



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:13 am GMT

PDB ID : 1AXK  
Title : ENGINEERED BACILLUS BIFUNCTIONAL ENZYME GLUXYN-1  
Authors : Ay, J.; Heinemann, U.  
Deposited on : 1997-10-16  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

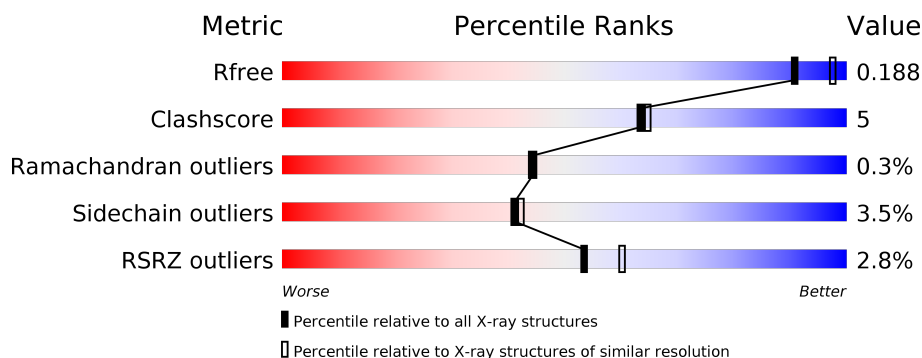
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	394	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	394	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6533 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 GLUXYN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3111	1988	515	601	7			
1	B	394	Total	C	N	O	S	0	0	0
			3108	1983	515	603	7			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

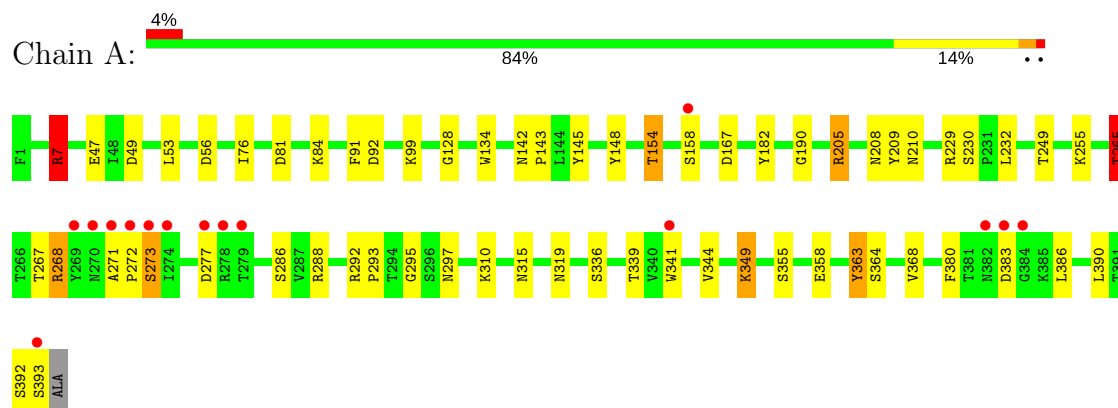
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	201	Total	O	0	0
			201	201		
3	B	111	Total	O	0	0
			111	111		

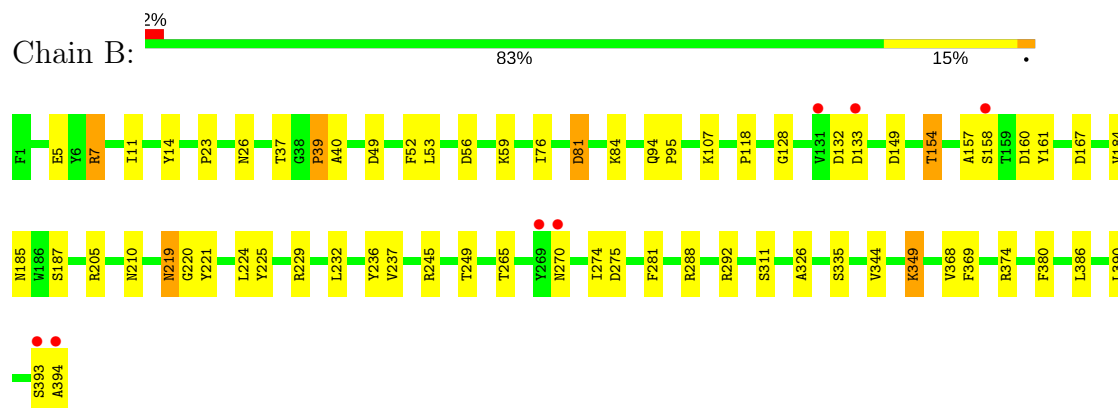
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: GLUXYN-1



