



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 07:08 PM BST

PDB ID : 4MS4
Title : Crystal structure of the extracellular domain of human GABA(B) receptor bound to the agonist baclofen
Authors : Geng, Y.; Bush, M.; Mosyak, L.; Wang, F.; Fan, Q.R.
Deposited on : 2013-09-18
Resolution : 1.90 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 : 2.13.1
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) : 2.13.1

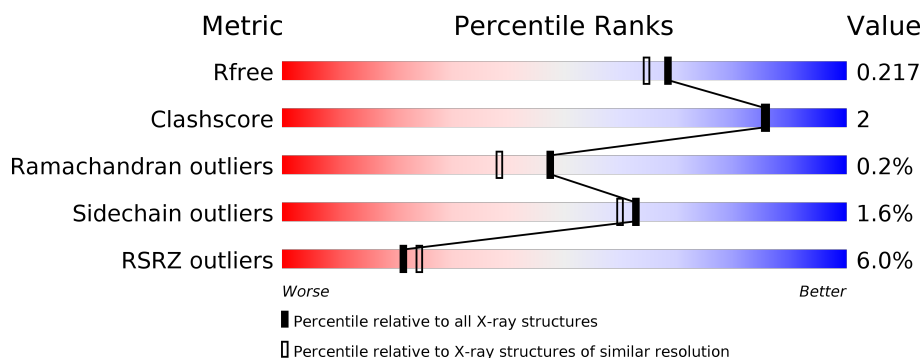
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	420	<div> <div>9%</div> <div>88%</div> <div>9%</div> <div>• •</div> </div>
2	B	433	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div>•</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7253 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 Gamma-aminobutyric acid type B receptor subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3280	2094	552	620	14	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ASP	-	expression tag	UNP Q9UBS5
A	461	TYR	-	expression tag	UNP Q9UBS5
A	462	LYS	-	expression tag	UNP Q9UBS5
A	463	ASP	-	expression tag	UNP Q9UBS5
A	464	ASP	-	expression tag	UNP Q9UBS5
A	465	ASP	-	expression tag	UNP Q9UBS5
A	466	ASP	-	expression tag	UNP Q9UBS5
A	467	LYS	-	expression tag	UNP Q9UBS5

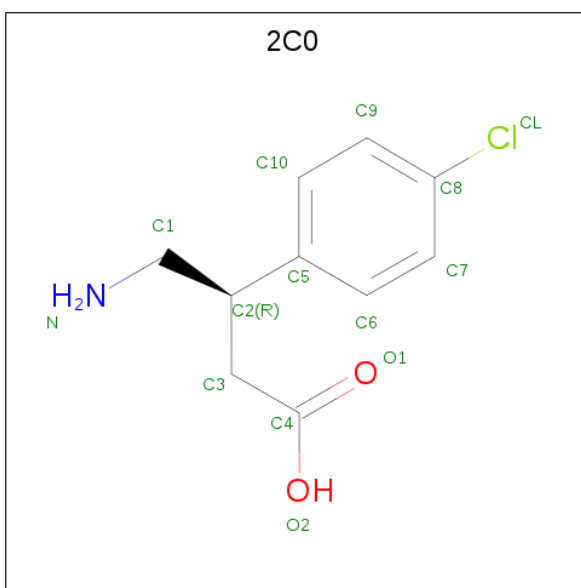
- Molecule 2 is a protein called Gamma-aminobutyric acid type B receptor subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	408	3255	2077	553	610	15	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

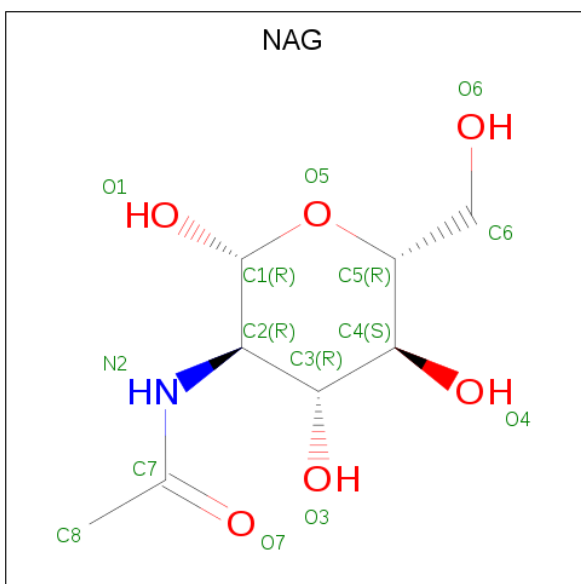
Chain	Residue	Modelled	Actual	Comment	Reference
B	467	ASP	-	expression tag	UNP O75899
B	468	TYR	-	expression tag	UNP O75899
B	469	LYS	-	expression tag	UNP O75899
B	470	ASP	-	expression tag	UNP O75899
B	471	ASP	-	expression tag	UNP O75899
B	472	ASP	-	expression tag	UNP O75899
B	473	ASP	-	expression tag	UNP O75899
B	474	LYS	-	expression tag	UNP O75899

