



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 11:58 pm BST

PDB ID : 6BM7  
Title : Crystal structure of Trypanosoma brucei AdoMetDC/prozyme heterodimer in complex with pyrimidineamine inhibitor UTSAM568  
Authors : Volkov, O.A.; Chen, Z.; Phillips, M.A.  
Deposited on : 2017-11-13  
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

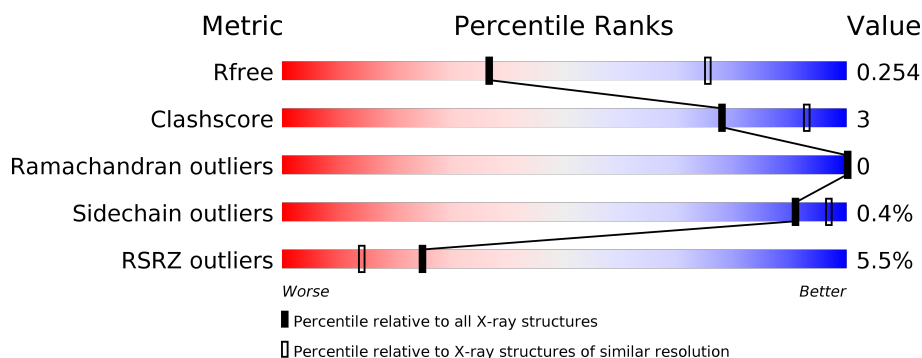
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	85	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>9%</div> </div> </div>
1	C	85	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>7%</div> </div> </div>
2	B	285	<div> <div>6%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
2	D	285	<div> <div>4%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
3	E	325	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>9%</div> <div>10%</div> </div> </div>
3	F	325	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>7%</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20224 atoms, of which 9907 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 S-adenosylmethionine decarboxylase beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	77	Total	C	H	N	O	S	0	0	0
			1217	391	600	105	117	4			
1	C	79	Total	C	H	N	O	S	0	0	0
			1263	403	626	111	119	4			

- Molecule 2 is a protein called S-adenosylmethionine decarboxylase alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	271	Total	C	H	N	O	S	0	0	0
			4214	1386	2047	354	411	16			
2	D	271	Total	C	H	N	O	S	0	0	0
			4215	1386	2048	354	411	16			

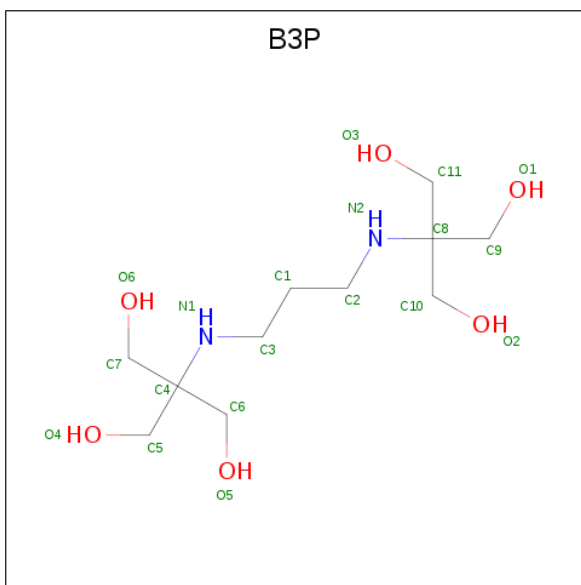
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	86	PYR	-	modified residue	UNP Q587A7
D	86	PYR	-	modified residue	UNP Q587A7

- Molecule 3 is a protein called Inactive S-adenosylmethionine decarboxylase prozyme.

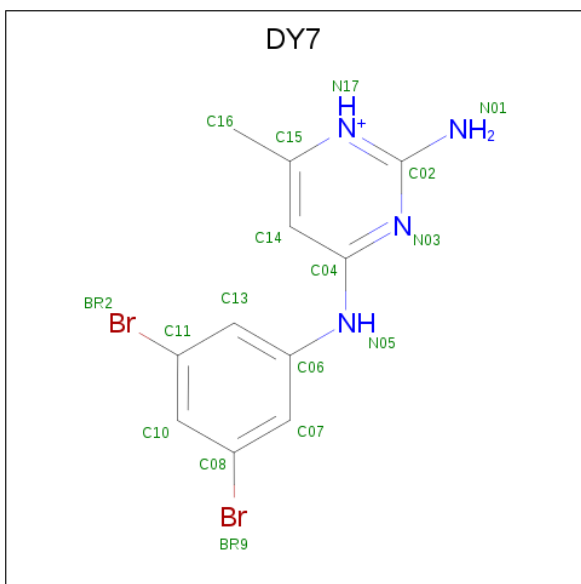
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	291	Total	C	H	N	O	S	0	0	0
			4536	1452	2227	405	438	14			
3	F	289	Total	C	H	N	O	S	0	0	0
			4511	1445	2215	403	434	14			

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: C<sub>11</sub>H<sub>26</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0
			45	11	26	2	6	
4	D	1	Total	C	H	N	O	0
			45	11	26	2	6	

- Molecule 5 is 2-amino-4-[(3,5-dibromophenyl)amino]-6-methylpyrimidin-1-ium (three-letter code: DY7) (formula: C<sub>11</sub>H<sub>11</sub>Br<sub>2</sub>N<sub>4</sub>) (labeled as "Ligand of Interest" by author).



