WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 07:59 AM EDT

PDB ID	:	6Y2I
Title	:	Crystal structure of M. tuberculosis KasA in complex with N-(1H-indazol-5-y l)butane-1-sulfonamide
Authors	:	Chung, C.
Deposited on	:	2020-02-16
Resolution	:	1.53 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

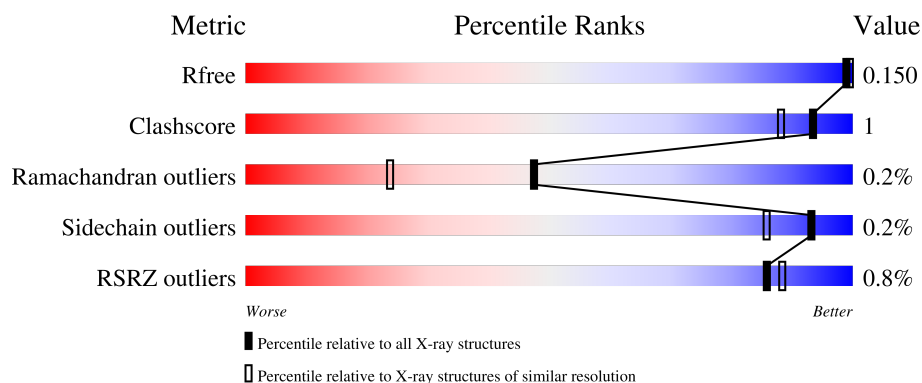|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

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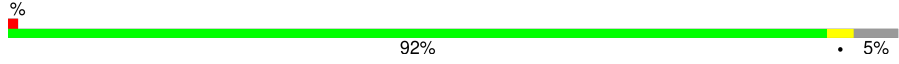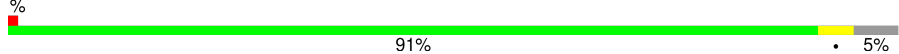*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.53 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	Percentile Ranks	Value
Rfree		0.150
Clashscore		1
Ramachandran outliers		0.2%
Sidechain outliers		0.2%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2556 (1.56-1.52)
Clashscore	141614	2634 (1.56-1.52)
Ramachandran outliers	138981	2580 (1.56-1.52)
Sidechain outliers	138945	2577 (1.56-1.52)
RSRZ outliers	127900	2524 (1.56-1.52)

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	AAA	435	% 92% · 5%
1	BBB	435	% 91% · 5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7243 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 3-oxoacyl-[acyl-carrier-protein] synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	413	Total	C	N	O	S	0	15	0
			3145	1960	560	607	18			
1	BBB	413	Total	C	N	O	S	0	12	0
			3123	1943	560	602	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-18	MET	-	initiating methionine	UNP P9WQD9
AAA	-17	GLY	-	expression tag	UNP P9WQD9
AAA	-16	SER	-	expression tag	UNP P9WQD9
AAA	-15	SER	-	expression tag	UNP P9WQD9
AAA	-14	HIS	-	expression tag	UNP P9WQD9
AAA	-13	HIS	-	expression tag	UNP P9WQD9
AAA	-12	HIS	-	expression tag	UNP P9WQD9
AAA	-11	HIS	-	expression tag	UNP P9WQD9
AAA	-10	HIS	-	expression tag	UNP P9WQD9
AAA	-9	HIS	-	expression tag	UNP P9WQD9
AAA	-8	SER	-	expression tag	UNP P9WQD9
AAA	-7	SER	-	expression tag	UNP P9WQD9
AAA	-6	GLY	-	expression tag	UNP P9WQD9
AAA	-5	LEU	-	expression tag	UNP P9WQD9
AAA	-4	VAL	-	expression tag	UNP P9WQD9
AAA	-3	PRO	-	expression tag	UNP P9WQD9
AAA	-2	ARG	-	expression tag	UNP P9WQD9
AAA	-1	GLY	-	expression tag	UNP P9WQD9
AAA	0	SER	-	expression tag	UNP P9WQD9
AAA	1	HIS	-	expression tag	UNP P9WQD9
BBB	-18	MET	-	initiating methionine	UNP P9WQD9
BBB	-17	GLY	-	expression tag	UNP P9WQD9
BBB	-16	SER	-	expression tag	UNP P9WQD9
BBB	-15	SER	-	expression tag	UNP P9WQD9
BBB	-14	HIS	-	expression tag	UNP P9WQD9

