wwPDB X-ray Structure Validation Summary Report (i)

Oct 3, 2023 – 06:10 AM EDT

PDB ID	:	6U6C
Title	:	Crystal structure of tryptophan synthase from M. tuberculosis - aminoacrylate- and GSK2-bound form
Authors	:	Chang, C.; Michalska, K.; Maltseva, N.I.; Jedrzejczak, R.; McCarren, P.; Nag, P.P.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-08-29
Resolution	:	2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 21418 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 Tryptophan synthase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	1	0
			1807	1134	324	343	6			
1	C	249	Total	C	N	O	S	0	1	0
			1811	1136	324	345	6			
1	E	245	Total	C	N	O	S	0	1	0
			1784	1120	320	338	6			
1	G	249	Total	C	N	O	S	0	2	0
			1818	1140	328	344	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	271	HIS	-	expression tag	UNP P9WFY1
A	272	HIS	-	expression tag	UNP P9WFY1
A	273	HIS	-	expression tag	UNP P9WFY1
A	274	HIS	-	expression tag	UNP P9WFY1
A	275	HIS	-	expression tag	UNP P9WFY1
A	276	HIS	-	expression tag	UNP P9WFY1
C	271	HIS	-	expression tag	UNP P9WFY1
C	272	HIS	-	expression tag	UNP P9WFY1
C	273	HIS	-	expression tag	UNP P9WFY1
C	274	HIS	-	expression tag	UNP P9WFY1
C	275	HIS	-	expression tag	UNP P9WFY1
C	276	HIS	-	expression tag	UNP P9WFY1
E	271	HIS	-	expression tag	UNP P9WFY1
E	272	HIS	-	expression tag	UNP P9WFY1
E	273	HIS	-	expression tag	UNP P9WFY1
E	274	HIS	-	expression tag	UNP P9WFY1
E	275	HIS	-	expression tag	UNP P9WFY1
E	276	HIS	-	expression tag	UNP P9WFY1
G	271	HIS	-	expression tag	UNP P9WFY1
G	272	HIS	-	expression tag	UNP P9WFY1
G	273	HIS	-	expression tag	UNP P9WFY1

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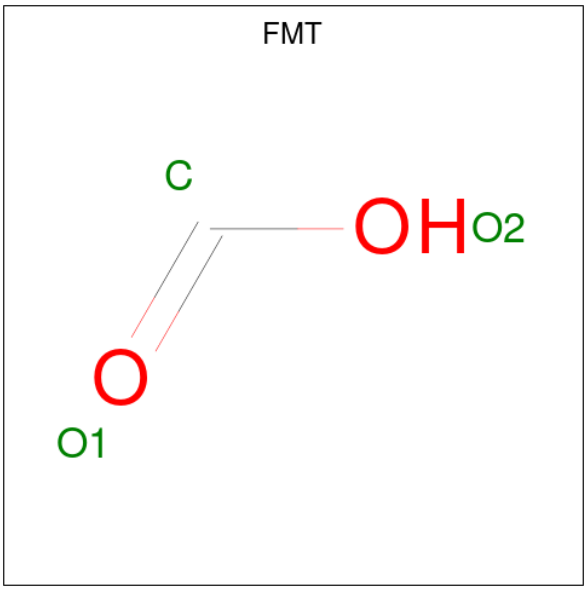
Chain	Residue	Modelled	Actual	Comment	Reference
G	274	HIS	-	expression tag	UNP P9WFY1
G	275	HIS	-	expression tag	UNP P9WFY1
G	276	HIS	-	expression tag	UNP P9WFY1

- Molecule 2 is a protein called Tryptophan synthase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	405	Total	C	N	O	S	0	8	0
			3083	1919	565	586	13			
2	D	404	Total	C	N	O	S	0	4	0
			3046	1901	553	579	13			
2	F	404	Total	C	N	O	S	0	3	0
			3036	1896	551	576	13			
2	H	404	Total	C	N	O	S	0	13	0
			3106	1940	564	588	14			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		
3	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	E	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	F	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	G	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

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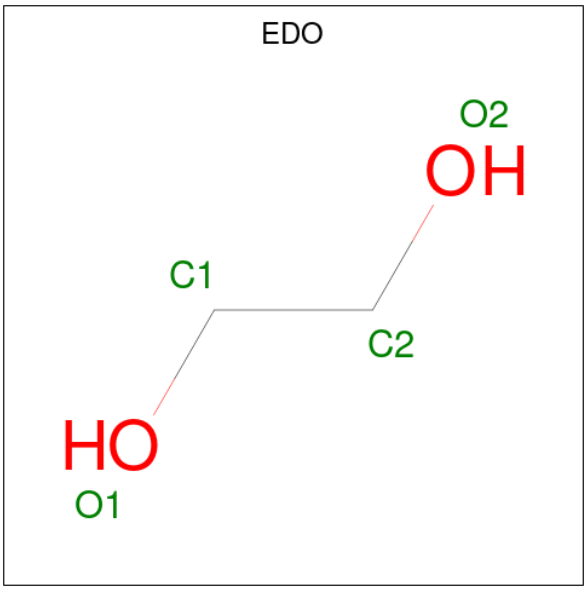
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0
3	H	1	Total C O 3 1 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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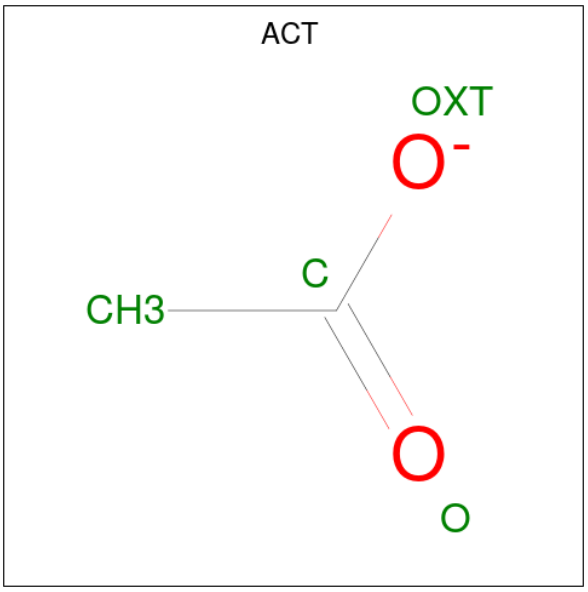
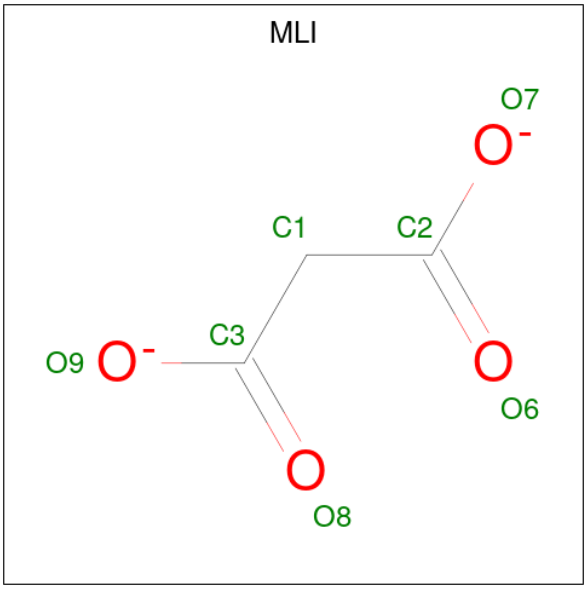
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



