



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

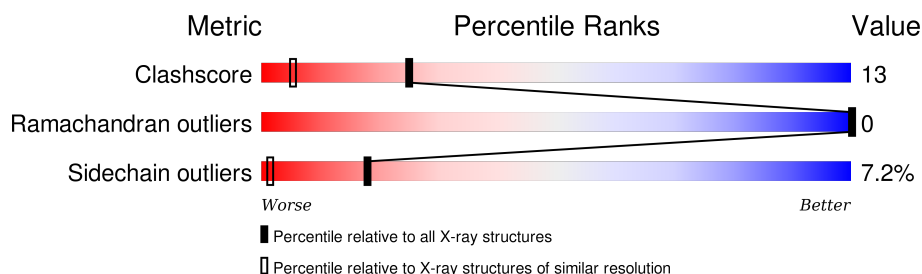
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 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	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	 71% 24% 5% 0%
1	B	152	 74% 19% 6% 1%
1	C	152	 70% 23% 5% 2%
1	D	152	 74% 20% 5% 1%
1	E	152	 64% 27% 6% 3%
1	F	152	 71% 23% 5% 1%

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
3	CDP	B	1603	X	-	-	-

## 2 Entry composition

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
1	A	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	B	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	C	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	D	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	E	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	F	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			

There are 18 discrepancies between the modelled and reference sequences:

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

*Continued on next page...*

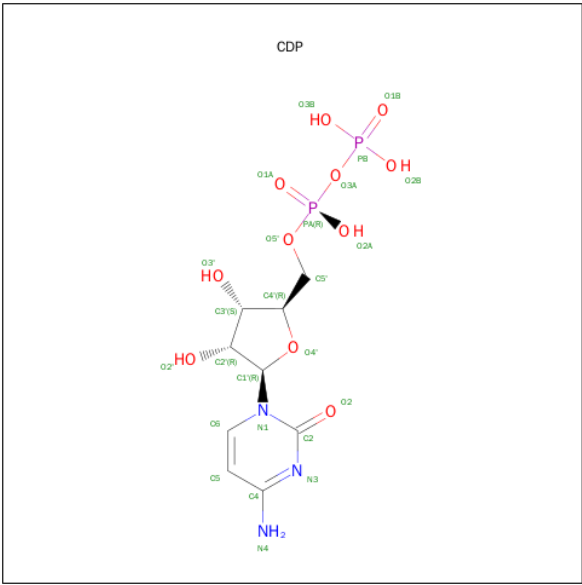
Continued from previous page...

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

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

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

- Molecule 3 is CYTIDINE-5'-DIPHOSPHATE (three-letter code: CDP) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>3</sub>O<sub>11</sub>P<sub>2</sub>).



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

Continued on next page...

*Continued from previous page...*

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

- Molecule 4 is water.

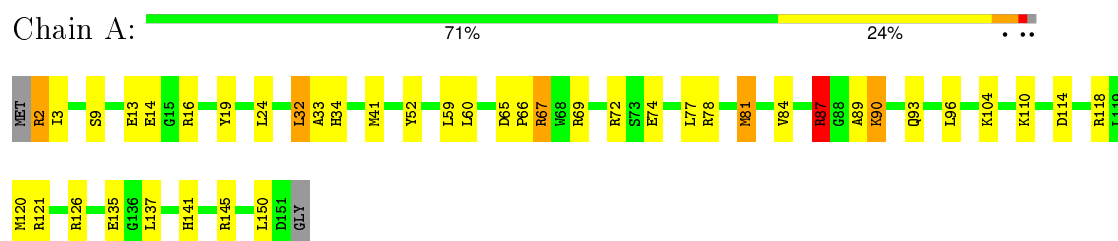
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	92	Total	O	0	0
			92	92		
4	C	76	Total	O	0	0
			76	76		
4	D	83	Total	O	0	0
			83	83		
4	E	77	Total	O	0	0
			77	77		
4	F	76	Total	O	0	0
			76	76		

### 3 Residue-property plots

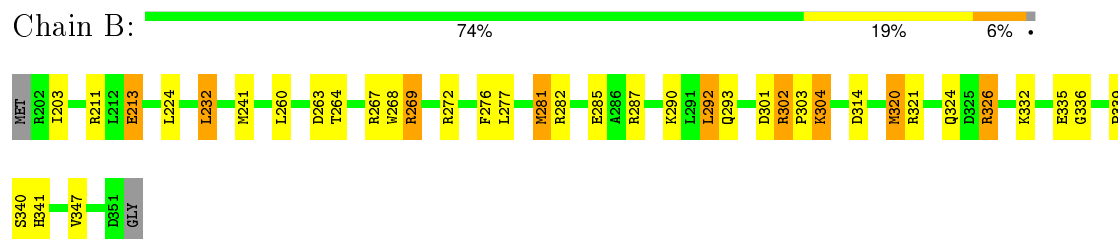
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

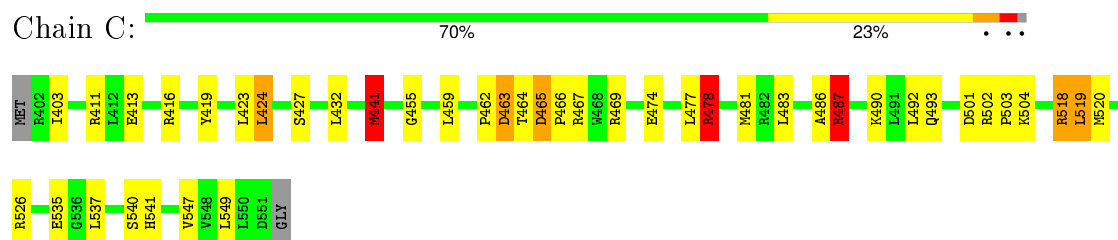
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



