Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 01:50 pm BST

PDB ID	:	7BAY / pdb_00007bay
Title	:	Crystal structure of CbpF from Streptococcus pneumoniae complexed with a Ytterbium derivative
Authors	:	Martinez Caballero, S.; Hermoso, J.A.
Deposited on	:	2020-12-16
Resolution	:	2.65 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:

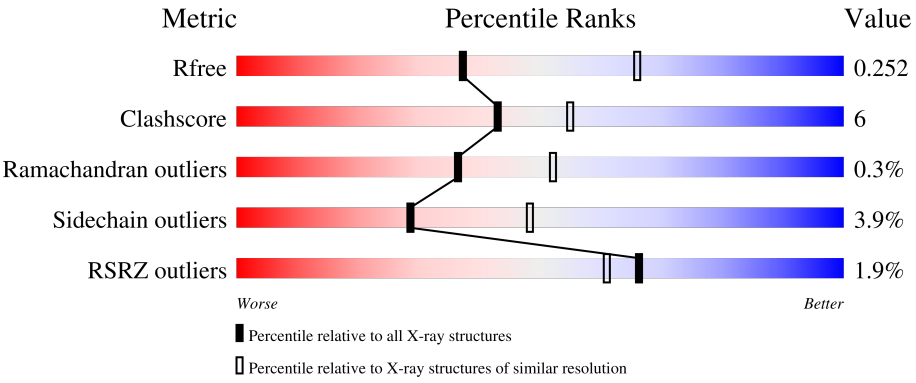
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 <=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	AA	311	2% 83% 16%

2 Entry composition

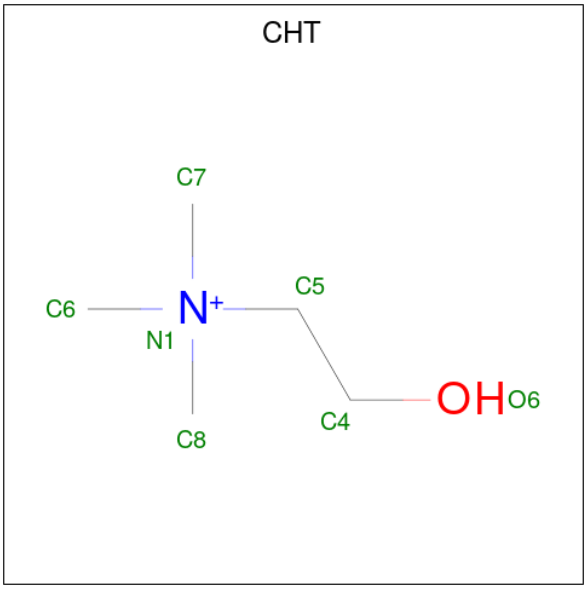
There are 6 unique types of molecules in this entry. The entry contains 2849 atoms, of which 122 are hydrogens and 0 are deuteriums.

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 Choline-binding protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	311	Total	C	N	O	S	0	0	0
			2580	1672	416	486	6			

- Molecule 2 is CHOLINE ION (CCD ID: CHT) (formula: $C_5H_{14}NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		