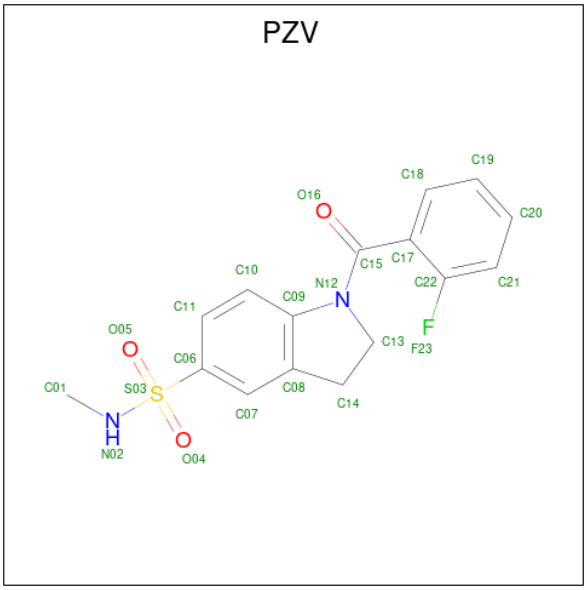
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	H	1	Total C O 4 2 2	0	0

- Molecule 6 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 3 4	0	0
6	C	1	Total C O 7 3 4	0	0
6	E	1	Total C O 7 3 4	0	0
6	F	1	Total C O 7 3 4	0	0
6	G	1	Total C O 7 3 4	0	0
6	H	1	Total C O 7 3 4	0	0

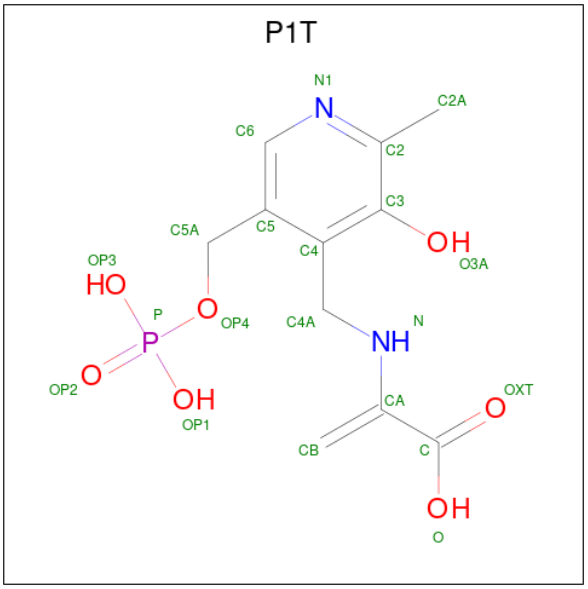
- Molecule 7 is 1-(2-fluorobenzene-1-carbonyl)-N-methyl-2,3-dihydro-1H-indole-5-sulfonamide (three-letter code: PZV) (formula: $C_{16}H_{15}FN_2O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C F N O S 23 16 1 2 3 1	0	0
7	D	1	Total C F N O S 23 16 1 2 3 1	0	0
7	F	1	Total C F N O S 23 16 1 2 3 1	0	0
7	H	1	Total C F N O S 23 16 1 2 3 1	0	0

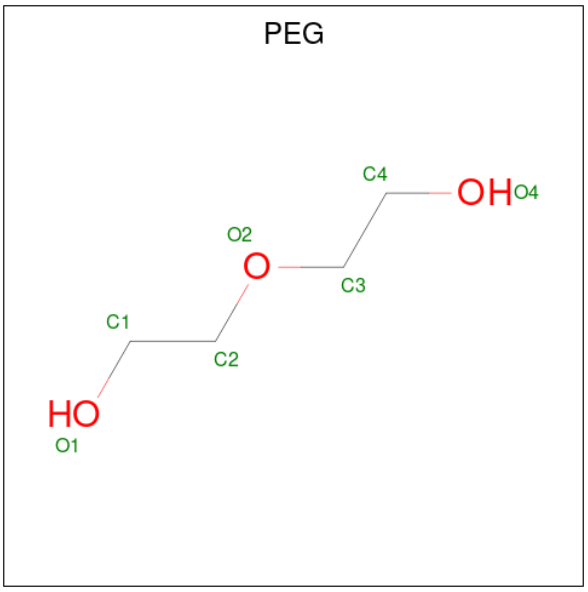
- Molecule 8 is 2-[({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PY

RIDIN-4-YL}METHYL)AMINO]ACRYLIC ACID (three-letter code: P1T) (formula: $C_{11}H_{15}N_2O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	D	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	F	1	Total	C	N	O	P	0	0
			21	11	2	7	1		
8	H	1	Total	C	N	O	P	0	0
			21	11	2	7	1		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

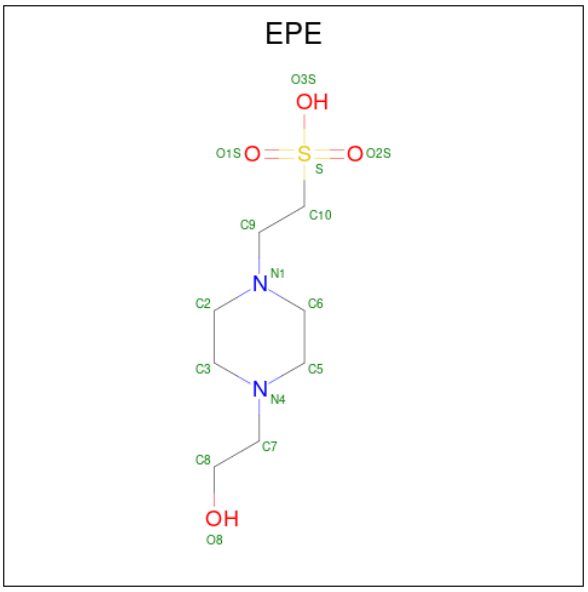


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 7 4 3	0	0
9	F	1	Total C O 7 4 3	0	0
9	G	1	Total C O 7 4 3	0	0
9	H	1	Total C O 7 4 3	0	0

- Molecule 10 is POTASSIUM ION (three-letter code: K) (formula: K).

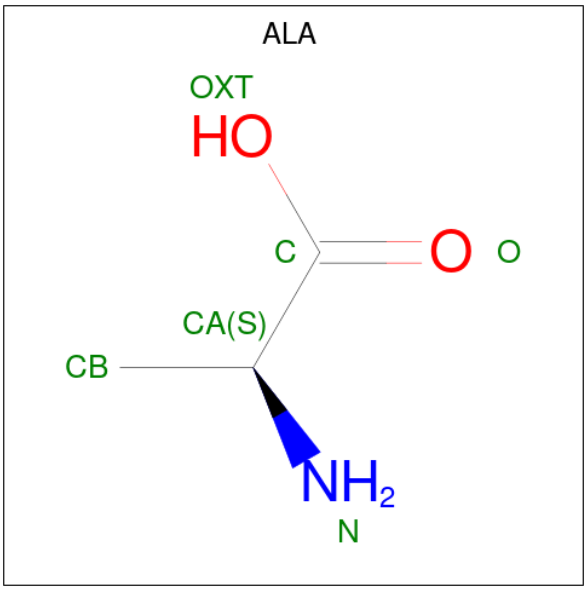
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total K 1 1	0	0
10	C	1	Total K 1 1	0	0
10	D	3	Total K 3 3	0	0
10	F	1	Total K 1 1	0	0
10	G	1	Total K 1 1	0	0
10	H	1	Total K 1 1	0	0

