



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:01 pm BST

PDB ID : 1UZ1
Title : Family 1 β -glucosidase from *Thermotoga maritima* in complex with isofagomine lactam
Authors : Gloster, T.M.; Macdonald, J.; Stick, R.V.; Davies, G.J.
Deposited on : 2004-03-03
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

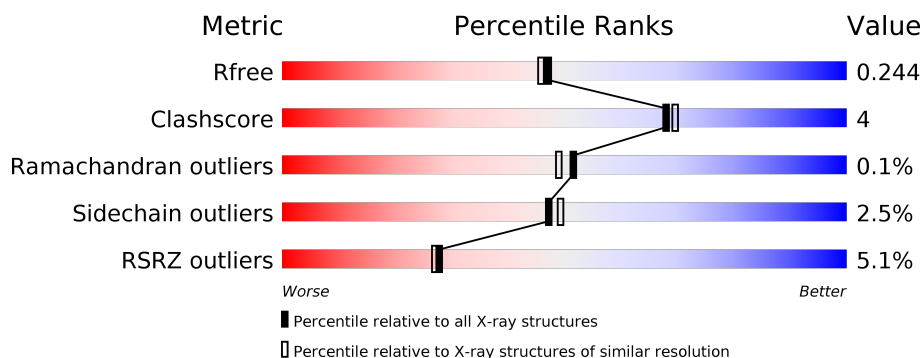
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 on 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	468	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 84%, grey 10%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 84% 10% 6% </div> </div>
1	B	468	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 9%, orange 1%, yellow 12%, green 82%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 9% 82% 12% 6% </div> </div>

2 Entry composition [i](#)

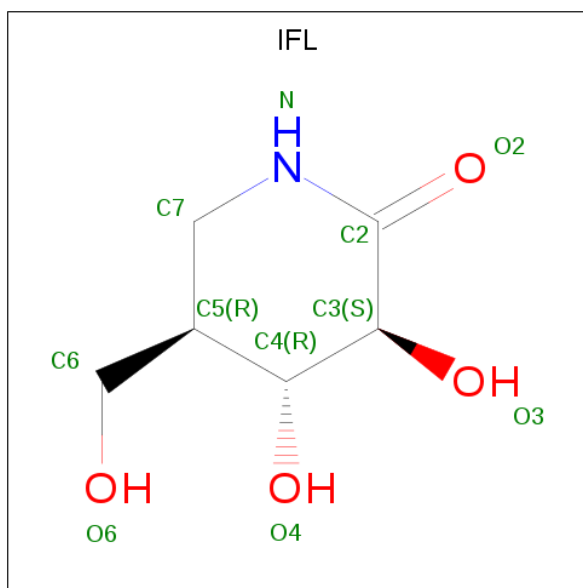
There are 3 unique types of molecules in this entry. The entry contains 7752 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-GLUCOSIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	4	0
			3621	2356	604	655	6			
1	B	440	Total	C	N	O	S	0	7	0
			3588	2330	597	654	7			

- Molecule 2 is (3S,4R,5R)-3,4-DIHYDROXY-5-(HYDROXYMETHYL)PIPERIDIN-2-ONE (three-letter code: IFL) (formula: C₆H₁₁NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		

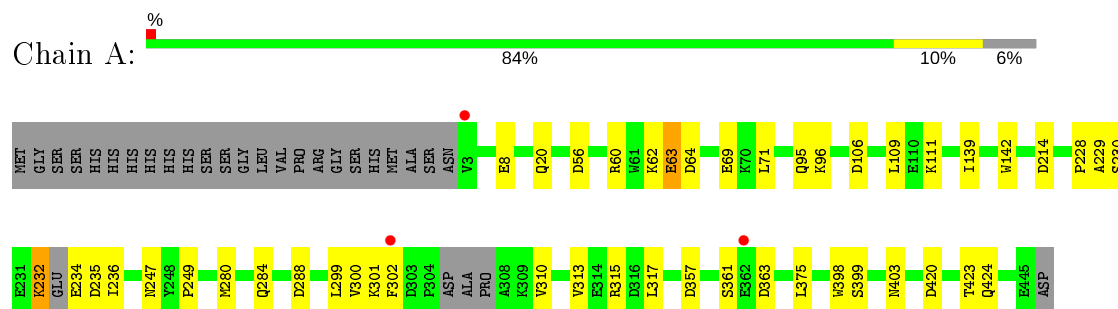
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	326	Total 326	O 326	0	0
3	B	195	Total 195	O 195	0	0

