



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 02:13 PM BST

PDB ID : 6WEV
Title : Crystal structures of human E-NPP 1: bound to N- $\{[1-(6,7\text{-dimethoxy-}5,8\text{-di}$
hydroquinazolin-4-yl)piperidin-4-yl]methyl\} sulfuric diamide
Authors : Peat, T.S.; Dennis, M.; Newman, J.
Deposited on : 2020-04-03
Resolution : 2.90 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 : 2.14.4.dev1
buster-report : 1.1.7 (2018)
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) : 2.14.4.dev1

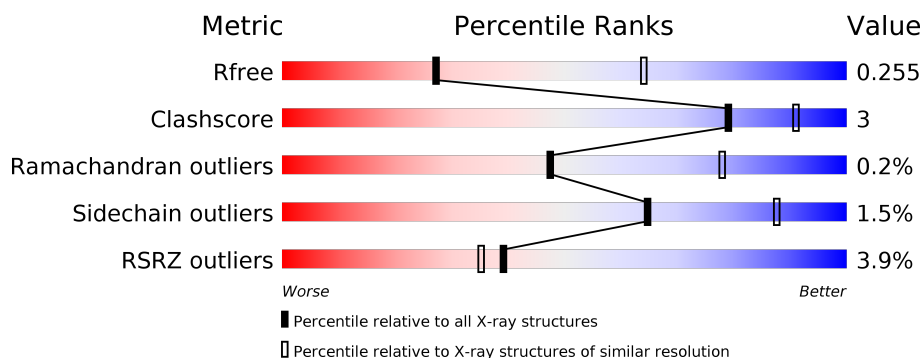
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	AbA	925	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>12%</div> </div> </div>
1	BbB	925	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> </div> </div>
2	AcA	4	<div> <div></div> <div>100%</div> </div>
3	AgA	3	<div> <div></div> <div>100%</div> </div>
3	BcB	3	<div> <div>33%</div> <div>67%</div> </div>
4	AkA	2	<div> <div></div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	BfB	2	

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	MAN	AcA	4	X	-	-	-
4	NAG	BfB	2	X	-	-	-

2 Entry composition [i](#)

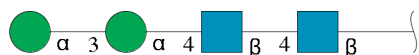
There are 10 unique types of molecules in this entry. The entry contains 13052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AbA	817	Total	C	N	O	S	0	1	0
			6536	4169	1110	1208	49			
1	BbB	796	Total	C	N	O	S	0	1	0
			6218	3971	1049	1151	47			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	AcA	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	AgA	3	Total	C	N	O	0	0	0
			39	22	2	15			
3	BcB	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	AkA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	BfB	2	Total	C	N	O	0	0	0
			28	16	2	10			

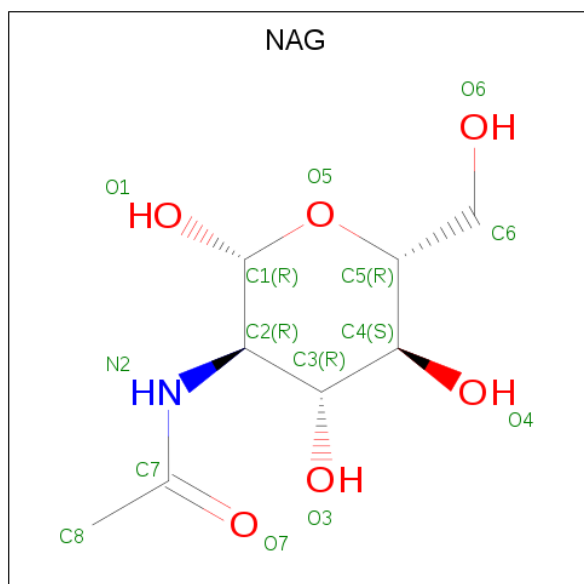
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AbA	1	Total	Zn	0	0
			1	1		
5	BbB	2	Total	Zn	0	0
			2	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

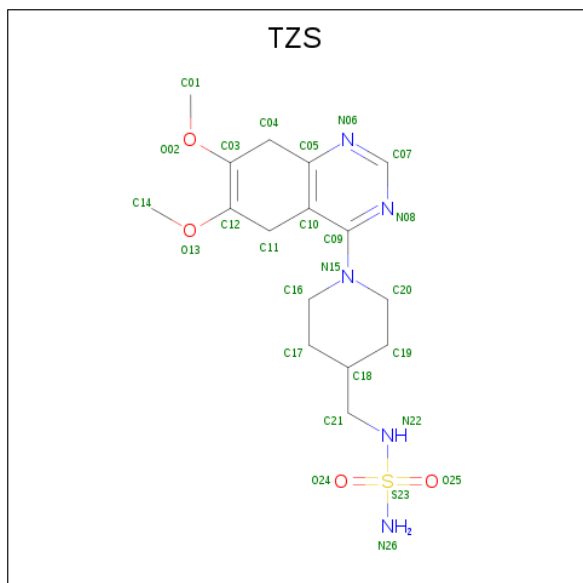
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AbA	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	AbA	1	Total	C	N	O	0	0
			14	8	1	5		
7	BbB	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is N-{[1-(6,7-dimethoxy-5,8-dihydroquinazolin-4-yl)piperidin-4-yl]methyl}sulfuric diamide (three-letter code: TZS) (formula: C₁₆H₂₅N₅O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	AbA	1	Total	C	N	O	S	0	0
			26	16	5	4	1		
8	BbB	1	Total	C	N	O	S	0	0
			26	16	5	4	1		

