wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2021 – 10:22 PM EDT

PDB ID	:	1IV2
Title	:	Structure of 2C-Methyl-D-erythritol-2,4-cyclodiphosphate Synthase (bound form CDP)
Authors	:	Kishida, H.; Wada, T.; Unzai, S.; Kuzuyama, T.; Terada, T.; Sirouzu, M.; Yokoyama, S.; Tame, J.R.H.; Park, S.-Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-03-11
Resolution	:	1.55 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 following versions of software and data (see references (1)) were used in the production of this report:

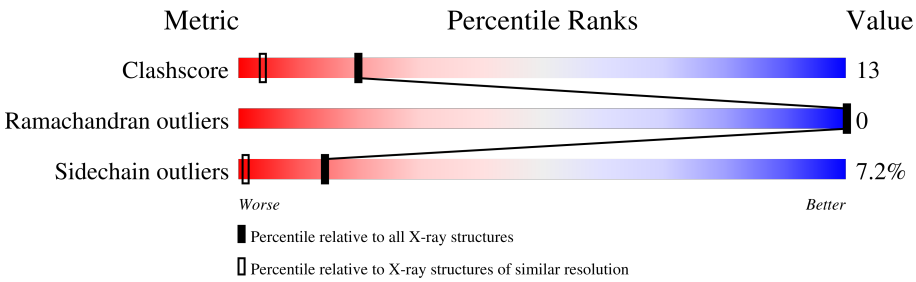
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.55 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	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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	152	71% 24% • ••
1	B	152	74% 19% 6% •
1	C	152	70% 23% • ••
1	D	152	74% 20% 5% •
1	E	152	64% 27% 6% ••
1	F	152	71% 23% 5% •

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CDP	B	1603	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7583 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	1152	726	213	209	4	0	0	0
1	B	150	1152	726	213	209	4	0	0	0
1	C	150	1152	726	213	209	4	0	0	0
1	D	150	1152	726	213	209	4	0	0	0
1	E	150	1152	726	213	209	4	0	0	0
1	F	150	1152	726	213	209	4	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	LEU	engineered mutation	UNP Q8RQP5
A	81	MET	LEU	engineered mutation	UNP Q8RQP5
A	120	MET	LEU	engineered mutation	UNP Q8RQP5
B	241	MET	LEU	engineered mutation	UNP Q8RQP5
B	281	MET	LEU	engineered mutation	UNP Q8RQP5
B	320	MET	LEU	engineered mutation	UNP Q8RQP5
C	441	MET	LEU	engineered mutation	UNP Q8RQP5
C	481	MET	LEU	engineered mutation	UNP Q8RQP5
C	520	MET	LEU	engineered mutation	UNP Q8RQP5
D	1041	MET	LEU	engineered mutation	UNP Q8RQP5
D	1081	MET	LEU	engineered mutation	UNP Q8RQP5
D	1120	MET	LEU	engineered mutation	UNP Q8RQP5
E	1241	MET	LEU	engineered mutation	UNP Q8RQP5
E	1281	MET	LEU	engineered mutation	UNP Q8RQP5
E	1320	MET	LEU	engineered mutation	UNP Q8RQP5
F	1441	MET	LEU	engineered mutation	UNP Q8RQP5
F	1481	MET	LEU	engineered mutation	UNP Q8RQP5

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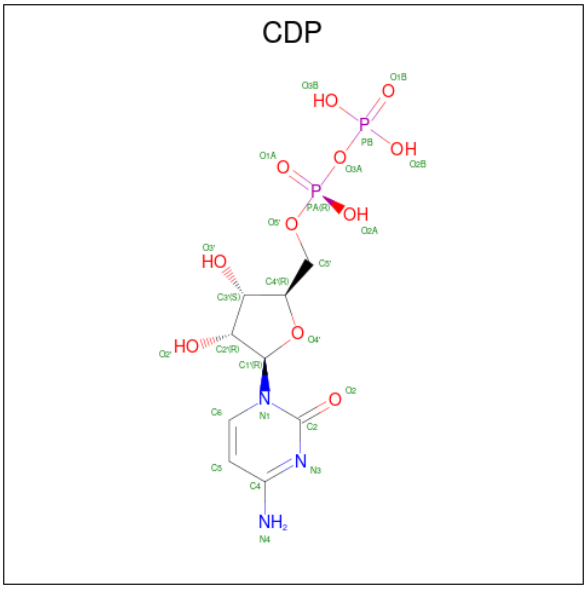
Chain	Residue	Modelled	Actual	Comment	Reference
F	1520	MET	LEU	engineered mutation	UNP Q8RQP5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	3	3	3	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	3	3	3	0	0
2	F	2	2	2	0	0

