



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:40 PM UTC

PDB ID : 5BX7 / pdb_00005bx7
Title : PKA in complex with a benzothiophene fragment compound.
Authors : Narayanan, D.; Alam, K.A.; Engh, R.A.
Deposited on : 2015-06-08
Resolution : 1.89 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

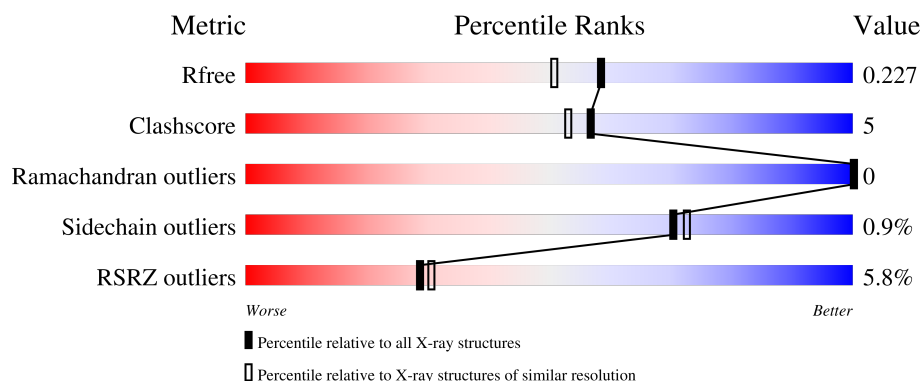
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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	351	5% 90% 8% ..
2	B	20	10% 80% 20%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3273 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	P	S	0	3	0
			2884	1862	488	523	3	8			

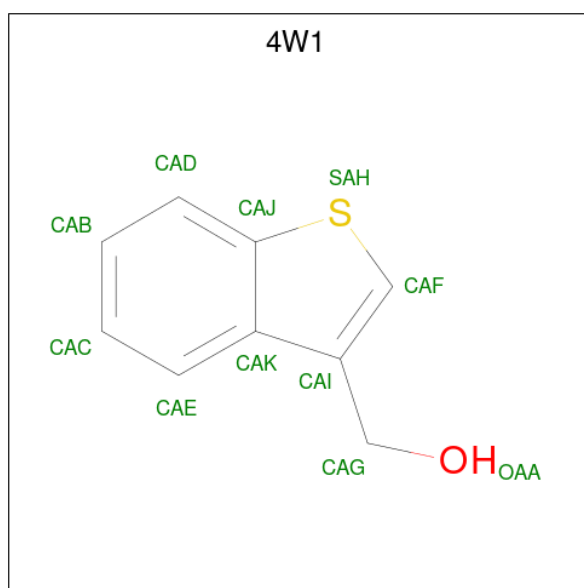
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	PHE	-	expression tag	UNP P17612

- Molecule 2 is a protein called cAMP-dependent protein kinase inhibitor alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	20	Total	C	N	O	0	0	0
			156	94	32	30			

- Molecule 3 is 1-benzothiophen-3-ylmethanol (CCD ID: 4W1) (formula: C₉H₈OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			11	9	1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

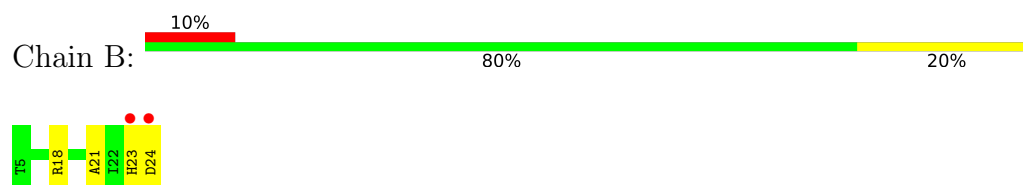


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	183	Total	O	0	0
			183	183		
6	B	19	Total	O	0	0
			19	19		

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.65Å 75.42Å 80.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.71 – 1.89 37.71 – 1.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (37.71-1.89) 98.3 (37.71-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.175 , 0.226 0.179 , 0.227	Depositor DCC
R_{free} test set	1838 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3273	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: SEP, MPD, EDO, 4W1, TPO

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	0.44	0/2923	0.72	0/3931
2	B	0.43	0/158	0.70	0/212
All	All	0.44	0/3081	0.72	0/4143

There are no bond length outliers.