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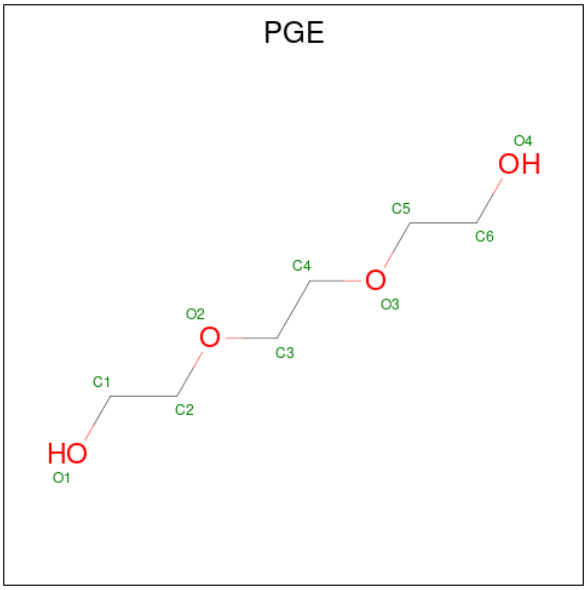
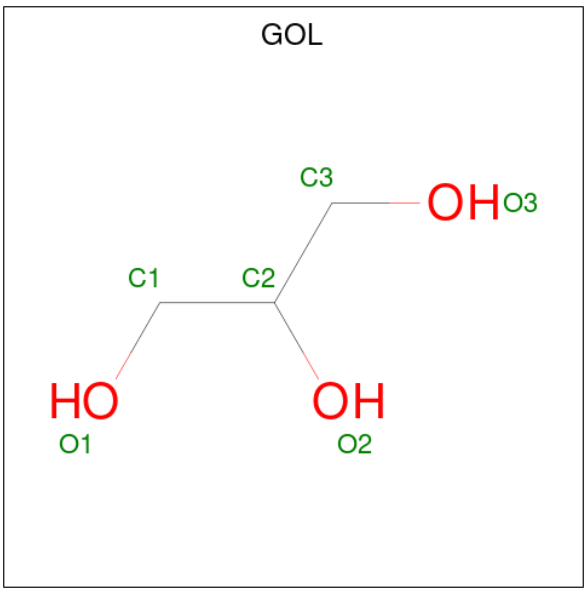
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AA	1	Total	C	H	N	O	0	0
			21	5	14	1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



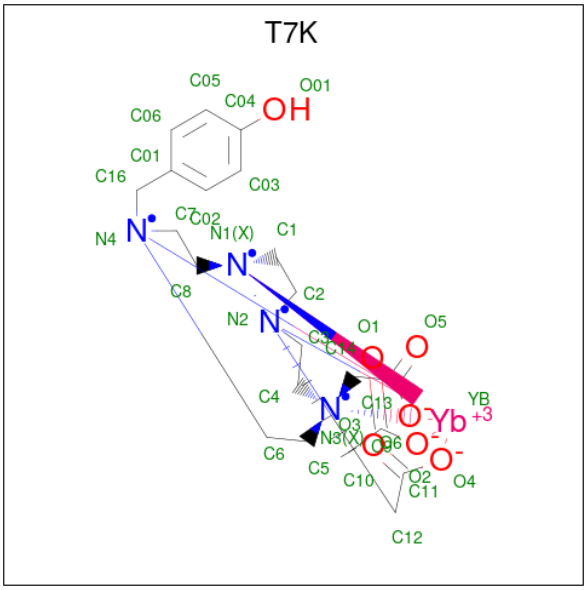
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AA	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AA	1	Total C H O 14 3 8 3	0	0
4	AA	1	Total C H O 14 3 8 3	0	0
4	AA	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is neutral Yb(III)-caged complex (CCD ID: T7K) (formula: $C_{21}H_{29}N_4O_7Yb$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AA	1	Total C N O Yb 33 21 4 7 1	0	0

- Molecule 6 is water.

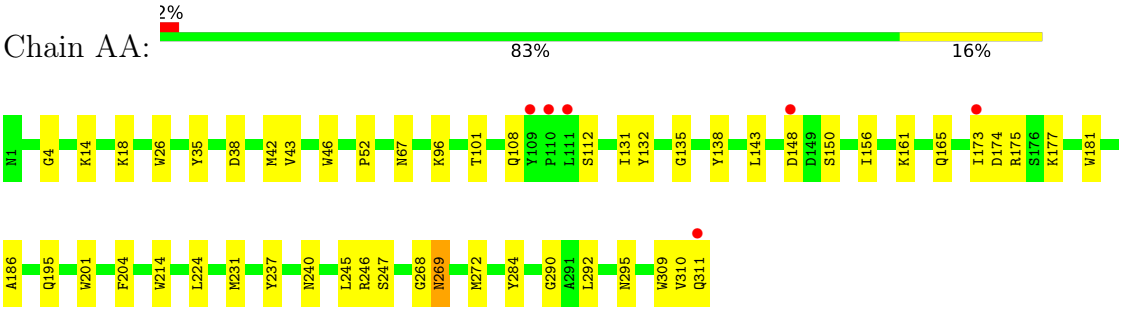
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AA	44	Total O 44 44	0	0