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: $C_9H_{15}N_3O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	25	9	3	11	2	0	0
3	B	1	25	9	3	11	2	0	0
3	B	1	25	9	3	11	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	D	1	25	9	3	11	2	0	0
			Total	C	N	O	P		
3	E	1	25	9	3	11	2	0	0
			Total	C	N	O	P		
3	E	1	25	9	3	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	105	105	105	0	0
			Total	O		
4	B	92	92	92	0	0
			Total	O		
4	C	76	76	76	0	0
			Total	O		
4	D	83	83	83	0	0
			Total	O		
4	E	77	77	77	0	0
			Total	O		
4	F	76	76	76	0	0

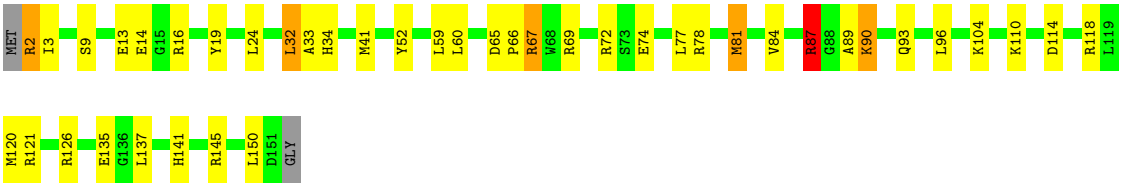
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

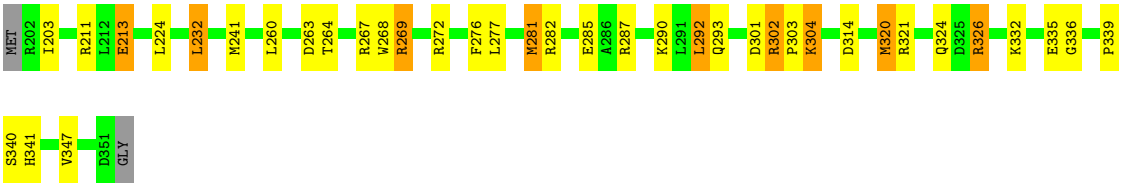
• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain A:



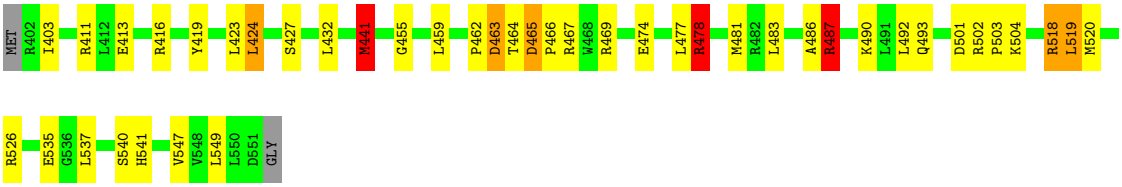
• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain B:



• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain C:

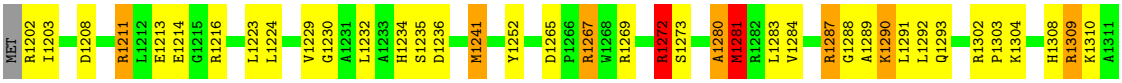


• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain D:

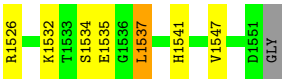
• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain E:



• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	106.10Å 106.10Å 149.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55	Depositor
% Data completeness (in resolution range)	90.9 (20.00-1.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.177 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7583	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.50	1/1173 (0.1%)	1.41	23/1587 (1.4%)
1	B	0.53	2/1173 (0.2%)	1.25	10/1587 (0.6%)
1	C	0.59	2/1173 (0.2%)	1.20	9/1587 (0.6%)
1	D	0.53	1/1173 (0.1%)	1.31	12/1587 (0.8%)
1	E	0.77	3/1173 (0.3%)	1.36	19/1587 (1.2%)
1	F	0.58	2/1173 (0.2%)	1.30	12/1587 (0.8%)
All	All	0.59	11/7038 (0.2%)	1.31	85/9522 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1281	MET	N-CA	16.21	1.78	1.46
1	E	1281	MET	CA-C	-11.46	1.23	1.52
1	C	481	MET	N-CA	9.71	1.65	1.46
1	F	1441	MET	N-CA	9.63	1.65	1.46
1	D	1120	MET	N-CA	8.25	1.62	1.46

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	1472	ARG	NE-CZ-NH2	-13.84	113.38	120.30
1	A	87	ARG	NE-CZ-NH1	10.60	125.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ARG	CD-NE-CZ	10.40	138.16	123.60
1	D	1072	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	E	1234	HIS	CA-CB-CG	9.53	129.79	113.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1208	ASP	Sidechain
1	E	1281	MET	Mainchain

5.2 Too-close contacts (i)

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	1152	0	1182	32	0
1	B	1152	0	1182	25	0
1	C	1152	0	1182	39	0
1	D	1152	0	1182	25	0
1	E	1152	0	1182	50	0
1	F	1152	0	1182	41	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	3	0	0	0	0
2	F	2	0	0	0	0
3	A	25	0	11	0	0
3	B	50	0	21	0	0
3	D	25	0	11	0	0
3	E	50	0	21	1	0
4	A	105	0	0	1	0
4	B	92	0	0	2	0
4	C	76	0	0	3	0
4	D	83	0	0	1	0
4	E	77	0	0	6	0
4	F	76	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7583	0	7156	180	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 13.

The worst 5 of 180 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:E:1281:MET:CA	1:E:1281:MET:N	1.78	1.45
1:F:1416:ARG:HH22	1:F:1432:LEU:CD1	1.54	1.19
1:F:1416:ARG:NH2	1:F:1432:LEU:HD13	1.63	1.12
1:E:1241:MET:HE1	1:E:1319:LEU:HD23	1.31	1.11
1:F:1416:ARG:HH22	1:F:1432:LEU:HD13	0.99	1.10

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	A	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	B	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	C	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
1	D	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	E	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	F	148/152 (97%)	144 (97%)	4 (3%)	0	100	100
All	All	888/912 (97%)	872 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	121/122 (99%)	113 (93%)	8 (7%)	16	1
1	B	121/122 (99%)	112 (93%)	9 (7%)	13	1
1	C	121/122 (99%)	110 (91%)	11 (9%)	9	1
1	D	121/122 (99%)	115 (95%)	6 (5%)	24	3
1	E	121/122 (99%)	110 (91%)	11 (9%)	9	1
1	F	121/122 (99%)	114 (94%)	7 (6%)	20	2
All	All	726/732 (99%)	674 (93%)	52 (7%)	14	1

5 of 52 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1011	ARG
1	E	1224	LEU
1	F	1472	ARG
1	D	1013	GLU
1	D	1069	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	1493	GLN
1	E	1343	GLN
1	D	1093	GLN
1	E	1341	HIS
1	C	541	HIS

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)

