wwPDB X-ray Structure Validation Summary Report (i)

Jan 27, 2024 – 03:00 PM EST

PDB ID	:	1AQX
Title	:	GLUTATHIONE S-TRANSFERASE IN COMPLEX WITH MEISENHEIMER COMPLEX
Authors	:	Prade, L.; Huber, R.; Manoharan, T.H.; Fahl, W.E.; Reuter, W.
Deposited on	:	1997-08-03
Resolution	:	2.00 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:

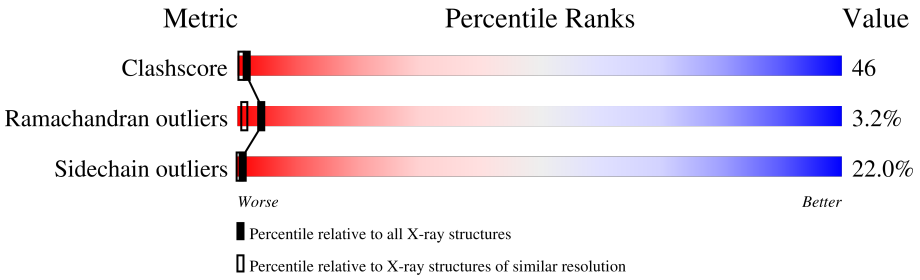
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	28% 57% 14%
1	B	209	29% 54% 16%
1	C	209	31% 57% 11%
1	D	209	33% 50% 16%

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	GTD	D	2401	-	-	X	-

2 Entry composition (i)

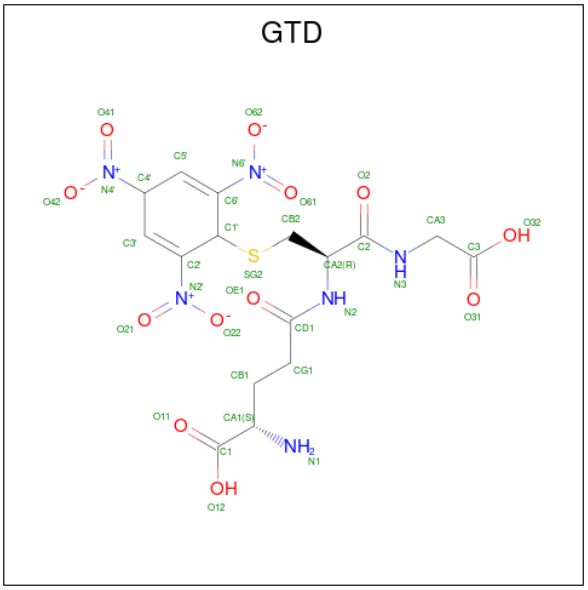
There are 4 unique types of molecules in this entry. The entry contains 7262 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	B	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	C	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			
1	D	208	Total	C	N	O	S	0	0	0
			1631	1047	271	307	6			

- Molecule 2 is 1-(S-GLUTATHIONYL)-2,4,6-TRINITROCYCLOHEXA-2,5-DIENE (three-letter code: GTD) (formula: $C_{16}H_{20}N_6O_{12}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			35	16	6	12	1		
2	B	1	Total	C	N	O	S	0	0
			35	16	6	12	1		

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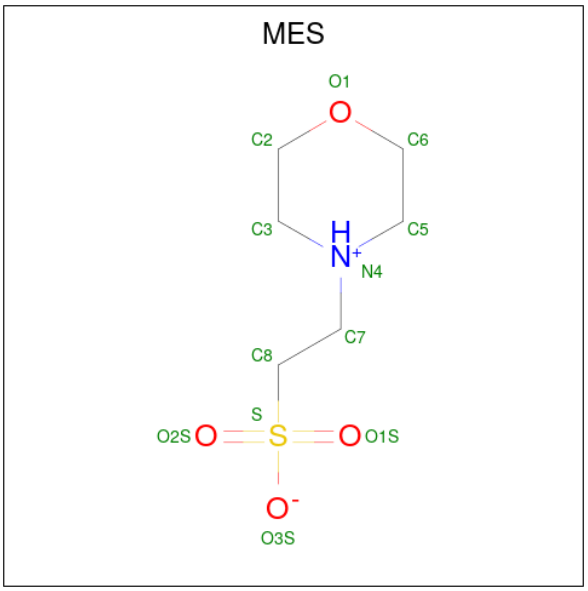
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O S 35 16 6 12 1	0	0
2	D	1	Total C N O S 35 16 6 12 1	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 12 6 1 4 1	0	0
3	B	1	Total C N O S 12 6 1 4 1	0	0
3	C	1	Total C N O S 12 6 1 4 1	0	0
3	D	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	135	Total O 135 135	0	0
4	B	127	Total O 127 127	0	0
4	C	144	Total O 144 144	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	144	Total	O	0	0
			144	144		

