wwPDB X-ray Structure Validation Summary Report (i)

Oct 16, 2021 – 11:01 PM EDT

PDB ID	:	1NT4
Title	:	Crystal structure of Escherichia coli periplasmic glucose-1-phosphatase H18A mutant complexed with glucose-1-phosphate
Authors	:	Lee, D.C.; Cottrill, M.A.; Forsberg, C.W.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2003-01-28
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 following versions of software and data (see references (1)) were used in the production of this report:

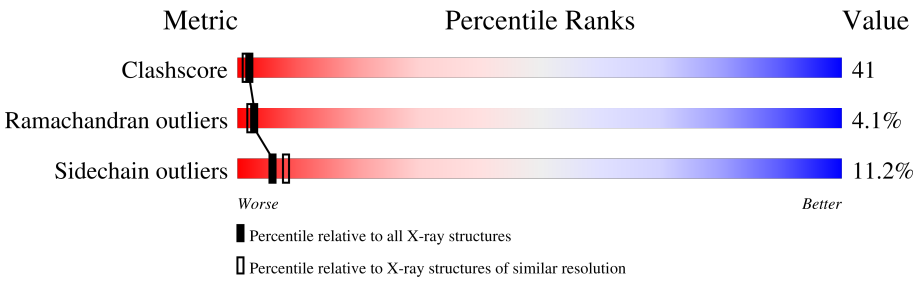
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	391	44% 46% 9% •
1	B	391	46% 43% 10% •

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	XGP	A	2000	-	-	X	-
2	XGP	B	2001	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6499 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.

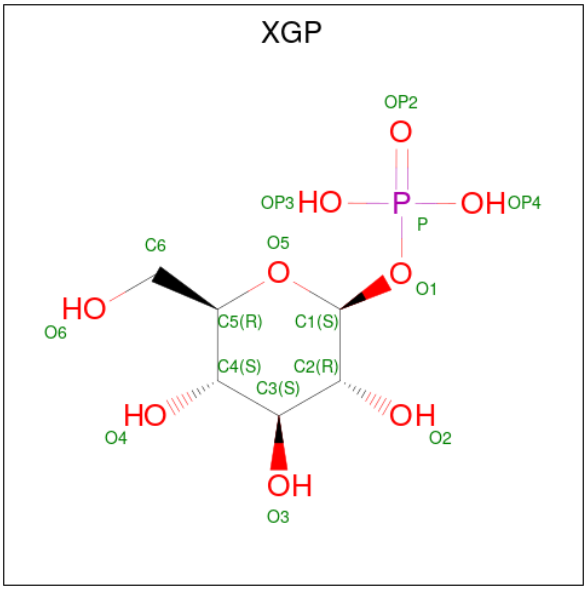
- Molecule 1 is a protein called Glucose-1-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	391	3058	1935	513	593	17	0	0	0
1	B	391	3058	1935	513	593	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	HIS	engineered mutation	UNP P19926
B	1018	ALA	HIS	engineered mutation	UNP P19926

- Molecule 2 is 1-O-phosphono-beta-D-glucopyranose (three-letter code: XGP) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	16	6	9	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	B	1	16	6	9	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	181	181	181	0	0
			Total	O		
3	B	170	170	170	0	0