- Molecule 11 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



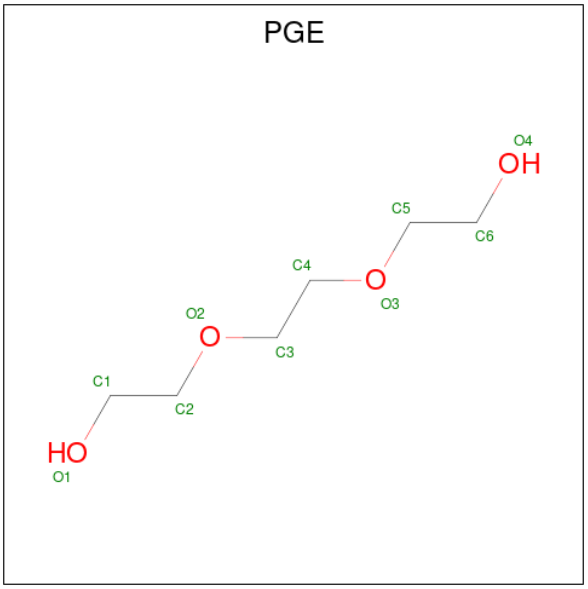
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C N O S 15 8 2 4 1	0	0
11	B	1	Total C N O S 15 8 2 4 1	0	0
11	F	1	Total C N O S 15 8 2 4 1	0	0
11	H	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 12 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	E	1	Total C N O 5 3 1 1	0	0

- Molecule 13 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	F	1	Total C O 10 6 4	0	0
13	F	1	Total C O 10 6 4	0	0