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	AbA	1	Total	O	P	0	0
			5	4	1		
9	BbB	1	Total	O	P	0	0
			5	4	1		

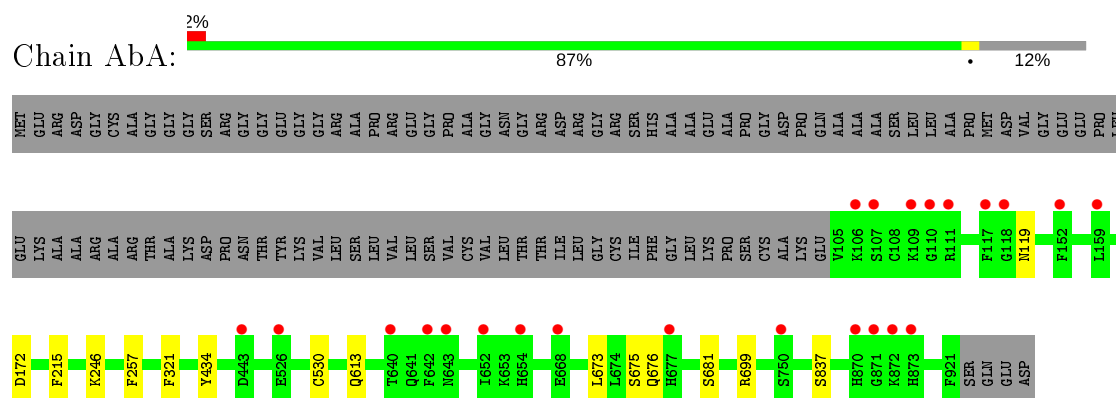
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	AbA	16	Total	O	0	0
			16	16		
10	BbB	4	Total	O	0	0
			4	4		

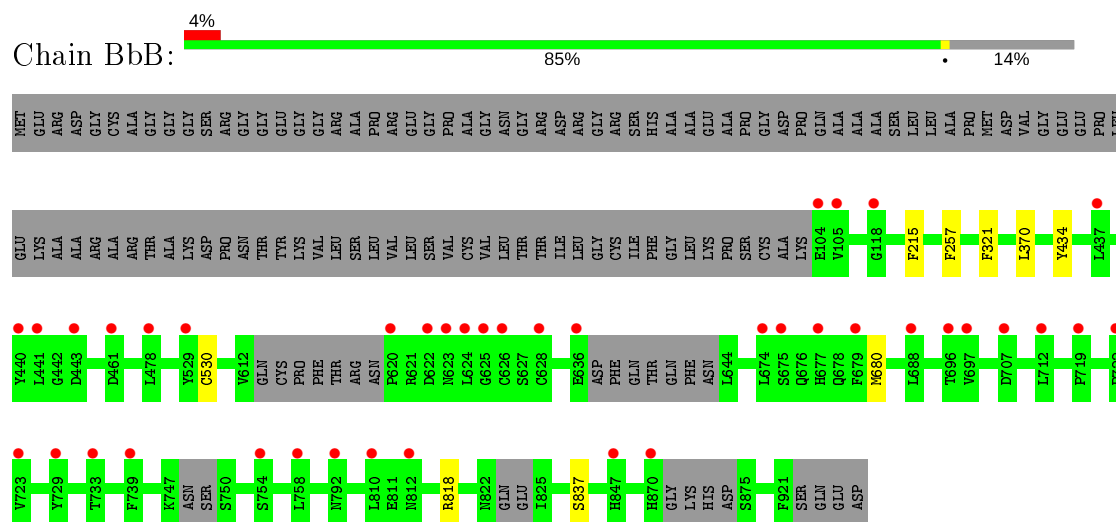
3 Residue-property plots

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: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1



- Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 1



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AcA: 



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AgA:  100%

MAG1
MAG2
EMAG3

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BcB:  33% 67%

MAG1
MAG2
EMAG3

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AkA:  100%

MAG1
MAG2

- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BfB:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 158.99Å 209.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.90 47.28 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.28-2.90) 99.9 (47.28-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.211 , 0.253 0.213 , 0.255	Depositor DCC
R_{free} test set	3122 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13052	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: ZN, BMA, NAG, PO4, TZS, CA, MAN

