



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 PM UTC

PDB ID : 5FJS / pdb_00005fjs
Title : Bacterial beta-glucosidase reveals the structural and functional basis of genetic defects in human glucocerebrosidase 2 (GBA2)
Authors : Charoenwattanasatien, R.; Pengthaisong, S.; Breen, I.; Mutoha, R.; Sansenya, S.; Hua, Y.; Tankrathok, A.; Wu, L.; Songsiriritthigul, C.; Tanaka, H.; Williams, S.J.; Davies, G.J.; Kurisu, G.; Ketudat Cairns, J.R.
Deposited on : 2015-10-12
Resolution : 2.60 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

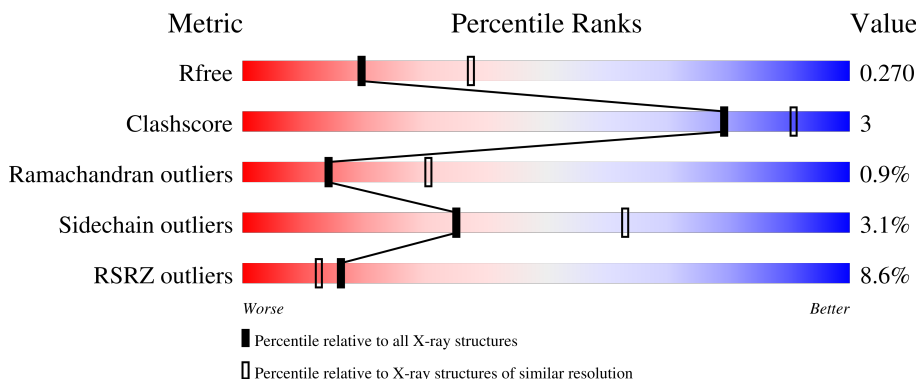
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	787	7% 86% 7% 7%
1	B	787	8% 79% 10% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11158 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 GLUCOSYLCERAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	733	Total	C	N	O	S	0	2	1
			5689	3672	919	1072	26			
1	B	702	Total	C	N	O	S	0	1	1
			5389	3480	870	1012	27			

There are 2 discrepancies between the modelled and reference sequences:

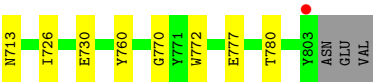
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP F6BL85
B	20	MET	-	expression tag	UNP F6BL85

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	22	Total	O	0	0
			22	22		



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	187.97Å 187.97Å 99.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	162.61 – 2.60 162.61 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (162.61-2.60) 99.8 (162.61-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.206 , 0.266 0.213 , 0.270	Depositor DCC
R_{free} test set	3081 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	60.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.031 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11158	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.91	2/5853 (0.0%)	0.97	3/7954 (0.0%)
1	B	0.86	1/5542 (0.0%)	0.96	4/7536 (0.1%)
All	All	0.88	3/11395 (0.0%)	0.97	7/15490 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	507	HIS	C-O	-5.12	1.18	1.24
1	B	391	LYS	N-CA	5.11	1.51	1.46
1	A	721	VAL	C-O	-5.09	1.19	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ASN	N-CA-C	6.35	118.75	108.34
1	A	778	ALA	N-CA-C	5.22	117.01	109.07
1	A	139	SER	N-CA-C	5.21	118.73	112.38
1	B	706	ASN	N-CA-C	5.18	118.88	112.24
1	B	713	ASN	N-CA-C	5.15	116.89	111.28
1	A	137	TYR	N-CA-C	5.05	121.56	110.80
1	B	480	ILE	N-CA-C	5.03	117.33	111.05

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	5689	0	5164	27	0
1	B	5389	0	4792	29	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	56	0	0	0	0
3	B	22	0	0	0	0
All	All	11158	0	9956	56	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 3.