- Molecule 14 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	F	1	Total Na 1 1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	107	Total O 107 107	0	0
15	B	201	Total O 201 201	0	0
15	C	113	Total O 113 113	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	202	Total O 202 202	0	0
15	E	71	Total O 71 71	0	0
15	F	181	Total O 181 181	0	0
15	G	124	Total O 124 124	0	0
15	H	196	Total O 196 196	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	135.11Å 159.23Å 164.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.40	Depositor
% Data completeness (in resolution range)	99.5 (29.88-2.40)	Depositor
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.153 , 0.195	Depositor
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.514	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
Total number of atoms	21418	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 155 ligands modelled in this entry, 9 are monoatomic - leaving 146 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	$\#\|Z\| > 2$
3	FMT	F	810	-	2,2,2	0.70	0	1,1,1	0.22	0
4	EDO	D	511	-	3,3,3	0.47	0	2,2,2	0.31	0
5	ACT	F	818	-	3,3,3	1.20	0	3,3,3	1.53	0
9	PEG	G	309	-	6,6,6	0.14	0	5,5,5	0.12	0
3	FMT	B	513	-	2,2,2	0.70	0	1,1,1	0.19	0
3	FMT	B	528	-	2,2,2	0.73	0	1,1,1	0.28	0
7	PZV	B	501	-	24,25,25	1.86	7 (29%)	32,37,37	3.03	8 (25%)
3	FMT	C	305	-	2,2,2	0.70	0	1,1,1	0.21	0
4	EDO	F	822	-	3,3,3	0.47	0	2,2,2	0.32	0
3	FMT	F	816	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	G	302	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	B	514	-	2,2,2	0.70	0	1,1,1	0.24	0
3	FMT	F	815	-	2,2,2	0.70	0	1,1,1	0.23	0
3	FMT	D	509	-	2,2,2	0.72	0	1,1,1	0.26	0
3	FMT	D	515	-	2,2,2	0.68	0	1,1,1	0.23	0
3	FMT	F	813	-	2,2,2	0.68	0	1,1,1	0.14	0
3	FMT	D	508	-	2,2,2	0.71	0	1,1,1	0.23	0
4	EDO	B	529	-	3,3,3	0.49	0	2,2,2	0.08	0
4	EDO	H	533	-	3,3,3	0.51	0	2,2,2	0.12	0
8	P1T	B	502	-	20,21,21	2.35	2 (10%)	28,30,30	1.73	4 (14%)
3	FMT	D	514	-	2,2,2	0.70	0	1,1,1	0.24	0
3	FMT	C	309	-	2,2,2	0.70	0	1,1,1	0.13	0
4	EDO	H	521	-	3,3,3	0.46	0	2,2,2	0.34	0
3	FMT	C	302	-	2,2,2	0.70	0	1,1,1	0.17	0
3	FMT	D	506	-	2,2,2	0.67	0	1,1,1	0.21	0
3	FMT	D	504	-	2,2,2	0.68	0	1,1,1	0.17	0
3	FMT	H	514	-	2,2,2	0.68	0	1,1,1	0.16	0
4	EDO	B	511	-	3,3,3	0.48	0	2,2,2	0.25	0
3	FMT	B	504	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	H	526	-	2,2,2	0.69	0	1,1,1	0.17	0
6	MLI	E	302	-	6,6,6	1.33	0	7,7,7	0.93	0
3	FMT	B	521	-	2,2,2	0.69	0	1,1,1	0.21	0
12	ALA	E	301	-	3,4,5	0.67	0	2,4,6	0.80	0
8	P1T	D	505	-	20,21,21	2.30	2 (10%)	28,30,30	1.85	4 (14%)
6	MLI	F	827	-	6,6,6	1.34	0	7,7,7	0.95	0
13	PGE	F	809	-	9,9,9	0.33	0	8,8,8	0.28	0
3	FMT	H	518	-	2,2,2	0.72	0	1,1,1	0.21	0
3	FMT	B	524	-	2,2,2	0.70	0	1,1,1	0.21	0
9	PEG	B	506	-	6,6,6	0.12	0	5,5,5	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FMT	G	306	-	2,2,2	0.66	0	1,1,1	0.16	0
4	EDO	A	304	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	C	303	10	3,3,3	0.42	0	2,2,2	0.35	0
3	FMT	B	519	-	2,2,2	0.71	0	1,1,1	0.23	0
6	MLI	H	530	-	6,6,6	1.31	0	7,7,7	1.00	0
3	FMT	A	308	-	2,2,2	0.70	0	1,1,1	0.29	0
4	EDO	F	812	-	3,3,3	0.44	0	2,2,2	0.34	0
3	FMT	G	307	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	H	516	-	2,2,2	0.70	0	1,1,1	0.21	0
3	FMT	E	304	-	2,2,2	0.72	0	1,1,1	0.24	0
3	FMT	H	517	-	2,2,2	0.69	0	1,1,1	0.17	0
3	FMT	H	501	-	2,2,2	0.64	0	1,1,1	0.13	0
3	FMT	G	305	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	D	502	-	2,2,2	0.67	0	1,1,1	0.18	0
3	FMT	B	512	-	2,2,2	0.71	0	1,1,1	0.23	0
3	FMT	D	513	-	2,2,2	0.69	0	1,1,1	0.21	0
4	EDO	E	305	-	3,3,3	0.48	0	2,2,2	0.29	0
3	FMT	A	307	-	2,2,2	0.72	0	1,1,1	0.25	0
3	FMT	B	518	-	2,2,2	0.68	0	1,1,1	0.20	0
4	EDO	B	526	-	3,3,3	0.48	0	2,2,2	0.26	0
11	EPE	B	530	-	15,15,15	1.76	1 (6%)	18,20,20	1.69	3 (16%)
3	FMT	H	529	-	2,2,2	0.71	0	1,1,1	0.23	0
4	EDO	G	310	-	3,3,3	0.54	0	2,2,2	0.14	0
3	FMT	H	511	-	2,2,2	0.69	0	1,1,1	0.21	0
5	ACT	H	506	-	3,3,3	1.36	1 (33%)	3,3,3	1.50	0
3	FMT	D	510	-	2,2,2	0.71	0	1,1,1	0.23	0
4	EDO	C	306	10	3,3,3	0.47	0	2,2,2	0.20	0
3	FMT	B	507	-	2,2,2	0.72	0	1,1,1	0.29	0
3	FMT	F	803	-	2,2,2	0.70	0	1,1,1	0.24	0
3	FMT	D	521	-	2,2,2	0.73	0	1,1,1	0.29	0
3	FMT	B	522	-	2,2,2	0.70	0	1,1,1	0.20	0
4	EDO	D	520	-	3,3,3	0.47	0	2,2,2	0.28	0
3	FMT	G	303	-	2,2,2	0.71	0	1,1,1	0.21	0
3	FMT	H	519	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	E	303	-	2,2,2	0.67	0	1,1,1	0.15	0
3	FMT	G	308	-	2,2,2	0.70	0	1,1,1	0.22	0
4	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.33	0
8	P1T	F	805	-	20,21,21	2.47	2 (10%)	28,30,30	1.68	4 (14%)
6	MLI	A	311	-	6,6,6	1.36	0	7,7,7	0.97	0
3	FMT	A	309	-	2,2,2	0.69	0	1,1,1	0.24	0
3	FMT	F	811	-	2,2,2	0.67	0	1,1,1	0.14	0
5	ACT	A	312	-	3,3,3	1.40	1 (33%)	3,3,3	1.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	G	312	-	3,3,3	0.59	0	2,2,2	0.19	0
3	FMT	B	531	-	2,2,2	0.72	0	1,1,1	0.24	0
3	FMT	B	508	-	2,2,2	0.70	0	1,1,1	0.23	0
4	EDO	H	512	-	3,3,3	0.52	0	2,2,2	0.02	0
3	FMT	B	523	-	2,2,2	0.68	0	1,1,1	0.19	0
9	PEG	F	829	-	6,6,6	0.12	0	5,5,5	0.09	0
4	EDO	F	819	-	3,3,3	0.48	0	2,2,2	0.25	0
3	FMT	G	301	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	B	520	-	2,2,2	0.69	0	1,1,1	0.14	0
11	EPE	F	830	-	15,15,15	2.02	1 (6%)	18,20,20	1.54	3 (16%)
3	FMT	H	507	-	2,2,2	0.70	0	1,1,1	0.18	0
3	FMT	H	524	-	2,2,2	0.68	0	1,1,1	0.19	0
3	FMT	A	301	-	2,2,2	0.70	0	1,1,1	0.19	0
3	FMT	D	516	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	H	522	-	2,2,2	0.70	0	1,1,1	0.18	0
5	ACT	A	310	-	3,3,3	1.35	0	3,3,3	1.52	0
3	FMT	H	508	-	2,2,2	0.68	0	1,1,1	0.14	0
11	EPE	B	527	-	15,15,15	1.99	1 (6%)	18,20,20	1.13	1 (5%)
3	FMT	F	814	-	2,2,2	0.66	0	1,1,1	0.13	0
3	FMT	H	503	-	2,2,2	0.69	0	1,1,1	0.19	0
3	FMT	H	523	-	2,2,2	0.68	0	1,1,1	0.16	0
6	MLI	G	311	-	6,6,6	1.31	0	7,7,7	0.97	0
3	FMT	D	517	-	2,2,2	0.70	0	1,1,1	0.23	0
3	FMT	D	512	-	2,2,2	0.70	0	1,1,1	0.16	0
7	PZV	F	802	-	24,25,25	1.85	5 (20%)	32,37,37	3.01	7 (21%)
11	EPE	H	532	-	15,15,15	1.90	1 (6%)	18,20,20	1.17	3 (16%)
4	EDO	B	510	-	3,3,3	0.51	0	2,2,2	0.15	0
3	FMT	F	817	-	2,2,2	0.69	0	1,1,1	0.21	0
3	FMT	H	509	-	2,2,2	0.69	0	1,1,1	0.20	0
3	FMT	F	806	-	2,2,2	0.74	0	1,1,1	0.31	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.44	0
4	EDO	C	301	-	3,3,3	0.49	0	2,2,2	0.16	0
6	MLI	C	307	-	6,6,6	1.33	0	7,7,7	1.04	0
3	FMT	B	505	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	F	828	-	2,2,2	0.68	0	1,1,1	0.20	0
3	FMT	B	515	-	2,2,2	0.68	0	1,1,1	0.20	0
3	FMT	F	807	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	A	306	-	2,2,2	0.70	0	1,1,1	0.22	0
7	PZV	D	501	-	24,25,25	1.83	4 (16%)	32,37,37	2.97	9 (28%)
3	FMT	G	304	-	2,2,2	0.70	0	1,1,1	0.19	0
4	EDO	H	520	-	3,3,3	0.54	0	2,2,2	0.03	0
3	FMT	A	302	-	2,2,2	0.68	0	1,1,1	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FMT	F	823	-	2,2,2	0.69	0	1,1,1	0.18	0
3	FMT	A	305	-	2,2,2	0.70	0	1,1,1	0.20	0
3	FMT	H	525	-	2,2,2	0.68	0	1,1,1	0.22	0
3	FMT	F	824	-	2,2,2	0.69	0	1,1,1	0.21	0
4	EDO	H	505	-	3,3,3	0.47	0	2,2,2	0.29	0
3	FMT	D	503	-	2,2,2	0.68	0	1,1,1	0.16	0
3	FMT	H	528	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	A	303	-	2,2,2	0.67	0	1,1,1	0.16	0
3	FMT	F	820	-	2,2,2	0.71	0	1,1,1	0.25	0
3	FMT	H	515	-	2,2,2	0.67	0	1,1,1	0.14	0
13	PGE	F	801	-	9,9,9	0.33	0	8,8,8	0.47	0
7	PZV	H	502	-	24,25,25	1.83	4 (16%)	32,37,37	3.30	8 (25%)
3	FMT	B	517	-	2,2,2	0.72	0	1,1,1	0.22	0
4	EDO	B	516	-	3,3,3	0.45	0	2,2,2	0.42	0
3	FMT	H	510	-	2,2,2	0.68	0	1,1,1	0.19	0
5	ACT	F	808	-	3,3,3	1.33	0	3,3,3	1.50	0
3	FMT	D	507	-	2,2,2	0.71	0	1,1,1	0.26	0
3	FMT	C	304	-	2,2,2	0.71	0	1,1,1	0.25	0
3	FMT	F	804	-	2,2,2	0.71	0	1,1,1	0.24	0
3	FMT	H	527	-	2,2,2	0.68	0	1,1,1	0.23	0
8	P1T	H	504	-	20,21,21	2.39	2 (10%)	28,30,30	1.73	4 (14%)
3	FMT	F	821	-	2,2,2	0.69	0	1,1,1	0.19	0
9	PEG	H	513	-	6,6,6	0.12	0	5,5,5	0.08	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	EDO	G	310	-	-	1/1/1/1	-
11	EPE	H	532	-	-	6/9/19/19	0/1/1/1
4	EDO	B	510	-	-	0/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
4	EDO	C	306	10	-	0/1/1/1	-
9	PEG	G	309	-	-	0/4/4/4	-
12	ALA	E	301	-	-	0/0/2/4	-
8	P1T	D	505	-	-	5/14/15/15	0/1/1/1
6	MLI	F	827	-	-	4/4/4/4	-
7	PZV	B	501	-	-	0/17/26/26	0/3/3/3
4	EDO	F	822	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PGE	F	809	-	-	6/7/7/7	-
4	EDO	D	520	-	-	0/1/1/1	-
4	EDO	B	503	-	-	0/1/1/1	-
4	EDO	C	301	-	-	0/1/1/1	-
6	MLI	C	307	-	-	0/4/4/4	-
9	PEG	B	506	-	-	0/4/4/4	-
8	P1T	F	805	-	-	5/14/15/15	0/1/1/1
4	EDO	B	509	-	-	0/1/1/1	-
4	EDO	B	529	-	-	0/1/1/1	-
6	MLI	A	311	-	-	2/4/4/4	-
7	PZV	D	501	-	-	0/17/26/26	0/3/3/3
4	EDO	H	533	-	-	1/1/1/1	-
8	P1T	B	502	-	-	5/14/15/15	0/1/1/1
4	EDO	A	304	-	-	0/1/1/1	-
4	EDO	H	520	-	-	0/1/1/1	-
4	EDO	C	303	10	-	0/1/1/1	-
4	EDO	H	505	-	-	0/1/1/1	-
6	MLI	H	530	-	-	4/4/4/4	-
4	EDO	G	312	-	-	0/1/1/1	-
4	EDO	F	812	-	-	0/1/1/1	-
4	EDO	H	512	-	-	0/1/1/1	-
4	EDO	H	521	-	-	1/1/1/1	-
9	PEG	F	829	-	-	1/4/4/4	-
4	EDO	F	819	-	-	0/1/1/1	-
11	EPE	F	830	-	-	2/9/19/19	0/1/1/1
13	PGE	F	801	-	-	3/7/7/7	-
7	PZV	H	502	-	-	0/17/26/26	0/3/3/3
4	EDO	B	516	-	-	1/1/1/1	-
4	EDO	B	511	-	-	0/1/1/1	-
11	EPE	B	527	-	-	5/9/19/19	0/1/1/1
8	P1T	H	504	-	-	5/14/15/15	0/1/1/1
4	EDO	E	305	-	-	0/1/1/1	-
6	MLI	E	302	-	-	2/4/4/4	-
4	EDO	B	526	-	-	0/1/1/1	-
11	EPE	B	530	-	-	3/9/19/19	0/1/1/1
6	MLI	G	311	-	-	0/4/4/4	-
9	PEG	H	513	-	-	1/4/4/4	-
7	PZV	F	802	-	-	0/17/26/26	0/3/3/3

