



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 11, 2019 – 07:37 PM EST

PDB ID : 1C30  
Title : CRYSTAL STRUCTURE OF CARBAMOYL PHOSPHATE SYNTHETASE:  
SMALL SUBUNIT MUTATION C269S  
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.  
Deposited on : 1999-07-24  
Resolution : 2.00 Å(reported)

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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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

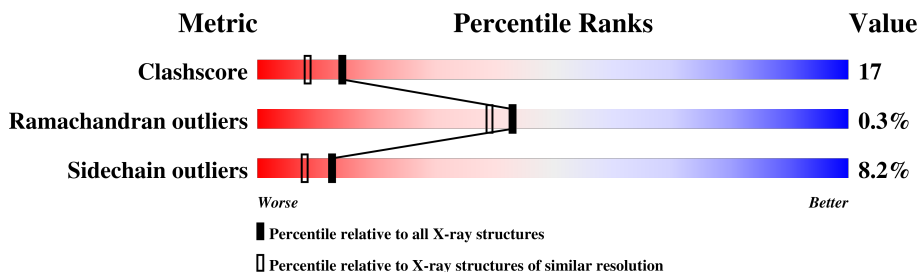
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1073	61% 30% 7% ..
1	C	1073	59% 31% 7% ..
1	E	1073	64% 28% 7% .
1	G	1073	52% 38% 8% ..
2	B	382	58% 35% 6% .
2	D	382	57% 35% 6% ..
2	F	382	53% 38% 8% .
2	H	382	45% 45% 8% .

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
6	PO4	C	4025	-	X	-	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 48668 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 CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1058	Total	C	N	O	S	0	6	0
			8189	5141	1429	1574	45			
1	C	1058	Total	C	N	O	S	0	1	0
			8165	5126	1422	1572	45			
1	E	1058	Total	C	N	O	S	0	6	0
			8188	5141	1426	1575	46			
1	G	1058	Total	C	N	O	S	0	4	0
			8178	5137	1424	1572	45			

- Molecule 2 is a protein called CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	D	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	F	379	Total	C	N	O	S	0	0	0
			2895	1825	508	553	9			
2	H	379	Total	C	N	O	S	0	1	0
			2900	1828	508	555	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	269	SER	CYS	engineered mutation	UNP P00907
D	269	SER	CYS	engineered mutation	UNP P00907
F	269	SER	CYS	engineered mutation	UNP P00907
H	269	SER	CYS	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	3	Total 3	Mn 3	0	0
3	A	3	Total 3	Mn 3	0	0
3	C	3	Total 3	Mn 3	0	0
3	E	3	Total 3	Mn 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	7	Total 7	K 7	0	0
4	D	1	Total 1	K 1	0	0
4	E	7	Total 7	K 7	0	0
4	H	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	C	7	Total 7	K 7	0	0
4	A	7	Total 7	K 7	0	0
4	F	1	Total 1	K 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

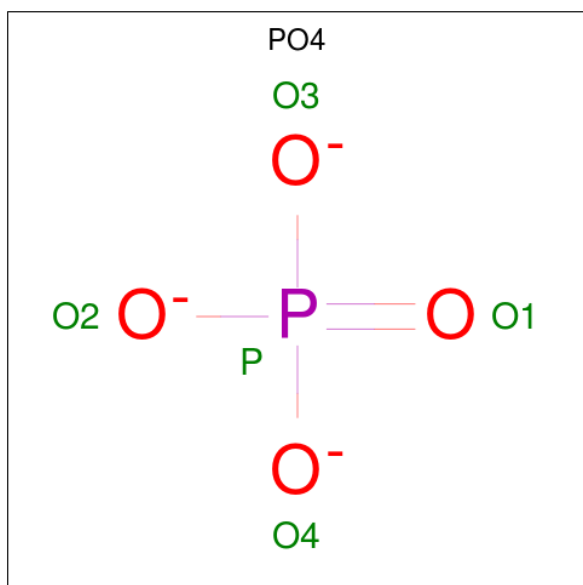
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	3	Total 3	Cl 3	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	3	Total 3	Cl 3	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	3	Total 3	Cl 3	0	0

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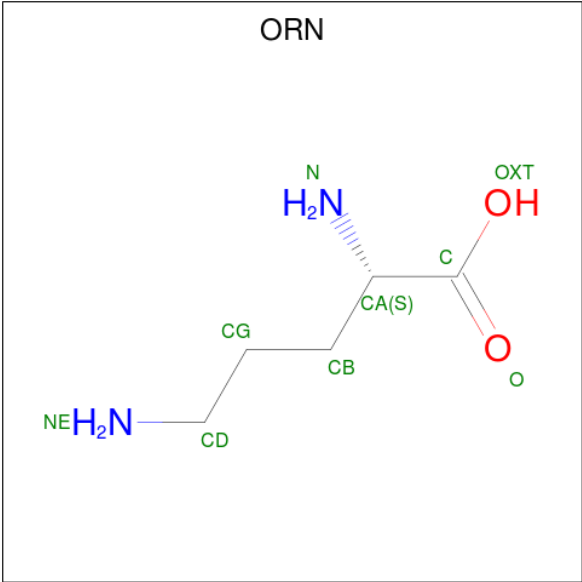
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



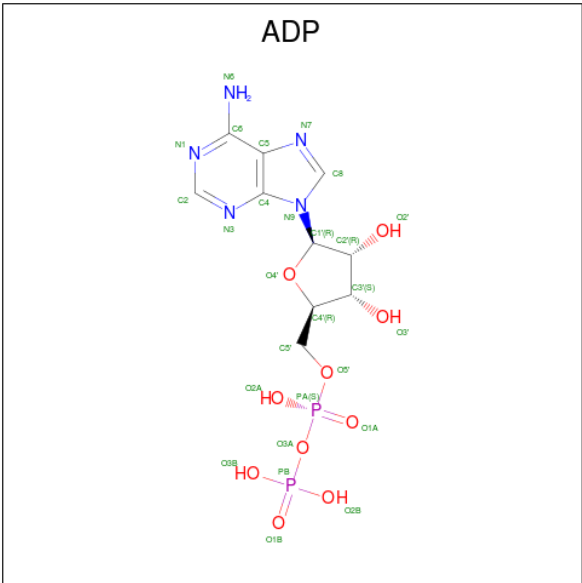
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		
6	G	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is L-ornithine (three-letter code: ORN) (formula: C<sub>5</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



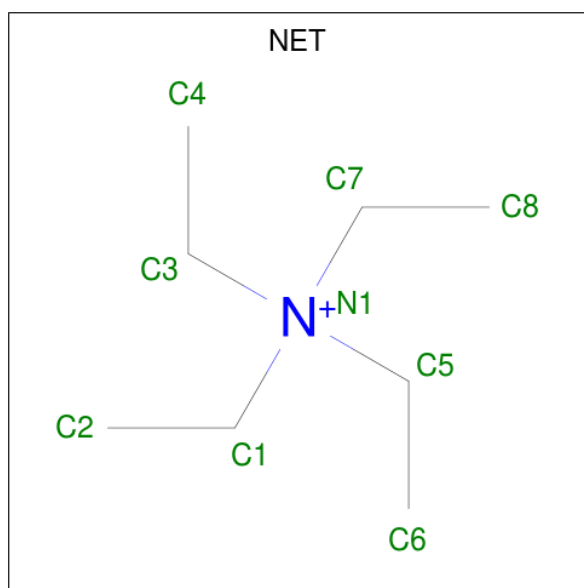
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			9	5	2	2		
7	A	1	Total	C	N	O	0	0
			8	5	2	1		
7	A	1	Total	C	N	O	0	0
			8	5	2	1		
7	A	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
8	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (three-letter code: NET) (formula:  $C_8H_{20}N$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	N	0	0
			9	8	1		
9	C	1	Total	C	N	0	0
			9	8	1		
9	E	1	Total	C	N	0	0
			9	8	1		
9	G	1	Total	C	N	0	0
			9	8	1		



- Molecule 10 is water.

