C:152:PRO:HG2	1.91	0.52
1:B:162:ARG:NE	1:B:164:LYS:O	2.42	0.52
1:C:79:TYR:CE2	1:C:81:TRP:HA	2.45	0.52
1:C:388:GLU:N	1:C:388:GLU:OE2	2.42	0.52
1:B:388:GLU:HG3	1:B:390:VAL:HG13	1.92	0.51
1:B:431:ILE:HG22	1:B:433:LEU:HD23	1.92	0.50
1:C:415:HIS:HA	1:C:491:LEU:O	2.11	0.50
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	0.50
1:A:135:VAL:HA	1:A:196:PHE:CE1	2.47	0.50
1:C:205:ASP:OD1	1:C:205:ASP:C	2.53	0.50
1:B:415:HIS:HA	1:B:491:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:NE	1:B:191:ASP:OD1	2.45	0.49
1:A:415:HIS:HA	1:A:491:LEU:O	2.12	0.49
1:B:79:TYR:CE2	1:B:81:TRP:HA	2.47	0.49
1:A:79:TYR:CE2	1:A:81:TRP:HA	2.46	0.49
1:C:95:VAL:HG13	1:C:103:ILE:HG12	1.94	0.48
1:A:214:GLY:HA3	1:A:238:SER:O	2.14	0.48
1:B:29:HIS:HB2	1:B:75:PHE:CD2	2.49	0.48
1:A:188:TYR:CD2	1:B:191:ASP:HB3	2.49	0.47
1:A:369:TYR:C	1:A:369:TYR:CD1	2.93	0.47
1:B:214:GLY:HA3	1:B:238:SER:O	2.14	0.47
1:B:439:GLY:O	1:B:496:GLY:N	2.46	0.47
1:A:162:ARG:NE	1:A:164:LYS:O	2.43	0.46
1:B:369:TYR:C	1:B:369:TYR:CD1	2.94	0.46
1:C:162:ARG:NE	1:C:164:LYS:O	2.43	0.46
1:B:92:LYS:CE	1:C:152:PRO:HG2	2.46	0.46
1:A:266:LEU:O	1:A:270:LEU:HG	2.16	0.46
1:C:214:GLY:HA3	1:C:238:SER:O	2.15	0.46
1:A:95:VAL:HG13	1:A:103:ILE:HG12	1.97	0.46
1:A:231:ALA:HB3	1:A:232:PRO:HD3	1.97	0.46
1:C:283:MET:O	1:C:287:ASP:N	2.49	0.46
1:C:266:LEU:O	1:C:270:LEU:HG	2.16	0.45
1:A:439:GLY:O	1:A:496:GLY:N	2.46	0.45
1:A:169:LYS:O	1:A:209:HIS:N	2.48	0.45
1:B:80:HIS:CE1	1:C:136:GLN:OE1	2.69	0.45
1:C:25:HIS:HB3	1:C:348:LEU:HD13	1.98	0.45
1:C:182:GLY:O	1:C:183:ASN:C	2.59	0.45
1:B:25:HIS:HB3	1:B:348:LEU:HD13	1.99	0.45
1:B:182:GLY:O	1:B:183:ASN:C	2.58	0.45
1:B:266:LEU:O	1:B:270:LEU:HG	2.16	0.45
1:C:439:GLY:O	1:C:496:GLY:N	2.47	0.45
1:A:283:MET:O	1:A:287:ASP:N	2.49	0.45
1:C:169:LYS:O	1:C:209:HIS:N	2.47	0.45
1:A:29:HIS:HB2	1:A:75:PHE:CD2	2.51	0.45
1:A:182:GLY:O	1:A:183:ASN:C	2.59	0.45
1:A:13[B]:ARG:HD3	1:A:385:ASP:HB2	1.98	0.44
1:A:364:LEU:C	1:A:364:LEU:HD12	2.42	0.44
1:C:364:LEU:C	1:C:364:LEU:HD12	2.42	0.44
1:C:29:HIS:HB2	1:C:75:PHE:CD2	2.52	0.44
1:B:271:PHE:O	1:B:272:MET:C	2.61	0.44
1:B:305:VAL:HG12	1:B:314:LEU:HA	1.99	0.44