There are no bond angle outliers.

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	2884	0	2866	26	0
2	B	156	0	146	4	0
3	A	11	0	0	0	0
4	A	8	0	14	2	0
4	B	8	0	14	0	0
5	A	4	0	6	0	0
6	A	183	0	0	7	1
6	B	19	0	0	2	0
All	All	3273	0	3046	28	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 (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:308[A]:ARG:NH2	6:A:502:HOH:O	2.13	0.82
1:A:54:PHE:CZ	1:A:84:GLN:HG3	2.20	0.77
1:A:5:ALA:N	6:A:503:HOH:O	2.21	0.73
1:A:10:SEP:O1P	6:A:501:HOH:O	2.11	0.67
1:A:83:LYS:NZ	2:B:24:ASP:OD2	2.28	0.64
1:A:194:ARG:NH2	6:A:506:HOH:O	2.33	0.62
1:A:123:VAL:HB	1:A:173:LEU:HD23	1.86	0.57
1:A:72:LYS:HE2	1:A:74:LEU:HD21	1.89	0.53
1:A:236:PRO:HG2	1:A:239:PHE:HB3	1.91	0.53
1:A:12:GLN:H	1:A:12:GLN:CD	2.17	0.52
1:A:71:MET:HE3	1:A:73:ILE:HD11	1.93	0.51
1:A:45[A]:ARG:NH1	6:A:504:HOH:O	2.29	0.50
1:A:54:PHE:HZ	1:A:84:GLN:HG3	1.73	0.50
1:A:45[A]:ARG:HD2	1:A:335:ILE:HD13	1.96	0.48
1:A:334:GLU:H	1:A:334:GLU:CD	2.20	0.48
1:A:55:GLY:HA3	1:A:73:ILE:O	2.14	0.48
1:A:9:GLY:N	1:A:12:GLN:OE1	2.47	0.46
1:A:134:ARG:HH11	4:A:402:MPD:HM3	1.80	0.46
1:A:134:ARG:HH11	4:A:402:MPD:CM	2.29	0.45
1:A:295:LYS:HG2	6:A:617:HOH:O	2.17	0.45
1:A:173:LEU:HD22	1:A:183:THR:HG21	2.00	0.44
1:A:303:ILE:HD12	1:A:303:ILE:H	1.83	0.43
1:A:45[A]:ARG:HG3	6:A:504:HOH:O	2.18	0.43
1:A:58:MET:HE2	1:A:58:MET:HB3	1.72	0.43
1:A:187:PHE:HE2	2:B:21:ALA:HB1	1.83	0.43
2:B:23:HIS:HD2	6:B:217:HOH:O	2.01	0.42
2:B:18:ARG:NH2	6:B:202:HOH:O	2.53	0.41
1:A:120:MET:HE3	1:A:120:MET:HB2	1.92	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)
6:A:594:HOH:O	6:A:601:HOH:O[3_454]	2.14	0.06

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	344/351 (98%)	333 (97%)	11 (3%)	0	100	100
2	B	18/20 (90%)	18 (100%)	0	0	100	100
All	All	362/371 (98%)	351 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	304/303 (100%)	301 (99%)	3 (1%)	68	70
2	B	15/15 (100%)	15 (100%)	0	100	100
All	All	319/318 (100%)	316 (99%)	3 (1%)	70	73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	334	GLU
1	A	335	ILE

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

Mol	Chain	Res	Type
1	A	245	GLN
2	B	23	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	$\# Z > 2$
1	SEP	A	10	1	8,9,10	1.69	2 (25%)	7,12,14	1.49	1 (14%)
1	SEP	A	338	1	8,9,10	1.51	1 (12%)	7,12,14	1.54	1 (14%)
1	TPO	A	197	1	8,10,11	1.07	0	10,14,16	1.84	2 (20%)