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-13	HIS	-	expression tag	UNP P9WQD9
BBB	-12	HIS	-	expression tag	UNP P9WQD9
BBB	-11	HIS	-	expression tag	UNP P9WQD9
BBB	-10	HIS	-	expression tag	UNP P9WQD9
BBB	-9	HIS	-	expression tag	UNP P9WQD9
BBB	-8	SER	-	expression tag	UNP P9WQD9
BBB	-7	SER	-	expression tag	UNP P9WQD9
BBB	-6	GLY	-	expression tag	UNP P9WQD9
BBB	-5	LEU	-	expression tag	UNP P9WQD9
BBB	-4	VAL	-	expression tag	UNP P9WQD9
BBB	-3	PRO	-	expression tag	UNP P9WQD9
BBB	-2	ARG	-	expression tag	UNP P9WQD9
BBB	-1	GLY	-	expression tag	UNP P9WQD9
BBB	0	SER	-	expression tag	UNP P9WQD9
BBB	1	HIS	-	expression tag	UNP P9WQD9

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0
2	BBB	1	Total 4	C 2	O 2	0	0

- Molecule 3 is {N}-(1 {H}-indazol-5-yl)butane-1-sulfonamide (three-letter code: O6Z) (formula: $C_{11}H_{15}N_3O_2S$) (labeled as "Ligand of Interest" by depositor).

O6Z
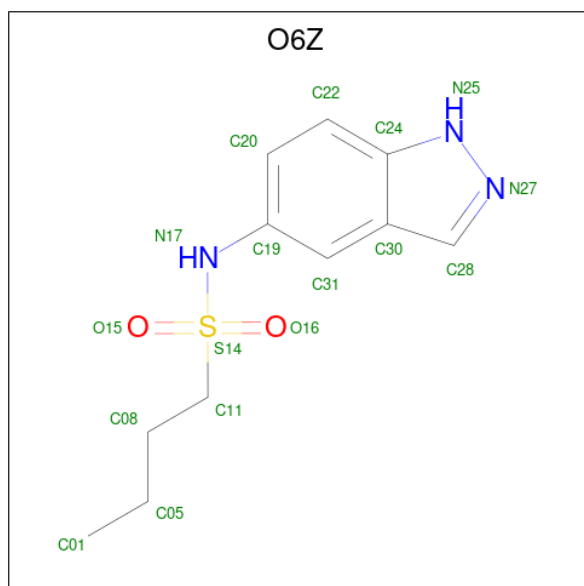
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	AAA	1	Total 17	C 11	N 3	O 2	S 1	0	0
3	BBB	1	Total 17	C 11	N 3	O 2	S 1	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	BBB	1	Total Na 1 1	0	0

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
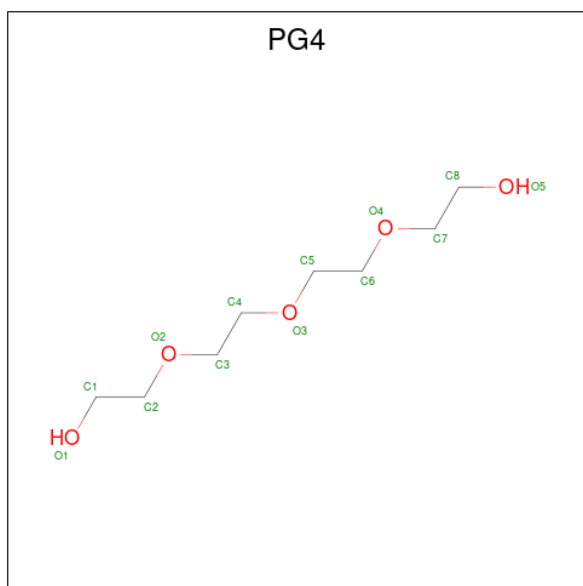
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total C O 13 8 5			0	0
5	BBB	1	Total C O 13 8 5			0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AAA	433	Total O 433 433		0	0
6	BBB	437	Total O 440 440		0	3