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	AbA	0.63	0/6722	0.79	0/9132
1	BbB	0.65	0/6390	0.77	0/8694
All	All	0.64	0/13112	0.78	0/17826

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	AbA	6536	0	6262	0	0
1	BbB	6218	0	5821	0	0
2	AcA	50	0	43	0	0
3	AgA	39	0	34	0	0
3	BcB	39	0	34	0	0
4	AkA	28	0	25	0	0
4	BfB	28	0	25	0	0
5	AbA	1	0	0	0	0
5	BbB	2	0	0	0	0
6	AbA	1	0	0	0	0
7	AbA	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	BbB	14	0	13	0	0
8	AbA	26	0	0	0	0
8	BbB	26	0	0	0	0
9	AbA	5	0	0	0	0
9	BbB	5	0	0	0	0
10	AbA	16	0	0	0	0
10	BbB	4	0	0	0	0
All	All	13052	0	12270	0	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.

There are no clashes within the asymmetric unit.

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	AbA	816/925 (88%)	777 (95%)	37 (4%)	2 (0%)	47	78
1	BbB	785/925 (85%)	745 (95%)	39 (5%)	1 (0%)	51	82
All	All	1601/1850 (86%)	1522 (95%)	76 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AbA	119	ASN
1	AbA	321	PHE
1	BbB	321	PHE

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	AbA	731/824 (89%)	718 (98%)	13 (2%)	59	85
1	BbB	668/824 (81%)	660 (99%)	8 (1%)	71	91
All	All	1399/1648 (85%)	1378 (98%)	21 (2%)	65	87

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AbA	172	ASP
1	AbA	215	PHE
1	AbA	246	LYS
1	AbA	257	PHE
1	AbA	434	TYR
1	AbA	530	CYS
1	AbA	613	GLN
1	AbA	673	LEU
1	AbA	675	SER
1	AbA	676	GLN
1	AbA	681	SER
1	AbA	699	ARG
1	AbA	837	SER
1	BbB	215	PHE
1	BbB	257	PHE
1	BbB	370	LEU
1	BbB	434	TYR
1	BbB	530	CYS
1	BbB	680	MET
1	BbB	818	ARG
1	BbB	837	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