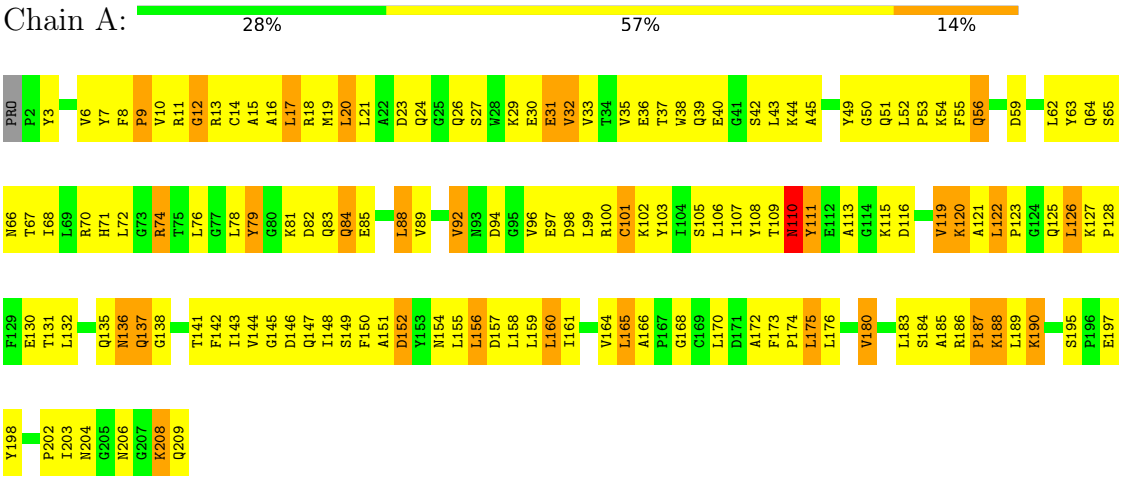
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

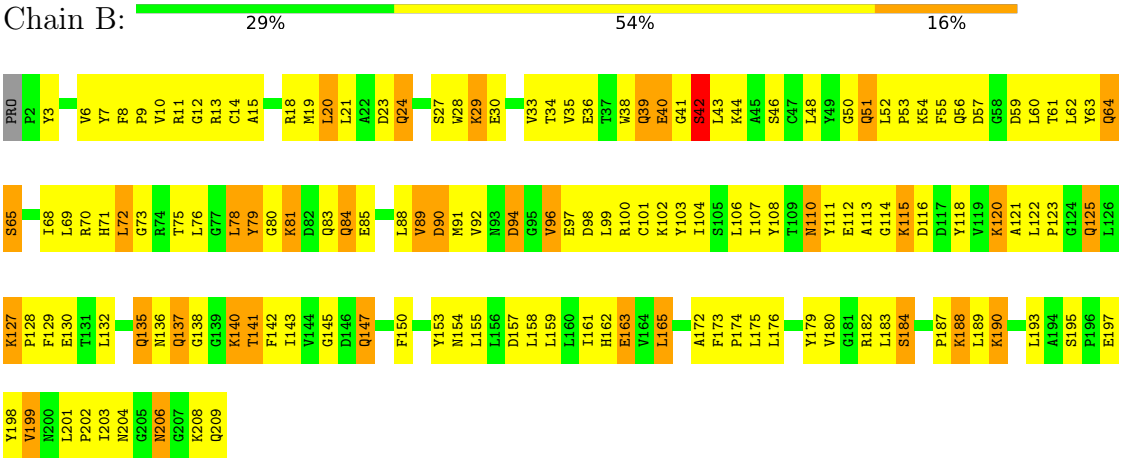
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain A:



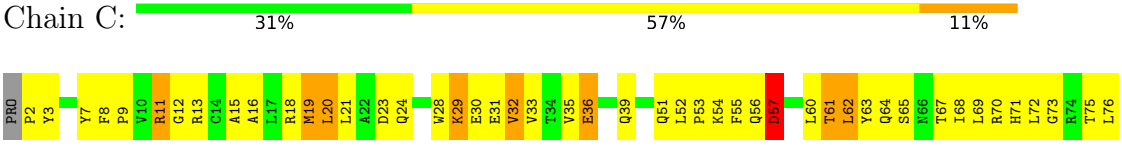
• Molecule 1: GLUTATHIONE S-TRANSFERASE

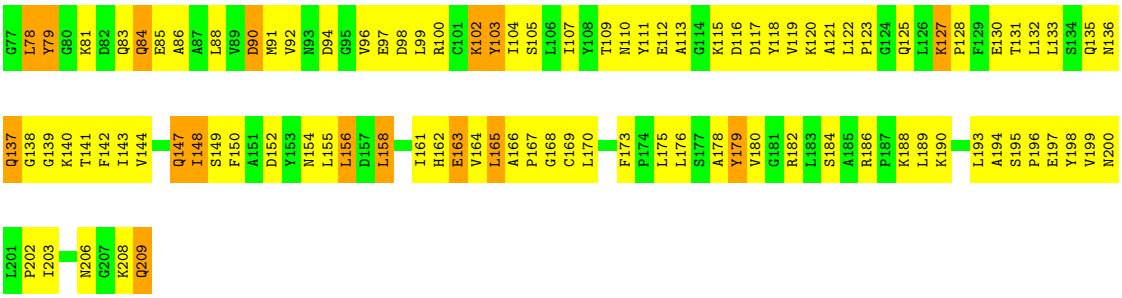
Chain B:



• Molecule 1: GLUTATHIONE S-TRANSFERASE

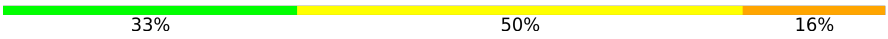
Chain C:

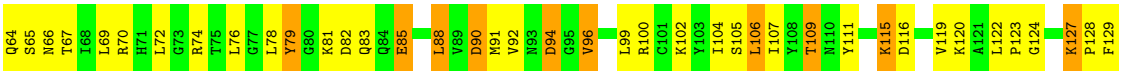


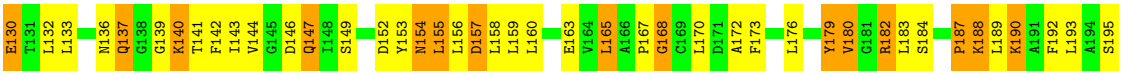


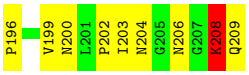
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain D:









4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.59Å 72.57Å 69.34Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	7.00 – 2.00	Depositor
% Data completeness (in resolution range)	90.0 (7.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, R_{free}	0.202 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7262	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTD, MES

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.41	0/1665	0.68	0/2257
1	B	0.42	0/1665	0.71	0/2257
1	C	0.41	0/1665	0.70	0/2257
1	D	0.42	0/1665	0.74	0/2257
All	All	0.41	0/6660	0.71	0/9028

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1631	0	1634	169	0
1	B	1631	0	1634	145	0
1	C	1631	0	1634	151	0
1	D	1631	0	1634	171	0
2	A	35	0	17	4	0
2	B	35	0	17	4	0
2	C	35	0	17	1	0
2	D	35	0	17	10	0
3	A	12	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	2	0
3	C	12	0	13	0	0
3	D	12	0	13	0	0
4	A	135	0	0	20	5
4	B	127	0	0	19	1
4	C	144	0	0	17	2
4	D	144	0	0	16	4
All	All	7262	0	6656	618	6

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 46.

The worst 5 of 618 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:C:92:VAL:HG11	1:C:143:ILE:HG12	1.36	1.06
1:B:110:ASN:HD21	1:B:113:ALA:HB3	1.25	1.01
1:D:36:GLU:HA	1:D:39:GLN:HB2	1.46	0.98
1:B:120:LYS:HE3	1:B:121:ALA:HB2	1.48	0.95
1:D:81:LYS:HD2	1:D:147:GLN:HE21	1.38	0.89

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3493:HOH:O	4:D:3102:HOH:O[2_656]	1.46	0.74
4:A:3209:HOH:O	4:D:3360:HOH:O[2_656]	1.81	0.39
4:B:3380:HOH:O	4:D:3121:HOH:O[1_455]	1.83	0.37
4:A:3152:HOH:O	4:C:3294:HOH:O[1_554]	1.96	0.24
4:A:3446:HOH:O	4:C:3299:HOH:O[1_554]	2.06	0.14