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
1	SEP	A	10	1	-	0/6/8/10	-
1	SEP	A	338	1	-	3/6/8/10	-
1	TPO	A	197	1	-	0/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	SEP	P-O1P	3.68	1.61	1.50
1	A	338	SEP	P-O1P	3.21	1.60	1.50
1	A	10	SEP	P-O3P	2.05	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TPO	P-OG1-CB	-4.51	111.08	123.33
1	A	338	SEP	OG-CB-CA	3.57	111.62	108.14
1	A	10	SEP	OG-CB-CA	3.34	111.40	108.14
1	A	197	TPO	CG2-CB-CA	-2.61	108.18	113.26

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	338	SEP	C-CA-CB-OG
1	A	338	SEP	CA-CB-OG-P
1	A	338	SEP	N-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	10	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
4	MPD	A	402	-	7,7,7	0.64	0	9,10,10	0.52	0
3	4W1	A	401	-	12,12,12	2.59	6 (50%)	12,16,16	3.92	4 (33%)
5	EDO	A	403	-	3,3,3	0.49	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MPD	B	101	-	7,7,7	0.64	0	9,10,10	0.34	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
4	MPD	A	402	-	-	5/5/5/5	-
3	4W1	A	401	-	-	0/2/2/2	0/2/2/2
5	EDO	A	403	-	-	0/1/1/1	-
4	MPD	B	101	-	-	3/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	4W1	CAK-CAI	-4.73	1.36	1.44
3	A	401	4W1	CAF-SAH	-3.80	1.67	1.72
3	A	401	4W1	CAK-CAJ	-3.35	1.36	1.41
3	A	401	4W1	CAD-CAJ	-3.23	1.34	1.39
3	A	401	4W1	CAE-CAK	-3.17	1.35	1.39
3	A	401	4W1	CAG-CAI	2.16	1.54	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	4W1	CAJ-SAH-CAF	9.17	96.14	91.16
3	A	401	4W1	CAI-CAF-SAH	-6.49	106.44	113.75
3	A	401	4W1	CAK-CAJ-SAH	-5.67	107.59	111.46
3	A	401	4W1	CAE-CAK-CAI	-4.03	127.84	133.85

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	402	MPD	C2-C3-C4-O4
4	B	101	MPD	C1-C2-C3-C4
4	B	101	MPD	CM-C2-C3-C4
4	A	402	MPD	C2-C3-C4-C5
4	A	402	MPD	O2-C2-C3-C4
4	B	101	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	A	402	MPD	C1-C2-C3-C4
4	A	402	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	MPD	2	0

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	343/351 (97%)	-0.09	19 (5%) 30 32	13, 24, 52, 98	3 (0%)
2	B	20/20 (100%)	0.04	2 (10%) 12 13	15, 21, 76, 94	0
All	All	363/371 (97%)	-0.08	21 (5%) 29 30	13, 24, 53, 98	3 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	54	PHE	7.1
1	A	9	GLY	6.0
1	A	6	ALA	4.7
1	A	7	LYS	4.6
2	B	23	HIS	4.1
1	A	55	GLY	4.0
2	B	24	ASP	3.6
1	A	318	PHE	3.4
1	A	8	LYS	3.0
1	A	5	ALA	3.0
1	A	12	GLN	2.7
1	A	53	SER	2.6
1	A	319	LYS	2.5
1	A	135	ILE	2.5
1	A	214	GLY	2.2
1	A	295	LYS	2.2
1	A	335	ILE	2.1
1	A	320	GLY	2.1
1	A	194	ARG	2.1
1	A	285	LYS	2.0
1	A	142	HIS	2.0

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($\text{\AA}^2$)	Q<0.9
1	SEP	A	10	10/11	0.74	0.17	49,71,95,165	0
1	SEP	A	338	10/11	0.96	0.07	29,33,37,42	0
1	TPO	A	197	11/12	0.99	0.04	15,17,19,21	0

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
5	EDO	A	403	4/4	0.70	0.22	44,48,49,52	0
4	MPD	A	402	8/8	0.82	0.14	37,41,46,54	0
4	MPD	B	101	8/8	0.83	0.18	57,61,62,64	0
3	4W1	A	401	11/11	0.89	0.12	11,30,42,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.