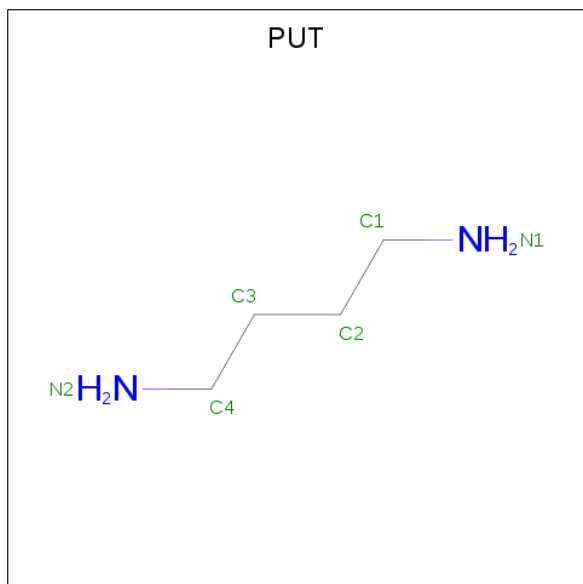
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Br	C	H	N	0
			28	2	11	11	4	

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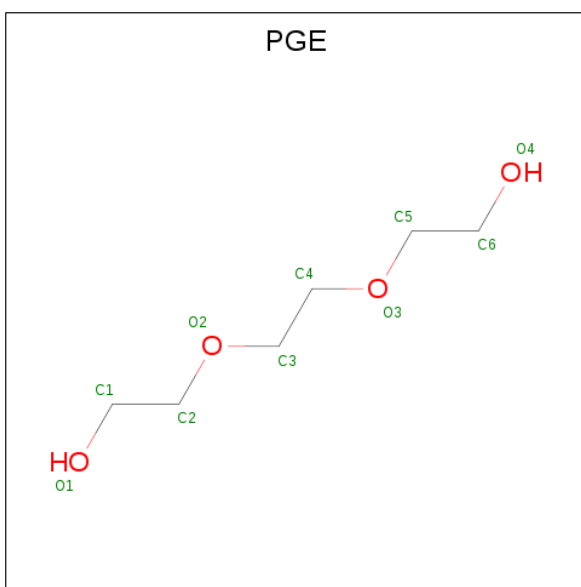
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	Br	C	H	N	0	0
			28	2	11	11	4		

- Molecule 6 is 1,4-DIAMINOBTANE (three-letter code: PUT) (formula:  $C_4H_{12}N_2$ ).



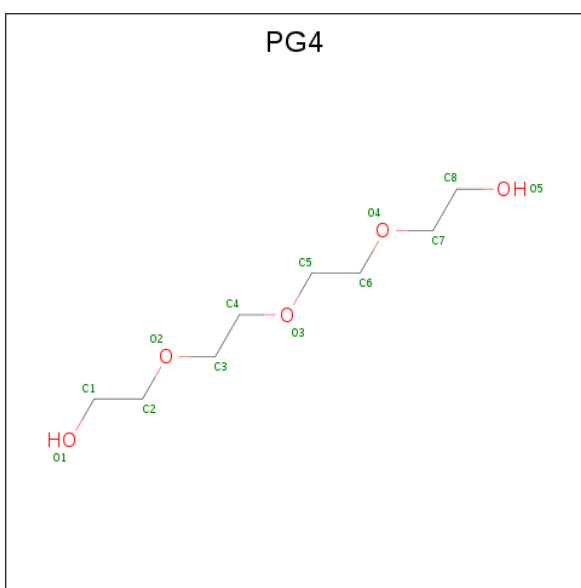
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	E	1	Total	C	H	N	0	0
			18	4	12	2		
6	F	1	Total	C	H	N	0	0
			18	4	12	2		

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	H	O	0	0
			24	6	14	4		
7	E	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	F	1	Total	C	H	O	0	0
			31	8	18	5		

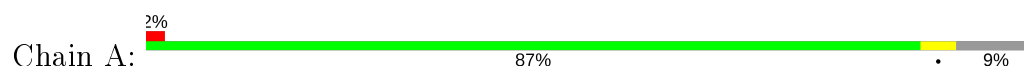
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	O 1	0	0
9	B	1	Total 1	O 1	0	0
9	C	1	Total 1	O 1	0	0
9	D	2	Total 2	O 2	0	0
9	F	2	Total 2	O 2	0	0

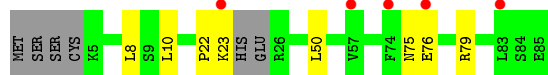
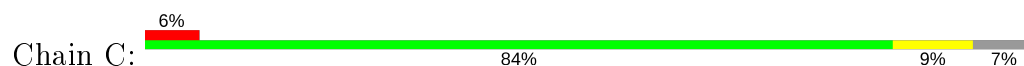
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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 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.

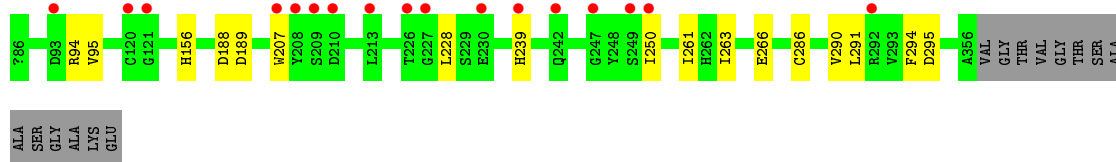
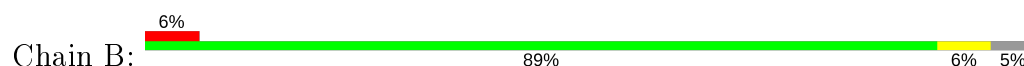
- Molecule 1: S-adenosylmethionine decarboxylase beta chain



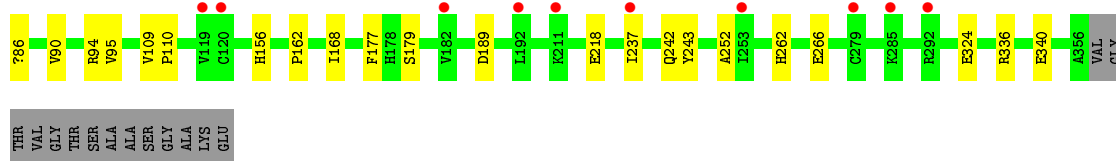
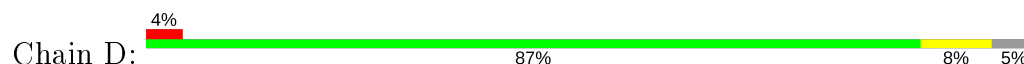
- Molecule 1: S-adenosylmethionine decarboxylase beta chain