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: Choline-binding protein F

Chain AA:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.90Å 52.21Å 73.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.65 47.53 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.53-2.65) 99.6 (47.53-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.18_3855	Depositor
R, R_{free}	0.201 , 0.242 0.209 , 0.252	Depositor DCC
R_{free} test set	614 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	55.2	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2849	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PGE, CHT, T7K, GOL

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	AA	0.08	0/2670	0.23	0/3630

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	AA	2580	0	2372	31	0
2	AA	42	84	84	2	0
3	AA	10	14	14	0	0
4	AA	18	24	24	1	0
5	AA	33	0	0	1	0
6	AA	44	0	0	1	0
All	All	2727	122	2494	32	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 6.

All (32) 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:AA:14:LYS:HD2	1:AA:42:MET:HE2	1.58	0.84
1:AA:14:LYS:HD2	1:AA:42:MET:CE	2.19	0.71
1:AA:173:ILE:HG22	1:AA:175:ARG:HD2	1.79	0.64
1:AA:132:TYR:OH	1:AA:135:GLY:HA2	1.98	0.62
1:AA:26:TRP:CD2	1:AA:52:PRO:HB3	2.41	0.56
1:AA:174:ASP:OD1	1:AA:177:LYS:HD2	2.05	0.56
1:AA:284:TYR:HB3	1:AA:292:LEU:HD11	1.90	0.54
1:AA:269:ASN:HB3	2:AA:1406:CHT:HC51	1.89	0.54
1:AA:165:GLN:HG3	1:AA:181:TRP:CE2	2.45	0.51
1:AA:246:ARG:HD3	4:AA:1409:GOL:H31	1.90	0.51
1:AA:46:TRP:CB	1:AA:101:THR:HG22	2.40	0.51
1:AA:108:GLN:HA	1:AA:108:GLN:OE1	2.10	0.51
1:AA:46:TRP:HB3	1:AA:101:THR:HG22	1.94	0.49
5:AA:1411:T7K:O2	5:AA:1411:T7K:C1	2.60	0.49
1:AA:272:MET:SD	1:AA:290:GLY:HA3	2.52	0.49
1:AA:26:TRP:CG	1:AA:52:PRO:HB3	2.47	0.48
1:AA:161:LYS:NZ	1:AA:186:ALA:O	2.46	0.48
1:AA:96:LYS:NZ	1:AA:156:ILE:O	2.46	0.48
1:AA:195:GLN:HB2	1:AA:204:PHE:HE2	1.79	0.47
1:AA:26:TRP:CE2	1:AA:52:PRO:HB3	2.49	0.46
1:AA:4:GLY:O	1:AA:18:LYS:HE3	2.15	0.46
1:AA:173:ILE:CG2	1:AA:175:ARG:HD2	2.45	0.45
1:AA:237:TYR:CZ	1:AA:240:ASN:HA	2.52	0.44
1:AA:67:ASN:HB2	6:AA:1512:HOH:O	2.16	0.43
1:AA:131:ILE:HD11	1:AA:138:TYR:HB2	1.99	0.43
1:AA:224:LEU:N	1:AA:224:LEU:HD22	2.34	0.43
1:AA:309:TRP:CZ2	1:AA:311:GLN:HG2	2.54	0.42
1:AA:132:TYR:CZ	1:AA:135:GLY:HA2	2.54	0.42
1:AA:165:GLN:HG3	1:AA:181:TRP:CD2	2.55	0.42
1:AA:214:TRP:CG	2:AA:1406:CHT:H72	2.56	0.41
1:AA:35:TYR:O	1:AA:43:VAL:HG22	2.21	0.40
1:AA:201:TRP:HB2	1:AA:231:MET:HE2	2.02	0.40