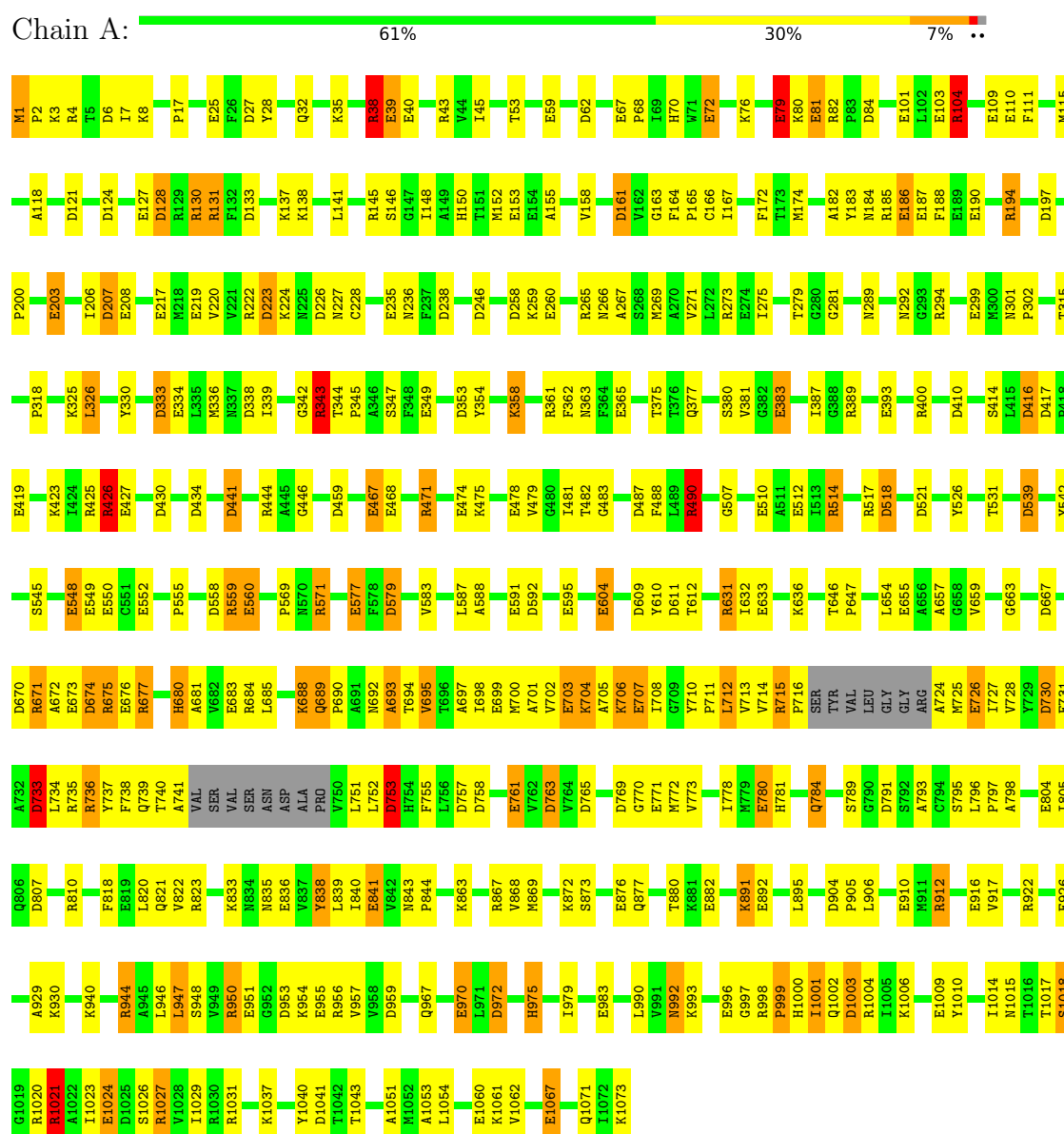
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	830	Total 830	O 830	0	0
10	B	230	Total 230	O 230	0	0
10	C	683	Total 683	O 683	0	0
10	D	238	Total 238	O 238	0	0
10	E	884	Total 884	O 884	0	0
10	F	272	Total 272	O 272	0	0
10	G	666	Total 666	O 666	0	0
10	H	184	Total 184	O 184	0	0

### 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 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.

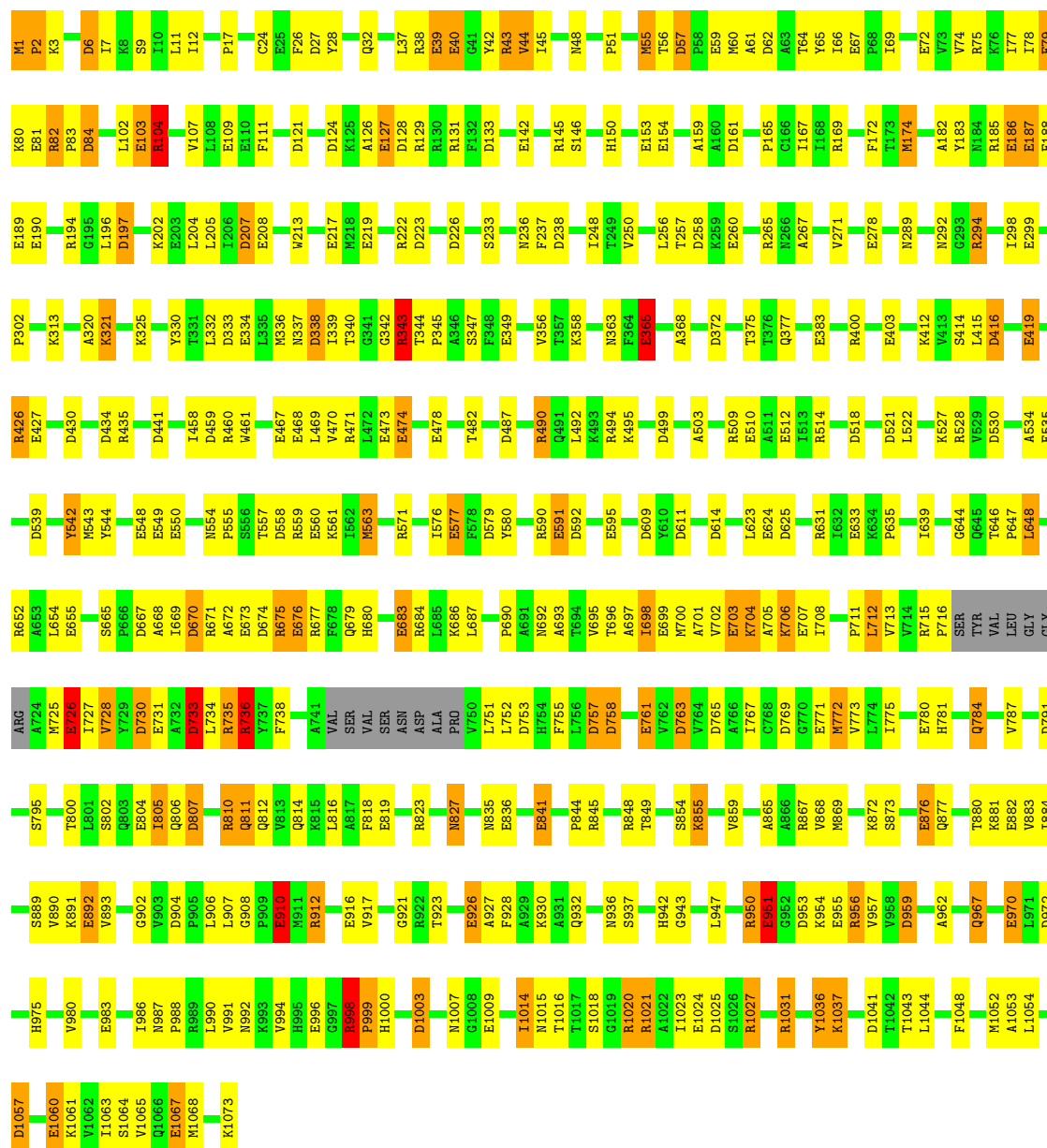
Note EDS was not executed.

#### • Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT



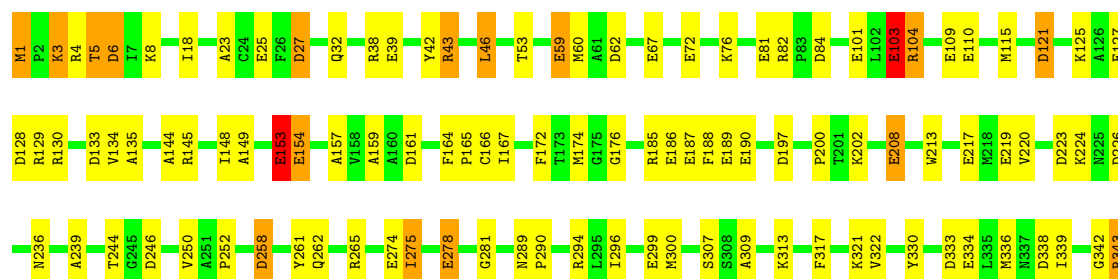
#### • Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain C:  59% 31% 7% ..



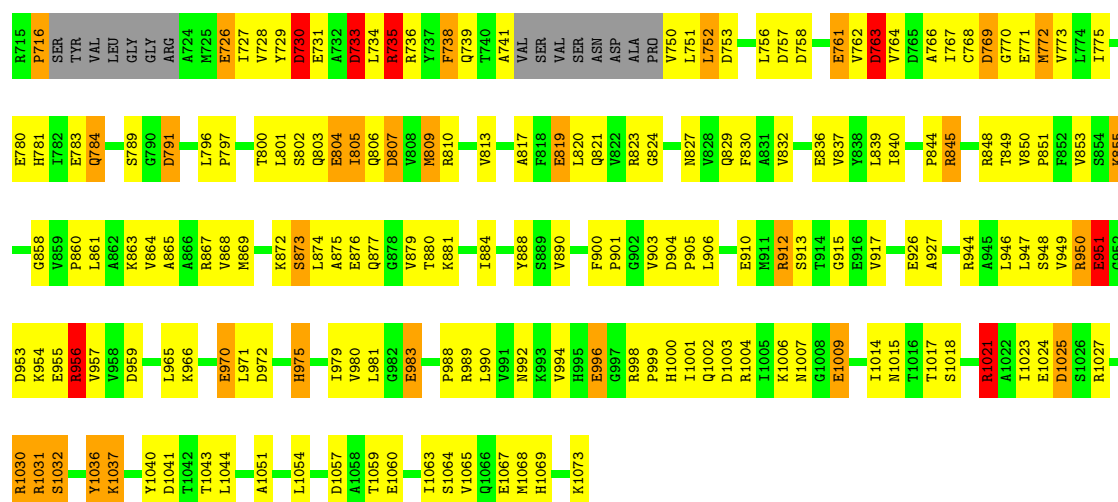
• Molecule 1: CARBAMOYL PHOSPHATE SYNTHETASE: LARGE SUBUNIT

Chain E:  64% 28% 7% ..