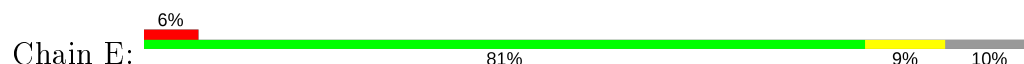
- Molecule 2: S-adenosylmethionine decarboxylase alpha chain



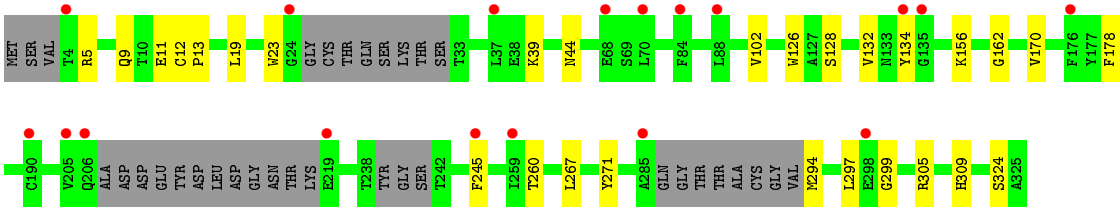
- Molecule 2: S-adenosylmethionine decarboxylase alpha chain



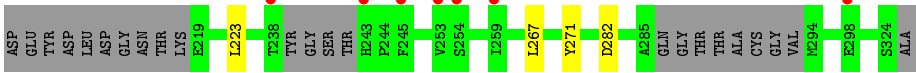
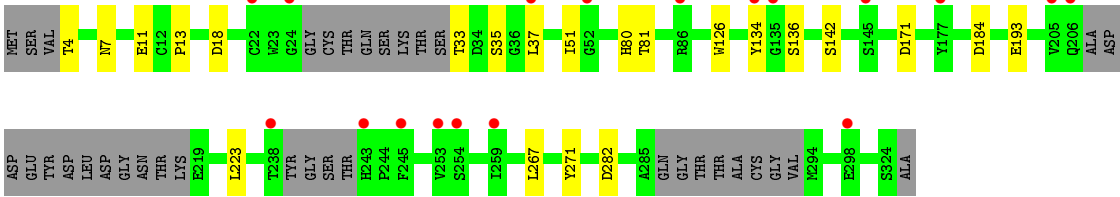
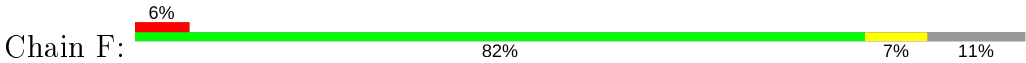
- Molecule 3: Inactive S-adenosylmethionine decarboxylase prozyme







● Molecule 3: Inactive S-adenosylmethionine decarboxylase prozyme



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.09Å 96.25Å 98.84Å 90.00° 102.43° 90.00°	Depositor
Resolution (Å)	48.26 – 2.98 48.26 – 2.98	Depositor EDS
% Data completeness (in resolution range)	84.6 (48.26-2.98) 98.0 (48.26-2.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.200 , 0.255 0.201 , 0.254	Depositor DCC
$R_{free}$ test set	1500 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.8	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 38.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	20224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.60% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: PGE, PYR, DY7, B3P, PG4, PUT

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	0.27	0/629	0.42	0/847
1	C	0.25	0/649	0.43	0/872
2	B	0.27	0/2229	0.44	0/3038
2	D	0.28	0/2229	0.45	0/3038
3	E	0.26	0/2358	0.45	0/3191
3	F	0.26	0/2345	0.44	0/3174
All	All	0.27	0/10439	0.44	0/14160

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 [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	617	600	600	5	0
1	C	637	626	626	6	0
2	B	2167	2047	2050	13	0
2	D	2167	2048	2050	15	0
3	E	2309	2227	2227	19	0
3	F	2296	2215	2215	15	0
4	B	19	26	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	19	26	26	0	0
5	B	17	11	0	0	0
5	D	17	11	0	1	0
6	E	6	12	12	0	0
6	F	6	12	12	3	0
7	E	20	28	28	0	0
8	F	13	18	18	1	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	2	0	0	0	0
9	F	2	0	0	0	0
All	All	10317	9907	9889	58	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 3.