14 monosaccharides 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$
2	NAG	AcA	1	1,2	14,14,15	0.66	0	17,19,21	1.68	3 (17%)
2	NAG	AcA	2	2	14,14,15	0.56	0	17,19,21	1.53	2 (11%)
2	MAN	AcA	3	2	11,11,12	0.49	0	15,15,17	1.54	3 (20%)
2	MAN	AcA	4	2	11,11,12	0.80	0	15,15,17	3.64	5 (33%)
3	NAG	AgA	1	1,3	14,14,15	0.58	0	17,19,21	1.97	3 (17%)
3	NAG	AgA	2	3	14,14,15	0.62	0	17,19,21	1.73	3 (17%)
3	BMA	AgA	3	3	11,11,12	0.43	0	15,15,17	1.24	1 (6%)
4	NAG	AkA	1	1,4	14,14,15	0.52	0	17,19,21	1.84	6 (35%)
4	NAG	AkA	2	4	14,14,15	0.31	0	17,19,21	0.93	1 (5%)
3	NAG	BcB	1	1,3	14,14,15	0.54	0	17,19,21	1.78	3 (17%)
3	NAG	BcB	2	3	14,14,15	0.43	0	17,19,21	0.75	0
3	BMA	BcB	3	3	11,11,12	0.32	0	15,15,17	1.03	1 (6%)
4	NAG	BfB	1	1,4	14,14,15	0.55	0	17,19,21	1.87	5 (29%)
4	NAG	BfB	2	4	14,14,15	0.31	0	17,19,21	0.90	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
2	NAG	AcA	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	AcA	2	2	-	1/6/23/26	0/1/1/1
2	MAN	AcA	3	2	-	2/2/19/22	1/1/1/1
2	MAN	AcA	4	2	1/1/4/5	2/2/19/22	1/1/1/1
3	NAG	AgA	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	AgA	2	3	-	5/6/23/26	0/1/1/1
3	BMA	AgA	3	3	-	1/2/19/22	0/1/1/1
4	NAG	AkA	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	AkA	2	4	-	2/6/23/26	0/1/1/1
3	NAG	BcB	1	1,3	-	3/6/23/26	0/1/1/1
3	NAG	BcB	2	3	-	2/6/23/26	0/1/1/1
3	BMA	BcB	3	3	-	2/2/19/22	0/1/1/1
4	NAG	BfB	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	BfB	2	4	1/1/5/7	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AcA	4	MAN	C1-C2-C3	-11.64	95.36	109.67
2	AcA	4	MAN	C1-O5-C5	-6.18	103.82	112.19
3	BcB	1	NAG	O5-C1-C2	-4.81	103.69	111.29
3	AgA	1	NAG	C8-C7-N2	-4.64	108.24	116.10
3	AgA	1	NAG	O5-C1-C2	-4.60	104.02	111.29
3	AgA	2	NAG	C8-C7-N2	-4.60	108.31	116.10
4	BfB	1	NAG	C1-O5-C5	4.46	118.23	112.19
4	AkA	1	NAG	C4-C3-C2	-4.35	104.64	111.02
4	BfB	1	NAG	C2-N2-C7	-3.70	117.64	122.90
2	AcA	1	NAG	C1-O5-C5	3.57	117.03	112.19
3	AgA	3	BMA	C1-O5-C5	3.57	117.03	112.19
3	AgA	2	NAG	O7-C7-N2	3.48	128.35	121.95
2	AcA	3	MAN	C3-C4-C5	-3.28	104.39	110.24
2	AcA	1	NAG	O5-C1-C2	-3.24	106.17	111.29
3	AgA	1	NAG	O7-C7-N2	3.23	127.90	121.95
3	BcB	1	NAG	C3-C4-C5	2.81	115.26	110.24
3	BcB	1	NAG	C1-C2-N2	2.75	115.18	110.49
2	AcA	4	MAN	O2-C2-C1	2.71	114.69	109.15
4	AkA	2	NAG	O5-C5-C6	2.71	111.45	107.20
2	AcA	2	NAG	C3-C4-C5	2.70	115.06	110.24
2	AcA	4	MAN	O5-C5-C6	2.63	111.33	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	BfB	1	NAG	C1-C2-N2	-2.61	106.02	110.49
4	AkA	1	NAG	O7-C7-N2	2.61	126.76	121.95
4	AkA	1	NAG	C2-N2-C7	2.60	126.60	122.90
3	BcB	3	BMA	C1-C2-C3	2.59	112.85	109.67
4	AkA	1	NAG	C8-C7-N2	-2.49	111.88	116.10
4	BfB	1	NAG	C8-C7-N2	-2.47	111.92	116.10
3	AgA	2	NAG	O5-C1-C2	-2.46	107.40	111.29
4	AkA	1	NAG	C1-O5-C5	-2.41	108.92	112.19
2	AcA	1	NAG	C3-C4-C5	2.40	114.52	110.24
2	AcA	2	NAG	C2-N2-C7	-2.26	119.69	122.90
4	BfB	1	NAG	O7-C7-N2	2.23	126.06	121.95
4	AkA	1	NAG	O5-C5-C4	-2.19	105.49	110.83
2	AcA	3	MAN	C1-O5-C5	2.06	114.98	112.19
2	AcA	3	MAN	O3-C3-C2	-2.04	106.09	109.99
2	AcA	4	MAN	O3-C3-C2	-2.01	106.14	109.99

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	BfB	2	NAG	C1
2	AcA	4	MAN	C1

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BcB	3	BMA	O5-C5-C6-O6
3	BcB	3	BMA	C4-C5-C6-O6
4	AkA	1	NAG	C8-C7-N2-C2
3	AgA	2	NAG	C8-C7-N2-C2
4	BfB	1	NAG	C8-C7-N2-C2
3	AgA	2	NAG	O5-C5-C6-O6
3	BcB	2	NAG	O5-C5-C6-O6
4	AkA	2	NAG	O5-C5-C6-O6
3	BcB	2	NAG	C4-C5-C6-O6
3	AgA	2	NAG	C4-C5-C6-O6
3	BcB	1	NAG	O5-C5-C6-O6
3	AgA	1	NAG	C8-C7-N2-C2
4	AkA	2	NAG	C4-C5-C6-O6
4	AkA	1	NAG	O7-C7-N2-C2
3	BcB	1	NAG	C4-C5-C6-O6
3	AgA	3	BMA	O5-C5-C6-O6
2	AcA	3	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	AgA	2	NAG	O7-C7-N2-C2
4	BfB	2	NAG	O5-C5-C6-O6
3	AgA	2	NAG	C3-C2-N2-C7
2	AcA	4	MAN	C4-C5-C6-O6
4	BfB	1	NAG	O7-C7-N2-C2
3	AgA	1	NAG	C1-C2-N2-C7
3	BcB	1	NAG	C8-C7-N2-C2
4	AkA	1	NAG	O5-C5-C6-O6
2	AcA	3	MAN	O5-C5-C6-O6
2	AcA	2	NAG	C4-C5-C6-O6
4	AkA	1	NAG	C3-C2-N2-C7
2	AcA	4	MAN	O5-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AcA	4	MAN	C1-C2-C3-C4-C5-O5
2	AcA	3	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
7	NAG	AbA	1003	1	14,14,15	0.49	0	17,19,21	1.20	1 (5%)
8	TZS	AbA	1004	-	24,28,28	2.42	12 (50%)	31,40,40	2.61	10 (32%)
9	PO4	AbA	1005	5	4,4,4	1.25	1 (25%)	6,6,6	0.37	0
7	NAG	BbB	1003	1	14,14,15	0.37	0	17,19,21	1.41	2 (11%)
9	PO4	BbB	1005	-	4,4,4	0.88	0	6,6,6	0.40	0
8	TZS	BbB	1004	-	24,28,28	2.54	13 (54%)	31,40,40	2.59	12 (38%)