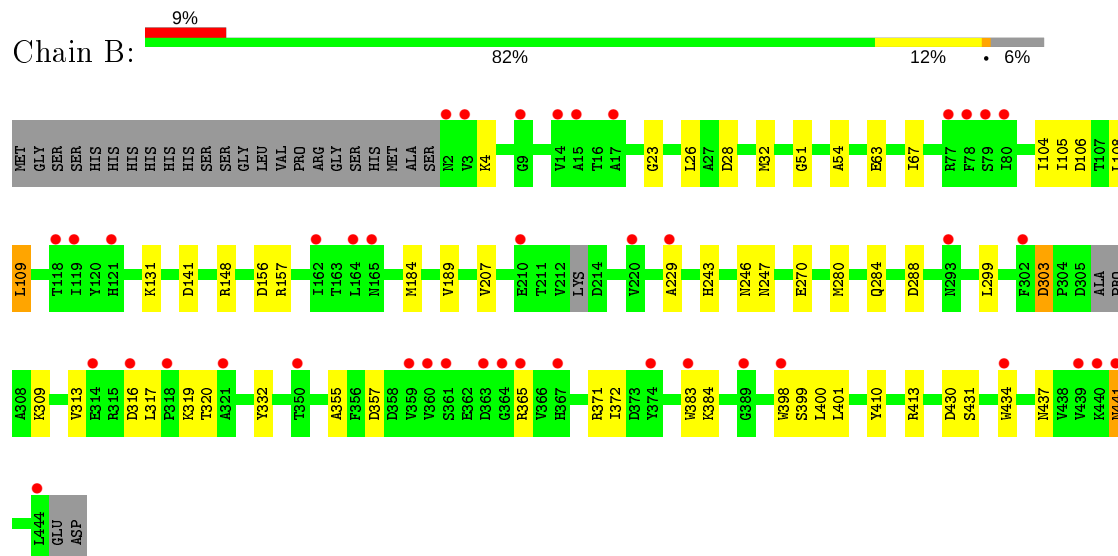
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: BETA-GLUCOSIDASE A



• Molecule 1: BETA-GLUCOSIDASE A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.41Å 94.33Å 113.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.55 – 2.00 29.83 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (72.55-2.00) 95.6 (29.83-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.194 , 0.244 0.194 , 0.244	Depositor DCC
R_{free} test set	3228 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7752	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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

Bond lengths and bond angles in the following residue types are not validated in this section: IFL

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	0.68	0/3751	0.77	6/5092 (0.1%)
1	B	0.57	0/3718	0.73	5/5059 (0.1%)
All	All	0.63	0/7469	0.75	11/10151 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	ASP	CB-CG-OD2	6.95	124.56	118.30
1	A	106	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	28	ASP	CB-CG-OD2	6.39	124.05	118.30
1	A	64	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	357	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	56	ASP	CB-CG-OD2	5.89	123.61	118.30
1	A	288	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	288	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	156	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	430	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	214	ASP	CB-CG-OD2	5.09	122.88	118.30

