



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 3, 2024 – 08:35 pm BST

PDB ID : 6TH7
Title : Structure of porcine pancreatic elastase in complex with tutuilamide
Authors : Koehnke, J.; Sikandar, A.
Deposited on : 2019-11-18
Resolution : 2.20 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

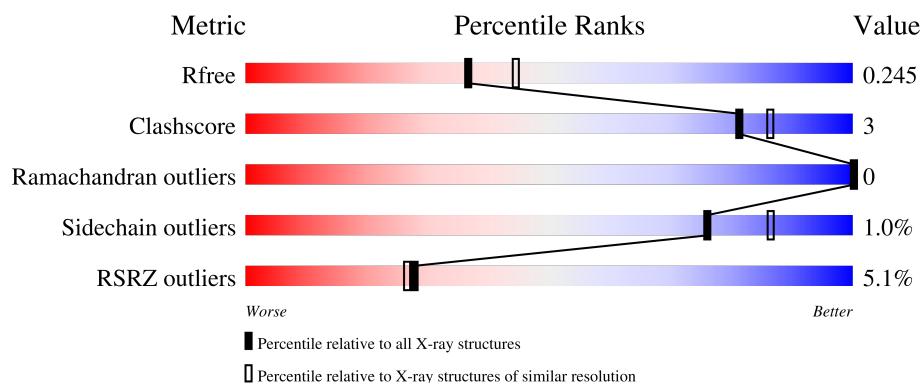
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	240	<div> <div>10%</div> <div>95% 5%</div> </div>
1	B	240	<div> <div>10%</div> <div>93% 7%</div> </div>
2	C	9	<div> <div>56% 33% 11%</div> </div>
3	D	9	<div> <div>56% 11% 33%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ABA	C	306	X	-	-	-
3	ABA	D	310	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7719 atoms, of which 3652 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 Chymotrypsin-like elastase family member 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	240	Total	C	H	N	O	S	0	0	0
			3579	1135	1757	329	348	10			
1	B	240	Total	C	H	N	O	S	0	0	0
			3578	1135	1757	329	347	10			

- Molecule 2 is a protein called Tutuilamide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	9	Total	C	Cl	H	N	O	0	0	0
			140	51	1	69	8	11			

- Molecule 3 is a protein called Tutuilamide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	9	Total	C	Cl	H	N	O	0	0	0
			140	51	1	69	8	11			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	170	Total	O	0	0
			170	170		
5	B	99	Total	O	0	0
			99	99		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	7	Total	O	0	0
			7	7		
5	D	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

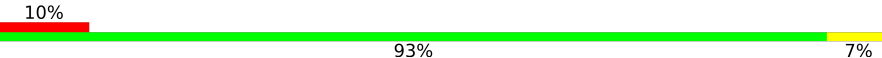
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

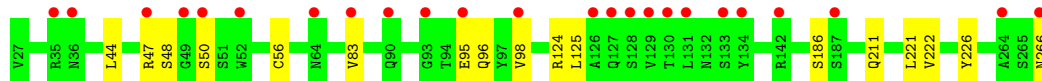
- Molecule 1: Chymotrypsin-like elastase family member 1

Chain A:  95% 5%



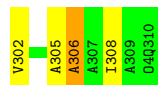
- Molecule 1: Chymotrypsin-like elastase family member 1

Chain B:  10% 93% 7%



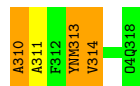
- Molecule 2: Tutuilamide

Chain C:  56% 33% 11%



- Molecule 3: Tutuilamide

Chain D:  56% 11% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.26Å 99.11Å 117.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.30 – 2.20 49.56 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.30-2.20) 99.1 (49.56-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.200 , 0.244 0.203 , 0.245	Depositor DCC
R_{free} test set	1786 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.4	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	0.94	EDS
Total number of atoms	7719	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: AA4, 5XU, N9K, O4Q, CA, ABA, YNM