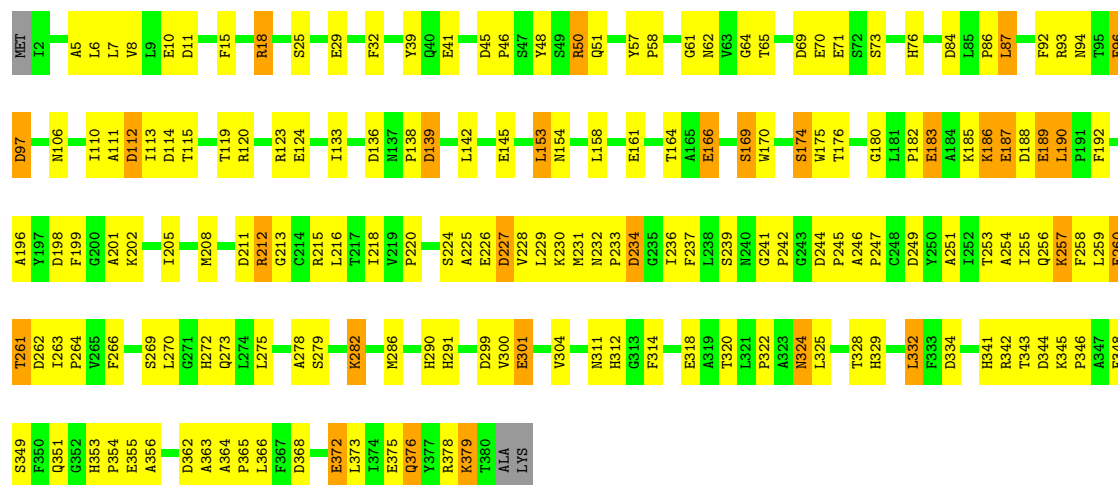




L654	M583	L492	A406	F286	Y183	E81	M1
E655	R571	K493	T407	R286	N184	R82	P2
A656	A657	R494		I296	E185	P83	K3
G658	E577		D410	I296	E186	D94	R4
V659	F578	D499	P411	P302	E188	A85	T5
P660	D579	V680	K412	R303	E189	V86	D6
I662	F580	L502	V413	F304	E190	L102	I7
G663	A588	L505	D416	K313	L196	E103	K8
T664	F589		D417	A314	D197	R104	S9
S665	R590	V608	P418	T315		Q105	I10
P666	R591	R509	E419		R202	E109	L11
D667	D592	E510	A420	A320	E203	E110	
A668	A511	A511	A420	K321	L204	F111	C24
E595	E512	E512	K423		L205	E111	E25
T596				K325	T206	A118	P96
	L516	L516	R426	L326	D207		D27
E604	R517	R517	E427	I328	E208	D121	Y28
E673	D518	L428	L428	V328			S29
D609	D519	K429	K429	G329	K214	D124	
R675	V610	Y620	D430	Y330	E215	K126	Q32
D611	D521	D521		T331		A126	
	L522	L522	D434	L332	E219	E127	
D614	R635	R635	R435	D333		D128	K35
R615	P524	P524	I436	E334	R222	R129	A36
H680	V525	V525	W437		D223	R130	L37
E619	Y626	Y626	Y438	D338	K224	R131	R38
	K527	K527	I439	I339	N295	F132	E39
	R528	R528	A440	T340	D226	D133	E40
E683	V629	V629		R434	E235	V134	G41
R684	L624	L624	R444	T344	N236	A135	Y42
L685	D624	D624	D450	P345	F237	K138	R43
K686	D625	T531			D238		V44
L687	V626		D450	E349			V46
	A534	A534	F453		D246	T143	
K688	E535	E535			D246	A144	M65
Q689	L628	L628	T456	D353	Q254	R145	T56
P690	P629	D539	M457	F354	T255	I148	D57
A691	R630		I458			A149	P58
N692	R631	Y642		K358	L256	H150	E59
A693	L632	N643	E467	I359	T257	E151	M60
T694	E633	Y644	E468	P360	D258	T152	A61
V695	K634	S545	L469	R361	K259	E153	D62
P696	P635	R545	V470	E365	E260	E154	A63
A697	K636	T546	V470		Y261		T64
I698	G637	Y547					
E699	V638	E548	E473	D372	R265	P165	
	F639	E549	E474	R373	K266	C166	E67
A701	V640	E550	K475	T376	A267	I167	P68
T702	G641	C551				H168	I69
E703	F642	E552	E478	T376	S268	R169	H70
K704	G643	A553	V479	E383	K269		W71
A705	G644	P554	G480	I481	A270	M174	E72
K706	G645	P555	I481	G388	V271	G175	V73
E707	T646	S556	T482	R389	L272		V74
T708	P647	T557	G483		E274	G176	R75
I709	L648	D558		E393	D275		K76
Y710		R559	D487			G180	
	A651	E560	F488			I181	E79
W713	R652	V661	I490	E400		A182	S80
	A652						

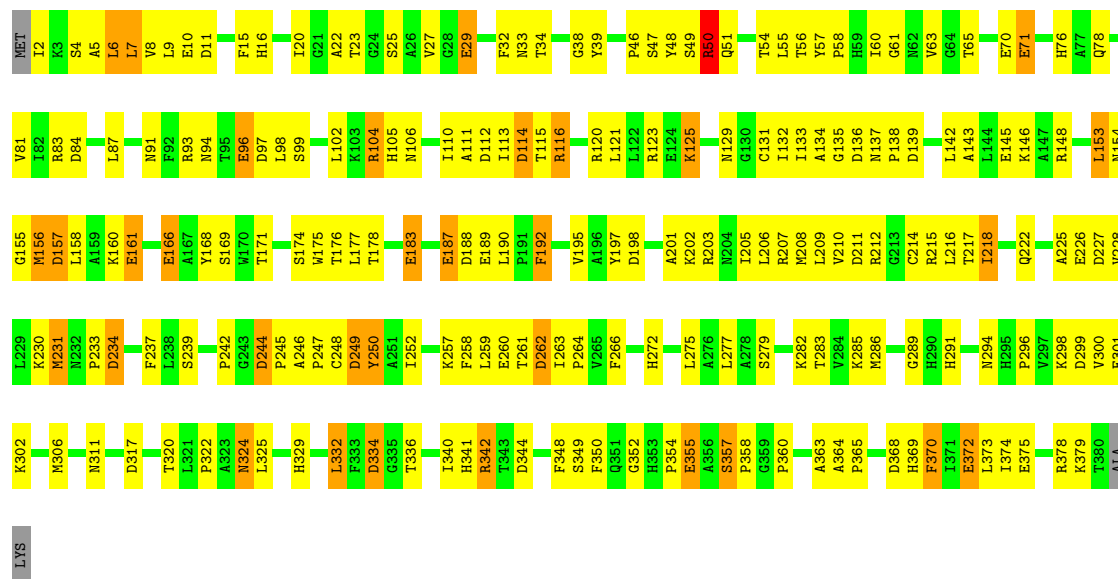


Chain F: 



### • Molecule 2: CARBAMOYL PHOSPHATE SYNTHETASE: SMALL SUBUNIT

Chain H: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.60Å 164.60Å 332.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.189 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	48668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CL, K, MN, ORN, NET, PO4

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	1.02	75/8339 (0.9%)	1.40	124/11273 (1.1%)
1	C	1.05	77/8295 (0.9%)	1.45	145/11214 (1.3%)
1	E	1.05	77/8338 (0.9%)	1.40	116/11270 (1.0%)
1	G	1.00	72/8320 (0.9%)	1.44	131/11246 (1.2%)
2	B	0.90	19/2957 (0.6%)	1.29	37/4016 (0.9%)
2	D	0.97	18/2957 (0.6%)	1.36	36/4016 (0.9%)
2	F	0.93	20/2957 (0.7%)	1.35	40/4016 (1.0%)
2	H	0.93	18/2966 (0.6%)	1.36	35/4028 (0.9%)
All	All	1.01	376/45129 (0.8%)	1.40	664/61079 (1.1%)

The worst 5 of 376 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CD-OE2	10.28	1.36	1.25
1	E	1009[A]	GLU	CD-OE2	9.59	1.36	1.25
1	E	1009[B]	GLU	CD-OE2	9.59	1.36	1.25
1	C	955	GLU	CD-OE2	9.24	1.35	1.25
1	C	951	GLU	CD-OE2	8.93	1.35	1.25

The worst 5 of 664 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	261	TYR	CB-CG-CD2	-14.58	112.25	121.00
1	C	490	ARG	NE-CZ-NH1	11.23	125.91	120.30
1	G	43	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	E	609	ASP	CB-CG-OD2	-10.78	108.60	118.30
1	E	514	ARG	NE-CZ-NH2	-10.48	115.06	120.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8189	0	8227	251	0
1	C	8165	0	8199	238	0
1	E	8188	0	8225	212	0
1	G	8178	0	8221	338	0
2	B	2895	0	2861	107	0
2	D	2895	0	2861	99	0
2	F	2895	0	2861	113	0
2	H	2900	0	2863	144	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
4	C	7	0	0	0	0
4	D	1	0	0	0	0
4	E	7	0	0	0	0
4	F	1	0	0	0	0
4	G	7	0	0	0	0
4	H	1	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
5	D	1	0	0	0	0
5	E	3	0	0	1	0
5	F	1	0	0	0	0
5	G	3	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	1	0
6	E	10	0	0	0	0
6	G	5	0	0	0	0
7	A	34	0	44	2	0
8	A	54	0	24	2	0
8	C	54	0	24	0	0
8	E	54	0	24	4	0
8	G	54	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	9	0	20	0	0
9	C	9	0	20	0	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	830	0	0	24	0
10	B	230	0	0	5	0
10	C	683	0	0	23	0
10	D	238	0	0	4	0
10	E	884	0	0	21	0
10	F	272	0	0	2	0
10	G	666	0	0	20	0
10	H	184	0	0	3	0
All	All	48668	0	44538	1483	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 17.