#### • Molecule 1: GLUXYN-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.27Å 133.70Å 77.95Å 90.00° 99.76° 90.00°	Depositor
Resolution (Å)	19.96 – 2.10 19.95 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.96-2.10) 91.3 (19.95-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.09 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.176 , 0.224 0.179 , 0.188	Depositor DCC
$R_{free}$ test set	2449 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.2	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA

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	0.70	0/3224	1.36	22/4408 (0.5%)
1	B	0.71	0/3214	1.42	35/4392 (0.8%)
All	All	0.70	0/6438	1.39	57/8800 (0.6%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	ARG	NE-CZ-NH1	-13.67	113.46	120.30
1	A	7	ARG	NE-CZ-NH2	13.22	126.91	120.30
1	B	374	ARG	NE-CZ-NH1	-10.54	115.03	120.30
1	B	7	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	292	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	A	145	TYR	CB-CG-CD2	-9.09	115.55	121.00
1	A	92	ASP	CB-CG-OD2	-8.52	110.64	118.30
1	B	205	ARG	CD-NE-CZ	8.50	135.50	123.60
1	B	205	ARG	NE-CZ-NH1	8.43	124.52	120.30
1	B	132	ASP	CB-CG-OD1	8.20	125.67	118.30
1	A	167	ASP	CB-CG-OD1	8.13	125.62	118.30
1	B	81	ASP	CB-CG-OD1	8.04	125.54	118.30
1	A	268	ARG	NE-CZ-NH2	-7.93	116.33	120.30
1	B	149	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	383	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	236	TYR	CB-CG-CD2	-7.32	116.61	121.00
1	A	205	ARG	CD-NE-CZ	7.28	133.79	123.60
1	B	288	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	167	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	245	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	363	TYR	CB-CG-CD1	-6.71	116.97	121.00
1	B	161	TYR	CB-CG-CD1	-6.69	116.99	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	A	383	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	167	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	275	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	236	TYR	CB-CG-CD1	6.09	124.65	121.00
1	B	133	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	374	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	B	245	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	182	TYR	N-CA-CB	5.69	120.83	110.60
1	B	37	THR	N-CA-CB	5.67	121.06	110.30
1	A	265	THR	N-CA-CB	-5.66	99.54	110.30
1	B	184	VAL	CB-CA-C	-5.64	100.69	111.40
1	B	149	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	311	SER	CB-CA-C	-5.60	99.46	110.10
1	A	358	GLU	OE1-CD-OE2	5.59	130.01	123.30
1	A	145	TYR	CB-CG-CD1	5.57	124.34	121.00
1	B	14	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	81	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	B	270	ASN	CB-CA-C	5.44	121.28	110.40
1	B	225	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	A	288	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	221	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	187	SER	N-CA-CB	-5.29	102.56	110.50
1	A	190	GLY	N-CA-C	-5.25	99.97	113.10
1	B	270	ASN	CA-C-O	5.25	131.12	120.10
1	A	286	SER	N-CA-CB	5.22	118.34	110.50
1	B	160	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	363	TYR	CB-CG-CD2	5.16	124.09	121.00
1	B	49	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	49	ASP	CB-CA-C	-5.09	100.22	110.40
1	B	326	ALA	CB-CA-C	-5.09	102.47	110.10
1	A	336	SER	N-CA-CB	5.05	118.07	110.50
1	B	40	ALA	CB-CA-C	-5.04	102.55	110.10
1	A	56	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	92	ASP	CB-CG-OD1	5.00	122.80	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	3111	0	2851	33	0
1	B	3108	0	2850	25	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	201	0	0	3	0
3	B	111	0	0	3	1
All	All	6533	0	5701	58	1

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 5.