- Molecule 3 is baclofen (three-letter code: 2C0) (formula: $C_{10}H_{12}ClNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			14	10	1	1	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

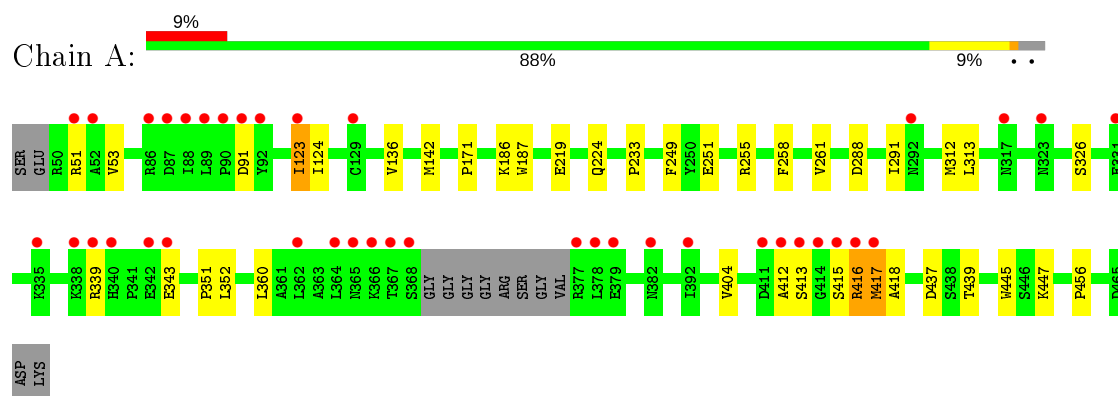
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	352	Total 352	O 352	0	0
5	B	338	Total 338	O 338	0	0

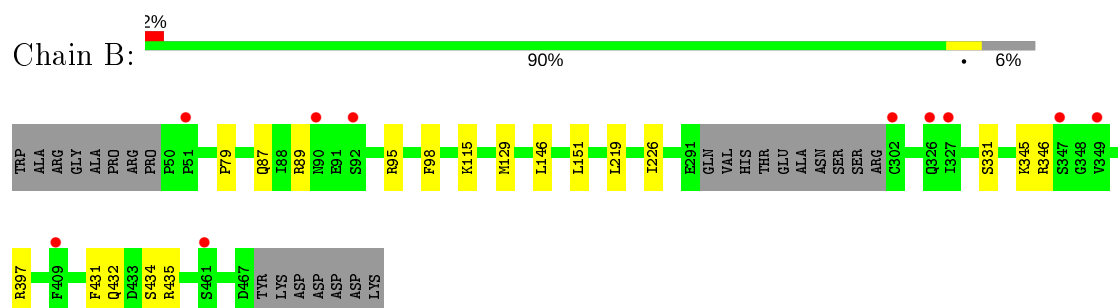
3 Residue-property plots [i](#)

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: Gamma-aminobutyric acid type B receptor subunit 1



- Molecule 2: Gamma-aminobutyric acid type B receptor subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.38 Å 140.39 Å 59.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.82 – 1.90 45.39 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (27.82-1.90) 95.2 (45.39-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 1.91 Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER	Depositor
R, R_{free}	0.190 , 0.216 0.189 , 0.217	Depositor DCC
R_{free} test set	3725 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: 2C0, NAG

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	0.51	0/3363	0.66	1/4560 (0.0%)
2	B	0.51	0/3332	0.60	0/4512
All	All	0.51	0/6695	0.63	1/9072 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	ARG	C-N-CA	5.02	134.25	121.70

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	3280	0	3196	21	0
2	B	3255	0	3202	8	0
3	A	14	0	11	0	0
4	B	14	0	13	0	0
5	A	352	0	0	3	0
5	B	338	0	0	0	0
All	All	7253	0	6422	28	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 2.