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.
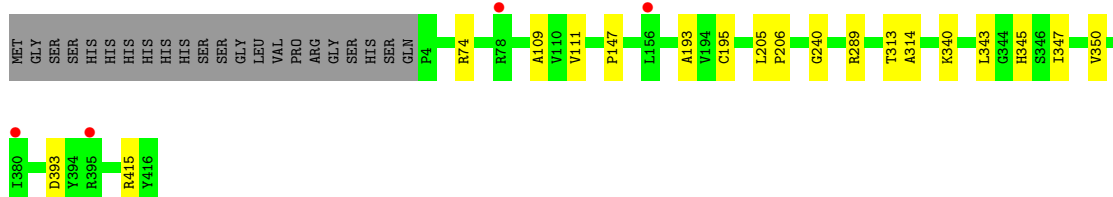
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1

Chain AAA:
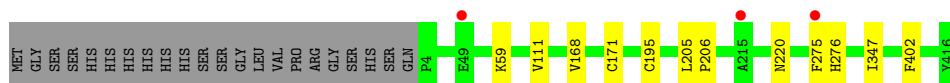
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 1

Chain BBB:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	75.31Å 75.31Å 149.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.22 – 1.53 65.22 – 1.53	Depositor EDS
% Data completeness (in resolution range)	99.4 (65.22-1.53) 100.0 (65.22-1.53)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 1.53Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.122 , 0.136 0.136 , 0.150	Depositor DCC
R_{free} test set	6993 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.1	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,l 0.019 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
Reported twinning fraction	0.841 for H, K, L 0.159 for K, H, -L	Depositor
Outliers	0 of 142070 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7243	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: NA, PG4, EDO, O6Z

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	AAA	0.63	0/3210	0.68	0/4355
1	BBB	0.63	0/3184	0.67	0/4319
All	All	0.63	0/6394	0.67	0/8674

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	AAA	3145	0	3082	7	0
1	BBB	3123	0	3064	12	0
2	AAA	20	0	30	0	0
2	BBB	20	0	30	0	0
3	AAA	17	0	0	0	0
3	BBB	17	0	0	0	0
4	AAA	1	0	0	0	0
4	BBB	1	0	0	0	0
5	AAA	13	0	18	0	0
5	BBB	13	0	18	0	0
6	AAA	433	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	440	0	0	0	0
All	All	7243	0	6242	18	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 1.

The worst 5 of 18 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:BBB:393[A]:ASP:OD1	1:BBB:415:ARG:NH1	2.36	0.58
1:BBB:74[B]:ARG:HD3	1:BBB:74[B]:ARG:O	2.04	0.57
1:AAA:275[A]:PHE:CD2	1:AAA:276[A]:HIS:HB2	2.40	0.56
1:BBB:289[B]:ARG:HE	1:BBB:289[B]:ARG:HA	1.71	0.55
1:BBB:74[B]:ARG:HD3	1:BBB:74[B]:ARG:C	2.28	0.54

There are no symmetry-related clashes.

5.3   Torsion angles   ⓘ

5.3.1   Protein backbone   ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	426/435 (98%)	413 (97%)	12 (3%)	1 (0%)	47	24
1	BBB	423/435 (97%)	413 (98%)	9 (2%)	1 (0%)	47	24
All	All	849/870 (98%)	826 (97%)	21 (2%)	2 (0%)	47	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	347	ILE
1	BBB	347	ILE

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	AAA	320/324 (99%)	320 (100%)	0	100	100
1	BBB	317/324 (98%)	316 (100%)	1 (0%)	92	84
All	All	637/648 (98%)	636 (100%)	1 (0%)	93	86