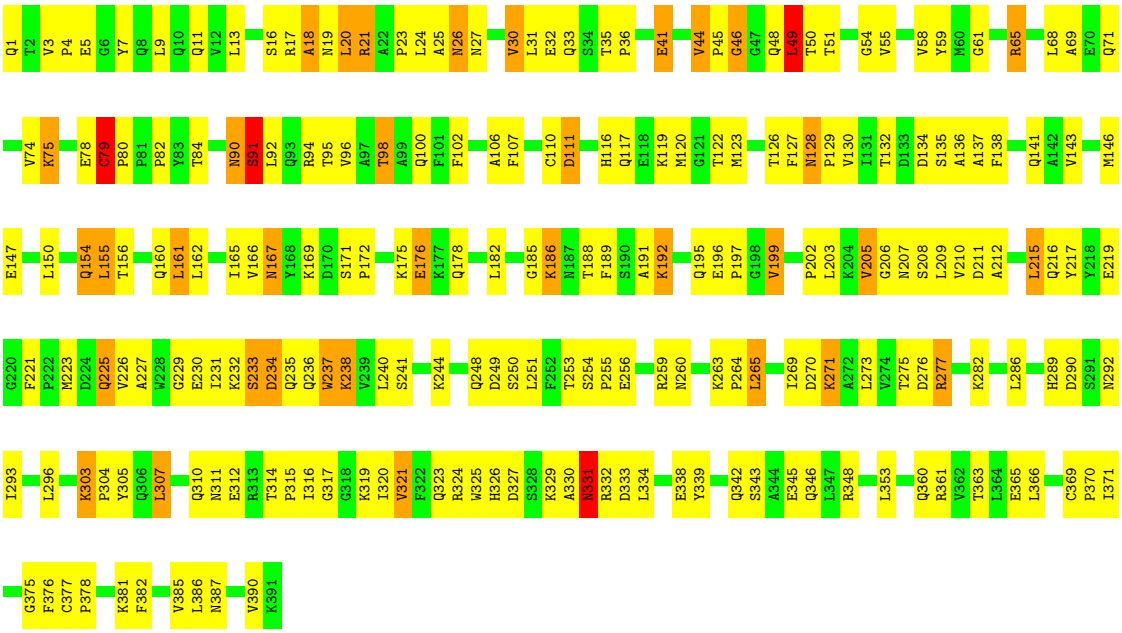
3 Residue-property plots (i)

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.