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
8	TZS	AbA	1004	-	-	7/13/36/36	0/3/3/3
7	NAG	AbA	1003	1	-	4/6/23/26	0/1/1/1
8	TZS	BbB	1004	-	-	6/13/36/36	0/3/3/3
7	NAG	BbB	1003	1	-	4/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	BbB	1004	TZS	C04-C05	-6.64	1.44	1.51
8	AbA	1004	TZS	C04-C05	-6.38	1.44	1.51
8	BbB	1004	TZS	C20-N15	4.62	1.54	1.46
8	BbB	1004	TZS	C16-N15	4.50	1.53	1.46
8	AbA	1004	TZS	C20-N15	4.16	1.53	1.46
8	AbA	1004	TZS	C16-N15	4.15	1.53	1.46
8	BbB	1004	TZS	C09-N15	3.88	1.47	1.37
8	AbA	1004	TZS	C09-N15	3.33	1.46	1.37
8	AbA	1004	TZS	C10-C05	-2.45	1.36	1.40
9	AbA	1005	PO4	P-O1	2.44	1.56	1.50
8	BbB	1004	TZS	C21-C18	2.43	1.56	1.51
8	AbA	1004	TZS	O02-C03	2.37	1.42	1.35
8	BbB	1004	TZS	C19-C18	-2.35	1.45	1.52
8	AbA	1004	TZS	C21-C18	2.35	1.56	1.51
8	AbA	1004	TZS	C19-C18	-2.31	1.46	1.52
8	AbA	1004	TZS	O13-C12	2.29	1.42	1.35
8	BbB	1004	TZS	C17-C18	-2.29	1.46	1.52
8	AbA	1004	TZS	C05-N06	2.28	1.37	1.34
8	BbB	1004	TZS	O13-C12	2.26	1.42	1.35
8	BbB	1004	TZS	S23-N22	2.26	1.71	1.62
8	BbB	1004	TZS	C10-C05	-2.22	1.37	1.40
8	BbB	1004	TZS	C05-N06	2.18	1.37	1.34
8	BbB	1004	TZS	O02-C03	2.18	1.42	1.35
8	AbA	1004	TZS	C17-C18	-2.16	1.46	1.52
8	AbA	1004	TZS	S23-N22	2.10	1.70	1.62
8	BbB	1004	TZS	C10-C09	2.09	1.45	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	BbB	1004	TZS	O25-S23-O24	-8.07	101.49	119.96
8	AbA	1004	TZS	O25-S23-O24	-7.79	102.12	119.96
8	AbA	1004	TZS	C10-C05-N06	-5.39	118.90	123.48
8	BbB	1004	TZS	C10-C05-N06	-5.03	119.21	123.48
8	AbA	1004	TZS	C09-C10-C05	4.92	118.27	115.80
8	BbB	1004	TZS	C09-C10-C05	4.62	118.12	115.80
8	AbA	1004	TZS	N08-C07-N06	-4.56	121.46	128.60
8	BbB	1004	TZS	N08-C07-N06	-4.55	121.49	128.60
8	BbB	1004	TZS	C07-N08-C09	3.89	120.94	111.75
8	AbA	1004	TZS	C07-N08-C09	3.67	120.43	111.75
7	BbB	1003	NAG	C1-C2-N2	3.43	116.34	110.49
8	AbA	1004	TZS	C05-C04-C03	3.00	120.20	112.71
8	BbB	1004	TZS	C05-C04-C03	3.00	120.19	112.71
8	AbA	1004	TZS	C04-C05-N06	2.88	121.08	116.41
7	BbB	1003	NAG	O5-C5-C6	2.86	111.69	107.20
8	AbA	1004	TZS	C14-O13-C12	-2.55	114.17	119.20
8	BbB	1004	TZS	C04-C05-N06	2.54	120.54	116.41
7	AbA	1003	NAG	C1-O5-C5	-2.51	108.79	112.19
8	BbB	1004	TZS	O24-S23-N22	2.45	111.69	106.88
8	AbA	1004	TZS	C01-O02-C03	-2.16	114.94	119.20
8	AbA	1004	TZS	O24-S23-N22	2.15	111.11	106.88
8	BbB	1004	TZS	O25-S23-N22	2.14	111.08	106.88
8	BbB	1004	TZS	C14-O13-C12	-2.12	115.02	119.20
8	BbB	1004	TZS	C01-O02-C03	-2.08	115.09	119.20
8	BbB	1004	TZS	O24-S23-N26	2.03	111.66	107.38