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	345	HIS

Sometimes 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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	$\#|Z| > 2$
2	EDO	AAA	504	-	3,3,3	0.06	0	2,2,2	0.10	0
2	EDO	BBB	502	-	3,3,3	0.06	0	2,2,2	0.12	0
2	EDO	BBB	504	-	3,3,3	0.05	0	2,2,2	0.09	0
2	EDO	AAA	503	-	3,3,3	0.04	0	2,2,2	0.17	0
2	EDO	AAA	501	-	3,3,3	0.09	0	2,2,2	0.28	0
2	EDO	BBB	501	-	3,3,3	0.04	0	2,2,2	0.13	0
3	O6Z	AAA	506	-	16,18,18	0.69	0	19,25,25	0.74	0
5	PG4	AAA	508	-	12,12,12	0.16	0	11,11,11	0.13	0
3	O6Z	BBB	506	-	16,18,18	0.70	0	19,25,25	0.83	1 (5%)
2	EDO	BBB	505	-	3,3,3	0.13	0	2,2,2	0.14	0
5	PG4	BBB	508	-	12,12,12	0.18	0	11,11,11	0.12	0
2	EDO	AAA	505	-	3,3,3	0.07	0	2,2,2	0.13	0
2	EDO	BBB	503	-	3,3,3	0.05	0	2,2,2	0.12	0
2	EDO	AAA	502	-	3,3,3	0.07	0	2,2,2	0.12	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	EDO	AAA	504	-	-	1/1/1/1	-
2	EDO	BBB	502	-	-	0/1/1/1	-
2	EDO	BBB	504	-	-	0/1/1/1	-
2	EDO	AAA	503	-	-	0/1/1/1	-
2	EDO	AAA	501	-	-	1/1/1/1	-
2	EDO	BBB	501	-	-	0/1/1/1	-
3	O6Z	AAA	506	-	-	0/10/10/10	0/2/2/2
5	PG4	AAA	508	-	-	3/10/10/10	-
3	O6Z	BBB	506	-	-	0/10/10/10	0/2/2/2
2	EDO	BBB	505	-	-	0/1/1/1	-
5	PG4	BBB	508	-	-	5/10/10/10	-
2	EDO	AAA	505	-	-	0/1/1/1	-
2	EDO	BBB	503	-	-	0/1/1/1	-
2	EDO	AAA	502	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BBB	506	O6Z	C11-S14-N17	2.23	109.88	106.72

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	508	PG4	O2-C3-C4-O3
5	AAA	508	PG4	O3-C5-C6-O4
5	BBB	508	PG4	O2-C3-C4-O3
5	BBB	508	PG4	O4-C7-C8-O5
5	BBB	508	PG4	O1-C1-C2-O2

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 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 O6Z AAA 506