All (58) 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)
2:D:86:PYR:H32	2:D:262:HIS:CE1	2.26	0.70
1:C:75:ASN:OD1	1:C:76:GLU:N	2.33	0.61
1:C:10:LEU:HD11	3:E:19:LEU:HG	1.82	0.61
2:B:94:ARG:NH2	4:B:401:B3P:O5	2.37	0.58
2:D:218:GLU:N	2:D:218:GLU:OE1	2.36	0.58
1:A:82:VAL:HG23	2:B:239:HIS:ND1	2.21	0.56
3:E:156:LYS:NZ	3:E:162:GLY:O	2.42	0.52
1:C:50:LEU:HD21	2:D:95:VAL:HG22	1.91	0.52
3:E:134:TYR:HH	3:E:245:PHE:HE1	1.59	0.51
3:F:184:ASP:HA	8:F:402:PG4:H22	1.93	0.51
3:E:13:PRO:HG2	3:E:19:LEU:HD13	1.94	0.50
1:A:82:VAL:HG23	2:B:239:HIS:CE1	2.47	0.49
3:F:33:THR:O	3:F:142:SER:OG	2.26	0.49
2:D:94:ARG:NH1	2:D:189:ASP:OD2	2.45	0.49
3:F:267:LEU:O	3:F:271:TYR:N	2.43	0.48
2:D:242:GLN:NE2	2:D:243:TYR:O	2.45	0.47
2:B:291:LEU:O	2:B:295:ASP:N	2.39	0.47
1:C:79:ARG:HB2	2:D:90:VAL:HB	1.97	0.47
3:F:37:LEU:HD11	3:F:134:TYR:HB3	1.97	0.47
3:E:267:LEU:HD11	3:E:297:LEU:HD13	1.97	0.46
2:B:94:ARG:NH1	2:B:189:ASP:OD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:VAL:HG23	2:B:239:HIS:HD1	1.81	0.44
3:E:128:SER:HA	3:E:178:PHE:O	2.17	0.44
3:E:11:GLU:HA	3:F:4:THR:O	2.18	0.44
2:B:263:ILE:HD13	2:B:294:PHE:HE1	1.81	0.44
3:E:44:ASN:HB2	3:E:126:TRP:HB3	2.00	0.44
2:D:266:GLU:OE2	5:D:402:DY7:N17	2.51	0.44
3:E:132:VAL:HG12	3:E:134:TYR:CE2	2.53	0.44
3:E:267:LEU:O	3:E:271:TYR:N	2.42	0.43
2:D:109:VAL:HB	2:D:110:PRO:HD3	2.01	0.43
3:F:81:THR:OG1	3:F:223:LEU:HD13	2.19	0.43
1:C:22:PRO:O	1:C:23:LYS:HB2	2.18	0.43
2:D:340:GLU:OE1	3:E:305:ARG:NH1	2.32	0.43
2:D:324:GLU:OE1	2:D:324:GLU:N	2.44	0.43
3:E:19:LEU:HD12	3:E:23:TRP:CG	2.54	0.43
2:D:237:ILE:O	2:D:252:ALA:HA	2.19	0.43
1:A:73:GLU:HG2	2:B:239:HIS:CD2	2.54	0.42
3:E:299:GLY:C	3:E:324:SER:HB2	2.39	0.42
2:B:250:ILE:CG2	2:B:261:ILE:HB	2.50	0.42
2:D:177:PHE:CZ	2:D:179:SER:HB3	2.55	0.42
3:F:193:GLU:HB3	6:F:401:PUT:HN22	1.83	0.42
2:D:162:PRO:HG2	3:E:170:VAL:HB	2.02	0.42
3:E:39:LYS:NZ	3:E:102:VAL:O	2.47	0.42
3:E:5:ARG:NH1	3:F:11:GLU:HG3	2.34	0.42
3:E:260:THR:HG22	3:E:294:MET:HG2	2.01	0.42
2:D:336:ARG:HB2	3:E:309:HIS:HB2	2.02	0.41
3:F:35:SER:HB2	3:F:134:TYR:CZ	2.55	0.41
3:F:126:TRP:CE2	6:F:401:PUT:H32	2.55	0.41
3:F:13:PRO:HB3	3:F:18:ASP:HB2	2.02	0.41
3:E:9:GLN:NE2	3:F:7:ASN:OD1	2.53	0.41
1:A:36:GLU:HA	2:B:95:VAL:O	2.21	0.41
3:F:51:ILE:HG22	3:F:80:HIS:CE1	2.56	0.41
2:B:286:CYS:O	2:B:290:VAL:HG23	2.21	0.41
2:B:207:TRP:CH2	2:B:228:LEU:HD11	2.56	0.41
2:B:266:GLU:N	2:B:266:GLU:OE1	2.50	0.41
3:F:136:SER:HB2	3:F:171:ASP:HA	2.02	0.40
1:C:8:LEU:HD22	2:D:168:ILE:HD13	2.03	0.40
3:F:282:ASP:OD1	6:F:401:PUT:N2	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
1	C	75/85 (88%)	71 (95%)	4 (5%)	0	100	100
2	B	268/285 (94%)	256 (96%)	12 (4%)	0	100	100
2	D	268/285 (94%)	264 (98%)	4 (2%)	0	100	100
3	E	281/325 (86%)	276 (98%)	5 (2%)	0	100	100
3	F	279/325 (86%)	275 (99%)	4 (1%)	0	100	100
All	All	1244/1390 (90%)	1213 (98%)	31 (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	68/76 (90%)	68 (100%)	0	100	100
1	C	70/76 (92%)	70 (100%)	0	100	100
2	B	243/251 (97%)	241 (99%)	2 (1%)	81	92
2	D	243/251 (97%)	242 (100%)	1 (0%)	91	97
3	E	254/281 (90%)	253 (100%)	1 (0%)	91	97
3	F	253/281 (90%)	253 (100%)	0	100	100
All	All	1131/1216 (93%)	1127 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	156	HIS
2	B	188	ASP
2	D	156	HIS
3	E	12	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	$\# Z  > 2$
6	PUT	F	401	-	5,5,5	0.15	0	4,4,4	0.48	0
5	DY7	D	402	-	18,18,18	2.42	8 (44%)	24,25,25	2.40	6 (25%)
4	B3P	D	401	-	18,18,18	2.86	6 (33%)	21,23,23	1.70	7 (33%)
7	PGE	E	403	-	9,9,9	0.47	0	8,8,8	0.39	0
5	DY7	B	402	-	18,18,18	2.53	8 (44%)	24,25,25	2.39	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PUT	E	401	-	5,5,5	0.26	0	4,4,4	0.55	0
8	PG4	F	402	-	12,12,12	0.50	0	11,11,11	0.39	0
7	PGE	E	402	-	9,9,9	0.51	0	8,8,8	0.31	0
4	B3P	B	401	-	18,18,18	2.36	6 (33%)	21,23,23	1.61	7 (33%)