The worst 5 of 1483 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:993:LYS:CE	1:E:993:LYS:NZ	1.67	1.55
1:G:695:VAL:HG11	1:G:701:ALA:HB2	1.28	1.12
1:C:998:ARG:HG3	1:C:999:PRO:HA	1.30	1.11
1:C:695:VAL:HG11	1:C:701:ALA:HB2	1.34	1.09
2:H:187:GLU:HG2	2:H:215:ARG:HD2	1.31	1.07

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	1058/1073 (99%)	1012 (96%)	42 (4%)	4 (0%)	36	31
1	C	1053/1073 (98%)	996 (95%)	51 (5%)	6 (1%)	27	21
1	E	1058/1073 (99%)	1014 (96%)	44 (4%)	0	100	100
1	G	1056/1073 (98%)	1000 (95%)	50 (5%)	6 (1%)	27	21
2	B	377/382 (99%)	361 (96%)	16 (4%)	0	100	100
2	D	377/382 (99%)	364 (97%)	13 (3%)	0	100	100
2	F	377/382 (99%)	358 (95%)	18 (5%)	1 (0%)	43	39
2	H	378/382 (99%)	355 (94%)	23 (6%)	0	100	100
All	All	5734/5820 (98%)	5460 (95%)	257 (4%)	17 (0%)	43	39

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	558	ASP
1	A	975	HIS
1	C	698	ILE
1	A	693	ALA
1	C	758	ASP

### 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	871/878 (99%)	808 (93%)	63 (7%)	16	10
1	C	866/878 (99%)	799 (92%)	67 (8%)	14	9
1	E	871/878 (99%)	805 (92%)	66 (8%)	14	9
1	G	869/878 (99%)	791 (91%)	78 (9%)	10	6
2	B	308/310 (99%)	284 (92%)	24 (8%)	14	9
2	D	308/310 (99%)	284 (92%)	24 (8%)	14	9
2	F	308/310 (99%)	279 (91%)	29 (9%)	9	5
2	H	309/310 (100%)	271 (88%)	38 (12%)	5	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4710/4752 (99%)	4321 (92%)	389 (8%)	12 7

5 of 389 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	366	LEU
1	E	735	ARG
2	H	125	LYS
1	E	46	LEU
1	E	428	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	222	GLN
1	E	784	GLN
2	H	51	GLN
2	D	324	ASN
1	E	457	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 82 ligands modelled in this entry, 60 are monoatomic - leaving 22 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
8	ADP	A	4000	3	24,29,29	1.06	2 (8%)	25,45,45	1.27	2 (8%)
6	PO4	A	4005	3,4	4,4,4	2.29	2 (50%)	6,6,6	1.24	0
8	ADP	A	4006	3,4	24,29,29	1.15	3 (12%)	25,45,45	1.33	3 (12%)
7	ORN	A	4010	-	4,8,8	0.57	0	3,9,9	1.03	0
9	NET	A	4011	-	8,8,8	0.66	0	10,10,10	0.55	0
7	ORN	A	4030	-	7,7,8	1.00	1 (14%)	3,7,9	1.87	1 (33%)
7	ORN	A	4051	-	7,7,8	1.31	2 (28%)	3,7,9	0.73	0
7	ORN	A	4072	-	4,8,8	0.35	0	3,9,9	0.73	0
8	ADP	C	4020	3	24,29,29	1.30	3 (12%)	25,45,45	1.30	2 (8%)
6	PO4	C	4025	3,4	4,4,4	2.35	4 (100%)	6,6,6	1.09	0
8	ADP	C	4026	3,4	24,29,29	1.33	4 (16%)	25,45,45	1.11	3 (12%)
9	NET	C	4031	-	8,8,8	0.54	0	10,10,10	0.49	0
6	PO4	C	4040	-	4,4,4	1.25	0	6,6,6	0.79	0
8	ADP	E	4041	3	24,29,29	1.50	4 (16%)	25,45,45	1.35	4 (16%)
6	PO4	E	4046	3,4	4,4,4	2.01	2 (50%)	6,6,6	1.05	0
8	ADP	E	4047	3,4	24,29,29	1.51	4 (16%)	25,45,45	1.05	3 (12%)
9	NET	E	4052	-	8,8,8	0.66	0	10,10,10	0.61	0
6	PO4	E	4061	-	4,4,4	2.24	3 (75%)	6,6,6	0.91	0
8	ADP	G	4062	3	24,29,29	1.26	2 (8%)	25,45,45	1.14	3 (12%)
6	PO4	G	4067	3,4	4,4,4	2.30	2 (50%)	6,6,6	1.11	0
8	ADP	G	4068	3,4	24,29,29	1.31	5 (20%)	25,45,45	1.17	3 (12%)
9	NET	G	4073	-	8,8,8	0.77	0	10,10,10	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	A	4000	3	-	0/12/32/32	0/3/3/3
8	ADP	A	4006	3,4	-	3/12/32/32	0/3/3/3
7	ORN	A	4010	-	-	4/4/8/8	-
9	NET	A	4011	-	-	0/12/12/12	-
7	ORN	A	4030	-	-	4/4/6/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ORN	A	4051	-	-	3/4/6/8	-
7	ORN	A	4072	-	-	4/4/8/8	-
8	ADP	C	4020	3	-	2/12/32/32	0/3/3/3
8	ADP	C	4026	3,4	-	0/12/32/32	0/3/3/3
9	NET	C	4031	-	-	0/12/12/12	-
8	ADP	E	4041	3	-	1/12/32/32	0/3/3/3
8	ADP	E	4047	3,4	-	2/12/32/32	0/3/3/3
9	NET	E	4052	-	-	3/12/12/12	-
8	ADP	G	4062	3	-	0/12/32/32	0/3/3/3
8	ADP	G	4068	3,4	-	3/12/32/32	0/3/3/3
9	NET	G	4073	-	-	0/12/12/12	-

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	4047	ADP	PB-O3A	4.42	1.66	1.60
8	E	4041	ADP	PB-O3A	3.93	1.66	1.60
8	C	4026	ADP	PB-O3A	3.87	1.65	1.60
6	G	4067	PO4	P-O2	-3.62	1.43	1.54
8	G	4062	ADP	PB-O3A	3.46	1.65	1.60

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	4020	ADP	C5-C6-N6	4.83	127.96	120.38
8	A	4000	ADP	C5-C6-N6	4.25	127.06	120.38
8	A	4006	ADP	C5-C6-N6	4.09	126.81	120.38
8	E	4041	ADP	C5-C6-N6	4.09	126.80	120.38
8	G	4068	ADP	C5-C6-N6	3.00	125.09	120.38