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	0.43	0/1862	0.63	0/2543
1	B	0.38	0/1861	0.59	0/2543
2	C	2.37	1/24 (4.2%)	1.77	0/28
3	D	2.52	1/24 (4.2%)	1.51	0/28
All	All	0.49	2/3771 (0.1%)	0.63	0/5142

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	1	0
3	D	1	0
All	All	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	314	VAL	C-O	10.67	1.43	1.23
2	C	302	VAL	C-O	9.84	1.42	1.23

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	306	ABA	CA
3	D	310	ABA	CA

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	1822	1757	1757	8	0
1	B	1821	1757	1757	10	0
2	C	71	69	47	1	0
3	D	71	69	59	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	170	0	0	1	0
5	B	99	0	0	0	0
5	C	7	0	0	0	0
5	D	4	0	0	0	0
All	All	4067	3652	3620	19	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 (19) 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:261:ASN:ND2	5:A:401:HOH:O	2.31	0.64
1:B:98:VAL:HG21	1:B:125:LEU:HD13	1.82	0.61
1:B:124:ARG:NH1	1:B:266:ASN:OD1	2.34	0.61
1:B:47:ARG:HH12	1:B:50:SER:HA	1.71	0.55
1:A:235:VAL:HG22	2:C:306:ABA:HG2	1.90	0.54
1:A:214:SER:HA	1:A:232:THR:HB	1.88	0.54
1:B:222:VAL:O	1:B:222:VAL:HG23	2.12	0.49
1:B:211:GLN:HA	3:D:310:ABA:O	2.13	0.48
1:B:221:LEU:HD21	1:B:226:TYR:CD2	2.48	0.47
1:B:44:LEU:HD23	1:B:56:CYS:HB2	1.95	0.47
1:B:83:VAL:CG2	1:B:96:GLN:HB2	2.45	0.47
1:A:98:VAL:HG21	1:A:129:VAL:HG12	1.97	0.46
1:A:27:VAL:N	1:A:213:ASP:OD2	2.49	0.45
1:B:221:LEU:HD21	1:B:226:TYR:CE2	2.51	0.45
1:B:83:VAL:O	1:B:95:GLU:HA	2.18	0.44
1:A:76:GLU:O	1:A:77:LEU:HD23	2.18	0.44
3:D:313:YNM:HM3C	3:D:314:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:PHE:CZ	1:A:248:VAL:HG11	2.53	0.42
1:A:234:PHE:CE1	1:A:248:VAL:HG21	2.55	0.41

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	238/240 (99%)	231 (97%)	7 (3%)	0	100	100
1	B	238/240 (99%)	226 (95%)	12 (5%)	0	100	100
3	D	1/9 (11%)	1 (100%)	0	0	100	100
All	All	477/489 (98%)	458 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	198/198 (100%)	197 (100%)	1 (0%)	88	94
1	B	198/198 (100%)	196 (99%)	2 (1%)	76	86
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0
3	D	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	402/402 (100%)	398 (99%)	4 (1%)	76	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	B	48	SER
1	B	186	SER
2	C	308	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

9 non-standard protein/DNA/RNA residues 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	5XU	D	317	3	3,4,4	1.00	0	2,4,4	0.21	0
2	AA4	C	305	2	6,7,8	2.97	1 (16%)	2,7,9	0.57	0
3	ABA	D	310	3	4,5,6	3.34	1 (25%)	1,5,7	4.50	1 (100%)
2	5XU	C	309	2	3,4,4	0.77	0	2,4,4	0.69	0
2	ABA	C	307	2	4,5,6	0.57	0	1,5,7	1.92	0
3	AA4	D	311	3	6,7,8	2.28	1 (16%)	2,7,9	0.70	0
2	ABA	C	306	2	4,5,6	3.17	1 (25%)	1,5,7	3.40	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ABA	D	315	3	4,5,6	0.38	0	1,5,7	0.16	0
3	YNM	D	313	3	12,13,14	1.11	2 (16%)	15,16,18	1.38	2 (13%)