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	3621	0	3473	22	0
1	B	3588	0	3362	31	0
2	A	11	0	11	0	0
2	B	11	0	11	0	0
3	A	326	0	0	3	0
3	B	195	0	0	2	0
All	All	7752	0	6857	53	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 (53) 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:63[B]:GLU:OE2	3:A:2090:HOH:O	1.69	1.08
1:B:104:ILE:O	1:B:108:LEU:HD23	1.68	0.94
1:B:372:ILE:CD1	1:B:431:SER:HA	2.03	0.87
1:B:105:ILE:O	1:B:109:LEU:HD22	1.83	0.78
1:B:372:ILE:HD11	1:B:431:SER:HA	1.68	0.76
1:B:372:ILE:HD13	1:B:431:SER:HA	1.67	0.76
1:B:270[B]:GLU:HG2	3:B:2140:HOH:O	1.87	0.74
1:B:229:ALA:HA	1:B:299:LEU:HD11	1.73	0.70
1:B:434:TRP:O	1:B:437:ASN:HB2	1.92	0.70
1:A:299:LEU:HD23	1:A:313:VAL:HB	1.82	0.62
1:A:229:ALA:HB3	1:A:301:LYS:HB3	1.83	0.60
1:A:60:ARG:O	1:A:63[C]:GLU:HG2	2.01	0.60
1:A:361:SER:HB2	1:A:363:ASP:OD1	2.03	0.57
1:B:26:LEU:HD21	1:B:32:MET:HG2	1.87	0.56
1:B:372:ILE:HD12	1:B:434:TRP:CB	2.35	0.56
1:A:228:PRO:HG3	1:A:236:ILE:HD13	1.89	0.54
1:A:299:LEU:HB2	1:A:315:ARG:HD3	1.88	0.54
1:B:316:ASP:O	1:B:317:LEU:HG	2.10	0.53
1:B:299:LEU:HD23	1:B:313:VAL:HG22	1.92	0.52
1:B:109:LEU:HD21	1:B:157:ARG:HB3	1.92	0.52
1:A:62:LYS:NZ	3:A:2086:HOH:O	2.41	0.52
1:B:441:ASN:HD22	1:B:441:ASN:N	2.07	0.51
1:A:20:GLN:O	1:A:403:ASN:HB2	2.11	0.51
1:A:69:GLU:OE2	1:A:111:LYS:HG3	2.12	0.50
1:B:372:ILE:HD11	1:B:431:SER:CA	2.41	0.50
1:B:372:ILE:CD1	1:B:434:TRP:HB3	2.43	0.49
1:B:371:ARG:HH11	1:B:371:ARG:HB2	1.77	0.49
1:B:184[A]:MET:SD	1:B:189:VAL:HG11	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:LEU:HG	1:B:401:LEU:HG	1.99	0.45
1:B:4:LYS:HD2	1:B:383:TRP:CE3	2.51	0.45
1:A:230:SER:C	1:A:232:LYS:H	2.20	0.44
1:A:420:ASP:O	1:A:424:GLN:N	2.49	0.44
1:B:280:MET:O	1:B:284:GLN:HG3	2.16	0.44
1:B:23:GLY:HA2	1:B:51:GLY:O	2.17	0.44
1:B:243:HIS:O	1:B:247:ASN:HB2	2.18	0.44
1:A:234:GLU:HG3	1:A:302:PHE:HB3	2.00	0.44
1:A:247:ASN:C	1:A:249:PRO:CD	2.85	0.44
1:A:398:TRP:HA	1:A:399:SER:HA	1.83	0.44
1:B:148:ARG:HB2	1:B:207:VAL:HG11	1.99	0.43
1:B:355:ALA:HA	1:B:413:ARG:O	2.17	0.43
1:B:63:GLU:O	1:B:67:ILE:HG13	2.18	0.43
1:A:423:THR:O	1:A:424:GLN:HB2	2.19	0.43
1:B:398:TRP:HA	1:B:399:SER:HA	1.80	0.42
1:A:95:GLN:NE2	3:A:2126:HOH:O	2.52	0.42
1:A:280:MET:O	1:A:284:GLN:HG3	2.20	0.42
1:A:300:VAL:HG13	1:A:310:VAL:HG13	2.02	0.41
1:A:139:ILE:HA	1:A:142:TRP:CE3	2.56	0.41
1:B:131:LYS:HE3	3:B:2083:HOH:O	2.21	0.40
1:B:320:THR:HB	1:B:355:ALA:O	2.20	0.40
1:B:54:ALA:HA	1:B:410:TYR:OH	2.21	0.40
1:B:303:ASP:O	1:B:309:LYS:HA	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	438/468 (94%)	427 (98%)	11 (2%)	0	100	100
1	B	441/468 (94%)	427 (97%)	13 (3%)	1 (0%)	47	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	879/936 (94%)	854 (97%)	24 (3%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	ASP