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
6	PUT	F	401	-	-	1/3/3/3	-
5	DY7	D	402	-	-	2/4/4/4	0/2/2/2
4	B3P	D	401	-	-	2/28/28/28	-
7	PGE	E	403	-	-	4/7/7/7	-
5	DY7	B	402	-	-	2/4/4/4	0/2/2/2
6	PUT	E	401	-	-	0/3/3/3	-
8	PG4	F	402	-	-	8/10/10/10	-
7	PGE	E	402	-	-	1/7/7/7	-
4	B3P	B	401	-	-	5/28/28/28	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	B3P	C7-C4	7.63	1.62	1.53
4	D	401	B3P	C11-C8	6.48	1.61	1.53
4	B	401	B3P	C11-C8	6.31	1.61	1.53
5	D	402	DY7	C02-N17	5.33	1.44	1.35
5	B	402	DY7	C02-N17	5.26	1.44	1.35
4	B	401	B3P	C7-C4	5.14	1.59	1.53
5	B	402	DY7	BR9-C08	3.91	1.98	1.90
4	D	401	B3P	C6-C4	3.81	1.58	1.53
5	B	402	DY7	BR2-C11	3.73	1.97	1.90
5	D	402	DY7	C15-N17	3.72	1.41	1.34
4	D	401	B3P	C10-C8	3.59	1.57	1.53
5	B	402	DY7	C15-N17	3.49	1.41	1.34
5	D	402	DY7	BR9-C08	3.48	1.97	1.90
5	D	402	DY7	BR2-C11	3.39	1.97	1.90
5	B	402	DY7	C06-N05	3.35	1.48	1.40
5	D	402	DY7	C06-N05	3.06	1.47	1.40
5	B	402	DY7	C04-N05	3.02	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	401	B3P	C10-C8	2.71	1.56	1.53
5	B	402	DY7	C07-C06	2.54	1.43	1.39
5	D	402	DY7	C04-N05	2.49	1.43	1.38
5	D	402	DY7	C07-C06	2.47	1.43	1.39
5	B	402	DY7	C14-C15	-2.31	1.34	1.38
5	D	402	DY7	C14-C15	-2.31	1.34	1.38
4	B	401	B3P	C6-C4	2.28	1.56	1.53
4	B	401	B3P	C3-N1	2.19	1.49	1.46
4	D	401	B3P	C3-N1	2.19	1.49	1.46
4	D	401	B3P	C2-N2	2.16	1.49	1.46
4	B	401	B3P	C2-N2	2.06	1.49	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	DY7	C16-C15-C14	5.64	130.42	121.81
5	D	402	DY7	C16-C15-C14	5.54	130.25	121.81
5	B	402	DY7	C14-C04-N03	-4.93	112.97	123.41
5	D	402	DY7	C14-C04-N03	-4.76	113.32	123.41
5	D	402	DY7	N01-C02-N03	4.46	124.19	117.25
5	B	402	DY7	N01-C02-N03	4.38	124.06	117.25
5	D	402	DY7	C02-N03-C04	3.99	123.75	114.68
5	B	402	DY7	C02-N03-C04	3.89	123.53	114.68
5	D	402	DY7	C16-C15-N17	-3.84	110.43	116.56
5	B	402	DY7	C16-C15-N17	-3.80	110.49	116.56
4	D	401	B3P	C3-N1-C4	-3.05	111.75	116.08
4	D	401	B3P	C2-N2-C8	-2.97	111.87	116.08
5	D	402	DY7	N03-C02-N17	-2.87	120.92	125.42
4	B	401	B3P	C2-N2-C8	-2.54	112.48	116.08
5	B	402	DY7	N03-C02-N17	-2.48	121.53	125.42
4	D	401	B3P	O5-C6-C4	-2.46	106.66	111.63
4	B	401	B3P	O4-C5-C4	-2.40	106.78	111.63
4	D	401	B3P	O1-C9-C8	-2.37	106.83	111.63
4	B	401	B3P	C3-N1-C4	-2.37	112.71	116.08
4	B	401	B3P	O2-C10-C8	-2.33	106.93	111.63
4	B	401	B3P	O5-C6-C4	-2.32	106.93	111.63
4	D	401	B3P	O2-C10-C8	-2.31	106.95	111.63
4	B	401	B3P	C7-C4-C5	-2.11	105.58	110.04
4	D	401	B3P	O4-C5-C4	-2.10	107.38	111.63
4	D	401	B3P	O3-C11-C8	-2.08	107.43	111.63
4	B	401	B3P	O6-C7-C4	-2.02	107.53	111.63

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	401	B3P	O3-C11-C8-C10
7	E	403	PGE	O2-C3-C4-O3
4	B	401	B3P	C2-C1-C3-N1
8	F	402	PG4	O2-C3-C4-O3
4	B	401	B3P	O3-C11-C8-N2
4	B	401	B3P	O3-C11-C8-C9
8	F	402	PG4	O4-C7-C8-O5
4	D	401	B3P	C1-C3-N1-C4
6	F	401	PUT	C2-C3-C4-N2
8	F	402	PG4	C6-C5-O3-C4
8	F	402	PG4	C3-C4-O3-C5
8	F	402	PG4	C8-C7-O4-C6
4	D	401	B3P	C6-C4-C5-O4
8	F	402	PG4	O3-C5-C6-O4
7	E	403	PGE	C1-C2-O2-C3
5	B	402	DY7	C14-C04-N05-C06
8	F	402	PG4	C5-C6-O4-C7
4	B	401	B3P	O2-C10-C8-C9
7	E	403	PGE	C4-C3-O2-C2
8	F	402	PG4	O1-C1-C2-O2
5	D	402	DY7	N03-C04-N05-C06
5	B	402	DY7	N03-C04-N05-C06
5	D	402	DY7	C14-C04-N05-C06
7	E	402	PGE	O2-C3-C4-O3
7	E	403	PGE	C6-C5-O3-C4