Bond lengths

Bond angles

Torsions

Rings

Ligand O6Z BBB 506

Bond lengths

Bond angles

Torsions

Rings
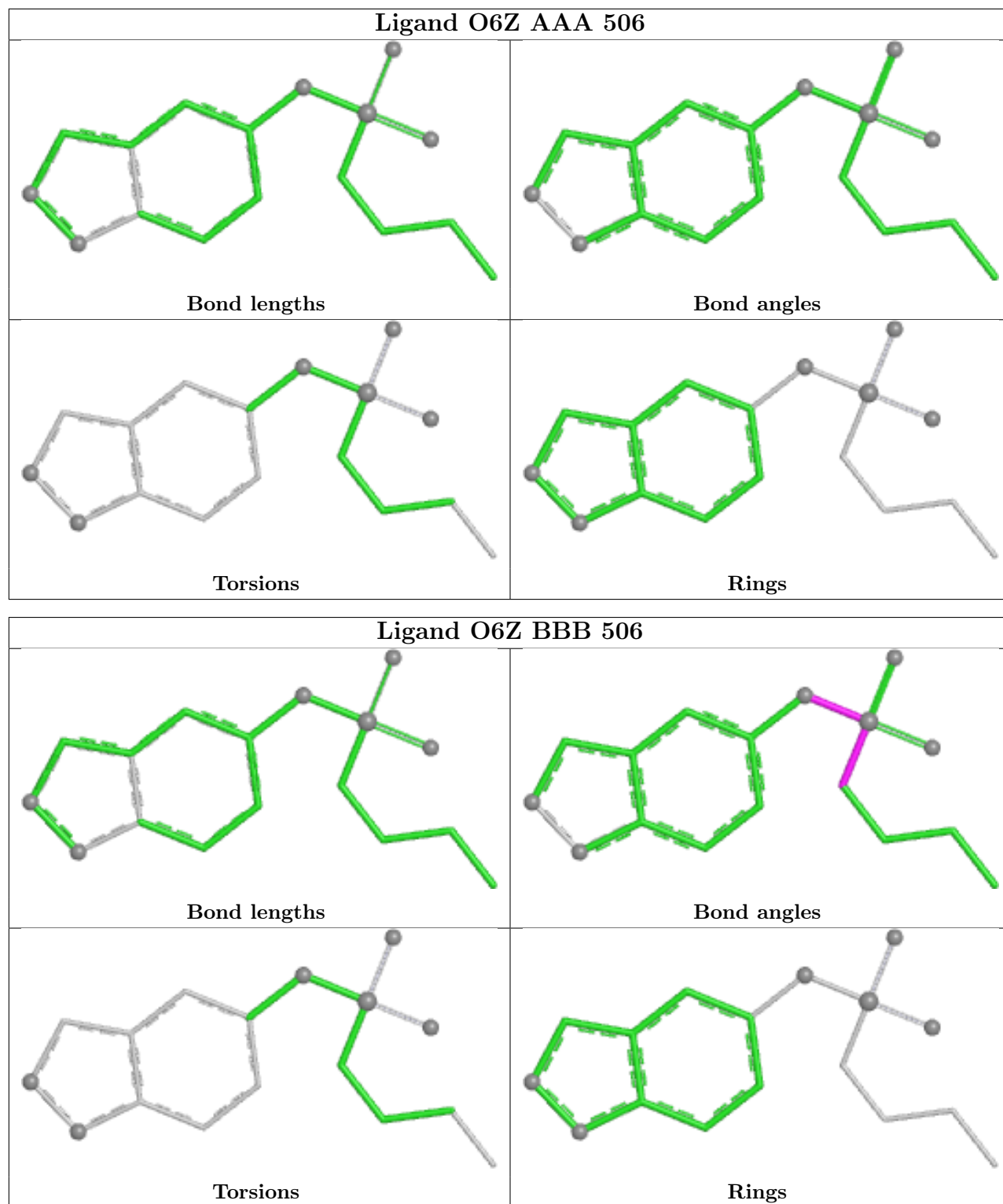
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	AAA	413/435 (94%)	-0.04	3 (0%)	87	90	14, 19, 29, 40	1 (0%)
1	BBB	413/435 (94%)	-0.01	4 (0%)	82	85	14, 20, 32, 38	1 (0%)
All	All	826/870 (94%)	-0.02	7 (0%)	86	88	14, 20, 31, 40	2 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	275[A]	PHE	3.1
1	BBB	78	ARG	3.1
1	BBB	156	LEU	2.4
1	AAA	49	GLU	2.3
1	AAA	215	ALA	2.3