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	AbA	1003	NAG	C8-C7-N2-C2
7	AbA	1003	NAG	O7-C7-N2-C2
8	AbA	1004	TZS	C17-C18-C21-N22
8	AbA	1004	TZS	C19-C18-C21-N22
8	AbA	1004	TZS	C04-C03-O02-C01
8	AbA	1004	TZS	C21-N22-S23-O24
8	AbA	1004	TZS	C21-N22-S23-O25
8	BbB	1004	TZS	C12-C03-O02-C01
8	BbB	1004	TZS	C21-N22-S23-O24
7	BbB	1003	NAG	O5-C5-C6-O6
7	BbB	1003	NAG	C4-C5-C6-O6
7	BbB	1003	NAG	C8-C7-N2-C2
7	AbA	1003	NAG	C4-C5-C6-O6

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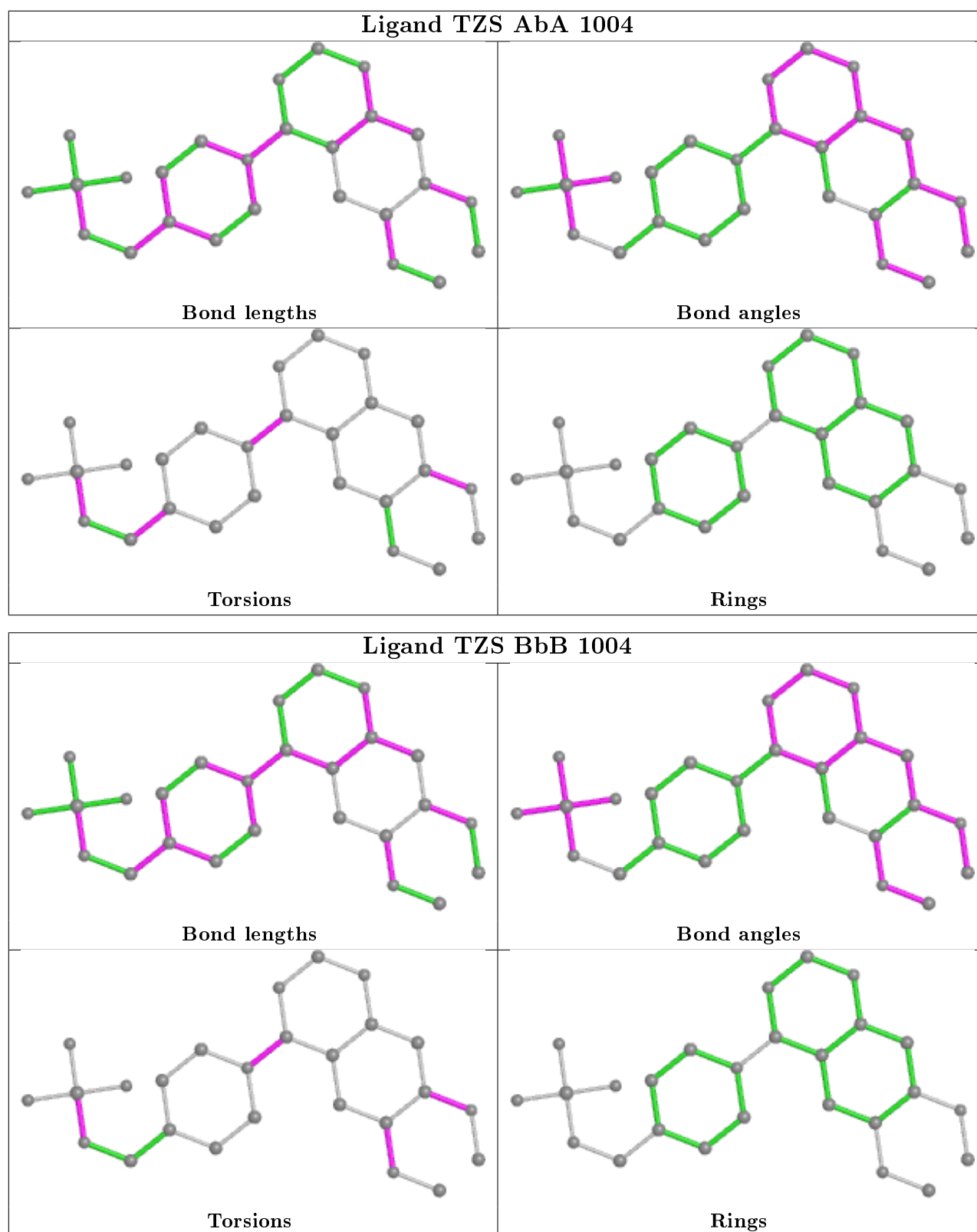
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Mol	Chain	Res	Type	Atoms
8	BbB	1004	TZS	C11-C12-O13-C14
7	BbB	1003	NAG	O7-C7-N2-C2
7	AbA	1003	NAG	O5-C5-C6-O6
8	AbA	1004	TZS	C12-C03-O02-C01
8	BbB	1004	TZS	C04-C03-O02-C01
8	BbB	1004	TZS	C21-N22-S23-O25
8	BbB	1004	TZS	N08-C09-N15-C16
8	AbA	1004	TZS	N08-C09-N15-C16

