



Full wwPDB X-ray Structure Validation Report i

Feb 3, 2021 – 03:04 PM GMT

PDB ID : 6ZTA
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 i symbol.

The following versions of software and data (see references ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.16
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) : 2.16

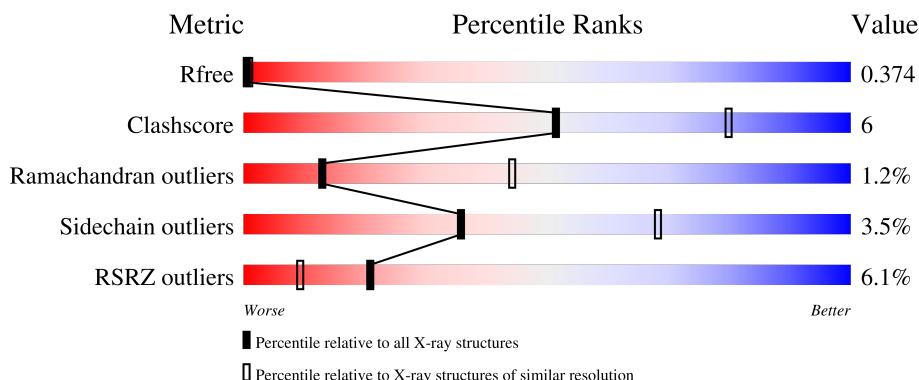
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

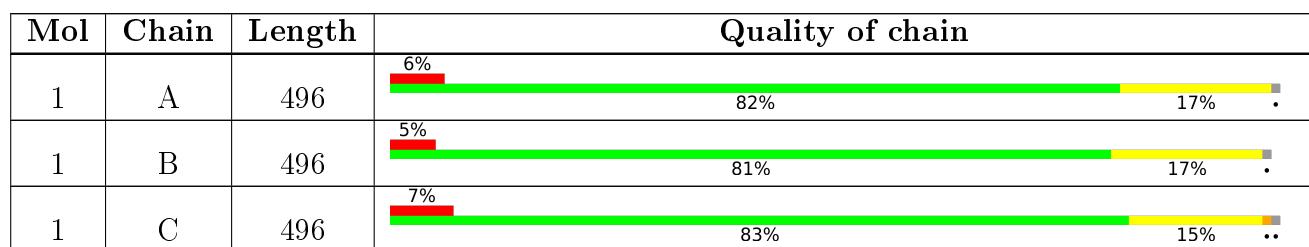
The reported resolution of this entry is 3.10 Å.

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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.



2 Entry composition (i)

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			

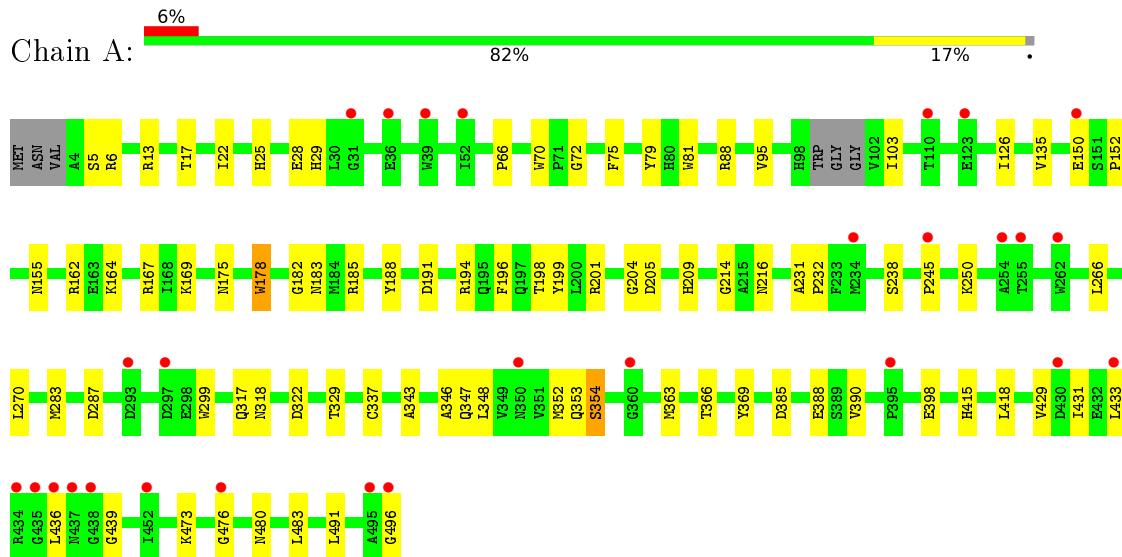
There are 9 discrepancies between the modelled and reference sequences:

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

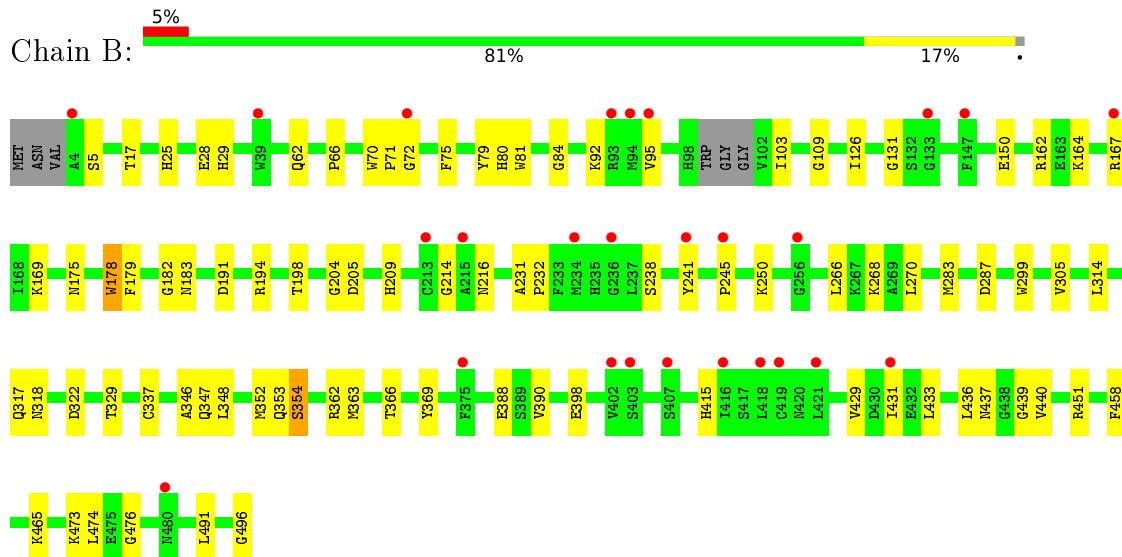
3 Residue-property plots

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.

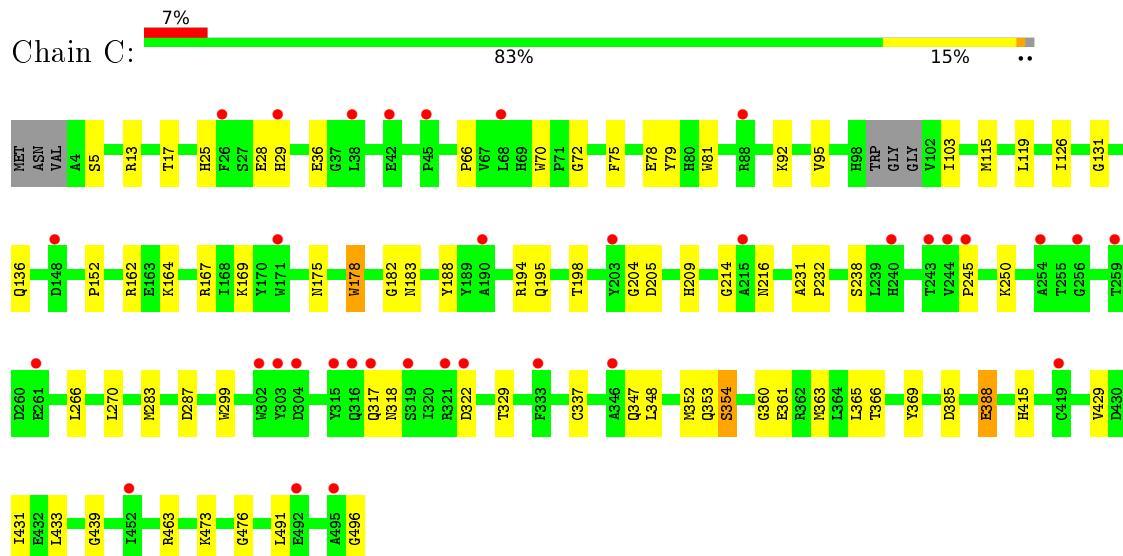
- Molecule 1: Alpha-L-arabinofuranosidase