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

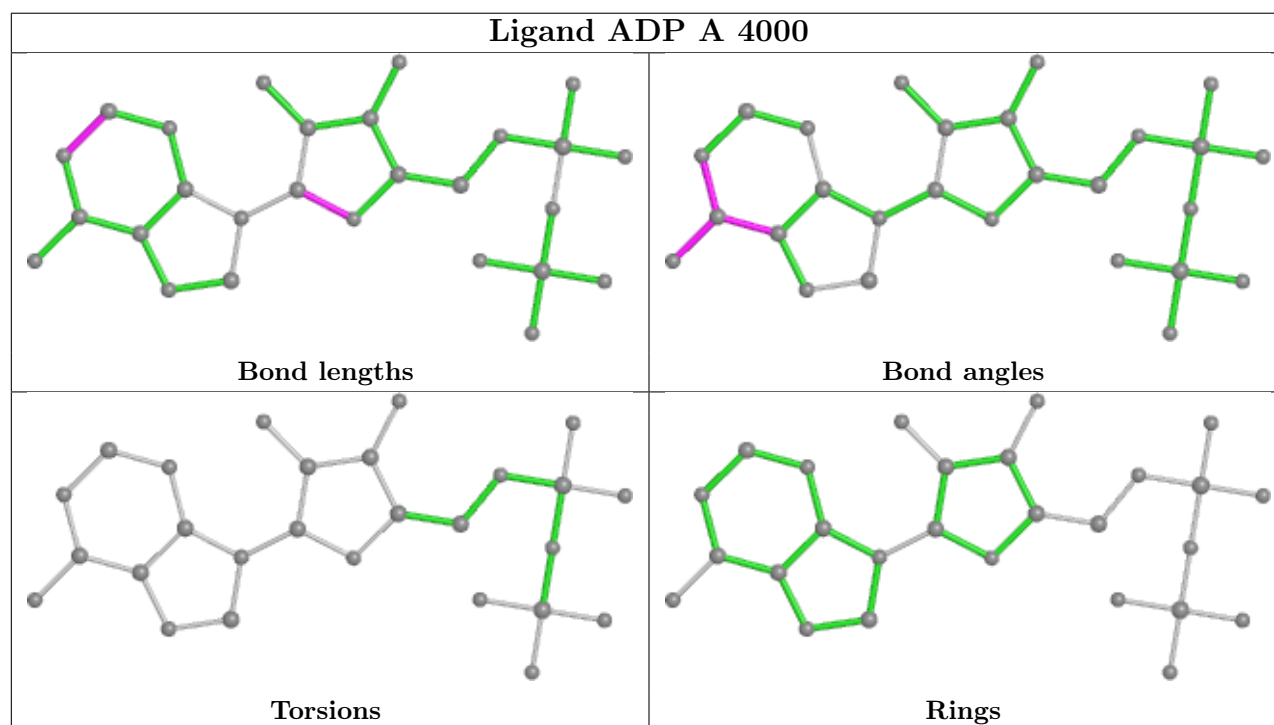
Mol	Chain	Res	Type	Atoms
7	A	4030	ORN	N-CA-CB-CG
7	A	4030	ORN	C-CA-CB-CG
8	G	4068	ADP	C5'-O5'-PA-O3A
7	A	4010	ORN	N-CA-CB-CG
7	A	4010	ORN	C-CA-CB-CG

There are no ring outliers.

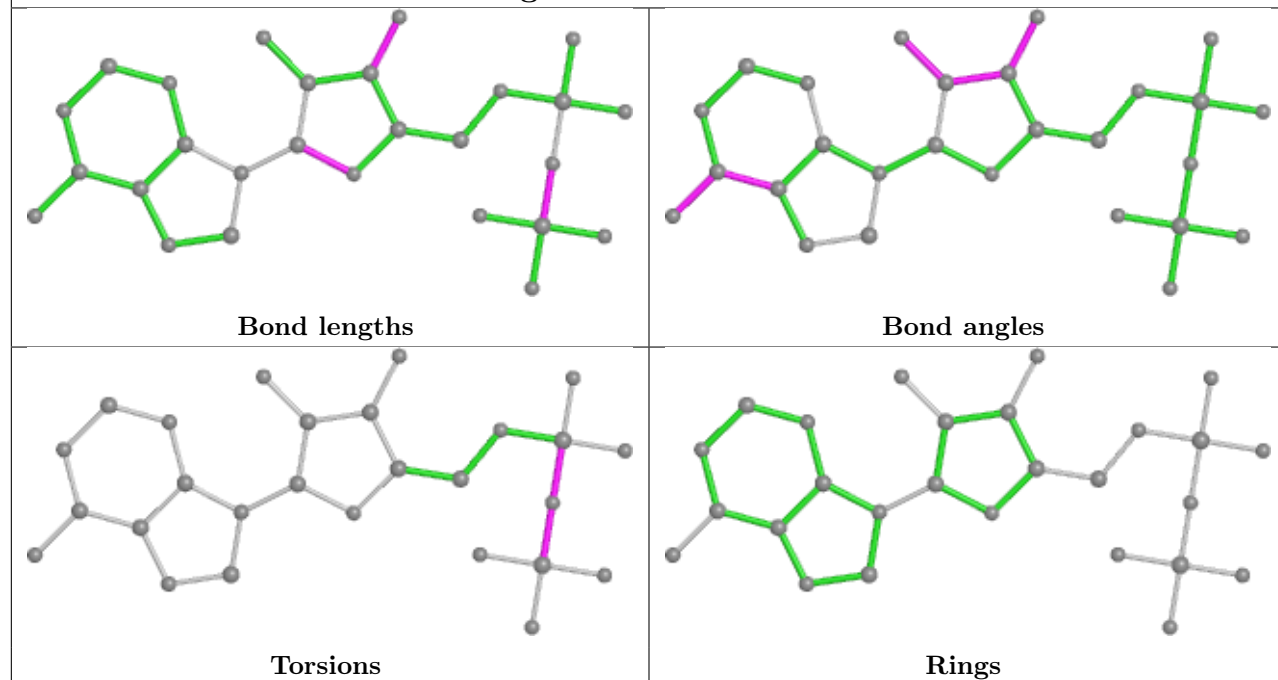
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4000	ADP	1	0
8	A	4006	ADP	1	0
7	A	4030	ORN	1	0
7	A	4051	ORN	1	0
8	E	4041	ADP	2	0
8	E	4047	ADP	2	0
8	G	4062	ADP	1	0

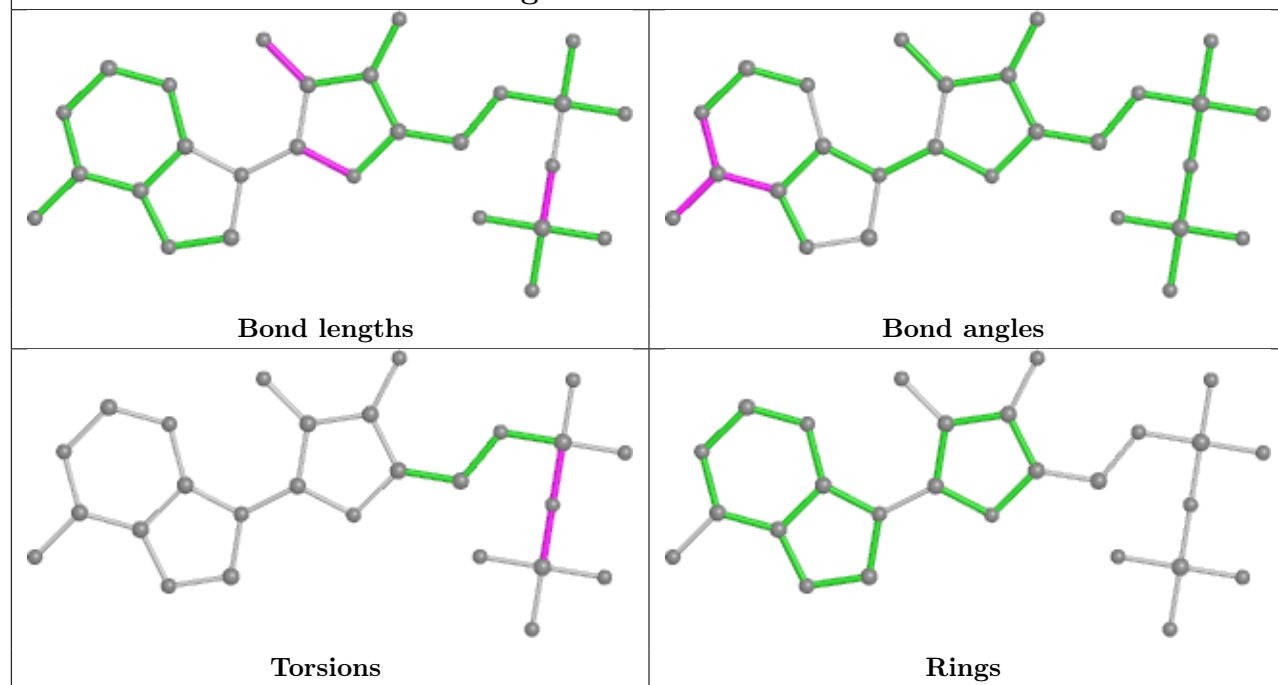
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand ADP A 4006