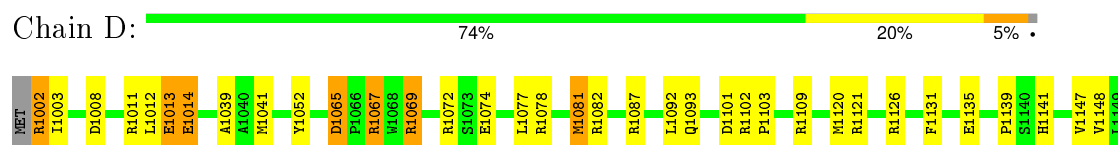
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



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



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



L1150  
D1151  
GLY

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

Chain E:  64% 27% 6% ..

MET R1202 I1203 D1208 R1211 L1212 E1213 E1214 G1215 R1216 L1223 L1224 V1229 G1230 A1231 L1232 A1233 H1234 S1235 D1236 M1241 Y1252 D1265 P1266 R1267 W1268 R1269 R1272 S1273 A1280 M1281 R1282 L1283 V1284 R1287 G1288 A1289 K1290 L1291 L1292 Q1293 R1302 P1303 K1304 H1308 R1309 K1310 A1311  
 L1312 L1316 S1317 R1318 L1319 R1320 R1321 L1322 R1326 F1331 K1332 E1335 G1336 H1341 R1345 D1351 GLY

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

Chain F:  71% 23% 5% ..

MET R1402 I1403 S1409 H1410 R1411 L1412 E1413 R1416 I1425 L1432 D1436 M1441 Y1452 G1455 L1459 L1460 D1463 T1464 D1465 P1466 R1467 W1468 R1469 R1472 S1473 E1474 R1478 M1481 A1489 K1490 Q1493 L1496 T1499 K1510 A1511 L1512 R1518 L1519 M1520  
 R1526 K1532 T1533 S1534 E1535 G1536 L1537 H1541 V1547 D1551 GLY



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: MG, CDP

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(°)	Ideal(°)
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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

*Continued on next page...*

*Continued from previous page...*

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:N	1:E:1281:MET:CA	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 ⓘ

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%)	21	2
1	B	121/122 (99%)	112 (93%)	9 (7%)	17	1
1	C	121/122 (99%)	110 (91%)	11 (9%)	12	1
1	D	121/122 (99%)	115 (95%)	6 (5%)	30	4
1	E	121/122 (99%)	110 (91%)	11 (9%)	12	1
1	F	121/122 (99%)	114 (94%)	7 (6%)	25	3
All	All	726/732 (99%)	674 (93%)	52 (7%)	18	1

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

Mol	Chain	Res	Type
1	C	490	LYS
1	D	1013	GLU
1	F	1467	ARG
1	C	502	ARG
1	C	519	LEU

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

Mol	Chain	Res	Type
1	C	541	HIS
1	D	1093	GLN
1	E	1341	HIS
1	C	508	HIS
1	E	1343	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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	A	1601	2	19,26,26	2.10	3 (15%)	27,40,40	2.92	13 (48%)
3	CDP	B	1602	2	19,26,26	2.03	3 (15%)	27,40,40	2.70	11 (40%)
3	CDP	B	1603	2	19,26,26	1.98	4 (21%)	27,40,40	3.07	14 (51%)
3	CDP	D	1604	2	19,26,26	1.98	4 (21%)	27,40,40	2.82	12 (44%)
3	CDP	E	1605	2	19,26,26	2.24	5 (26%)	27,40,40	2.89	12 (44%)
3	CDP	E	1606	2	19,26,26	2.05	5 (26%)	27,40,40	2.93	12 (44%)

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	A	1601	2	-	0/12/32/32	0/2/2/2
3	CDP	B	1602	2	-	0/12/32/32	0/2/2/2
3	CDP	B	1603	2	1/1/6/6	0/12/32/32	0/2/2/2
3	CDP	D	1604	2	-	0/12/32/32	0/2/2/2
3	CDP	E	1605	2	-	0/12/32/32	0/2/2/2
3	CDP	E	1606	2	-	0/12/32/32	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1601	CDP	PA-O2A	-2.55	1.44	1.54
3	E	1606	CDP	PA-O2A	-2.49	1.44	1.54
3	B	1602	CDP	PA-O2A	-2.49	1.44	1.54
3	E	1605	CDP	PA-O2A	-2.41	1.44	1.54
3	D	1604	CDP	PA-O2A	-2.37	1.44	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1603	CDP	O4'-C1'-N1	-8.86	89.40	108.08
3	E	1606	CDP	O4'-C1'-N1	-8.50	90.16	108.08
3	A	1601	CDP	O4'-C1'-N1	-8.41	90.35	108.08
3	E	1605	CDP	O4'-C1'-N1	-8.28	90.62	108.08
3	B	1602	CDP	O4'-C1'-N1	-8.01	91.18	108.08

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	1603	CDP	C3'

There are no torsion outliers.

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

## 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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.