- Molecule 1: Alpha-L-arabinofuranosidase



- Molecule 1: Alpha-L-arabinofuranosidase



4 Data and refinement statistics (i)

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 48.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.01-3.10) 99.9 (48.96-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.66 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R , R_{free}	0.345 , 0.375 0.347 , 0.374	Depositor DCC
R_{free} test set	499 reflections (0.99%)	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)	0.31 , 40.5	EDS
L-test for twinning ²	$< L > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	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 $< |L| >$, $< L^2 >$ 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	0.36	0/4060	0.58	0/5508
1	B	0.36	0/4066	0.58	0/5516
1	C	0.36	0/4058	0.57	0/5504
All	All	0.36	0/12184	0.58	0/16528

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	3944	0	3794	52	0
1	B	3947	0	3798	45	0
1	C	3942	0	3797	43	0
All	All	11833	0	11389	129	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 (129) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13[B]:ARG:HH11	1:A:13[B]:ARG:HG3	1.06	1.12
1:A:13[B]:ARG:NH1	1:A:13[B]:ARG:HG3	1.85	0.84
1:A:13[B]:ARG:NH1	1:A:13[B]:ARG:CG	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:HG2	1:A:88[B]:ARG:HH21	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:HG2	1:A:13[B]:ARG:HH11	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: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:388:GLU:N	1:C:388:GLU:OE2	2.42	0.52
1:C:79:TYR:CE2	1:C:81:TRP:HA	2.45	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:A:135:VAL:HA	1:A:196:PHE:CE1	2.47	0.50
1:B:415:HIS:HA	1:B:491:LEU:O	2.12	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:ASP:OD1	1:A:205:ASP:C	2.52	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: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:205:ASP:C	1:C:205:ASP:OD1	2.53	0.46
1:B:205:ASP:OD1	1:B:205:ASP:C	2.54	0.45
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:241:TYR:OH	1:B:268:LYS:O	2.29	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:B:266:LEU:O	1:B:270:LEU:HG	2.16	0.45
1:B:25:HIS:HB3	1:B:348:LEU:HD13	1.99	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:13[B]:ARG:HD3	1:A:385:ASP:HB2	1.98	0.44
1:C:29:HIS:HB2	1:C:75:PHE:CD2	2.52	0.44
1:B:305:VAL:HG12	1:B:314:LEU:HA	1.99	0.44
1:A:88[B]:ARG:HB3	1:A:88[B]:ARG:HH21	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: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: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:B:169:LYS:O	1:B:209:HIS:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:194:ARG:O	1:B:198:THR:OG1	2.37	0.43
1:B:95:VAL:HG22	1:B:103:ILE:HG23	2.01	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:A:369:TYR:CD1	1:A:369:TYR:C	2.93	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:CB	1:A:88[B]:ARG:HH21	2.32	0.42
1:A:194:ARG:O	1:A:198:THR:OG1	2.37	0.42
1:B:369:TYR:C	1:B:369:TYR:CD1	2.94	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:436:LEU:HA	1:A:436:LEU:HD13	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: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:A:182:GLY:O	1:A:183:ASN:C	2.59	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:182:GLY:O	1:C:183:ASN:C	2.59	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:182:GLY:O	1:B:183:ASN:C	2.58	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:O	1:B:109:GLY:HA3	2.21	0.40
1:B:70:TRP:CD1	1:B:71:PRO:HA	2.56	0.40
1:A:191:ASP:HB3	1:C:188:TYR:CD2	2.56	0.40
1:C:178:TRP:CE2	1:C:216:ASN:HB2	2.56	0.40
1:C:36:GLU:OE2	1:C:360:GLY:N	2.54	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	490/496 (99%)	437 (89%)	47 (10%)	6 (1%)	13 44
1	B	491/496 (99%)	439 (89%)	46 (9%)	6 (1%)	13 44
1	C	490/496 (99%)	435 (89%)	49 (10%)	6 (1%)	13 44
All	All	1471/1488 (99%)	1311 (89%)	142 (10%)	18 (1%)	13 44

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

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Mol	Chain	Res	Type
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 [\(i\)](#)

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	420/420 (100%)	405 (96%)	15 (4%)	35 67
1	B	421/420 (100%)	405 (96%)	16 (4%)	33 66
1	C	420/420 (100%)	406 (97%)	14 (3%)	38 69
All	All	1261/1260 (100%)	1216 (96%)	45 (4%)	36 67

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	17	THR
1	A	152	PRO
1	A	167	ARG
1	A	175	ASN
1	A	178	TRP
1	A	250	LYS
1	A	322	ASP
1	A	337	CYS
1	A	354	SER
1	A	363	MET
1	A	398	GLU
1	A	473	LYS
1	A	480[A]	ASN
1	A	480[B]	ASN
1	B	17	THR