All (56) 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:360:TYR:CE2	1:B:360:TYR:CG	2.69	0.77
1:B:454:ARG:NH1	1:B:473:MET:HE3	2.15	0.61
1:A:595:TRP:O	1:A:596:SER:HB3	2.01	0.60
1:B:192:VAL:HG21	1:B:375:ALA:HB2	1.85	0.58
1:B:182:PRO:HG2	1:B:389:TRP:CD2	2.38	0.57
1:A:668:GLN:HG3	1:A:669:LEU:HG	1.86	0.57
1:A:80:ALA:HB1	1:A:191:PRO:HB3	1.87	0.57
1:A:386:ILE:HA	1:A:389:TRP:CD1	2.41	0.55
1:A:306:ASP:O	1:A:307:ASP:HB2	2.08	0.54
1:A:62:TYR:HB2	1:A:63:PRO:HD2	1.92	0.52
1:B:218:MET:HB2	1:B:265:TYR:CZ	2.45	0.51
1:B:292:LEU:O	1:B:296:PHE:CB	2.59	0.51
1:B:544:ARG:HB2	1:B:678:LEU:HD11	1.93	0.51
1:B:473:MET:HE2	1:B:473:MET:HA	1.94	0.49
1:B:543:TYR:CE2	1:B:680:LEU:HD21	2.47	0.49
1:B:106:VAL:HG21	1:B:218:MET:HE3	1.94	0.49
1:B:182:PRO:HD2	1:B:389:TRP:CD1	2.48	0.48
1:B:181:ILE:HG22	1:B:182:PRO:O	2.13	0.48
1:B:71:GLN:OE1	1:B:93:ARG:HD3	2.15	0.46
1:A:279:TYR:O	1:A:279:TYR:CG	2.68	0.46
1:A:595:TRP:O	1:A:596:SER:CB	2.64	0.46
1:A:386:ILE:HA	1:A:389:TRP:HD1	1.80	0.45
1:B:341:ASP:OD1	1:B:357:TYR:OH	2.31	0.45
1:A:655:ASP:OD1	1:A:655:ASP:C	2.58	0.45
1:B:356:MET:HE1	1:B:435:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ALA:HB3	1:B:216:GLN:HB2	1.99	0.44
1:A:156:TYR:CG	1:A:157:PRO:HA	2.52	0.44
1:A:351:ASP:CG	1:A:515:LEU:HD22	2.42	0.44
1:B:726:ILE:O	1:B:730:GLU:HG3	2.17	0.44
1:A:279:TYR:O	1:A:279:TYR:CD2	2.71	0.44
1:B:770:GLY:HA2	1:B:772:TRP:CZ3	2.53	0.44
1:A:568:LEU:HD11	1:A:615:ALA:HB2	1.99	0.43
1:A:515:LEU:HD12	1:A:519:LYS:CD	2.49	0.43
1:B:396:ASN:OD1	1:B:396:ASN:C	2.61	0.43
1:A:595:TRP:CE2	1:A:728:ALA:HB2	2.54	0.43
1:B:450:THR:HG23	1:B:507:HIS:CE1	2.53	0.43
1:B:295:GLU:HA	1:B:296:PHE:CB	2.47	0.43
1:A:505:ILE:HD13	1:A:506:PRO:HD2	2.01	0.42
1:B:539:VAL:HG22	1:B:564:VAL:HG13	2.00	0.42
1:A:760:TYR:CD1	1:A:760:TYR:C	2.97	0.42
1:B:414:LEU:HD22	1:B:461:LEU:HD21	2.02	0.42
1:A:579:ASP:OD1	1:A:579:ASP:C	2.60	0.42
1:A:515:LEU:HD12	1:A:519:LYS:HD2	2.01	0.41
1:B:411:LEU:O	1:B:412:TYR:C	2.63	0.41
1:A:407:LEU:HD21	1:A:800:GLU:HG3	2.01	0.41
1:A:713:ASN:HD21	1:A:732:TRP:CD1	2.38	0.41
1:A:136:GLY:O	1:A:137:TYR:O	2.38	0.41
1:B:272:VAL:O	1:B:274:GLY:N	2.53	0.41
1:A:546:TYR:HB2	1:A:557:LEU:HD21	2.03	0.41
1:A:441:GLU:OE2	1:A:790:TYR:OH	2.38	0.41
1:B:191:PRO:HB2	1:B:340:TRP:CD1	2.56	0.41
1:B:452:ASP:HB2	1:B:591:THR:HB	2.03	0.41
1:A:462:VAL:HG13	1:A:463:MET:HG3	2.03	0.40
1:A:110:GLN:OE1	1:A:129:TYR:HB2	2.22	0.40
1:B:459:PHE:HA	1:B:462:VAL:HG12	2.04	0.40
1:B:760:TYR:CD2	1:B:760:TYR:C	2.97	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	713/787 (91%)	658 (92%)	51 (7%)	4 (1%)	21	42
1	B	671/787 (85%)	611 (91%)	52 (8%)	8 (1%)	10	23
All	All	1384/1574 (88%)	1269 (92%)	103 (7%)	12 (1%)	14	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	TYR
1	A	307	ASP
1	B	35	HIS
1	B	144	ASP
1	B	273	PRO
1	B	296	PHE
1	B	297	SER
1	B	348	GLY
1	A	272	VAL
1	B	281	ALA
1	A	271	LYS
1	B	143	TRP

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	547/675 (81%)	533 (97%)	14 (3%)	40	68
1	B	505/675 (75%)	486 (96%)	19 (4%)	29	56
All	All	1052/1350 (78%)	1019 (97%)	33 (3%)	35	63