All (28) 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:171:PRO:HA	1:A:415:SER:HB2	1.29	1.10
1:A:288:ASP:HB3	1:A:291:ILE:HG12	1.70	0.73
2:B:219:LEU:HD12	2:B:226:ILE:HD11	1.87	0.57
1:A:445:TRP:HD1	1:A:447:LYS:HE2	1.71	0.56
1:A:312:MET:HE2	1:A:352:LEU:HD11	1.87	0.55
1:A:123:ILE:HD12	1:A:124:ILE:HG22	1.90	0.54
2:B:432:GLN:O	2:B:435:ARG:HG2	2.08	0.53
1:A:439:THR:HG23	5:A:644:HOH:O	2.08	0.52
1:A:51:ARG:HG3	5:A:924:HOH:O	2.11	0.51
1:A:351:PRO:HB3	1:A:404:VAL:HG23	1.93	0.50
1:A:224:GLN:HB3	1:A:233:PRO:HB3	1.94	0.50
1:A:258:PHE:HA	1:A:261:VAL:HB	1.94	0.49
1:A:142:MET:HB3	2:B:115:LYS:HD2	1.96	0.48
1:A:418:ALA:HB1	1:A:437:ASP:OD1	2.12	0.48
2:B:79:PRO:HG2	2:B:346:ARG:HB3	1.96	0.47
1:A:251:GLU:OE2	1:A:255:ARG:NH2	2.47	0.47
1:A:124:ILE:HD13	1:A:360:LEU:HD13	1.96	0.47
2:B:87:GLN:OE1	2:B:331:SER:HB2	2.16	0.46
1:A:53:VAL:HG13	1:A:123:ILE:HG12	1.97	0.46
1:A:313:LEU:HG	1:A:326:SER:HB3	1.98	0.45
2:B:146:LEU:HB3	2:B:151:LEU:O	2.17	0.45
1:A:186:LYS:HE2	1:A:445:TRP:CE2	2.53	0.44
1:A:187:TRP:CD1	1:A:456:PRO:HG2	2.53	0.44
2:B:431:PHE:CZ	2:B:434:SER:HA	2.54	0.42
2:B:89:ARG:HE	2:B:98:PHE:HB2	1.84	0.42
1:A:123:ILE:H	1:A:123:ILE:HG13	1.68	0.41
1:A:219:GLU:HG2	5:A:949:HOH:O	2.20	0.41
1:A:339:ARG:HD2	1:A:343:GLU:OE2	2.21	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	404/420 (96%)	389 (96%)	13 (3%)	2 (0%)	29	18
2	B	404/433 (93%)	390 (96%)	14 (4%)	0	100	100
All	All	808/853 (95%)	779 (96%)	27 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	MET
1	A	412	ALA

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	355/362 (98%)	348 (98%)	7 (2%)	55	51
2	B	354/375 (94%)	350 (99%)	4 (1%)	73	73
All	All	709/737 (96%)	698 (98%)	11 (2%)	62	60

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ASP
1	A	123	ILE
1	A	136	VAL
1	A	249	PHE
1	A	413	SER
1	A	416	ARG
1	A	417	MET
2	B	95	ARG
2	B	129	MET
2	B	345	LYS

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Mol	Chain	Res	Type
2	B	397	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	98	HIS
1	A	107	GLN

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](#)

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	$\# Z > 2$
3	2C0	A	501	-	10,14,14	1.16	0	11,18,18	1.25	2 (18%)
4	NAG	B	501	2	14,14,15	0.29	0	17,19,21	0.62	0

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
3	2C0	A	501	-	-	0/8/10/10	0/1/1/1
4	NAG	B	501	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	2C0	C3-C2-C5	-2.66	107.67	111.52
3	A	501	2C0	C9-C10-C5	-2.15	119.04	121.20

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C8-C7-N2-C2
4	B	501	NAG	O7-C7-N2-C2

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, 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	408/420 (97%)	0.41	39 (9%) 8 9	10, 24, 60, 83	0
2	B	408/433 (94%)	0.08	10 (2%) 57 60	13, 23, 47, 79	0
All	All	816/853 (95%)	0.24	49 (6%) 21 24	10, 23, 53, 83	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	413	SER	8.7
1	A	412	ALA	7.7
1	A	88	ILE	5.9
1	A	343	GLU	5.8
1	A	415	SER	5.8
1	A	338	LYS	5.4
1	A	317	ASN	5.0
1	A	51	ARG	5.0
1	A	342	GLU	4.5
1	A	367	THR	4.4
1	A	91	ASP	4.2
2	B	347	SER	4.2
1	A	417	MET	4.1
1	A	86	ARG	4.0
2	B	461	SER	4.0
1	A	377	ARG	3.8
1	A	379	GLU	3.8
1	A	392	ILE	3.8
1	A	368	SER	3.7
1	A	87	ASP	3.7
1	A	416	ARG	3.5
1	A	411	ASP	3.3
1	A	89	LEU	3.3
1	A	340	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	92	TYR	3.2
1	A	335	LYS	3.2
1	A	90	PRO	3.1
2	B	92	SER	3.1
1	A	129	CYS	3.1
1	A	414	GLY	3.1
2	B	326	GLN	3.0
1	A	366	LYS	2.7
2	B	90	ASN	2.7
1	A	378	LEU	2.7
2	B	327	ILE	2.7
1	A	331	GLU	2.5
1	A	123	ILE	2.4
1	A	339	ARG	2.4
1	A	292	ASN	2.4
2	B	51	PRO	2.3
2	B	349	VAL	2.2
1	A	52	ALA	2.2
1	A	364	LEU	2.1
1	A	382	ASN	2.1
1	A	362	LEU	2.1
2	B	302	CYS	2.1
1	A	323	ASN	2.1
2	B	409	PHE	2.0
1	A	365	ASN	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 monosaccharides 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
4	NAG	B	501	14/15	0.86	0.16	32,37,43,47	0
3	2C0	A	501	14/14	0.97	0.10	11,13,14,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.