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	AA	309/311 (99%)	292 (94%)	16 (5%)	1 (0%)	36 52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	268	GLY

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	AA	259/259 (100%)	249 (96%)	10 (4%)	28 48

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	38	ASP
1	AA	112	SER
1	AA	143	LEU
1	AA	148	ASP
1	AA	150	SER
1	AA	245	LEU
1	AA	247	SER
1	AA	269	ASN
1	AA	295	ASN
1	AA	310	VAL

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

Mol	Chain	Res	Type
1	AA	198	ASN
1	AA	228	ASN
1	AA	280	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	PGE	AA	1404	-	9,9,9	0.31	0	8,8,8	0.34	0
4	GOL	AA	1407	-	5,5,5	0.82	0	5,5,5	0.92	0
4	GOL	AA	1410	-	5,5,5	0.77	0	5,5,5	1.00	0
4	GOL	AA	1409	-	5,5,5	0.72	0	5,5,5	1.02	0
2	CHT	AA	1405	-	6,6,6	0.40	0	8,8,8	0.12	0
2	CHT	AA	1401	-	6,6,6	0.41	0	8,8,8	0.13	0
2	CHT	AA	1403	-	6,6,6	0.40	0	8,8,8	0.10	0
2	CHT	AA	1408	-	6,6,6	0.41	0	8,8,8	0.11	0
2	CHT	AA	1406	-	6,6,6	0.41	0	8,8,8	0.14	0
5	T7K	AA	1411	-	30,40,40	2.94	8 (26%)	34,79,79	1.96	7 (20%)
2	CHT	AA	1402	-	6,6,6	0.40	0	8,8,8	0.10	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	PGE	AA	1404	-	-	3/7/7/7	-
4	GOL	AA	1407	-	-	1/4/4/4	-
4	GOL	AA	1410	-	-	2/4/4/4	-
4	GOL	AA	1409	-	-	2/4/4/4	-
2	CHT	AA	1405	-	-	0/4/4/4	-
2	CHT	AA	1401	-	-	0/4/4/4	-
2	CHT	AA	1403	-	-	1/4/4/4	-
2	CHT	AA	1408	-	-	0/4/4/4	-
2	CHT	AA	1406	-	-	0/4/4/4	-
5	T7K	AA	1411	-	-	0/4/144/144	0/1/8/8
2	CHT	AA	1402	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AA	1411	T7K	C06-C05	8.95	1.55	1.38
5	AA	1411	T7K	C02-C01	7.64	1.55	1.38
5	AA	1411	T7K	C03-C04	7.42	1.53	1.38
5	AA	1411	T7K	C06-C01	-3.51	1.31	1.38
5	AA	1411	T7K	C03-C02	-3.31	1.32	1.38
5	AA	1411	T7K	C05-C04	-3.02	1.33	1.38
5	AA	1411	T7K	C16-C01	2.35	1.56	1.51
5	AA	1411	T7K	O01-C04	2.22	1.42	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AA	1411	T7K	O2-C9-O1	-5.37	119.39	124.58
5	AA	1411	T7K	O2-C9-C10	5.07	123.05	116.83
5	AA	1411	T7K	O6-C13-O5	-4.83	119.91	124.58
5	AA	1411	T7K	O4-C11-O3	-4.75	119.99	124.58
5	AA	1411	T7K	C9-C10-N1	2.64	117.05	112.01
5	AA	1411	T7K	O4-C11-C12	2.53	119.94	116.83
5	AA	1411	T7K	O6-C13-C14	2.47	119.86	116.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AA	1410	GOL	C1-C2-C3-O3
3	AA	1404	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	AA	1407	GOL	O1-C1-C2-C3
4	AA	1409	GOL	O1-C1-C2-C3
4	AA	1410	GOL	O2-C2-C3-O3
2	AA	1403	CHT	O6-C4-C5-N1
4	AA	1409	GOL	O1-C1-C2-O2
3	AA	1404	PGE	O3-C5-C6-O4
3	AA	1404	PGE	C1-C2-O2-C3
2	AA	1402	CHT	O6-C4-C5-N1