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	377/399 (94%)	366 (97%)	11 (3%)	42	43
1	B	366/399 (92%)	356 (97%)	10 (3%)	44	46
All	All	743/798 (93%)	722 (97%)	21 (3%)	47	44

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	63[A]	GLU
1	A	63[B]	GLU
1	A	63[C]	GLU
1	A	71	LEU
1	A	96	LYS
1	A	109	LEU
1	A	232	LYS
1	A	235	ASP
1	A	317	LEU
1	A	375	LEU
1	B	109	LEU
1	B	141	ASP
1	B	246[A]	ASN
1	B	246[B]	ASN
1	B	319	LYS
1	B	332	TYR

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Mol	Chain	Res	Type
1	B	357	ASP
1	B	365	ARG
1	B	384	LYS
1	B	441	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	B	441	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IFL	A	1446	-	10,11,11	0.92	0	9,15,15	1.53	2 (22%)
2	IFL	B	1445	-	10,11,11	1.55	1 (10%)	9,15,15	1.38	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IFL	A	1446	-	-	0/2/19/19	0/1/1/1
2	IFL	B	1445	-	-	0/2/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1445	IFL	C3-C2	4.20	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1445	IFL	O4-C4-C5	3.04	115.22	110.08
2	A	1446	IFL	O4-C4-C5	2.23	113.86	110.08
2	A	1446	IFL	O4-C4-C3	-2.19	105.50	109.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	439/468 (93%)	-0.11	3 (0%) 87 87	20, 31, 51, 64	0
1	B	440/468 (94%)	0.47	42 (9%) 8 7	21, 43, 65, 75	0
All	All	879/936 (93%)	0.18	45 (5%) 28 27	20, 36, 61, 75	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	361	SER	4.4
1	B	364	GLY	4.3
1	B	229	ALA	4.1
1	B	359	VAL	4.1
1	B	318	PRO	3.9
1	A	3	VAL	3.9
1	B	441	ASN	3.7
1	B	439	VAL	3.4
1	B	398	TRP	3.3
1	B	15	ALA	3.3
1	B	316	ASP	3.2
1	B	302	PHE	3.1
1	B	164	LEU	3.1
1	B	389	GLY	3.1
1	B	350	THR	3.1
1	B	363	ASP	3.0
1	B	383	TRP	2.9
1	B	9	GLY	2.9
1	B	444	LEU	2.9
1	B	17	ALA	2.8
1	B	118	THR	2.7
1	B	2	ASN	2.7
1	B	119	ILE	2.6
1	B	367	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	374	TYR	2.4
1	B	80	ILE	2.4
1	B	77	ARG	2.4
1	B	314	GLU	2.4
1	B	293	ASN	2.4
1	B	434	TRP	2.4
1	B	78	PHE	2.3
1	A	302	PHE	2.3
1	B	365	ARG	2.3
1	B	3	VAL	2.3
1	B	321	ALA	2.3
1	B	165	ASN	2.3
1	A	362	GLU	2.2
1	B	14	VAL	2.1
1	B	79	SER	2.1
1	B	121	HIS	2.1
1	B	162	ILE	2.1
1	B	220	VAL	2.1
1	B	360	VAL	2.1
1	B	210	GLU	2.0
1	B	440	LYS	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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IFL	B	1445	11/11	0.94	0.22	28,31,34,36	0
2	IFL	A	1446	11/11	0.97	0.14	24,26,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.