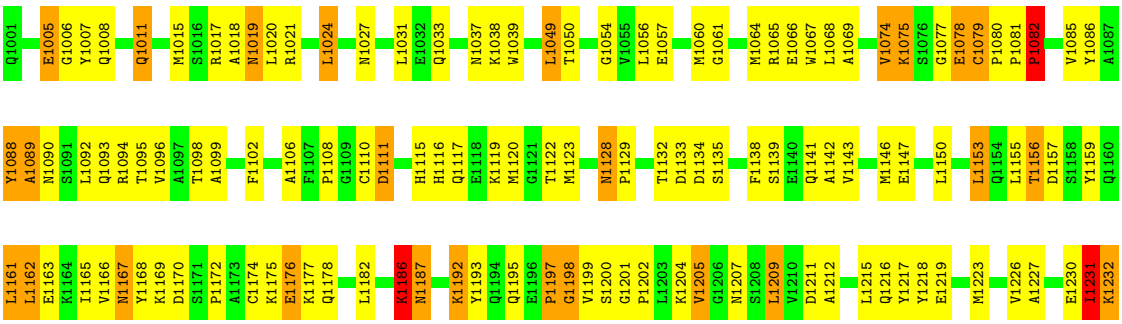
• Molecule 1: Glucose-1-phosphatase

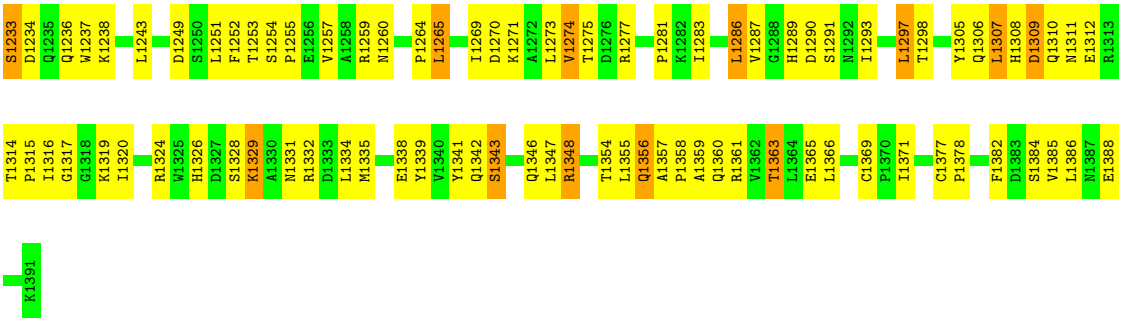
Chain A: 44% 46% 9%



• Molecule 1: Glucose-1-phosphatase

Chain B: 46% 43% 10%




S1233
D1234
Q1235
Q1236
W1237
K1238
L1243
D1249
S1250
L1251
F1252
T1253
S1254
P1255
E1256
V1257
A1258
R1259
N1260
P1264
L1265
I1269
D1270
K1271
A1272
L1273
V1274
T1275
D1276
R1277
P1281
K1282
I1283
L1286
V1287
G1288
H1289
D1290
S1291
N1292
I1293
L1297
T1298
Y1305
Q1306
L1307
H1308
D1309
Q1310
N1311
E1312
R1313
T1314
P1315
I1316
G1317
G1318
K1319
I1320
R1324
W1325
H1326
D1327
S1328
K1329
A1330
N1331
R1332
D1333
L1334
M1335
E1338
Y1339
V1340
Y1341
Q1342
S1343
Q1346
L1347
R1348
T1354
L1355
Q1356
A1357
P1358
A1359
Q1360
R1361
V1362
T1363
L1364
E1365
L1366
C1369
P1370
I1371
C1377
P1378
F1382
D1383
S1384
V1385
L1386
N1387
E1388
K1391

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	156.26Å 156.26Å 84.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	91.9 (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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: XGP

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	0.39	0/3128	0.66	1/4248 (0.0%)
1	B	0.40	0/3128	0.68	1/4248 (0.0%)
All	All	0.40	0/6256	0.67	2/8496 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	49	LEU	CA-CB-CG	6.42	130.07	115.30
1	B	1356	GLN	N-CA-C	-5.17	97.06	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3058	0	2996	243	0
1	B	3058	0	2993	256	0
2	A	16	0	10	6	0
2	B	16	0	10	6	0
3	A	181	0	0	21	0
3	B	170	0	0	14	0
All	All	6499	0	6009	501	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 41.

The worst 5 of 501 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:A:332:ARG:HH12	1:A:334:LEU:HD11	1.17	1.08
1:A:223:MET:HB3	1:A:232:LYS:HD2	1.37	1.07
1:A:186:LYS:H	1:A:186:LYS:HD2	1.19	1.03
1:B:1231:ILE:CD1	1:B:1232:LYS:H	1.73	1.02
1:B:1277:ARG:HD2	1:B:1324:ARG:HH21	1.26	1.00

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	389/391 (100%)	352 (90%)	22 (6%)	15 (4%)	3 2
1	B	389/391 (100%)	347 (89%)	25 (6%)	17 (4%)	2 2
All	All	778/782 (100%)	699 (90%)	47 (6%)	32 (4%)	3 2

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	CYS
1	A	91	SER
1	A	111	ASP
1	A	176	GLU
1	A	234	ASP

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	335/335 (100%)	294 (88%)	41 (12%)	5 6
1	B	335/335 (100%)	301 (90%)	34 (10%)	7 11
All	All	670/670 (100%)	595 (89%)	75 (11%)	6 8

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1186	LYS
1	B	1339	TYR
1	B	1205	VAL
1	B	1274	VAL
1	A	192	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1116	HIS
1	B	1310	GLN
1	B	1128	ASN
1	B	1195	GLN
1	B	1331	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)

2 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	$\#\|Z\| > 2$
2	XGP	B	2001	-	15,16,16	1.34	2 (13%)	23,24,24	0.82	1 (4%)
2	XGP	A	2000	-	15,16,16	1.11	1 (6%)	23,24,24	0.82	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	XGP	B	2001	-	-	1/7/27/27	0/1/1/1
2	XGP	A	2000	-	-	1/7/27/27	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	XGP	P-OP2	2.76	1.59	1.50
2	B	2001	XGP	C4-C3	2.07	1.57	1.52
2	A	2000	XGP	C4-C3	2.06	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	XGP	O5-C1-O1	-2.71	107.82	111.36
2	A	2000	XGP	O5-C1-O1	-2.70	107.83	111.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	XGP	C2-C1-O1-P
2	B	2001	XGP	C2-C1-O1-P