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	805	P1T	CA-C	-10.65	1.34	1.49
8	H	504	P1T	CA-C	-10.30	1.34	1.49
8	B	502	P1T	CA-C	-10.11	1.34	1.49
8	D	505	P1T	CA-C	-9.89	1.35	1.49
11	F	830	EPE	C10-S	-7.55	1.66	1.77

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	502	PZV	O05-S03-O04	-14.27	102.00	119.55
7	B	501	PZV	O05-S03-O04	-13.02	103.55	119.55
7	F	802	PZV	O05-S03-O04	-12.99	103.58	119.55
7	D	501	PZV	O05-S03-O04	-12.32	104.41	119.55
7	D	501	PZV	O05-S03-N02	6.26	114.14	107.08

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

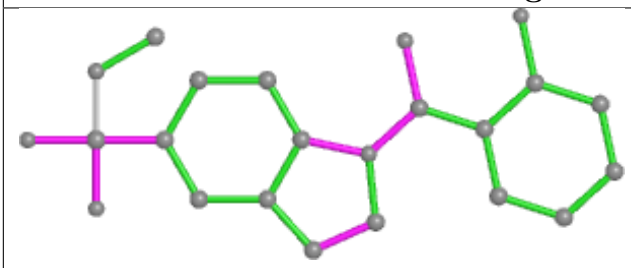
Mol	Chain	Res	Type	Atoms
8	B	502	P1T	C5-C4-C4A-N
8	D	505	P1T	C5-C4-C4A-N
8	D	505	P1T	C3-C4-C4A-N
8	F	805	P1T	C5-C4-C4A-N
8	H	504	P1T	C5-C4-C4A-N

There are no ring outliers.

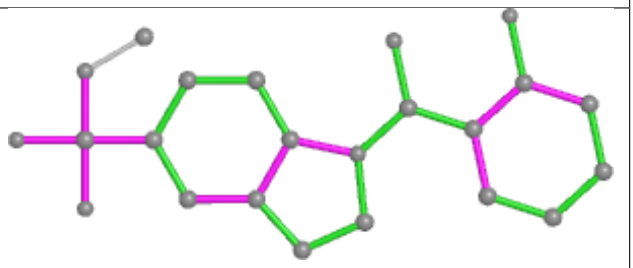
No monomer is involved in short contacts.

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.