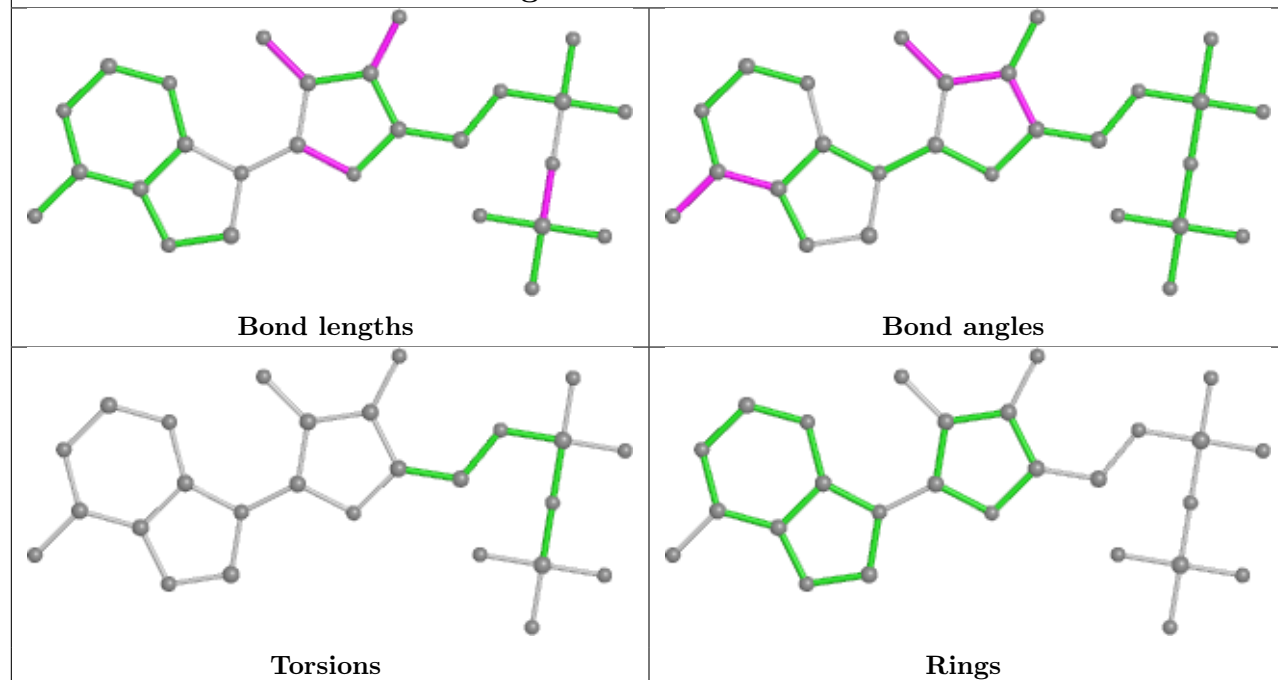


## Ligand ADP C 4020

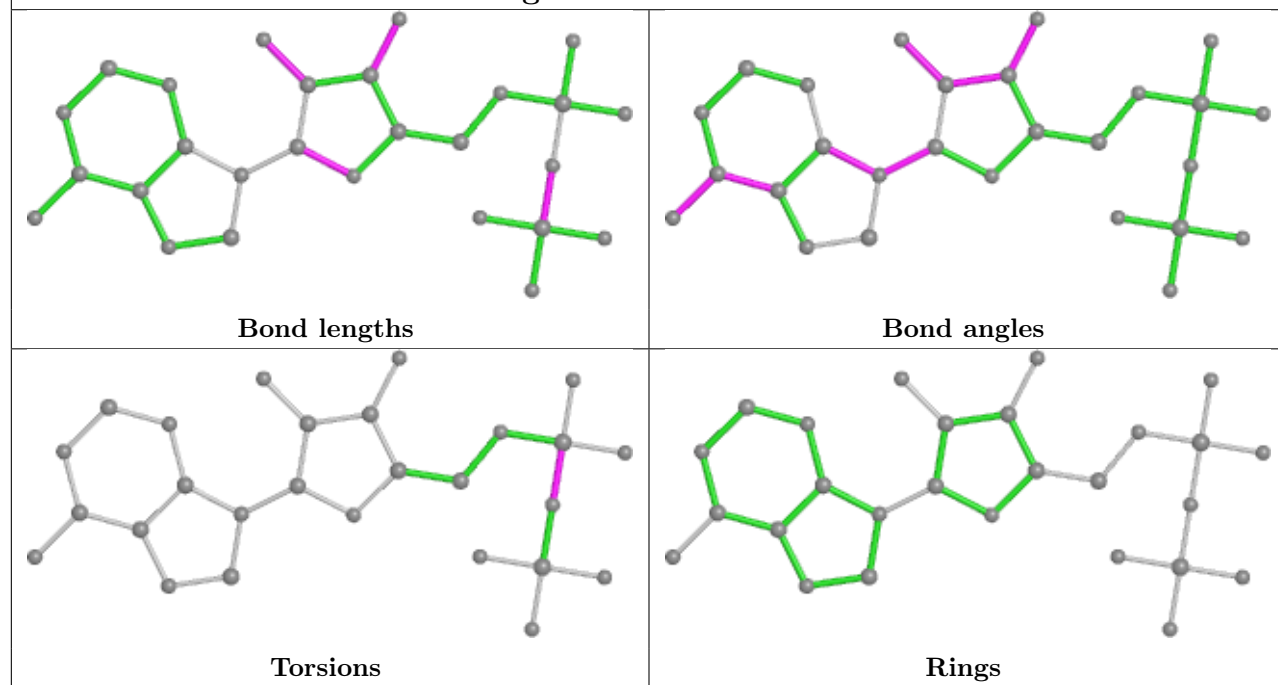




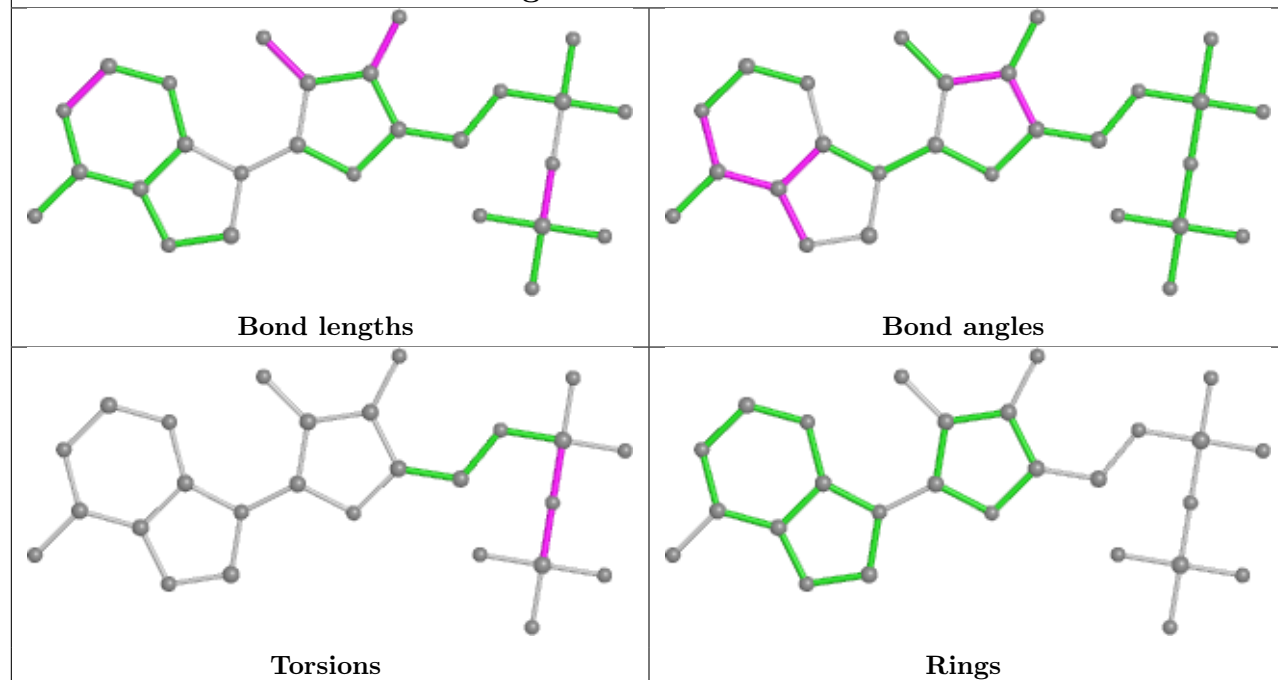
## Ligand ADP C 4026



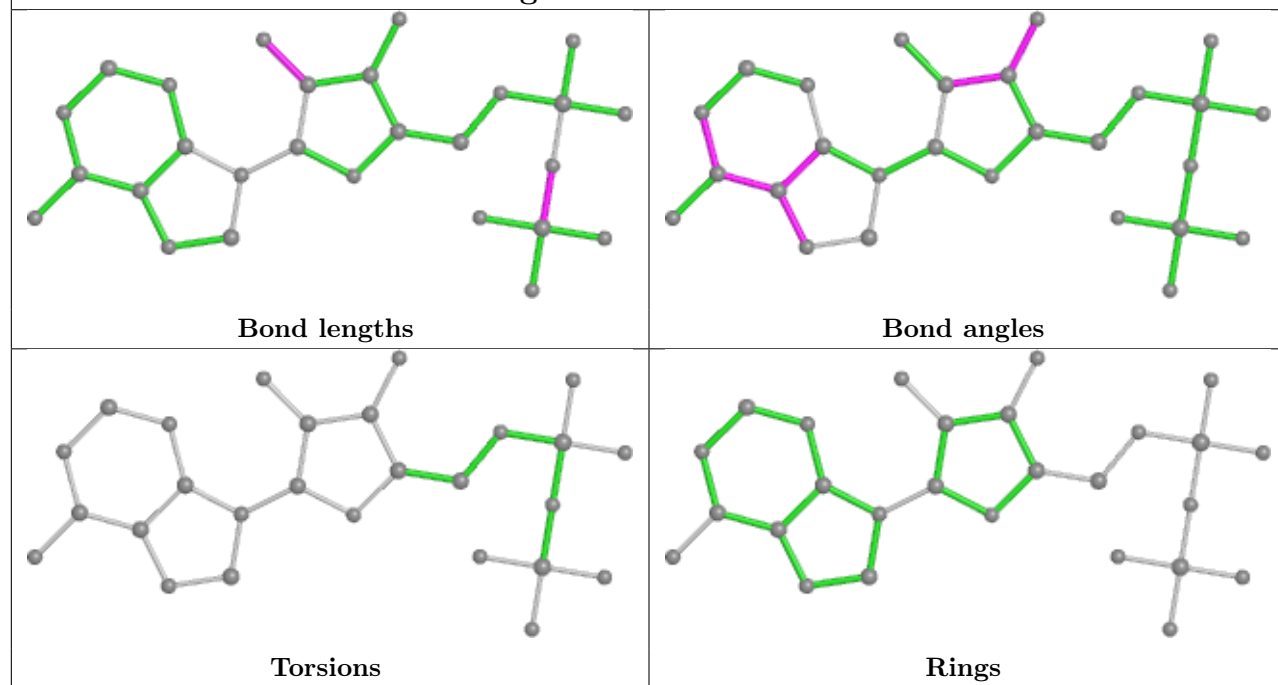