1:B:364:LEU:HD12	1:B:364:LEU:C	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88[B]:ARG:HH21	1:A:88[B]:ARG:HB3	1.83	0.44
1:B:283:MET:O	1:B:287:ASP:N	2.49	0.44
1:C:178:TRP:CZ2	1:C:216:ASN:HB2	2.53	0.44
1:C:193:TYR:CD1	1:C:193:TYR:C	2.95	0.44
1:C:194:ARG:O	1:C:198:THR:OG1	2.36	0.44
1:B:131:GLY:O	1:C:195:GLN:NE2	2.47	0.44
1:B:241:TYR:OH	1:B:268:LYS:O	2.29	0.44
1:B:5:SER:O	1:B:429:VAL:HA	2.18	0.43
1:B:440:VAL:HG23	1:B:474:LEU:HD21	2.00	0.43
1:A:28:GLU:HB3	1:A:347:GLN:HE22	1.83	0.43
1:A:193:TYR:CD1	1:A:193:TYR:C	2.97	0.43
1:B:169:LYS:O	1:B:209:HIS:N	2.48	0.43
1:B:352:MET:O	1:B:354:SER:N	2.52	0.43
1:A:25:HIS:HB3	1:A:348:LEU:HD13	1.99	0.43
1:C:5:SER:O	1:C:429:VAL:HA	2.19	0.43
1:C:271:PHE:O	1:C:272:MET:C	2.61	0.43
1:B:95:VAL:HG22	1:B:103:ILE:HG23	2.01	0.43
1:B:194:ARG:O	1:B:198:THR:OG1	2.37	0.43
1:A:346:ALA:HA	1:A:347:GLN:HA	1.76	0.43
1:B:28:GLU:HB3	1:B:347:GLN:HE22	1.83	0.43
1:B:346:ALA:HA	1:B:347:GLN:HA	1.78	0.43
1:A:352:MET:O	1:A:354:SER:N	2.52	0.42
1:C:28:GLU:HB3	1:C:347:GLN:HE22	1.84	0.42
1:B:436:LEU:HD13	1:B:436:LEU:HA	1.93	0.42
1:A:318:ASN:HB3	1:A:366:THR:HB	2.00	0.42
1:B:94:MET:HE3	1:C:147:PHE:CZ	2.55	0.42
1:A:199:TYR:OH	1:C:131:GLY:HA3	2.19	0.42
1:C:115[B]:MET:SD	1:C:119:LEU:HD11	2.60	0.42
1:A:88[B]:ARG:HH21	1:A:88[B]:ARG:CB	2.32	0.42
1:A:194:ARG:O	1:A:198:THR:OG1	2.37	0.42
1:A:5:SER:O	1:A:429:VAL:HA	2.19	0.42
1:A:431:ILE:HG22	1:A:433:LEU:CD2	2.50	0.42
1:A:271:PHE:O	1:A:272:MET:C	2.62	0.41
1:A:436:LEU:HD13	1:A:436:LEU:HA	1.94	0.41
1:C:231:ALA:HB3	1:C:232:PRO:HD3	2.01	0.41
1:C:318:ASN:HB3	1:C:366:THR:HB	2.01	0.41
1:B:178:TRP:CZ2	1:B:216:ASN:HB2	2.54	0.41
1:B:318:ASN:HB3	1:B:366:THR:HB	2.02	0.41
1:C:352:MET:O	1:C:354:SER:N	2.53	0.41
1:A:178:TRP:CZ2	1:A:216:ASN:HB2	2.56	0.41
1:B:375:PHE:O	1:B:376:LYS:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ILE:HG22	1:C:433:LEU:CD2	2.51	0.41
1:A:22:ILE:O	1:A:343:ALA:HB3	2.21	0.41
1:C:115[A]:MET:HE3	1:C:115[A]:MET:HB2	1.92	0.41
1:A:418:LEU:HB3	1:A:483:LEU:HD11	2.03	0.41
1:B:178:TRP:CE2	1:B:216:ASN:HB2	2.56	0.41
1:C:95:VAL:HG22	1:C:103:ILE:HG23	2.03	0.41
1:B:25:HIS:CB	1:B:348:LEU:HD13	2.51	0.41