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	AbA	817/925 (88%)	-0.10	23 (2%)	53 49	29, 53, 106, 158	0
1	BbB	796/925 (86%)	0.18	40 (5%)	28 25	32, 75, 137, 164	0
All	All	1613/1850 (87%)	0.04	63 (3%)	39 35	29, 59, 130, 164	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AbA	677	HIS	4.7
1	BbB	478	LEU	4.2
1	BbB	696	THR	4.0
1	BbB	722	PRO	3.9
1	AbA	111	ARG	3.9
1	AbA	526	GLU	3.6
1	AbA	750	SER	3.5
1	BbB	675	SER	3.5
1	BbB	712	LEU	3.5
1	BbB	441	LEU	3.4
1	AbA	642	PHE	3.4
1	AbA	110	GLY	3.4
1	BbB	847	HIS	3.4
1	BbB	754	SER	3.3
1	BbB	723	VAL	3.3
1	BbB	104	GLU	3.3
1	BbB	620	PRO	3.3
1	AbA	152	PHE	3.2
1	BbB	624	LEU	3.2
1	BbB	729	TYR	3.1
1	AbA	109	LYS	3.1
1	BbB	677	HIS	3.1
1	AbA	106	LYS	3.0
1	BbB	674	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	BbB	812	ASN	2.9
1	BbB	628	CYS	2.9
1	BbB	105	VAL	2.8
1	BbB	626	CYS	2.8
1	BbB	623	ASN	2.7
1	BbB	622	ASP	2.7
1	BbB	529	TYR	2.6
1	BbB	440	TYR	2.6
1	AbA	107	SER	2.6
1	AbA	443	ASP	2.6
1	AbA	117	PHE	2.6
1	BbB	625	GLY	2.5
1	AbA	873	HIS	2.5
1	BbB	118	GLY	2.5
1	BbB	719	PRO	2.5
1	AbA	870	HIS	2.5
1	AbA	871	GLY	2.5
1	AbA	159	LEU	2.5
1	BbB	707	ASP	2.4
1	BbB	461	ASP	2.4
1	AbA	640	THR	2.4
1	BbB	697	VAL	2.4
1	AbA	118	GLY	2.3
1	AbA	643	ASN	2.3
1	BbB	792	ASN	2.3
1	BbB	437	LEU	2.3
1	BbB	733	THR	2.2
1	AbA	654	HIS	2.2
1	BbB	679	PHE	2.2
1	BbB	739	PHE	2.2
1	AbA	668	GLU	2.2
1	AbA	872	LYS	2.2
1	BbB	810	LEU	2.2
1	AbA	652	ILE	2.2
1	BbB	870	HIS	2.1
1	BbB	636	GLU	2.1
1	BbB	758	LEU	2.1
1	BbB	688	LEU	2.0
1	BbB	443	ASP	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](#)

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	MAN	AcA	3	11/12	0.64	0.23	87,113,132,150	0
2	MAN	AcA	4	11/12	0.68	0.20	107,132,142,147	0
3	BMA	AgA	3	11/12	0.75	0.17	110,123,135,136	0
4	NAG	BfB	2	14/15	0.82	0.37	87,115,147,160	0
4	NAG	AkA	2	14/15	0.86	0.38	120,139,158,176	0
3	BMA	BcB	3	11/12	0.88	0.11	100,112,117,119	0
4	NAG	AkA	1	14/15	0.89	0.15	73,90,106,115	0
3	NAG	AgA	2	14/15	0.90	0.21	71,87,97,119	0
4	NAG	BfB	1	14/15	0.92	0.30	72,94,113,132	0
3	NAG	AgA	1	14/15	0.92	0.14	63,75,83,87	0
3	NAG	BcB	2	14/15	0.93	0.12	81,102,115,118	0
2	NAG	AcA	2	14/15	0.93	0.18	62,69,77,90	0
3	NAG	BcB	1	14/15	0.96	0.17	63,73,82,90	0
2	NAG	AcA	1	14/15	0.97	0.18	42,43,46,56	0