Of 18 ligands modelled in this entry, 12 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	$\#\|Z\| > 2$
3	CDP	E	1605	2	21,26,26	2.45	6 (28%)	28,40,40	2.73	11 (39%)
3	CDP	B	1603	2	21,26,26	2.18	5 (23%)	28,40,40	2.90	13 (46%)
3	CDP	E	1606	2	21,26,26	2.24	6 (28%)	28,40,40	2.79	11 (39%)
3	CDP	A	1601	2	21,26,26	2.30	5 (23%)	28,40,40	2.74	11 (39%)
3	CDP	B	1602	2	21,26,26	2.25	5 (23%)	28,40,40	2.77	11 (39%)
3	CDP	D	1604	2	21,26,26	2.18	5 (23%)	28,40,40	2.84	11 (39%)

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	CDP	E	1605	2	-	4/14/32/32	0/2/2/2
3	CDP	B	1603	2	1/1/6/6	2/14/32/32	0/2/2/2
3	CDP	E	1606	2	-	4/14/32/32	0/2/2/2
3	CDP	A	1601	2	-	2/14/32/32	0/2/2/2
3	CDP	B	1602	2	-	4/14/32/32	0/2/2/2
3	CDP	D	1604	2	-	3/14/32/32	0/2/2/2

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1605	CDP	C6-N1	7.81	1.45	1.35
3	A	1601	CDP	C6-N1	7.29	1.44	1.35
3	B	1602	CDP	C6-N1	6.83	1.44	1.35
3	E	1606	CDP	C6-N1	6.73	1.44	1.35
3	D	1604	CDP	C6-N1	6.55	1.43	1.35

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1604	CDP	O2'-C2'-C1'	-7.36	83.69	110.85
3	B	1603	CDP	O2'-C2'-C1'	-7.01	84.98	110.85
3	A	1601	CDP	O2'-C2'-C1'	-6.92	85.30	110.85
3	B	1602	CDP	O2'-C2'-C1'	-6.86	85.54	110.85
3	E	1606	CDP	O2'-C2'-C1'	-6.78	85.80	110.85

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1603	CDP	C3'

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1601	CDP	PA-O3A-PB-O3B
3	B	1602	CDP	PA-O3A-PB-O3B
3	B	1602	CDP	C2'-C1'-N1-C6
3	B	1603	CDP	PA-O3A-PB-O3B
3	D	1604	CDP	PA-O3A-PB-O3B

There are no ring outliers.

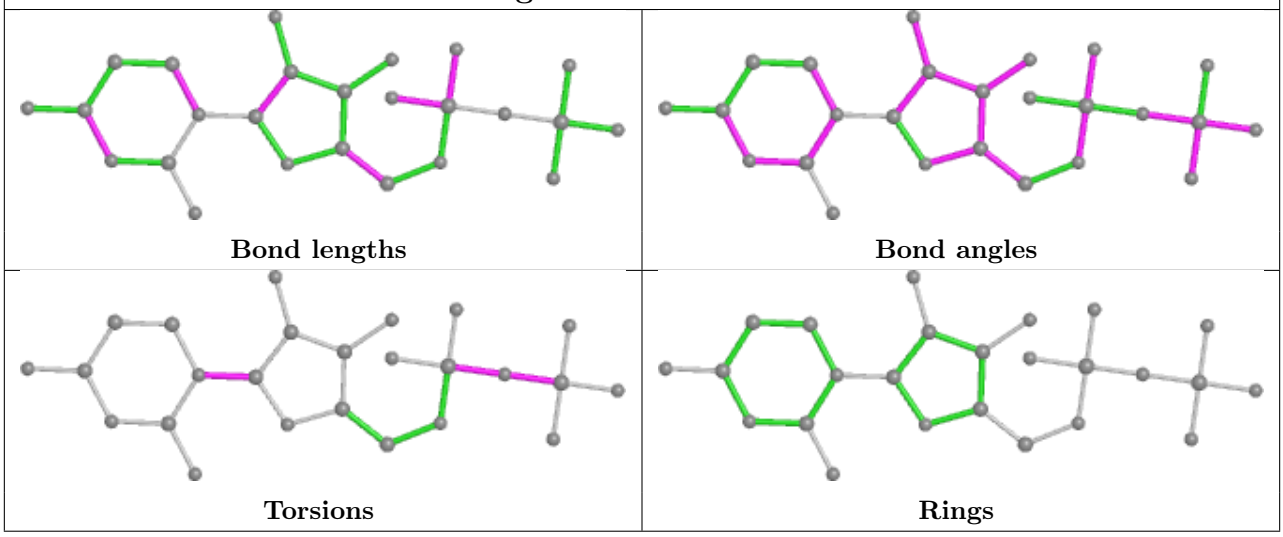
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1605	CDP	1	0