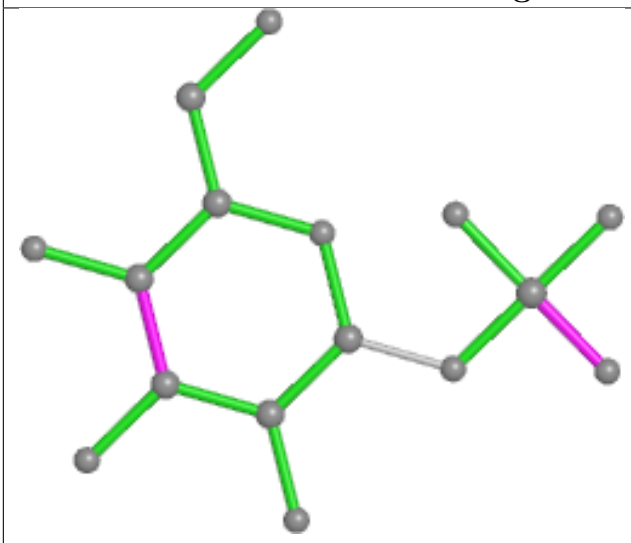
There are no ring outliers.

2 monomers are involved in 12 short contacts:

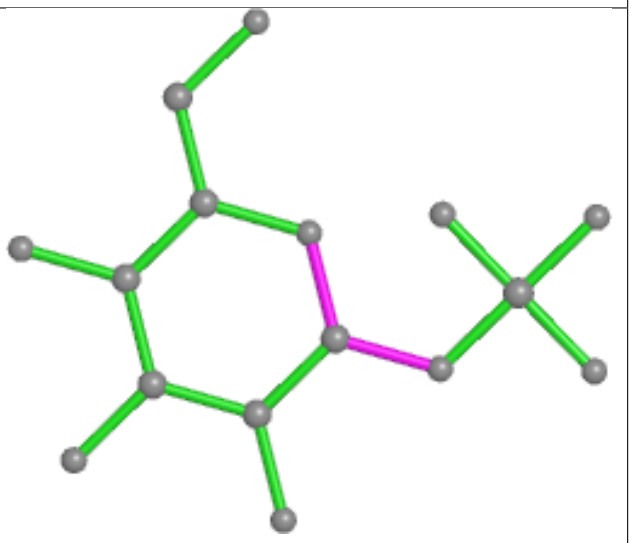
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	XGP	6	0
2	A	2000	XGP	6	0

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.