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	A	206/209 (99%)	189 (92%)	8 (4%)	9 (4%)	2	0
1	B	206/209 (99%)	191 (93%)	7 (3%)	8 (4%)	3	1
1	C	206/209 (99%)	192 (93%)	10 (5%)	4 (2%)	8	3
1	D	206/209 (99%)	188 (91%)	13 (6%)	5 (2%)	6	2
All	All	824/836 (99%)	760 (92%)	38 (5%)	26 (3%)	4	1

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	137	GLN
1	B	137	GLN
1	C	32	VAL
1	C	137	GLN

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	A	175/176 (99%)	138 (79%)	37 (21%)	1	0
1	B	175/176 (99%)	129 (74%)	46 (26%)	0	0
1	C	175/176 (99%)	138 (79%)	37 (21%)	1	0
1	D	175/176 (99%)	141 (81%)	34 (19%)	1	0
All	All	700/704 (99%)	546 (78%)	154 (22%)	1	0

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	165	LEU
1	D	149	SER
1	C	209	GLN
1	D	85	GLU

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Mol	Chain	Res	Type
1	D	182	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	93	ASN
1	D	125	GLN
1	B	110	ASN
1	B	93	ASN
1	D	154	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	MES	A	2500	-	12,12,12	2.87	5 (41%)	14,16,16	2.04	5 (35%)
2	GTD	D	2401	-	26,35,35	1.34	4 (15%)	25,48,48	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MES	B	2600	-	12,12,12	2.92	5 (41%)	14,16,16	2.03	4 (28%)
3	MES	D	2800	-	12,12,12	2.83	5 (41%)	14,16,16	1.91	4 (28%)
2	GTD	A	2101	-	26,35,35	1.41	4 (15%)	25,48,48	0.76	0
2	GTD	B	2201	-	26,35,35	1.42	4 (15%)	25,48,48	0.76	0
3	MES	C	2700	-	12,12,12	2.87	5 (41%)	14,16,16	1.89	4 (28%)
2	GTD	C	2301	-	26,35,35	1.42	4 (15%)	25,48,48	0.76	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	MES	A	2500	-	-	3/6/14/14	0/1/1/1
2	GTD	D	2401	-	-	7/31/55/55	0/1/1/1
3	MES	B	2600	-	-	3/6/14/14	0/1/1/1
3	MES	D	2800	-	-	4/6/14/14	0/1/1/1
2	GTD	A	2101	-	-	2/31/55/55	0/1/1/1
2	GTD	B	2201	-	-	2/31/55/55	0/1/1/1
3	MES	C	2700	-	-	4/6/14/14	0/1/1/1
2	GTD	C	2301	-	-	2/31/55/55	0/1/1/1

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2600	MES	O3S-S	5.73	1.67	1.47
3	A	2500	MES	O3S-S	5.71	1.67	1.47
3	D	2800	MES	O3S-S	5.67	1.67	1.47
3	C	2700	MES	O3S-S	5.62	1.67	1.47
3	C	2700	MES	O2S-S	4.91	1.59	1.45

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2500	MES	O2S-S-C8	4.52	112.35	106.92
3	B	2600	MES	O2S-S-C8	4.03	111.77	106.92
3	D	2800	MES	O2S-S-C8	3.81	111.50	106.92
3	C	2700	MES	O2S-S-C8	3.54	111.17	106.92
3	C	2700	MES	O1S-S-C8	2.94	110.45	106.92

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2101	GTD	C2-CA2-CB2-SG2
2	B	2201	GTD	C2-CA2-CB2-SG2
2	C	2301	GTD	C2-CA2-CB2-SG2
2	D	2401	GTD	C2-CA2-CB2-SG2
3	A	2500	MES	C7-C8-S-O1S

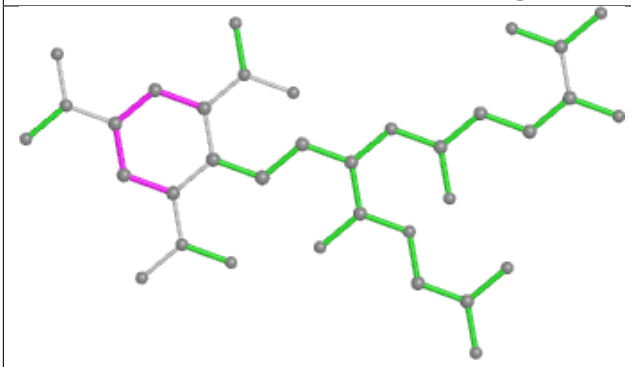
There are no ring outliers.