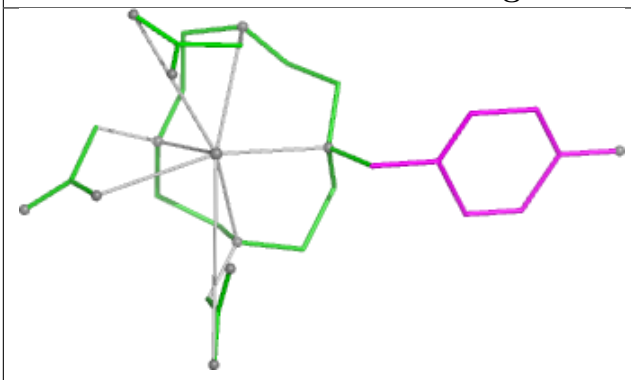
There are no ring outliers.

3 monomers are involved in 4 short contacts:

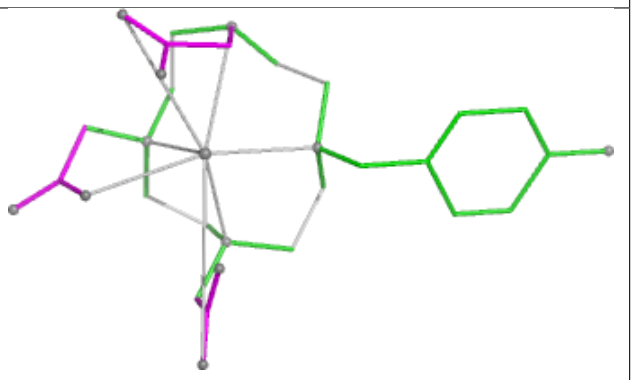
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AA	1409	GOL	1	0
2	AA	1406	CHT	2	0
5	AA	1411	T7K	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