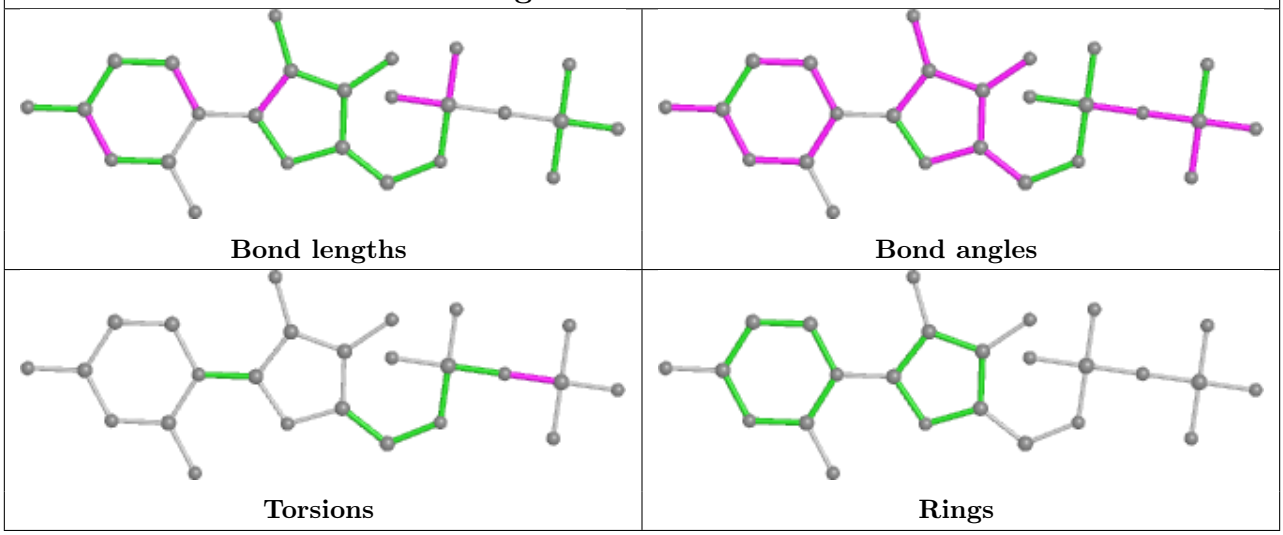
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