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Mol	Chain	Res	Type
1	B	62	GLN
1	B	167	ARG
1	B	175	ASN
1	B	178	TRP
1	B	179	PHE
1	B	250	LYS
1	B	322	ASP
1	B	337	CYS
1	B	354	SER
1	B	363	MET
1	B	398	GLU
1	B	437	ASN
1	B	451	ARG
1	B	465	LYS
1	B	473	LYS
1	C	17	THR
1	C	92	LYS
1	C	167	ARG
1	C	175	ASN
1	C	178	TRP
1	C	250	LYS
1	C	322	ASP
1	C	337	CYS
1	C	354	SER
1	C	361	GLU
1	C	363	MET
1	C	388	GLU
1	C	463	ARG
1	C	473	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	96	ASN
1	A	98	HIS
1	A	155	ASN
1	A	437	ASN
1	B	48	ASN
1	B	80	HIS
1	B	96	ASN
1	B	98	HIS

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	437	ASN
1	C	48	ASN
1	C	80	HIS
1	C	96	ASN
1	C	98	HIS
1	C	437	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 monosaccharides 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 [\(i\)](#)

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	490/496 (98%)	0.54	28 (5%) 23 11	52, 82, 113, 138	0
1	B	490/496 (98%)	0.67	26 (5%) 26 12	50, 93, 127, 148	0
1	C	490/496 (98%)	0.69	35 (7%) 16 6	45, 92, 120, 150	0
All	All	1470/1488 (98%)	0.63	89 (6%) 21 9	45, 89, 122, 150	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	254	ALA	5.6
1	B	419	CYS	5.1
1	B	402	VAL	5.0
1	B	256	GLY	4.6
1	C	316	GLN	3.9
1	C	303	TYR	3.9
1	B	215	ALA	3.9
1	A	438	GLY	3.8
1	C	346	ALA	3.5
1	C	88	ARG	3.5
1	A	436	LEU	3.4
1	A	110	THR	3.4
1	C	243	THR	3.4
1	C	261	GLU	3.4
1	A	36	GLU	3.3
1	B	147	PHE	3.2
1	A	452	ILE	3.2
1	B	480[A]	ASN	3.2
1	C	302	TRP	3.1
1	A	437	ASN	3.1
1	B	93	ARG	3.1
1	B	167	ARG	3.0
1	B	236	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	2.9
1	C	245	PRO	2.8
1	B	245	PRO	2.8
1	A	39	TRP	2.7
1	A	435	GLY	2.7
1	C	317	GLN	2.6
1	A	350	ASN	2.6
1	A	254	ALA	2.6
1	A	496	GLY	2.6
1	C	322	ASP	2.6
1	C	29	HIS	2.5
1	B	421	LEU	2.5
1	C	171	TRP	2.4
1	A	31	GLY	2.4
1	C	256	GLY	2.4
1	B	241	TYR	2.4
1	A	234	MET	2.4
1	C	45	PRO	2.4
1	C	315	TYR	2.4
1	B	94	MET	2.3
1	B	418	LEU	2.3
1	C	495	ALA	2.3
1	B	403	SER	2.3
1	C	240	HIS	2.3
1	B	416	ILE	2.3
1	C	244	VAL	2.3
1	C	38	LEU	2.3
1	B	407	SER	2.3
1	C	452	ILE	2.3
1	A	52	ILE	2.3
1	C	304	ASP	2.2
1	A	150	GLU	2.2
1	C	492	GLU	2.2
1	C	42	GLU	2.2
1	A	255	THR	2.2
1	C	215	ALA	2.2
1	A	245	PRO	2.2
1	B	95	VAL	2.2
1	C	321	ARG	2.2
1	C	68	LEU	2.2
1	A	430	ASP	2.2
1	A	433	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	495	ALA	2.1
1	A	297	ASP	2.1
1	C	190	ALA	2.1
1	C	319	SER	2.1
1	A	293	ASP	2.1
1	A	262	TRP	2.1
1	B	4	ALA	2.1
1	A	476	GLY	2.1
1	B	375	PHE	2.1
1	C	333	PHE	2.1
1	B	39	TRP	2.1
1	C	203	TYR	2.1
1	A	434	ARG	2.1
1	B	234	MET	2.1
1	A	123	GLU	2.1
1	C	259	THR	2.1
1	C	148	ASP	2.1
1	C	419	CYS	2.0
1	B	133	GLY	2.0
1	C	26	PHE	2.0
1	A	360	GLY	2.0
1	A	395	PRO	2.0
1	B	213	CYS	2.0
1	B	72	GLY	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 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.