6 monomers are involved in 23 short contacts:

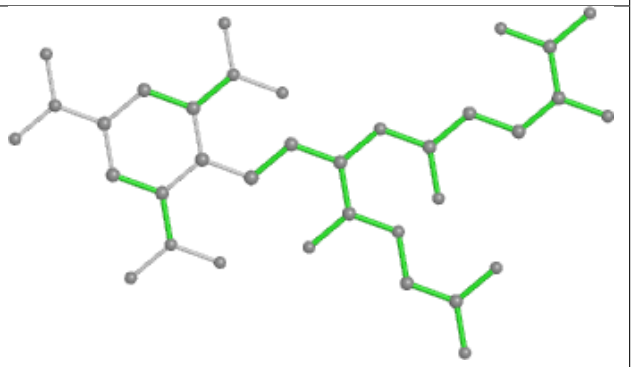
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2500	MES	2	0
2	D	2401	GTD	10	0
3	B	2600	MES	2	0
2	A	2101	GTD	4	0
2	B	2201	GTD	4	0
2	C	2301	GTD	1	0

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.

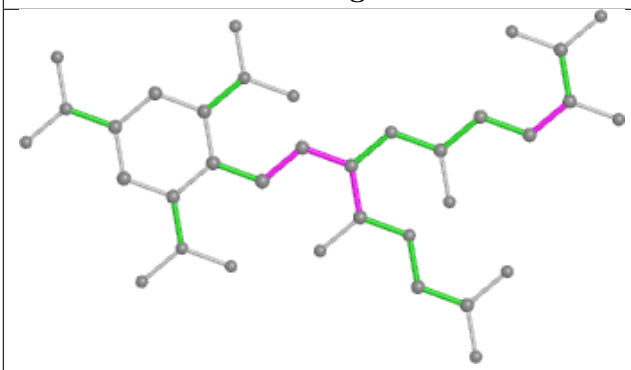
Ligand GTD D 2401



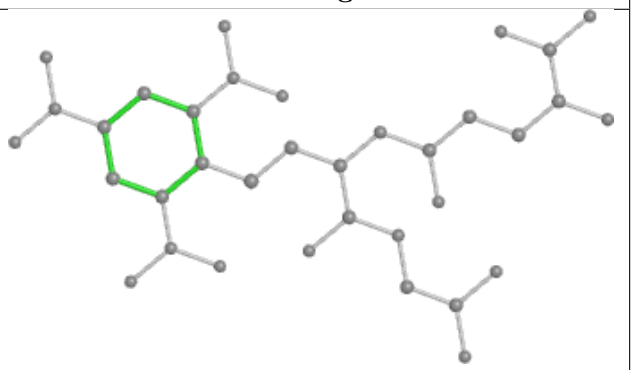