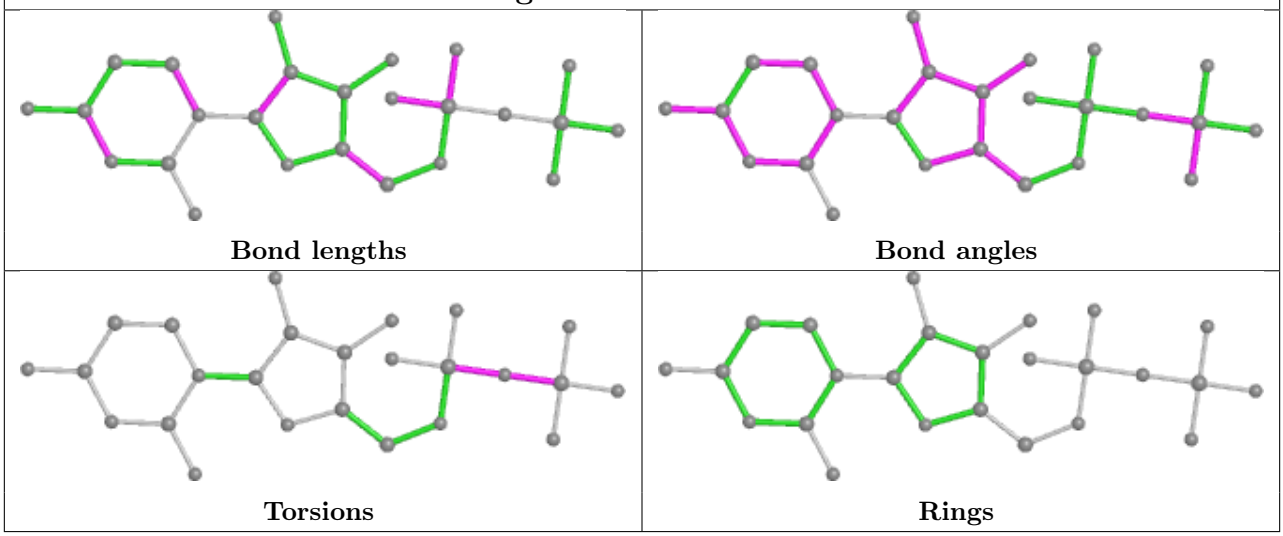
Ligand CDP E 1605



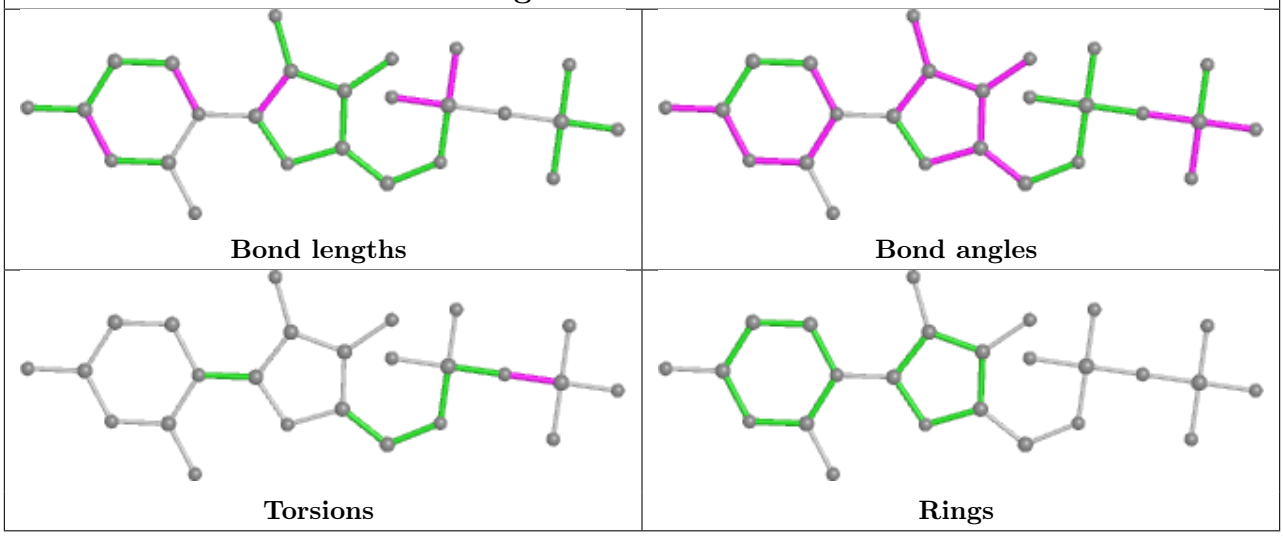
Ligand CDP B 1603



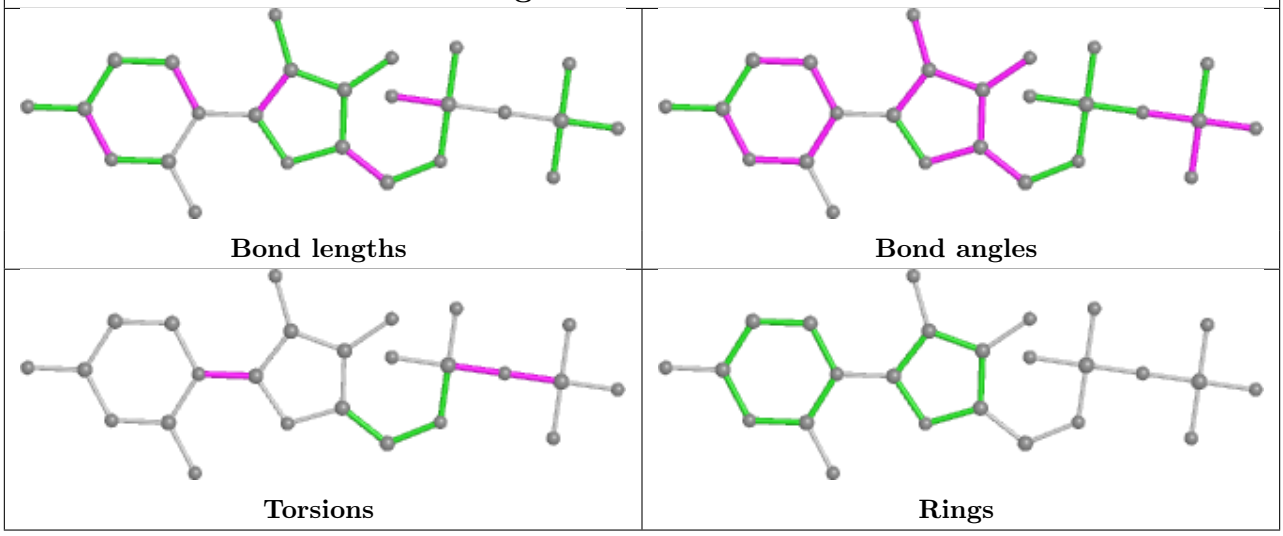
Ligand CDP E 1606

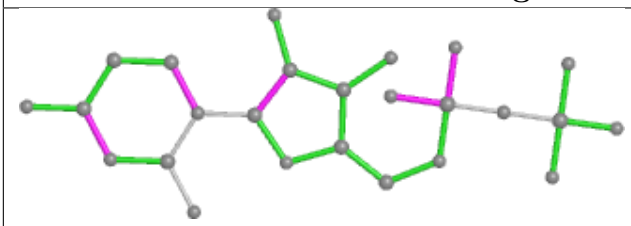