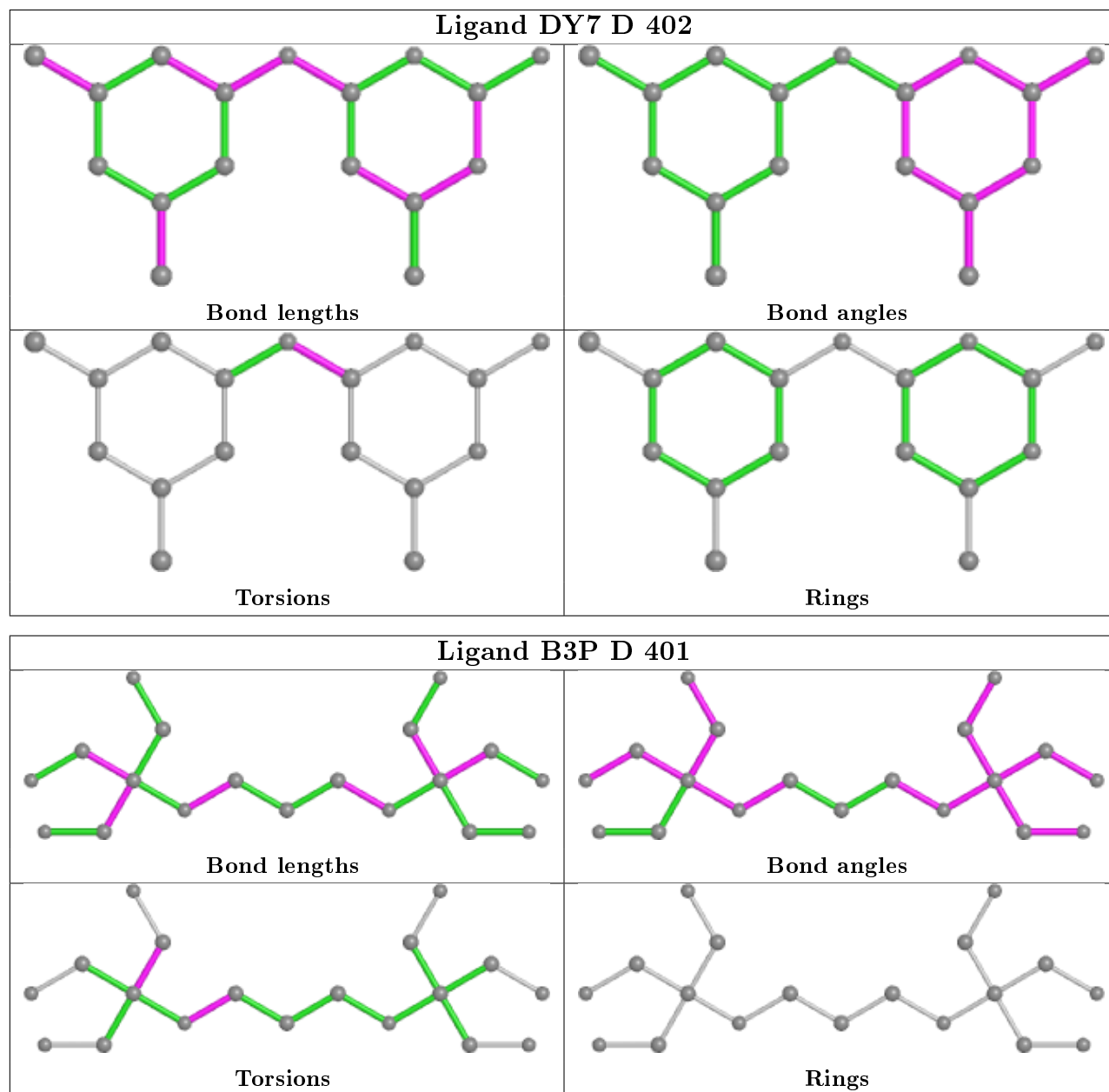
There are no ring outliers.

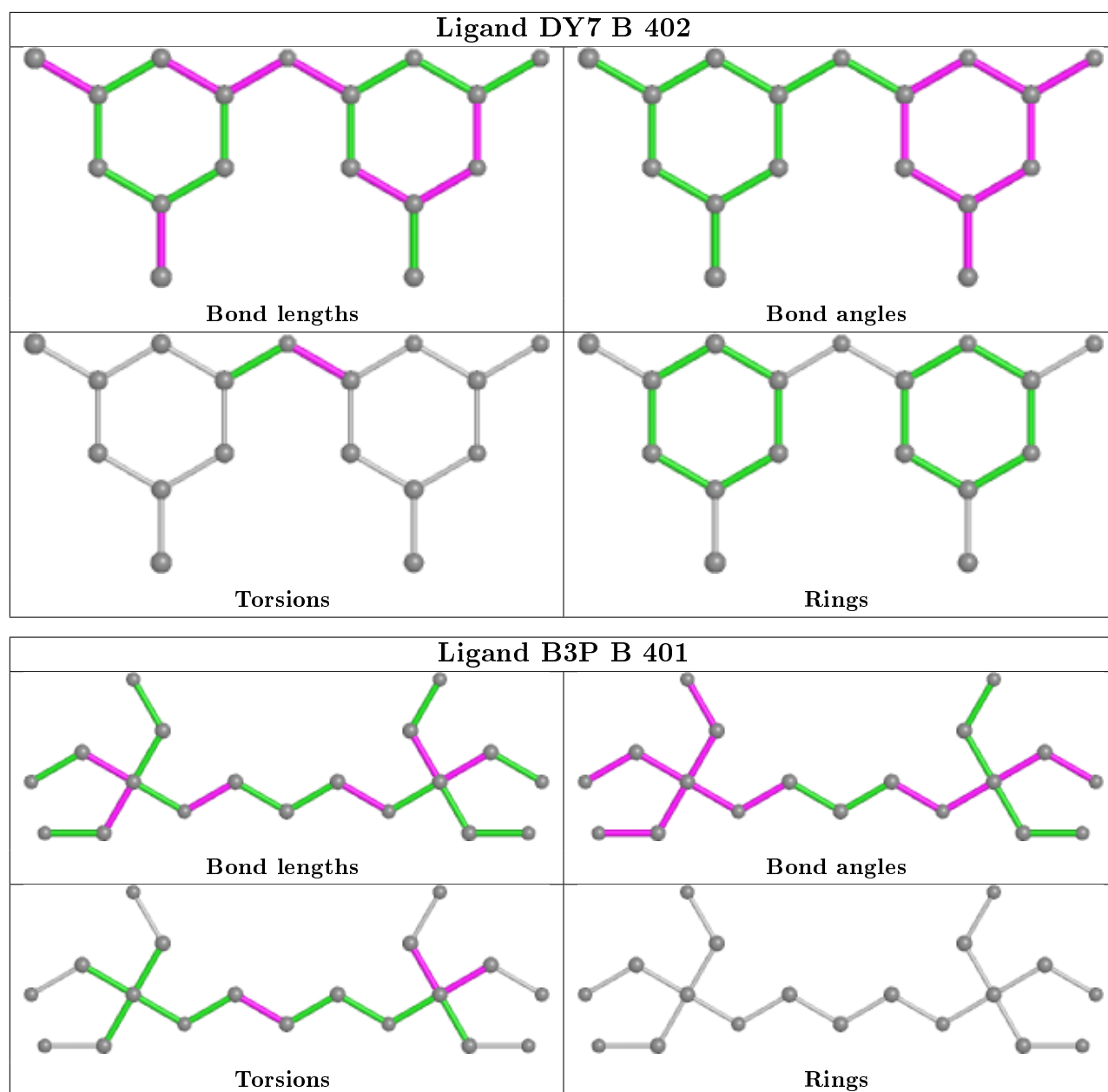
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	401	PUT	3	0
5	D	402	DY7	1	0
8	F	402	PG4	1	0
4	B	401	B3P	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 than 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.