1:B:231:ALA:HB3	1:B:232:PRO:HD3	2.03	0.40
1:C:25:HIS:CB	1:C:348:LEU:HD13	2.52	0.40
1:C:13[A]:ARG:HD3	1:C:385:ASP:HB2	2.02	0.40
1:C:13[A]:ARG:NH1	1:C:385:ASP:OD2	2.47	0.40
1:A:95:VAL:HG22	1:A:103:ILE:HG23	2.03	0.40
1:A:191:ASP:HB3	1:C:188:TYR:CD2	2.56	0.40
1:B:70:TRP:CD1	1:B:71:PRO:HA	2.56	0.40
1:B:84:GLY:O	1:B:109:GLY:HA3	2.21	0.40
1:C:36:GLU:OE2	1:C:360:GLY:N	2.54	0.40
1:C:178:TRP:CE2	1:C:216:ASN:HB2	2.56	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	490/496 (99%)	437 (89%)	47 (10%)	6 (1%)	10	37
1	B	491/496 (99%)	439 (89%)	46 (9%)	6 (1%)	10	37
1	C	490/496 (99%)	435 (89%)	49 (10%)	6 (1%)	10	37
All	All	1471/1488 (99%)	1311 (89%)	142 (10%)	18 (1%)	10	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	476	GLY
1	A	353	GLN
1	A	476	GLY
1	B	353	GLN
1	B	476	GLY
1	C	353	GLN
1	C	204	GLY
1	A	72	GLY
1	A	204	GLY
1	B	66	PRO
1	B	72	GLY
1	B	204	GLY
1	C	66	PRO
1	C	72	GLY
1	A	66	PRO
1	A	245	PRO
1	C	245	PRO
1	B	245	PRO

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	420/420 (100%)	407 (97%)	13 (3%)	35	64
1	B	421/420 (100%)	404 (96%)	17 (4%)	28	60
1	C	420/420 (100%)	404 (96%)	16 (4%)	29	60
All	All	1261/1260 (100%)	1215 (96%)	46 (4%)	30	62

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	78	GLU
1	A	102	VAL
1	A	152	PRO
1	A	167	ARG

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Mol	Chain	Res	Type
1	A	175	ASN
1	A	250	LYS
1	A	324	LEU
1	A	354	SER
1	A	363	MET
1	A	398	GLU
1	A	404	VAL
1	A	433	LEU
1	B	17	THR
1	B	62	GLN
1	B	89	GLU
1	B	102	VAL
1	B	167	ARG
1	B	175	ASN
1	B	317	GLN
1	B	324	LEU
1	B	349	VAL
1	B	354	SER
1	B	363	MET
1	B	398	GLU
1	B	404	VAL
1	B	433	LEU
1	B	451	ARG
1	B	465	LYS
1	B	473	LYS
1	C	17	THR
1	C	89	GLU
1	C	92	LYS
1	C	94	MET
1	C	102	VAL
1	C	167	ARG
1	C	175	ASN
1	C	324	LEU
1	C	349	VAL
1	C	354	SER
1	C	361	GLU
1	C	363	MET
1	C	404	VAL
1	C	433	LEU
1	C	463	ARG
1	C	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	48	ASN
1	A	98	HIS
1	A	155	ASN
1	A	175	ASN
1	A	229	GLN
1	A	437	ASN
1	B	10	ASN
1	B	48	ASN
1	B	62	GLN
1	B	80	HIS
1	B	98	HIS
1	B	175	ASN
1	B	229	GLN
1	B	347	GLN
1	B	437	ASN
1	C	10	ASN
1	C	48	ASN