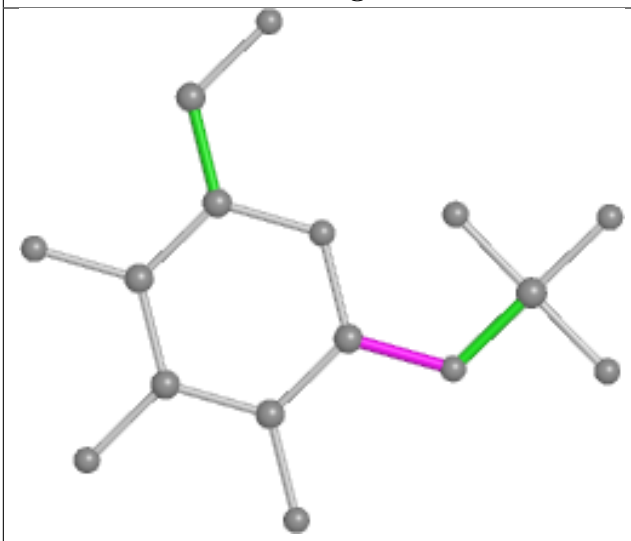
Ligand XGP B 2001



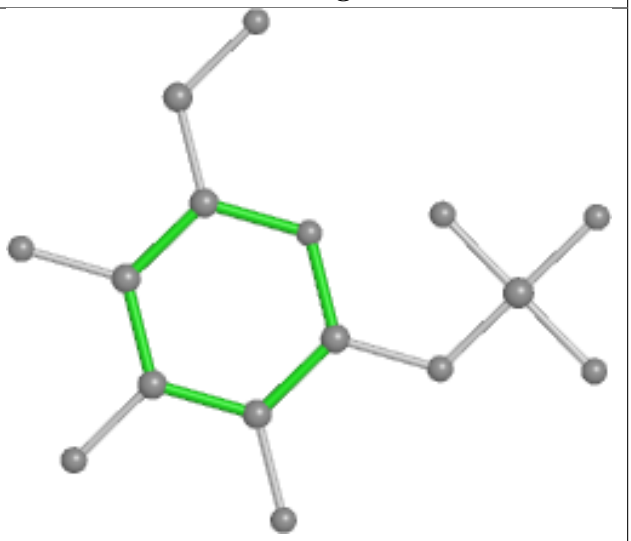
Bond lengths



Bond angles

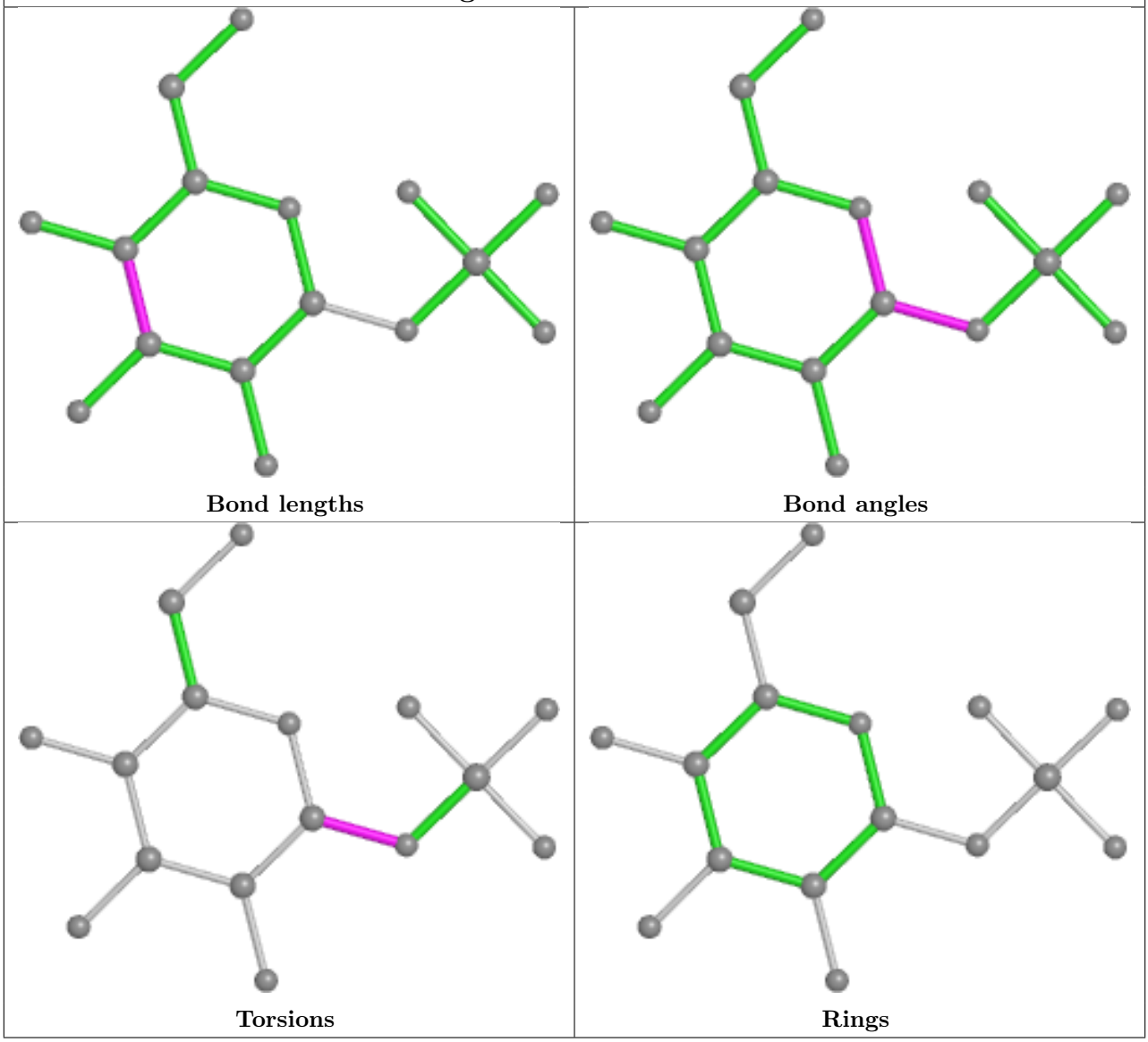


Torsions



Rings

Ligand XGP A 2000



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.