## 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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	77/85 (90%)	0.51	2 (2%) 56 36	32, 61, 82, 93	0
1	C	79/85 (92%)	0.63	5 (6%) 20 10	35, 63, 91, 101	0
2	B	270/285 (94%)	0.48	17 (6%) 20 10	29, 50, 75, 100	0
2	D	270/285 (94%)	0.47	10 (3%) 41 25	28, 54, 77, 86	0
3	E	291/325 (89%)	0.52	18 (6%) 20 11	25, 50, 86, 98	0
3	F	289/325 (88%)	0.46	18 (6%) 20 11	25, 44, 79, 106	0
All	All	1276/1390 (91%)	0.49	70 (5%) 25 14	25, 51, 82, 106	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	24	GLY	5.6
1	C	74	PHE	4.3
2	B	120	CYS	4.3
3	F	22	CYS	4.3
3	E	206	GLN	4.1
3	E	205	VAL	4.0
3	F	134	TYR	3.9
2	D	120	CYS	3.5
3	F	37	LEU	3.4
2	D	292	ARG	3.4
2	B	208	TYR	3.4
3	E	37	LEU	3.3
3	F	238	THR	3.3
3	E	134	TYR	3.2
3	F	206	GLN	3.2
3	F	245	PHE	3.1
3	F	205	VAL	3.0
3	E	190	CYS	2.9
3	E	24	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	23	LYS	2.9
2	B	209	SER	2.9
1	C	83	LEU	2.8
3	F	259	ILE	2.8
2	B	226	THR	2.8
2	B	213	LEU	2.8
2	D	192	LEU	2.7
3	F	86	ARG	2.7
3	E	135	GLY	2.7
3	E	259	ILE	2.7
2	B	207	TRP	2.7
2	D	119	VAL	2.7
3	E	84	PHE	2.6
2	D	182	VAL	2.6
3	F	253	VAL	2.6
2	B	242	GLN	2.6
3	F	243	HIS	2.6
2	D	279	CYS	2.5
2	B	210	ASP	2.5
2	D	237	ILE	2.5
1	A	82	VAL	2.5
1	C	57	VAL	2.5
2	B	292	ARG	2.5
1	C	76	GLU	2.5
2	B	121	GLY	2.5
3	E	245	PHE	2.5
3	E	70	LEU	2.4
3	F	298	GLU	2.4
3	E	285	ALA	2.4
3	E	298	GLU	2.3
2	B	239	HIS	2.3
2	D	285	LYS	2.3
3	E	219	GLU	2.3
3	F	177	TYR	2.2
3	F	254	SER	2.2
3	E	68	GLU	2.2
3	E	4	THR	2.2
3	F	52	GLY	2.2
2	B	247	GLY	2.1
2	D	253	ILE	2.1
2	B	227	GLY	2.1
2	B	230	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	F	135	GLY	2.1
2	B	249	SER	2.1
2	B	250	ILE	2.1
3	E	176	PHE	2.1
2	B	93	ASP	2.1
2	D	211	LYS	2.0
3	E	88	LEU	2.0
3	F	145	SER	2.0
1	A	40	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

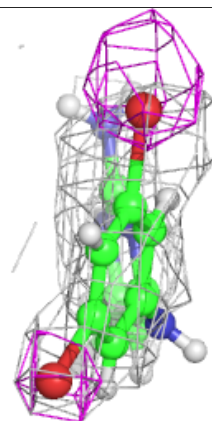
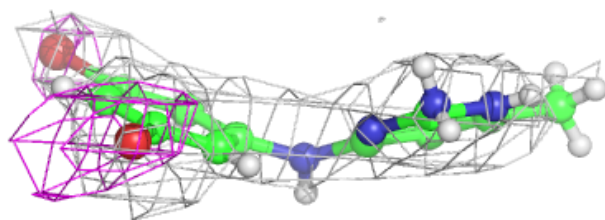
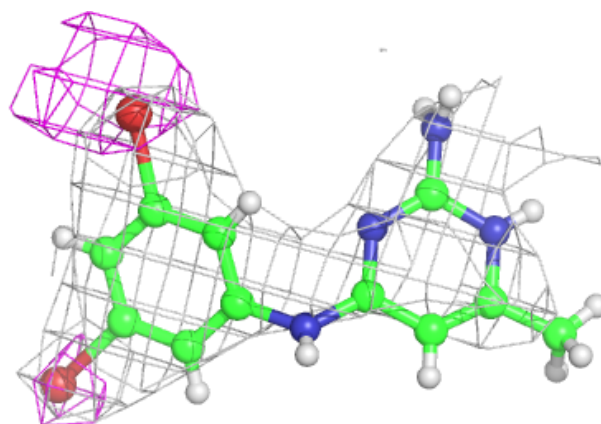
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	PGE	E	403	10/10	0.61	0.20	65,88,103,103	0
7	PGE	E	402	10/10	0.64	0.38	46,69,77,82	0
8	PG4	F	402	13/13	0.68	0.33	41,58,72,72	0
5	DY7	D	402	17/17	0.81	0.32	60,85,107,133	0
4	B3P	D	401	19/19	0.85	0.21	49,71,93,100	0
5	DY7	B	402	17/17	0.86	0.30	57,76,99,122	0
4	B3P	B	401	19/19	0.93	0.21	35,55,72,87	0
6	PUT	E	401	6/6	0.95	0.25	35,46,57,57	0
6	PUT	F	401	6/6	0.97	0.22	25,32,48,48	0