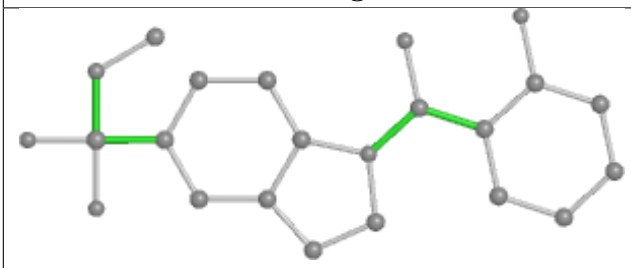
Ligand PZV B 501



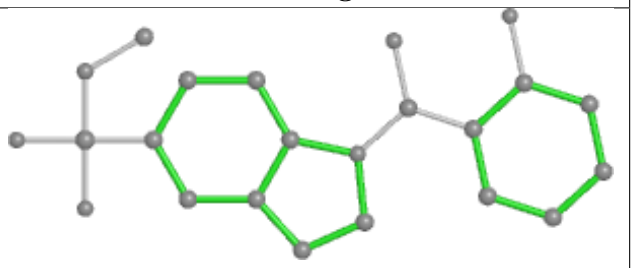
Bond lengths



Bond angles

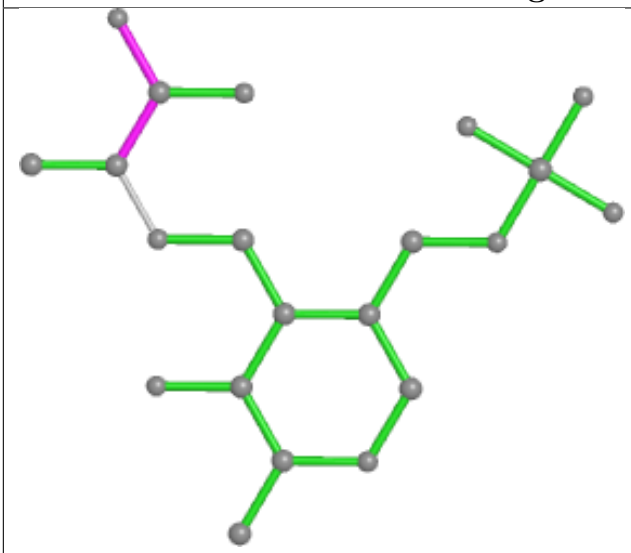


Torsions

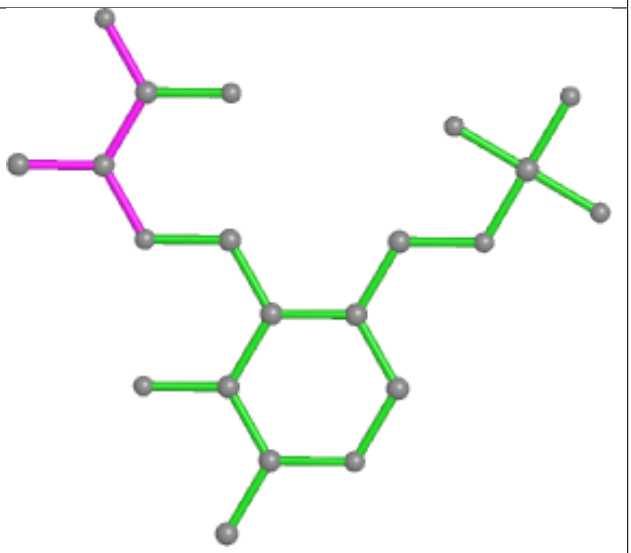


Rings

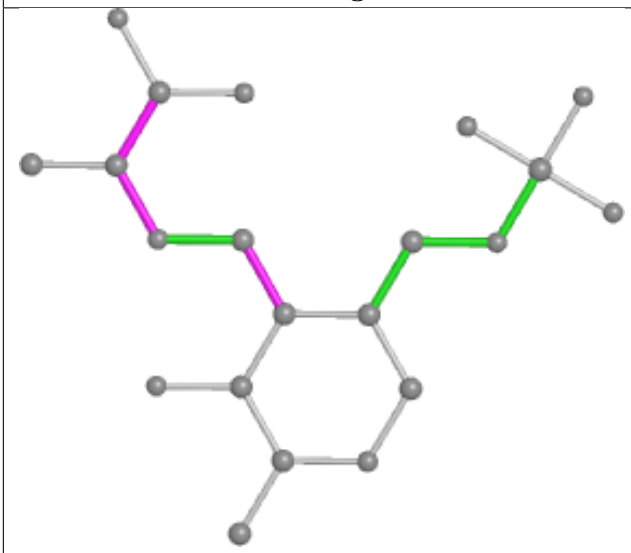
Ligand P1T B 502



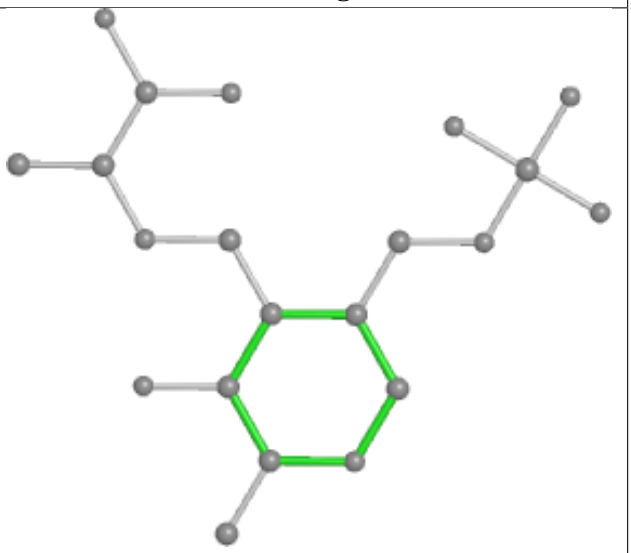
Bond lengths



Bond angles

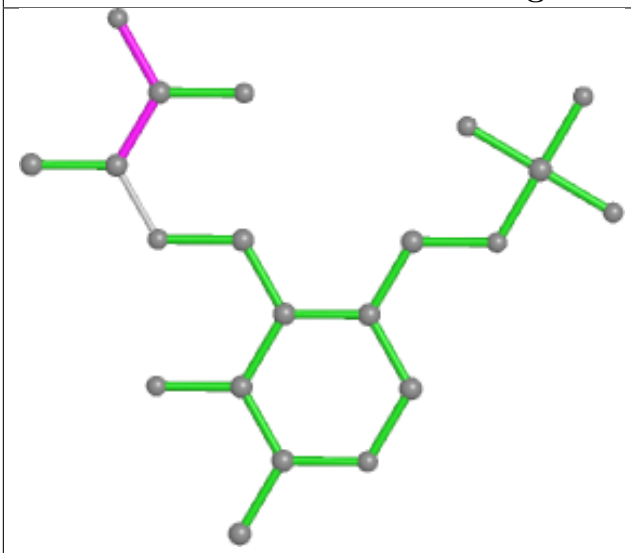


Torsions

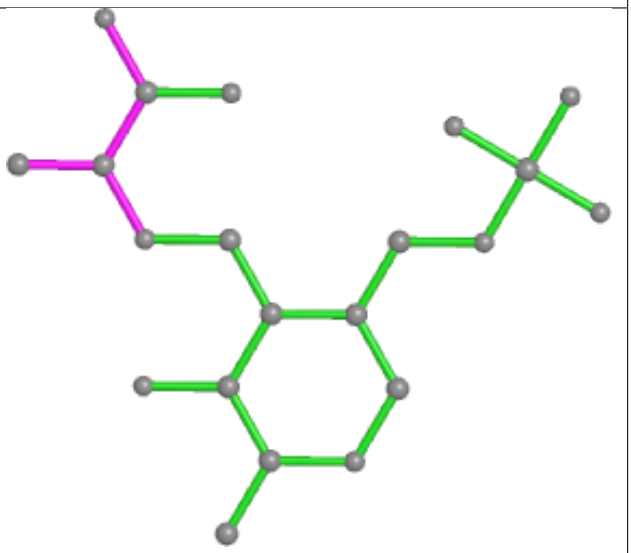


Rings

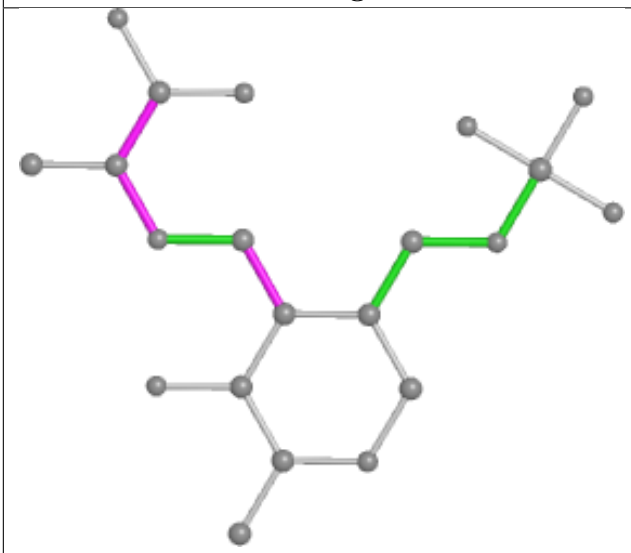
Ligand P1T D 505



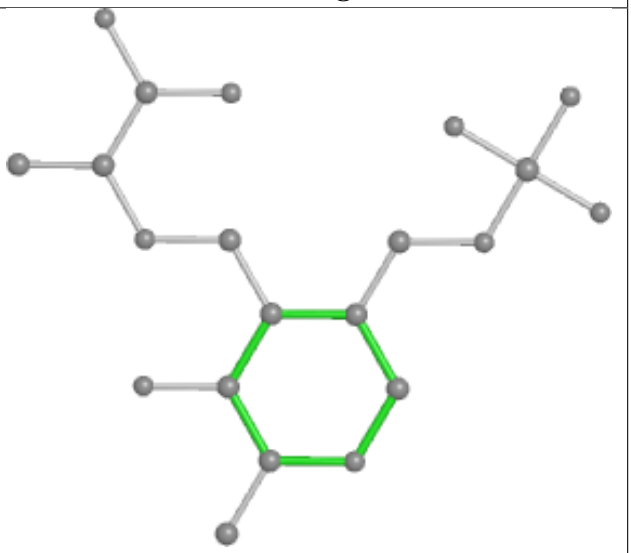
Bond lengths



Bond angles

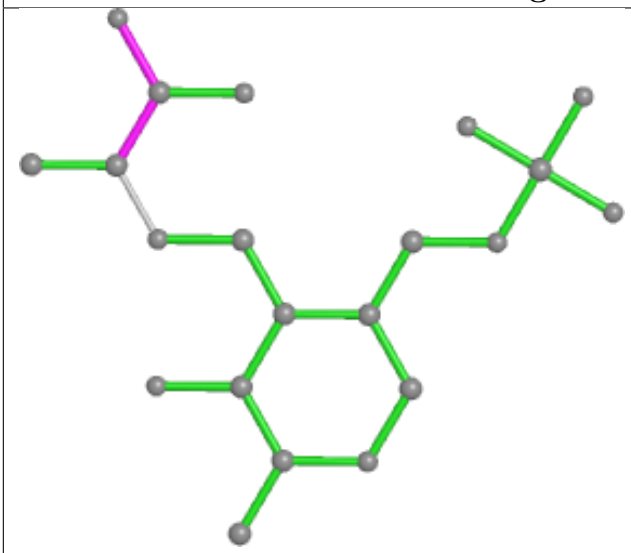