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR

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Mol	Chain	Res	Type
1	A	167	ASP
1	A	212	MET
1	A	257	ASP
1	A	278	SER
1	A	286	THR
1	A	291	ASP
1	A	381	LYS
1	A	451	LEU
1	A	505	ILE
1	A	669	LEU
1	A	679	ARG
1	A	698	GLU
1	A	715	MET
1	B	172	LEU
1	B	198	THR
1	B	270	LYS
1	B	306	ASP
1	B	331	THR
1	B	333	GLU
1	B	364	ASN
1	B	416	ASP
1	B	512	SER
1	B	542	VAL
1	B	571	LEU
1	B	625	ASN
1	B	674	TYR
1	B	679	ARG
1	B	683	ILE
1	B	691	LYS
1	B	706	ASN
1	B	777	GLU
1	B	780	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	616	GLN
1	A	625	ASN
1	B	229	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 oligosaccharides 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, 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	733/787 (93%)	0.42	57 (7%) 19 15	27, 53, 91, 112	33 (4%)
1	B	702/787 (89%)	0.62	66 (9%) 14 11	21, 59, 93, 108	53 (7%)
All	All	1435/1574 (91%)	0.52	123 (8%) 16 12	21, 57, 92, 112	86 (5%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	ASN	12.2
1	B	34	SER	9.3
1	B	243	ASP	9.0
1	B	38	ASP	8.8
1	A	135	ASN	8.8
1	A	327	GLN	8.7
1	B	35	HIS	8.4
1	A	303	ASP	8.0
1	B	313	GLN	7.6
1	B	247	VAL	7.6
1	B	303	ASP	7.4
1	A	271	LYS	6.9
1	B	274	GLY	6.8
1	B	165	ASN	6.8
1	B	283	PHE	6.7
1	A	314	ASP	6.6
1	A	803	TYR	6.4
1	A	168	LEU	6.4
1	B	310	PRO	6.3
1	B	366	LYS	6.2
1	B	307	ASP	6.0
1	B	244	SER	6.0
1	B	284	VAL	6.0
1	A	209	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	327	GLN	5.8
1	B	293	TRP	5.6
1	A	313	GLN	5.5
1	B	312	LYS	5.5
1	A	328	PRO	5.5
1	A	321	ALA	5.4
1	B	297	SER	5.4
1	B	330	GLN	5.4
1	B	331	THR	5.3
1	B	328	PRO	5.3
1	A	169	PRO	5.1
1	B	305	LYS	5.1
1	A	257	ASP	4.9
1	B	263	GLY	4.7
1	B	254	ILE	4.7
1	A	251	MET	4.6
1	B	298	LYS	4.6
1	A	295	GLU	4.5
1	B	36	LYS	4.5
1	A	36	LYS	4.5
1	A	326	LEU	4.5
1	B	333	GLU	4.3
1	B	304	ASN	4.2
1	B	324	PHE	4.2
1	B	288	ASP	4.2
1	B	319	ALA	4.2
1	A	293	TRP	4.2
1	B	141	TRP	4.2
1	B	271	LYS	4.1
1	B	332	ILE	3.8
1	A	222	PHE	3.8
1	B	627	ALA	3.7
1	B	323	ASN	3.7
1	B	131	GLY	3.6
1	A	215	TRP	3.5
1	A	207	VAL	3.5
1	A	427	GLY	3.4
1	A	35	HIS	3.4
1	A	220	GLY	3.3
1	A	219	ILE	3.3
1	A	221	PHE	3.2
1	A	137	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	3.2
1	A	324	PHE	3.2
1	B	54	ASN	3.2
1	A	213	PHE	3.2
1	B	285	THR	3.1
1	B	321	ALA	3.0
1	A	113	VAL	3.0
1	B	325	LYS	3.0
1	B	351	ASP	3.0
1	B	317	GLY	2.9
1	B	170	VAL	2.9
1	B	567	ALA	2.9
1	B	57[A]	HIS	2.9
1	B	219	ILE	2.8
1	A	288	ASP	2.8
1	B	634	TRP	2.8
1	A	258	ASN	2.8
1	A	218	MET	2.7
1	A	294	HIS	2.7
1	A	338	LEU	2.7
1	B	433	THR	2.7
1	A	243	ASP	2.7
1	B	75	LEU	2.6
1	A	208	ASP	2.6
1	A	260	GLU	2.6
1	A	217	ASN	2.6
1	B	628	TYR	2.6
1	A	291	ASP	2.5
1	B	136	GLY	2.5
1	B	144	ASP	2.5
1	A	141	TRP	2.4
1	A	320	ILE	2.4
1	B	200	TYR	2.4
1	B	318	SER	2.4
1	A	167	ASP	2.4
1	A	283	PHE	2.4
1	A	114	PHE	2.2
1	A	262	ASN	2.2
1	B	428	GLU	2.2
1	A	282	LYS	2.2
1	A	38	ASP	2.2
1	A	247	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	375	ALA	2.1
1	A	250	VAL	2.1
1	B	108	ALA	2.1
1	A	165	ASN	2.1
1	B	631	TYR	2.1
1	A	170	VAL	2.1
1	B	174	VAL	2.1
1	A	239	ASP	2.0
1	B	233	PHE	2.1
1	A	286	THR	2.0
1	A	279	TYR	2.0
1	B	212	MET	2.0
1	A	330	GLN	2.0
1	B	194	VAL	2.0
1	B	803	TYR	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 oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
2	CA	B	1804	1/1	0.96	0.05	74,74,74,74	0
2	CA	A	1804	1/1	0.99	0.04	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.