Bond lengths



Bond angles

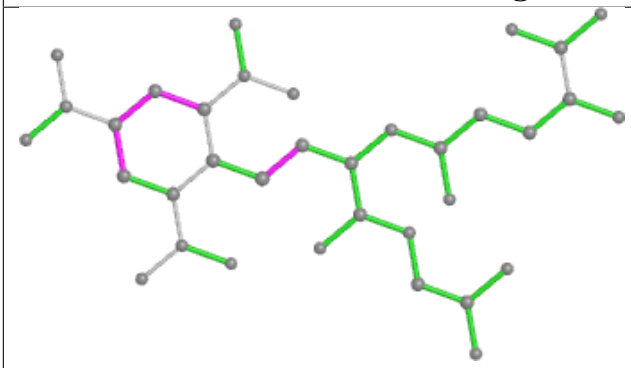


Torsions

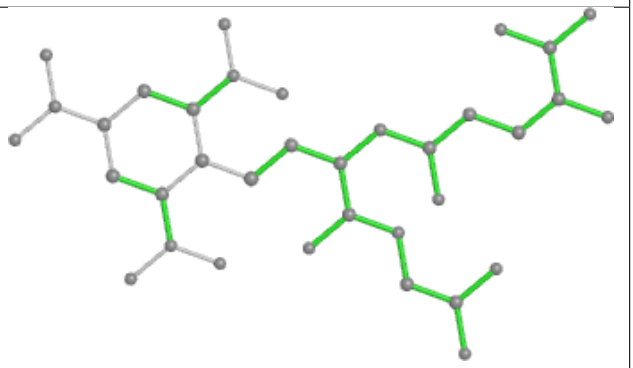


Rings

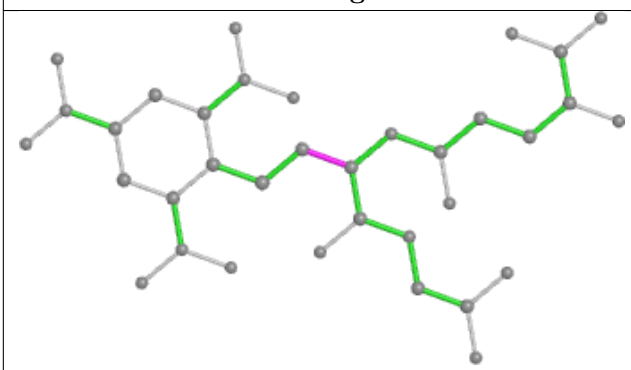
Ligand GTD A 2101



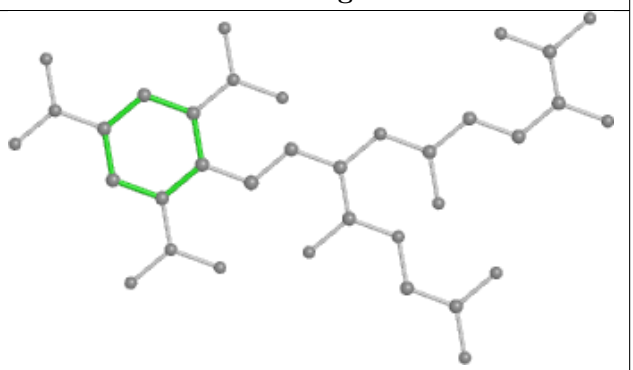
Bond lengths



Bond angles

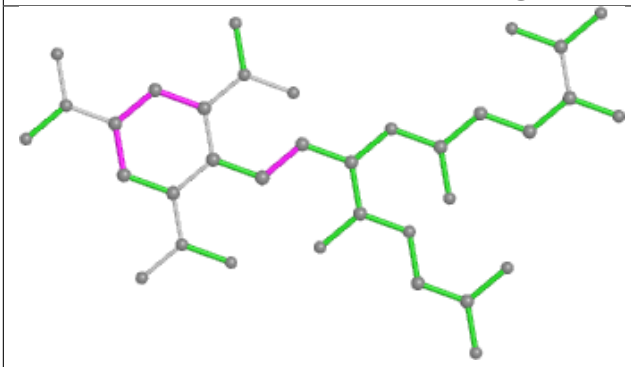


Torsions

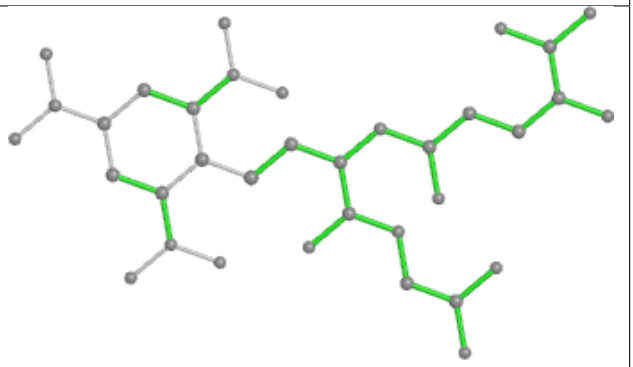


Rings