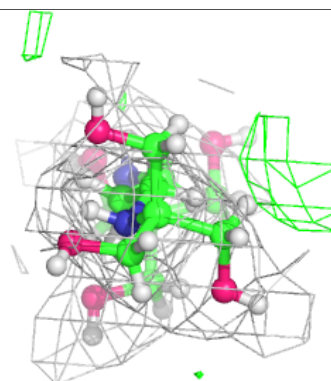
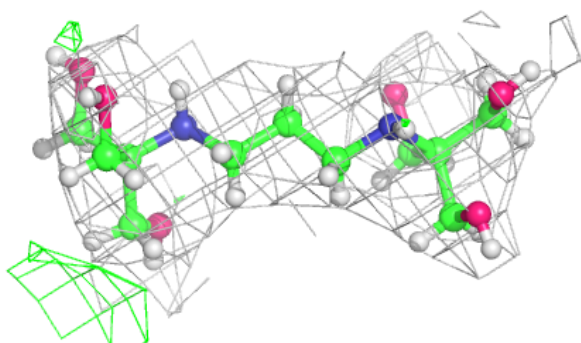
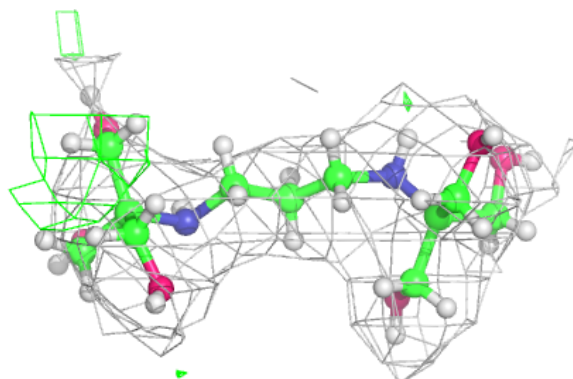
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around DY7 D 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around B3P D 401:**

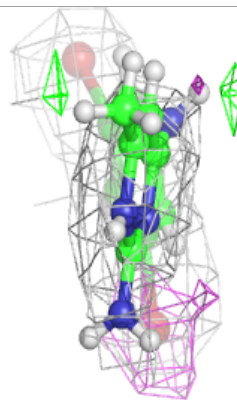
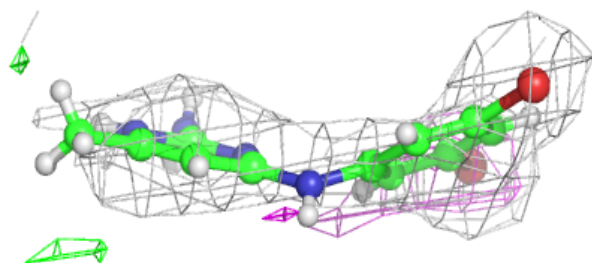
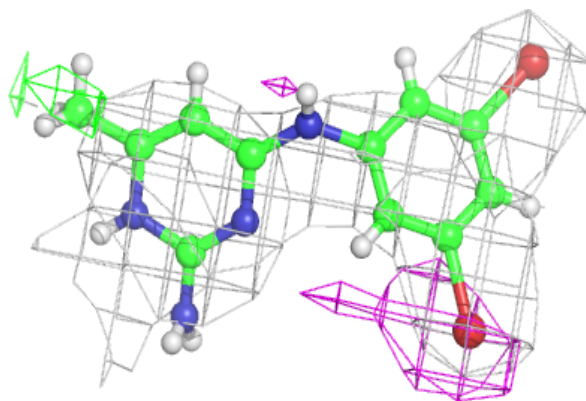
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



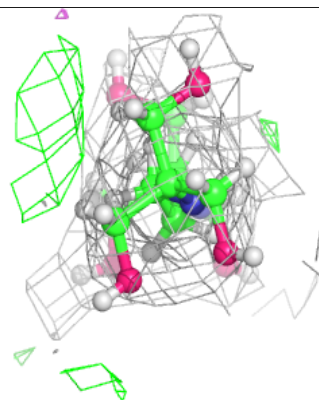
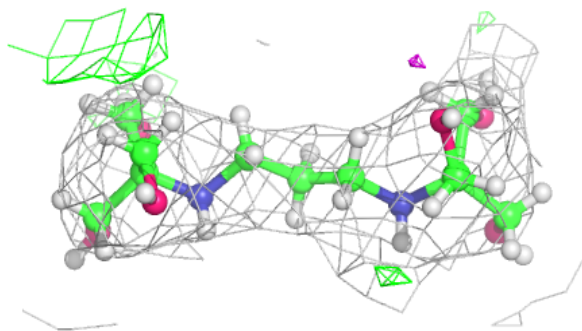
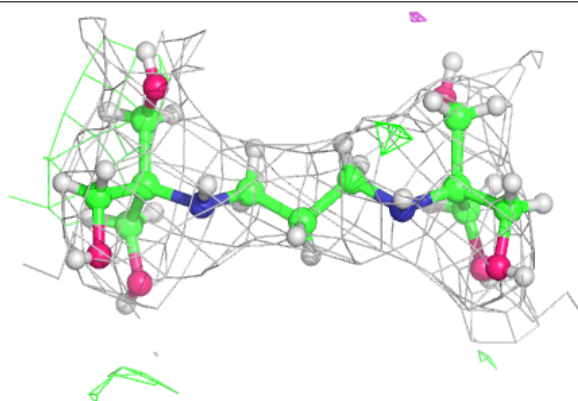


**Electron density around DY7 B 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around B3P B 401:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.