1	C	80	HIS
1	C	96	ASN
1	C	98	HIS
1	C	175	ASN
1	C	229	GLN
1	C	347	GLN
1	C	437	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

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	490/496 (98%)	1.11	63 (12%) 7 4	40, 82, 113, 138	4 (0%)
1	B	490/496 (98%)	1.06	73 (14%) 5 3	45, 93, 127, 148	5 (1%)
1	C	490/496 (98%)	1.18	80 (16%) 4 2	30, 92, 120, 150	4 (0%)
All	All	1470/1488 (98%)	1.12	216 (14%) 6 3	30, 89, 122, 150	13 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	PHE	5.1
1	B	419	CYS	4.3
1	C	29	HIS	4.1
1	A	110	THR	4.0
1	C	316	GLN	4.0
1	B	256	GLY	4.0
1	B	402	VAL	3.8
1	C	215	ALA	3.8
1	C	26	PHE	3.8
1	C	294	LEU	3.8
1	A	150	GLU	3.7
1	C	302	TRP	3.7
1	A	342	MET	3.6
1	C	243	THR	3.5
1	B	171	TRP	3.5
1	A	262	TRP	3.5
1	C	324	LEU	3.5
1	B	102	VAL	3.5
1	A	433	LEU	3.5
1	A	297	ASP	3.5
1	C	31	GLY	3.4
1	C	327	GLY	3.4
1	C	346	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	94	MET	3.4
1	B	347	GLN	3.3
1	A	171	TRP	3.3
1	C	405	SER	3.3
1	C	329	THR	3.3
1	C	421	LEU	3.3
1	C	419	CYS	3.3
1	B	192	LEU	3.3
1	B	375	PHE	3.3
1	A	11	ALA	3.3
1	B	364	LEU	3.2
1	C	88	ARG	3.2
1	C	322	ASP	3.2
1	B	315	TYR	3.2
1	B	416	ILE	3.2
1	A	129	ASN	3.2
1	C	353	GLN	3.2
1	C	325	VAL	3.1
1	A	294	LEU	3.1
1	B	141	TRP	3.1
1	A	315	TYR	3.1
1	C	128	GLY	3.0
1	A	293	ASP	3.0
1	A	451	ARG	3.0
1	A	334	HIS	3.0
1	C	239	LEU	2.9
1	B	403	SER	2.9
1	C	45	PRO	2.9
1	A	170	TYR	2.9
1	B	125	TYR	2.9
1	C	331	HIS	2.9
1	B	138	MET	2.9
1	C	68	LEU	2.8
1	A	234	MET	2.8
1	C	103	ILE	2.8
1	A	25	HIS	2.8
1	A	452	ILE	2.8
1	B	127	SER	2.8
1	B	103	ILE	2.8
1	B	242	TYR	2.8
1	C	93	ARG	2.8
1	A	163	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	2.8
1	B	345	ILE	2.8
1	C	211	ILE	2.8
1	A	75	PHE	2.7
1	A	128	GLY	2.7
1	C	171	TRP	2.7
1	C	38	LEU	2.7
1	B	458	PHE	2.7
1	C	236	GLY	2.7
1	C	312	GLY	2.7
1	A	245	PRO	2.6
1	A	416	ILE	2.6
1	A	237	LEU	2.6
1	B	418	LEU	2.6
1	C	130	VAL	2.6
1	A	333	PHE	2.6
1	B	133	GLY	2.6
1	A	186	ALA	2.6
1	C	340	VAL	2.6
1	A	103	ILE	2.6
1	C	315	TYR	2.6
1	B	417	SER	2.6
1	A	123	GLU	2.6
1	C	298	GLU	2.6
1	C	4	ALA	2.6
1	C	120	LEU	2.5
1	A	4	ALA	2.5
1	A	266	LEU	2.5
1	C	490	VAL	2.5
1	A	233	PHE	2.5
1	B	181	GLY	2.5