Torsions

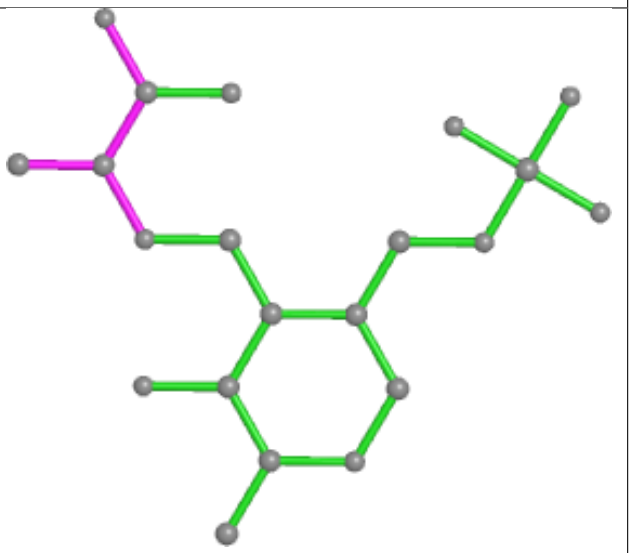


Rings

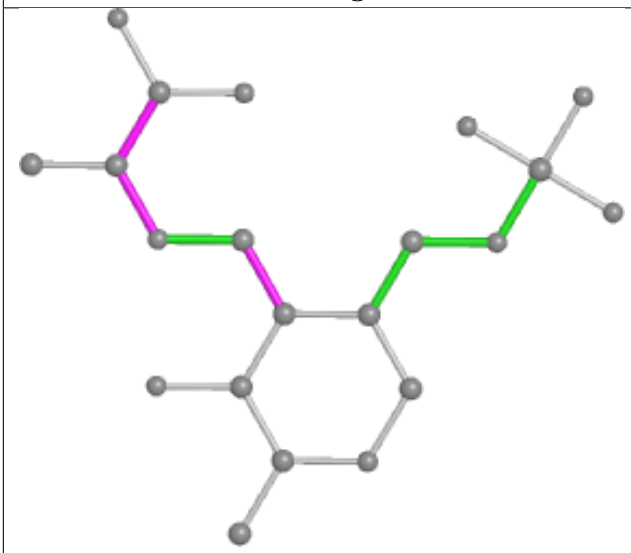
Ligand P1T F 805



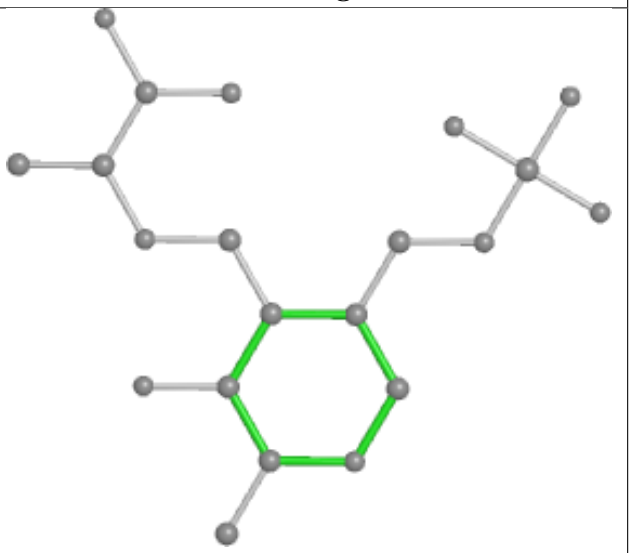
Bond lengths



Bond angles

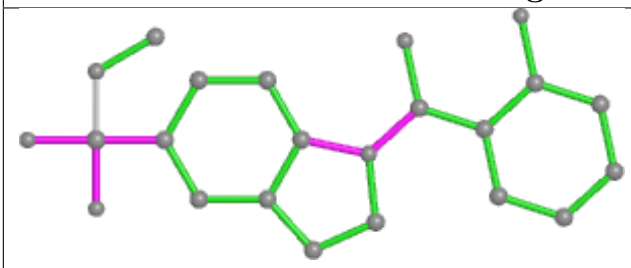


Torsions

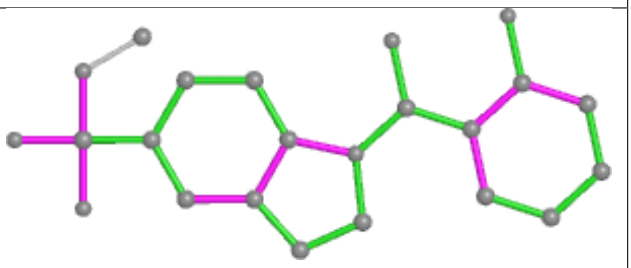


Rings

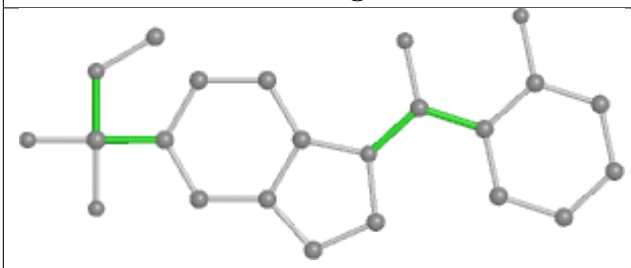
Ligand PZV F 802



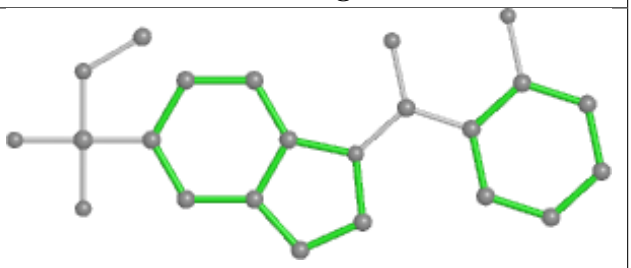
Bond lengths



Bond angles

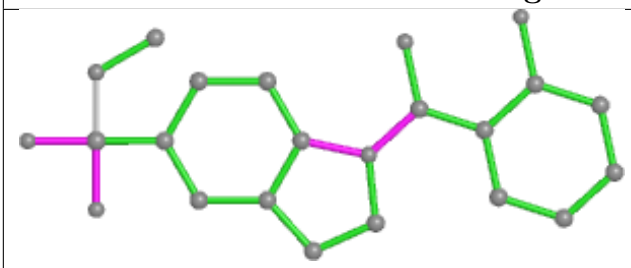


Torsions

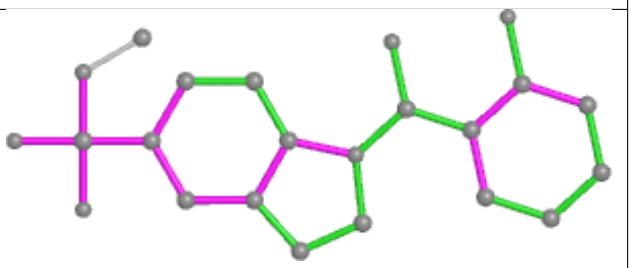


Rings

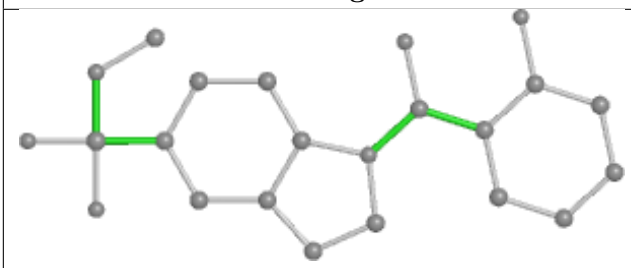
Ligand PZV D 501



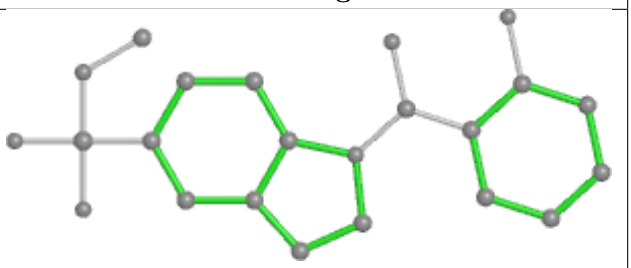