All (58) 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:B:154:THR:HB	1:B:344:VAL:HG22	1.61	0.80
1:A:272:PRO:HA	1:A:277:ASP:HA	1.67	0.75
1:B:81:ASP:HB3	1:B:84:LYS:HG2	1.77	0.67
1:A:265:THR:HG21	3:A:559:HOH:O	1.92	0.67
1:A:154:THR:HG21	3:A:498:HOH:O	1.95	0.67
1:B:394:ALA:HA	3:B:480:HOH:O	1.98	0.63
1:B:349:LYS:HG2	1:B:386:LEU:HB2	1.82	0.62
1:A:349:LYS:HG2	1:A:386:LEU:HB2	1.82	0.62
1:B:349:LYS:HG3	1:B:380:PHE:HE2	1.63	0.62
1:A:310:LYS:HG2	1:A:315:ASN:HD21	1.65	0.61
1:A:297:ASN:HB3	1:A:341[B]:TRP:CZ2	2.36	0.60
1:A:142:ASN:HB2	1:A:143:PRO:HA	1.83	0.60
1:B:349:LYS:HB2	1:B:349:LYS:HZ2	1.66	0.60
1:A:310:LYS:HG2	1:A:315:ASN:ND2	2.20	0.56
1:B:128:GLY:HA2	1:B:368:VAL:O	2.06	0.56
1:A:341[B]:TRP:CZ3	1:A:344:VAL:HG23	2.41	0.55
1:A:267:THR:O	1:A:268:ARG:HG2	2.07	0.54
1:A:271:ALA:HB1	1:A:272:PRO:HD2	1.90	0.54
1:A:232:LEU:HD21	1:A:273:SER:OG	2.08	0.54
1:B:94:GLN:HB3	1:B:95:PRO:HD2	1.90	0.53
1:B:39:PRO:HG3	3:B:498:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLU:OE2	1:B:7:ARG:NH1	2.43	0.50
1:B:154:THR:HG23	3:B:397:HOH:O	2.10	0.50
1:B:219:ASN:HD22	1:B:220:GLY:N	2.10	0.50
1:A:349:LYS:HG3	1:A:380:PHE:HE2	1.76	0.49
1:B:76:ILE:HD13	1:B:107:LYS:HB3	1.93	0.49
1:A:339:THR:HG21	1:A:341[A]:TRP:CZ2	2.48	0.49
1:B:157:ALA:O	1:B:158:SER:HB3	2.12	0.49
1:B:11:ILE:HD12	1:B:118:PRO:HB2	1.96	0.47
1:B:56:ASP:OD2	1:B:59:LYS:HD2	2.14	0.47
1:A:81:ASP:HB3	1:A:84:LYS:HG2	1.96	0.47
1:A:292:ARG:CG	1:A:293:PRO:HD2	2.44	0.47
1:B:185:ASN:ND2	1:B:335:SER:OG	2.48	0.47
1:B:349:LYS:CB	1:B:349:LYS:HZ2	2.26	0.47
1:A:210:ASN:HD21	1:A:295:GLY:C	2.18	0.46
1:A:208:ASN:HB3	1:A:341[B]:TRP:CZ2	2.51	0.46
1:A:364:SER:HB3	3:A:496:HOH:O	2.17	0.45
1:A:53:LEU:HD21	1:A:134:TRP:NE1	2.31	0.45
1:B:349:LYS:HG3	1:B:380:PHE:CE2	2.49	0.44
1:A:7:ARG:NH1	1:A:363:TYR:OH	2.39	0.44
1:A:47:GLU:OE2	1:A:49:ASP:OD1	2.36	0.43
1:A:208:ASN:HB3	1:A:341[B]:TRP:CE2	2.53	0.43
1:B:368:VAL:HG23	1:B:369:PHE:CD1	2.53	0.43
1:A:392:SER:O	1:A:393:SER:CB	2.65	0.43
1:B:232:LEU:HD23	1:B:281:PHE:HB3	2.01	0.43
1:B:157:ALA:O	1:B:158:SER:CB	2.64	0.42
1:B:224:LEU:HB3	1:B:237:VAL:HB	2.01	0.42
1:A:349:LYS:HB2	1:A:349:LYS:HE3	1.68	0.42
1:A:209:TYR:C	1:A:341[B]:TRP:HE1	2.22	0.42
1:A:392:SER:O	1:A:393:SER:HB2	2.20	0.42
1:A:128:GLY:HA2	1:A:368:VAL:O	2.20	0.42
1:A:229:ARG:HH11	1:A:229:ARG:HD2	1.63	0.41
1:A:148:TYR:HB2	1:A:386:LEU:HB3	2.01	0.41
1:A:91:PHE:HA	1:A:99:LYS:O	2.20	0.41
1:A:297:ASN:HB3	1:A:341[B]:TRP:HZ2	1.81	0.41
1:B:23:PRO:HG3	1:B:52:PHE:CG	2.55	0.41
1:B:229:ARG:CZ	1:B:274:ILE:HD12	2.51	0.41
1:A:208:ASN:HB3	1:A:341[B]:TRP:CH2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:484:HOH:O	3:B:505:HOH:O[1_655]	2.12	0.08