1	B	34	ILE	2.5
1	C	196	PHE	2.5
1	B	8	VAL	2.5
1	C	67	VAL	2.5
1	B	495	ALA	2.5
1	B	184	MET	2.5
1	B	294	LEU	2.5
1	B	236	GLY	2.4
1	A	63	MET	2.4
1	C	352	MET	2.4
1	A	299	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	330	LEU	2.4
1	C	216	ASN	2.4
1	C	464	VAL	2.4
1	B	11	ALA	2.4
1	B	352	MET	2.4
1	C	89	GLU	2.4
1	A	295	ILE	2.4
1	B	452	ILE	2.4
1	B	372	PHE	2.4
1	B	124	PRO	2.4
1	B	367	PRO	2.4
1	C	296	VAL	2.4
1	B	83	ASP	2.3
1	C	42	GLU	2.3
1	A	375	PHE	2.3
1	C	208	LEU	2.3
1	C	317	GLN	2.3
1	C	254	ALA	2.3
1	C	427	ALA	2.3
1	A	423	PHE	2.3
1	B	108	PHE	2.3
1	B	233	PHE	2.3
1	C	297	ASP	2.3
1	A	407	SER	2.3
1	B	142	VAL	2.3
1	B	245	PRO	2.3
1	B	406	ALA	2.3
1	B	421	LEU	2.3
1	C	57	LEU	2.3
1	A	23	TYR	2.3
1	C	23	TYR	2.3
1	A	30	LEU	2.2
1	A	418	LEU	2.2
1	C	314	LEU	2.2
1	B	147	PHE	2.2
1	B	405	SER	2.2
1	A	102	VAL	2.2
1	A	347	GLN	2.2
1	A	117	CYS	2.2
1	C	404	VAL	2.2
1	B	326	ALA	2.2
1	B	342	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	433	LEU	2.2
1	B	113	PHE	2.2
1	A	98	HIS	2.2
1	C	428	SER	2.2
1	A	276	VAL	2.2
1	B	126	ILE	2.2
1	B	431	ILE	2.2
1	B	71	PRO	2.2
1	B	328	ALA	2.2
1	B	433	LEU	2.2
1	A	189	TYR	2.2
1	C	188	TYR	2.2
1	C	142	VAL	2.2
1	B	139	SER	2.2
1	B	226	LEU	2.2
1	A	215	ALA	2.2
1	C	454	GLY	2.2
1	A	240	HIS	2.2
1	B	78	GLU	2.2
1	B	153	MET	2.2
1	C	272	MET	2.2
1	B	300	GLY	2.2
1	B	248	TRP	2.2
1	A	209	HIS	2.2
1	C	491	LEU	2.1
1	B	9	VAL	2.1
1	A	126	ILE	2.1
1	B	195	GLN	2.1
1	A	298	GLU	2.1
1	A	405	SER	2.1
1	A	435	GLY	2.1
1	B	150	GLU	2.1
1	B	490	VAL	2.1
1	B	193	TYR	2.1
1	B	479	LEU	2.1
1	C	303	TYR	2.1
1	A	409	ALA	2.1
1	C	203	TYR	2.1
1	C	313	PHE	2.1
1	C	27	SER	2.1
1	C	351	VAL	2.1
1	A	474	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	2.1
1	B	324	LEU	2.1
1	C	320	ILE	2.1
1	A	312	GLY	2.1
1	B	187[A]	GLU	2.1
1	C	108	PHE	2.1
1	C	85	VAL	2.0
1	C	417	SER	2.0
1	A	320	ILE	2.0
1	A	324	LEU	2.0
1	B	330	LEU	2.0
1	C	34	ILE	2.0
1	C	25	HIS	2.0
1	C	248	TRP	2.0
1	C	138	MET	2.0
1	A	271	PHE	2.0
1	A	317	GLN	2.0
1	C	192	LEU	2.0
1	B	27	SER	2.0
1	B	211	ILE	2.0
1	B	295	ILE	2.0
1	B	114	MET	2.0
1	C	98	HIS	2.0
1	A	67	VAL	2.0
1	C	140	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.