Bond lengths



Bond angles

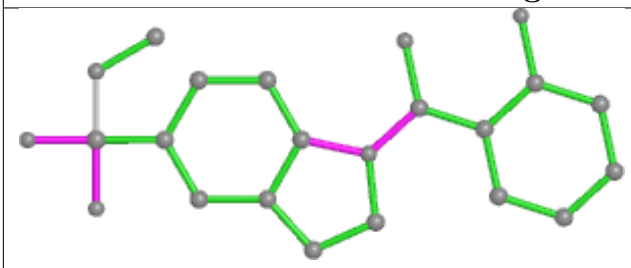


Torsions



Rings

Ligand PZV H 502



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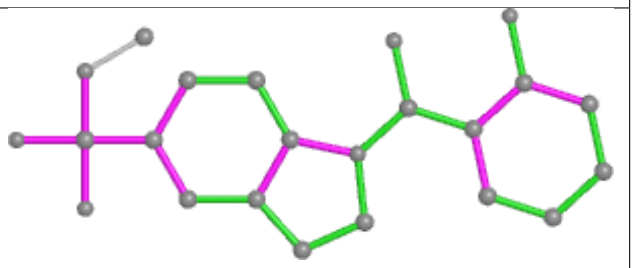
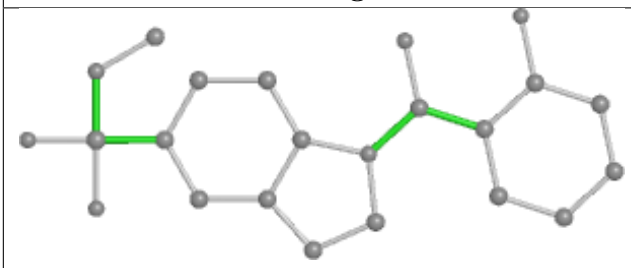
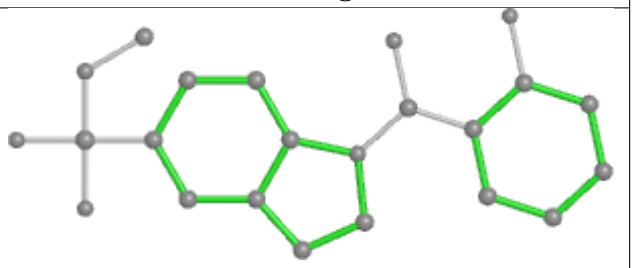


Bond angles

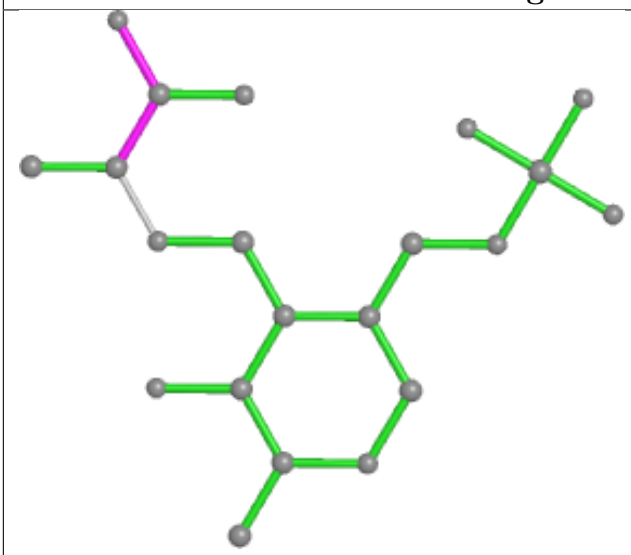


Torsions

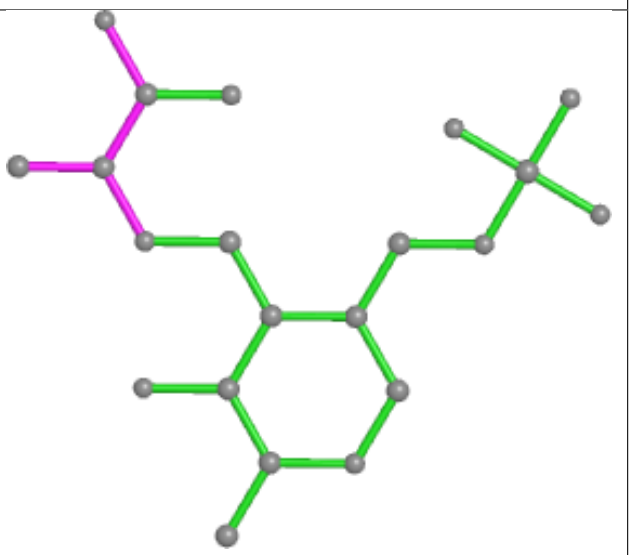


Rings

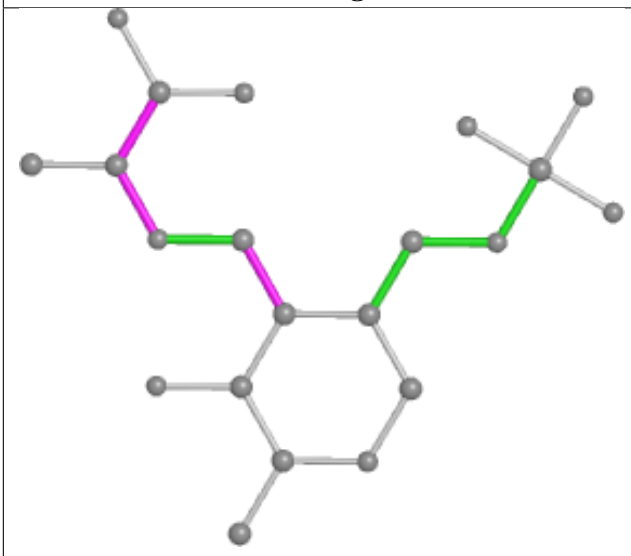
Ligand P1T H 504



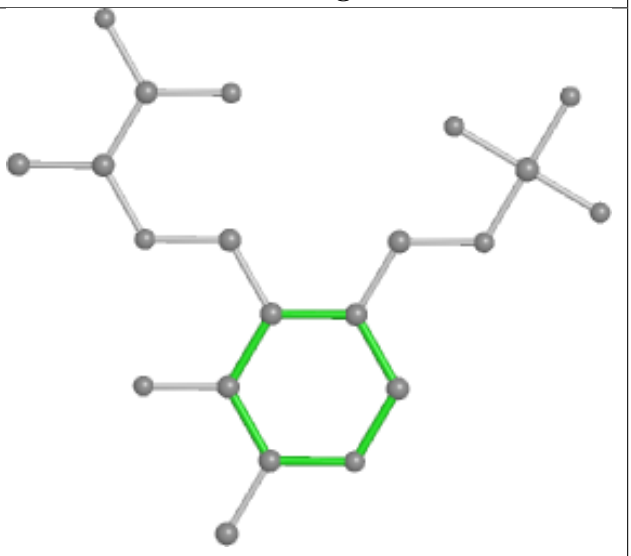
Bond lengths



Bond angles



Torsions



Rings

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.