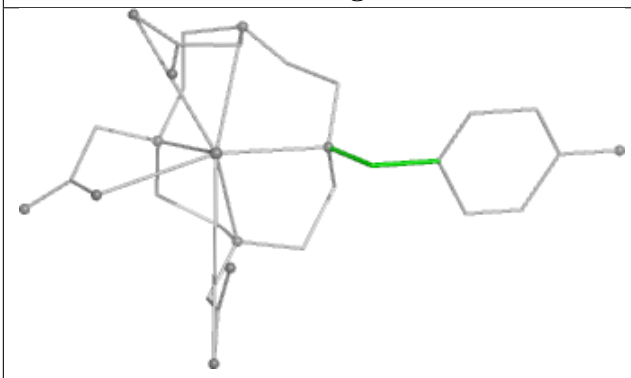
Ligand T7K AA 1411



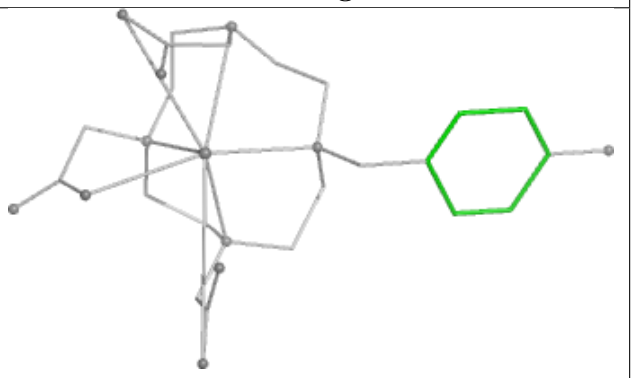
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	AA	311/311 (100%)	0.14	6 (1%) 66 61	38, 54, 88, 116	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AA	173	ILE	2.3
1	AA	311	GLN	2.3
1	AA	148	ASP	2.2
1	AA	109	TYR	2.2
1	AA	110	PRO	2.1
1	AA	111	LEU	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 oligosaccharides 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, 95^{th} 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
3	PGE	AA	1404	10/10	0.80	0.13	61,78,85,92	0

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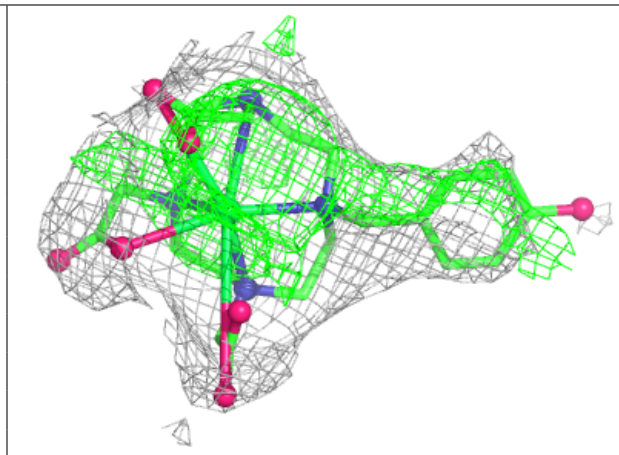
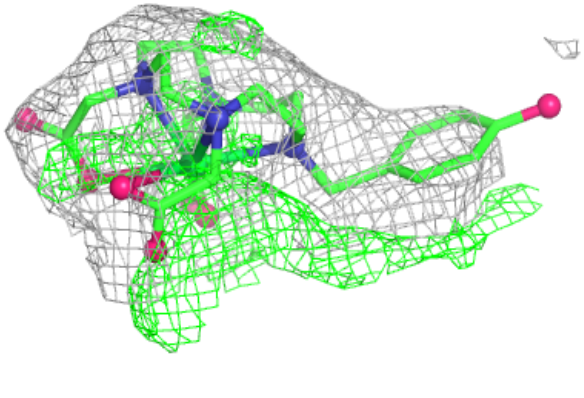
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	AA	1410	6/6	0.80	0.14	61,74,87,92	0
2	CHT	AA	1408	7/7	0.82	0.14	36,54,57,63	0
4	GOL	AA	1407	6/6	0.83	0.21	59,78,94,99	0
2	CHT	AA	1406	7/7	0.84	0.14	56,71,82,85	0
2	CHT	AA	1403	7/7	0.86	0.19	55,70,92,95	0
2	CHT	AA	1405	7/7	0.87	0.23	55,75,96,102	0
4	GOL	AA	1409	6/6	0.87	0.10	55,71,87,87	0
2	CHT	AA	1402	7/7	0.87	0.12	50,67,74,84	0
2	CHT	AA	1401	7/7	0.89	0.15	52,63,87,97	0
5	T7K	AA	1411	33/33	0.96	0.14	76,85,95,98	0

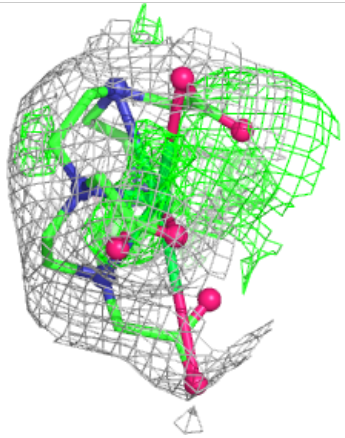
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around T7K AA 1411:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.