## 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	392/394 (100%)	374 (95%)	18 (5%)	0	100	100
1	B	392/394 (100%)	381 (97%)	9 (2%)	2 (0%)	32	28
All	All	784/788 (100%)	755 (96%)	27 (3%)	2 (0%)	44	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	SER
1	B	26	ASN

### 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	325/324 (100%)	311 (96%)	14 (4%)	33	32
1	B	324/324 (100%)	315 (97%)	9 (3%)	49	52
All	All	649/648 (100%)	626 (96%)	23 (4%)	41	42

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	76	ILE
1	A	154	THR
1	A	158	SER
1	A	205	ARG
1	A	230	SER
1	A	249	THR
1	A	255	LYS
1	A	265	THR
1	A	273	SER
1	A	319	ASN
1	A	349	LYS
1	A	355	SER
1	A	390	LEU
1	B	39	PRO
1	B	53	LEU
1	B	154	THR
1	B	210	ASN
1	B	219	ASN
1	B	249	THR
1	B	265	THR
1	B	349	LYS
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
1	A	210	ASN
1	A	315	ASN
1	A	319	ASN
1	B	41	HIS
1	B	164	ASN
1	B	185	ASN
1	B	210	ASN
1	B	219	ASN
1	B	312	HIS
1	B	315	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	393/394 (99%)	-0.10	15 (3%) 41 48	9, 19, 37, 77	0
1	B	394/394 (100%)	-0.25	7 (1%) 69 73	11, 19, 32, 47	0
All	All	787/788 (99%)	-0.18	22 (2%) 53 60	9, 19, 34, 77	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	ARG	8.4
1	A	277	ASP	6.3
1	A	393	SER	5.2
1	B	394	ALA	4.0
1	B	270	ASN	3.9
1	A	274	ILE	3.9
1	A	158	SER	3.8
1	A	279	THR	3.7
1	B	269	TYR	3.6
1	A	269	TYR	3.4
1	A	270	ASN	3.2
1	A	382	ASN	3.2
1	A	271	ALA	3.0
1	A	272	PRO	2.8
1	B	158	SER	2.6
1	B	133	ASP	2.5
1	B	393	SER	2.5
1	A	383	ASP	2.4
1	B	131	VAL	2.3
1	A	273	SER	2.3
1	A	341[A]	TRP	2.2
1	A	384	GLY	2.1

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	395	1/1	0.96	0.15	-0.31	40,40,40,40	0
2	CA	B	395	1/1	0.99	0.03	-2.33	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.