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
7	NAG	AbA	1003	14/15	0.85	0.38	93,101,112,131	0
6	CA	AbA	1002	1/1	0.86	0.14	121,121,121,121	0
7	NAG	BbB	1003	14/15	0.86	0.20	92,117,125,126	0
9	PO4	BbB	1005	5/5	0.86	0.20	86,86,104,107	0
8	TZS	BbB	1004	26/26	0.95	0.26	54,66,71,75	0
9	PO4	AbA	1005	5/5	0.96	0.11	71,72,77,91	0
8	TZS	AbA	1004	26/26	0.96	0.18	40,43,51,52	0
5	ZN	BbB	1002	1/1	0.97	0.25	103,103,103,103	1

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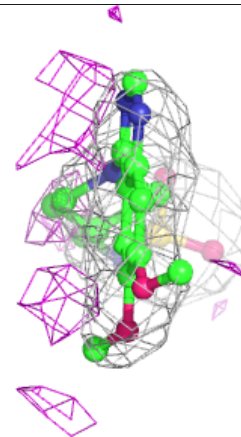
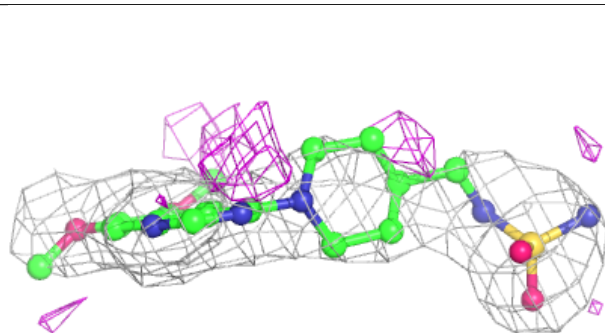
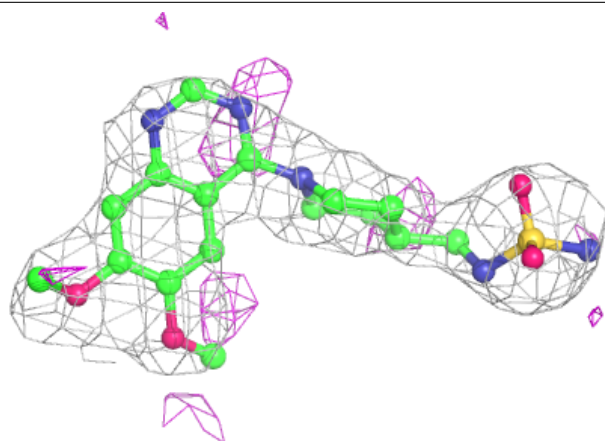
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	ZN	BbB	1001	1/1	0.99	0.02	64,64,64,64	0
5	ZN	AbA	1001	1/1	1.00	0.10	43,43,43,43	0

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.

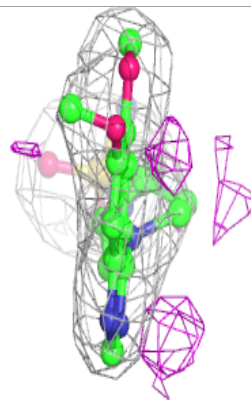
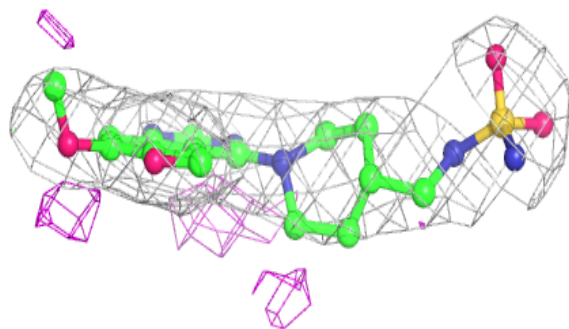
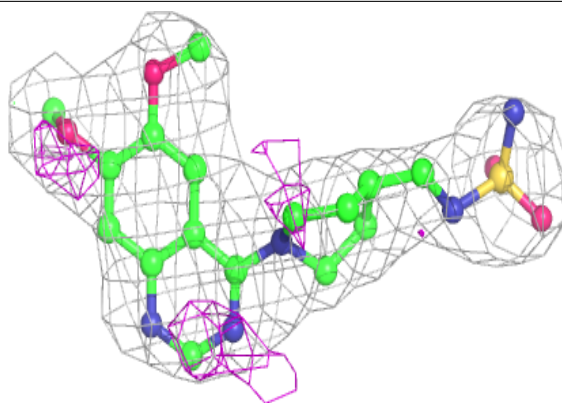
Electron density around TZS BbB 1004:

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



Electron density around TZS AbA 1004:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.