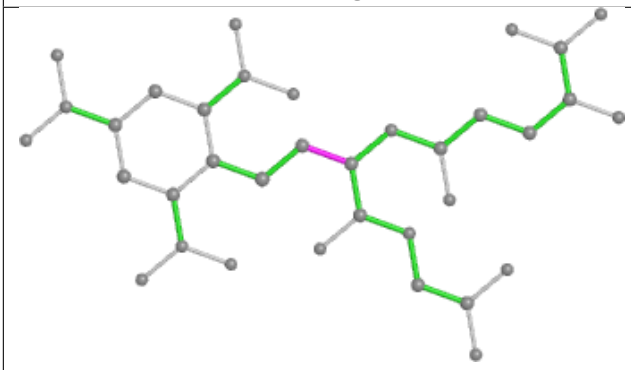
Ligand GTD B 2201



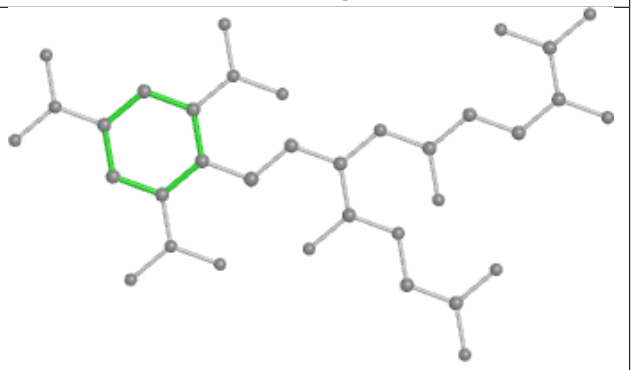
Bond lengths



Bond angles

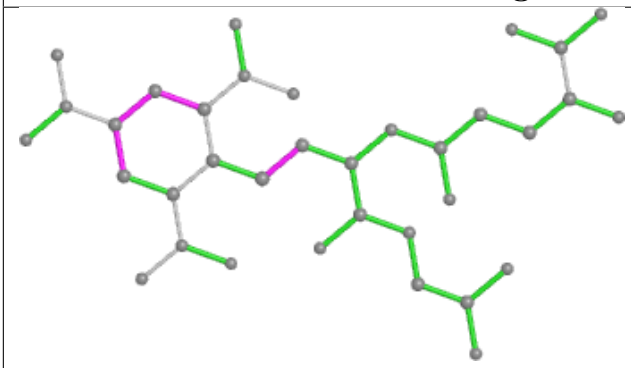


Torsions

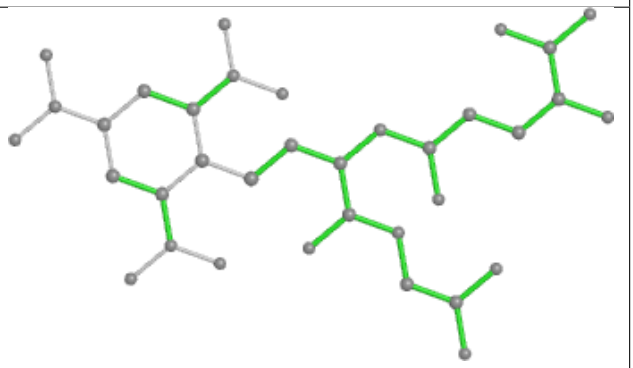


Rings

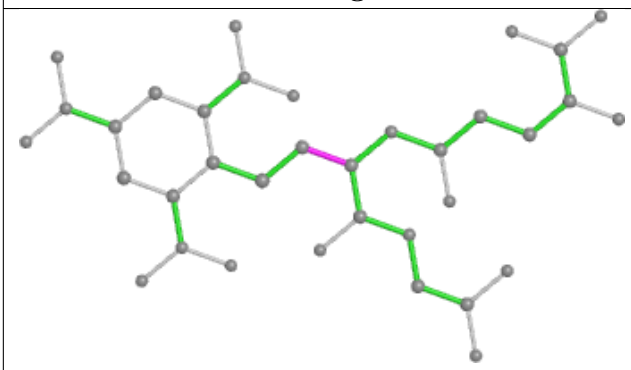
Ligand GTD C 2301



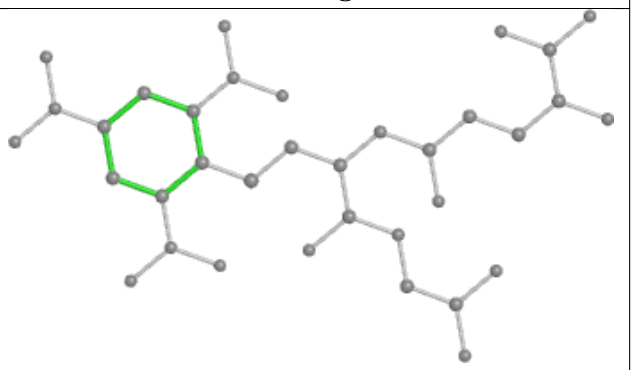
Bond lengths



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.