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 monosaccharides 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, 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	EDO	BBB	503	4/4	0.81	0.19	38,39,39,41	0
5	PG4	BBB	508	13/13	0.81	0.14	33,35,40,43	0
5	PG4	AAA	508	13/13	0.82	0.13	31,35,43,44	0
2	EDO	BBB	502	4/4	0.82	0.17	31,34,36,39	0
2	EDO	AAA	503	4/4	0.89	0.14	29,32,35,35	0
2	EDO	BBB	504	4/4	0.91	0.18	32,34,35,36	0
2	EDO	BBB	505	4/4	0.91	0.24	28,28,30,30	0
2	EDO	BBB	501	4/4	0.92	0.14	24,28,29,31	0
2	EDO	AAA	504	4/4	0.93	0.14	34,36,36,36	0
2	EDO	AAA	505	4/4	0.94	0.17	26,30,31,32	0
2	EDO	AAA	502	4/4	0.95	0.13	20,21,22,23	0
2	EDO	AAA	501	4/4	0.96	0.10	21,22,23,23	0
3	O6Z	AAA	506	17/17	0.98	0.08	18,19,20,20	0
3	O6Z	BBB	506	17/17	0.98	0.07	18,19,19,20	0
4	NA	AAA	507	1/1	0.99	0.07	16,16,16,16	0
4	NA	BBB	507	1/1	1.00	0.09	16,16,16,16	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.
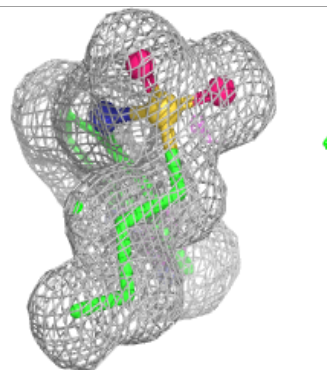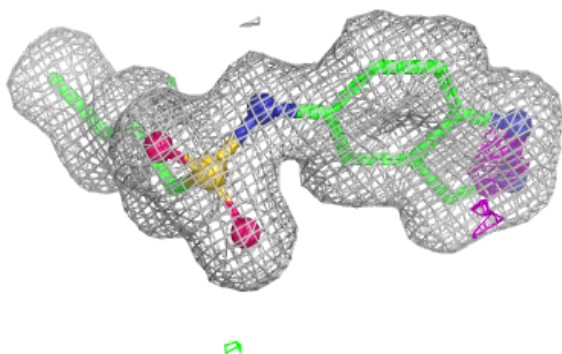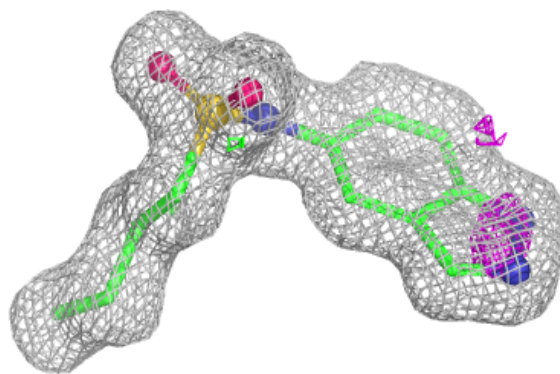

Electron density around O6Z AAA 506:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
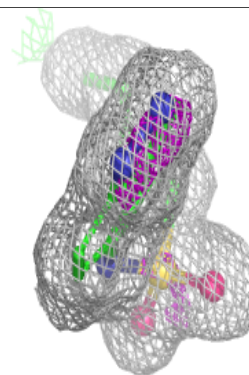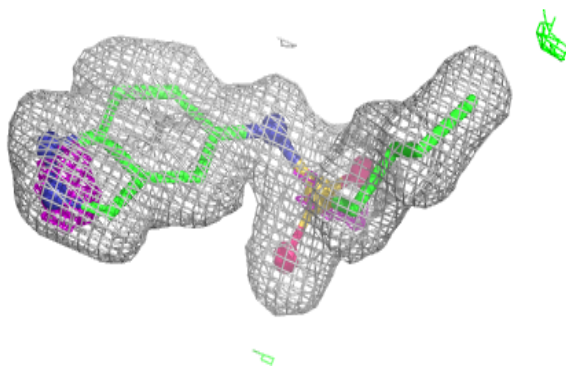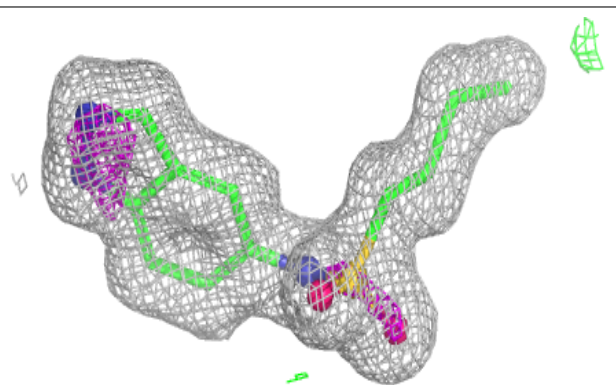
Electron density around O6Z BBB 506:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.