## Ligand ADP E 4041

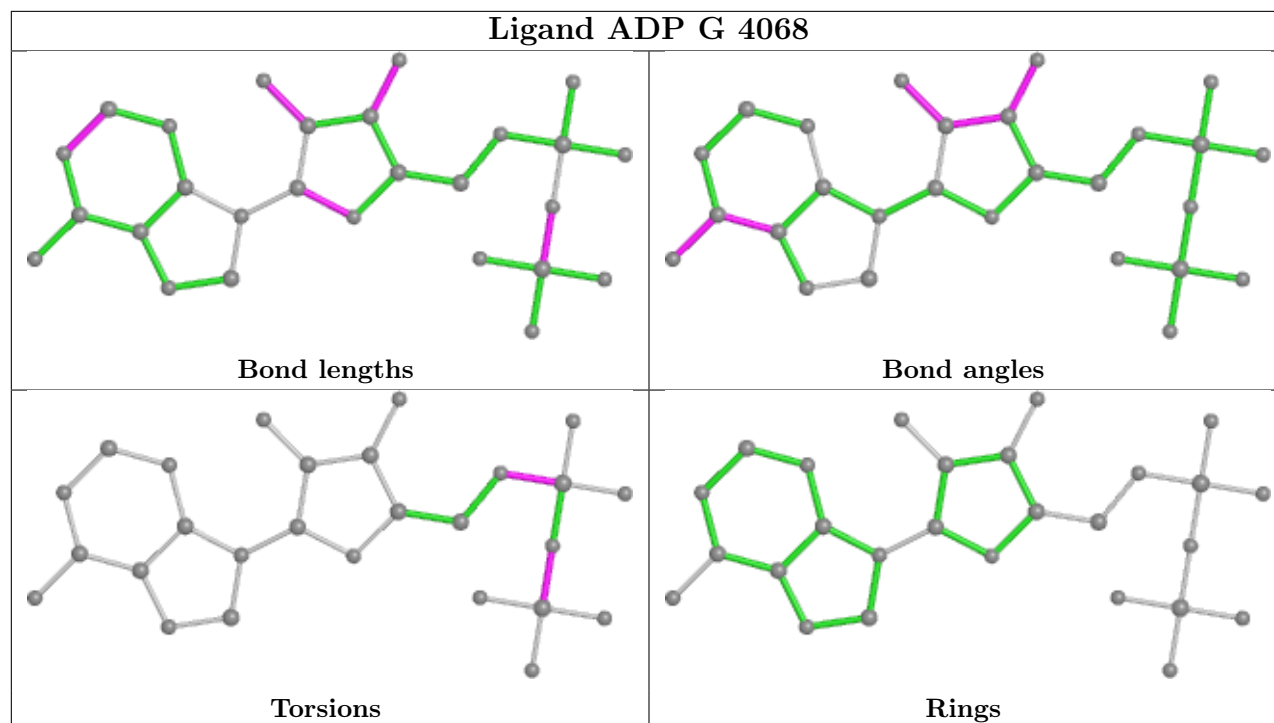


## Ligand ADP E 4047



## Ligand ADP G 4062





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.