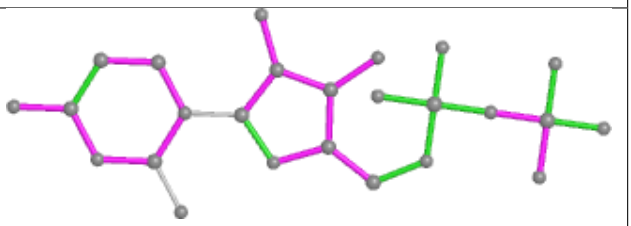
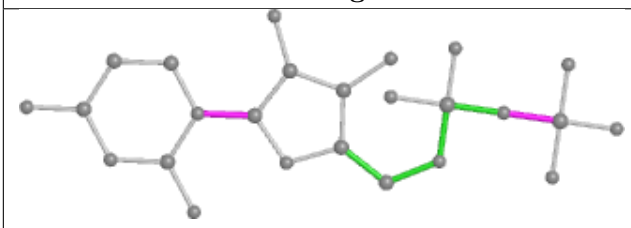
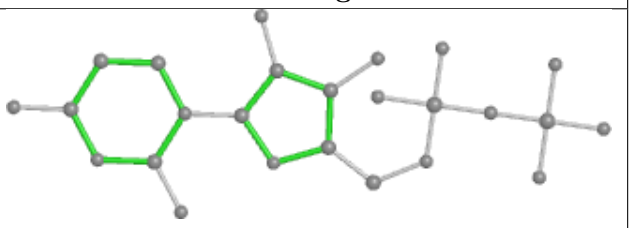


Ligand CDP A 1601



Ligand CDP B 1602



Ligand CDP D 1604	
 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.