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	5XU	D	317	3	-	0/0/2/2	-
2	AA4	C	305	2	-	1/5/6/8	-
3	ABA	D	310	3	1/1/1/2	1/3/4/6	-
2	ABA	C	307	2	-	1/3/4/6	-
2	5XU	C	309	2	-	0/0/2/2	-
3	AA4	D	311	3	-	1/5/6/8	-
2	ABA	C	306	2	1/1/1/2	1/3/4/6	-
3	ABA	D	315	3	-	0/3/4/6	-
3	YNM	D	313	3	-	0/5/8/10	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	305	AA4	CB-CA	-7.07	1.44	1.53
3	D	310	ABA	CB-CA	-6.62	1.34	1.52
2	C	306	ABA	CB-CA	-6.18	1.36	1.52
3	D	311	AA4	CB-CA	-5.33	1.46	1.53
3	D	313	YNM	CA-N	2.32	1.51	1.47
3	D	313	YNM	CB-CG	2.00	1.56	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	310	ABA	CG-CB-CA	4.50	123.72	113.42
2	C	306	ABA	CG-CB-CA	3.40	121.19	113.42
3	D	313	YNM	CG-CB-CA	-3.13	109.14	113.63
3	D	313	YNM	CM-N-CA	2.08	120.10	113.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	306	ABA	CA
3	D	310	ABA	CA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	305	AA4	O-C-CA-CB
2	C	306	ABA	N-CA-CB-CG
2	C	307	ABA	O-C-CA-CB
3	D	310	ABA	N-CA-CB-CG
3	D	311	AA4	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	310	ABA	1	0
2	C	306	ABA	1	0
3	D	313	YNM	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	240/240 (100%)	-0.10	1 (0%) 92 91	21, 35, 60, 103	0
1	B	240/240 (100%)	0.37	24 (10%) 7 6	28, 46, 85, 109	0
2	C	3/9 (33%)	0.16	0 100 100	29, 29, 33, 41	0
3	D	3/9 (33%)	0.52	0 100 100	39, 39, 42, 49	0
All	All	486/498 (97%)	0.14	25 (5%) 28 26	21, 40, 76, 109	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	TYR	4.2
1	B	49	GLY	3.6
1	B	133	SER	3.5
1	B	50	SER	3.4
1	B	83	VAL	3.3
1	B	264	ALA	3.3
1	B	266	ASN	3.2
1	B	129	VAL	3.2
1	B	47	ARG	3.1
1	B	130	THR	3.1
1	B	187	SER	3.0
1	B	128	SER	3.0
1	B	98	VAL	3.0
1	B	142	ARG	2.9
1	B	64	ASN	2.8
1	B	52	TRP	2.8
1	B	90	GLN	2.6
1	B	126	ALA	2.6
1	B	93	GLY	2.6
1	B	131	LEU	2.5
1	A	264	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	127	GLN	2.4
1	B	36	ASN	2.1
1	B	95	GLU	2.1
1	B	35	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	AA4	C	305	8/9	0.91	0.11	24,37,71,71	0
2	ABA	C	306	6/7	0.91	0.17	25,33,91,91	0
3	ABA	D	315	6/7	0.94	0.12	22,32,42,47	0
3	5XU	D	317	5/5	0.94	0.12	33,63,76,76	0
3	AA4	D	311	8/9	0.95	0.12	20,33,51,51	0
2	ABA	C	307	6/7	0.97	0.08	20,29,35,37	0
3	YNM	D	313	13/14	0.97	0.14	30,39,56,58	0
2	5XU	C	309	5/5	0.97	0.13	30,50,57,60	0
3	ABA	D	310	6/7	0.97	0.16	29,42,70,70	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(Å ²)	Q<0.9
4	CA	B	301	1/1	0.35	0.20	102,102,102,102	0
4	CA	A	301	1/1	0.90	0.13	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.