



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 04:57 PM GMT

PDB ID : 2BMC  
Title : AURORA-2 T287D T288D COMPLEXED WITH PHA-680632  
Authors : Cameron, A.D.; Izzo, G.; Sagliano, A.; Rusconi, L.; Storici, P.; Fancelli, D.; Berta, D.; Bindi, S.; Catana, C.; Forte, B.; Giordano, P.; Mantegani, S.; Meroni, M.; Moll, J.; Pittala, V.; Severino, D.; Tonani, R.; Varasi, M.; Vulpetti, A.; Vianello, P.  
Deposited on : 2005-03-11  
Resolution : 2.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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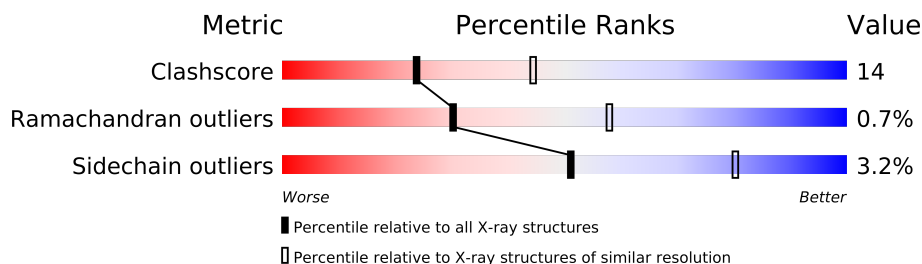
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	306	
1	B	306	
1	C	306	
1	D	306	
1	E	306	
1	F	306	

## 2 Entry composition i

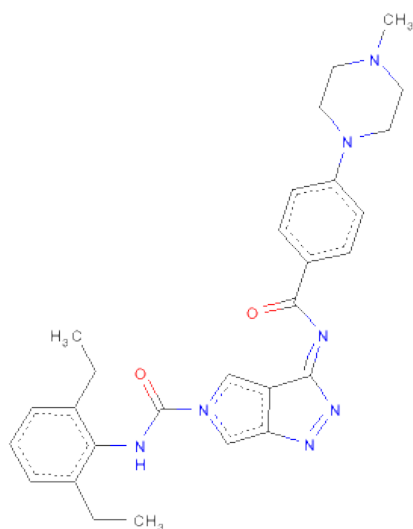
There are 3 unique types of molecules in this entry. The entry contains 13094 atoms, of which 0 are hydrogen and 0 are deuterium.

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 SERINE THREONINE-PROTEIN KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	B	258	Total	C	N	O	S	0	0	0
			2125	1367	373	379	6			
1	C	257	Total	C	N	O	S	0	0	0
			2116	1362	371	377	6			
1	D	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	E	256	Total	C	N	O	S	0	0	0
			2105	1355	367	377	6			
1	F	257	Total	C	N	O	S	0	0	0
			2116	1361	371	378	6			

- Molecule 2 is (3E)-N-(2,6-DIETHYLPHENYL)-3-{[4-(4-METHYLPYPERAZIN-1-YL)BENZOYL]IMINO}PYRROLO[3,4-C]PYRAZOLE-5(3H)-CARBOXAMIDE (three-letter code: MPY) (formula: C<sub>28</sub>H<sub>31</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			37	28	7	2		
2	B	1	Total	C	N	O	0	0
			37	28	7	2		
2	C	1	Total	C	N	O	0	0
			37	28	7	2		
2	D	1	Total	C	N	O	0	0
			37	28	7	2		
2	E	1	Total	C	N	O	0	0
			37	28	7	2		
2	F	1	Total	C	N	O	0	0
			37	28	7	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	37	Total	O	0	0
			37	37		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		
3	E	29	Total	O	0	0
			29	29		
3	F	37	Total	O	0	0
			37	37		

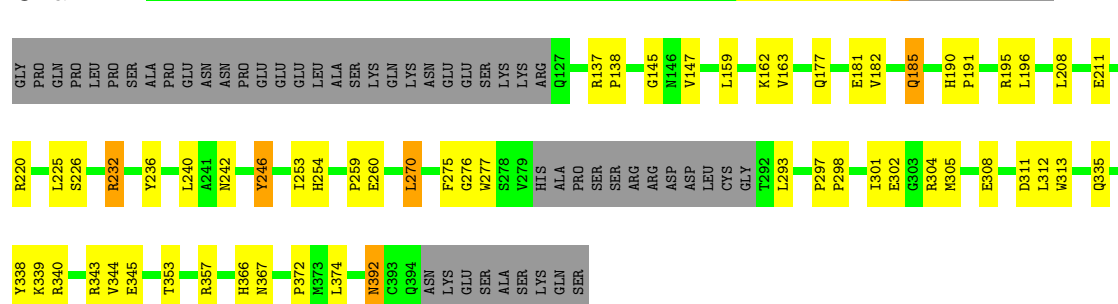
### 3 Residue-property plots

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.

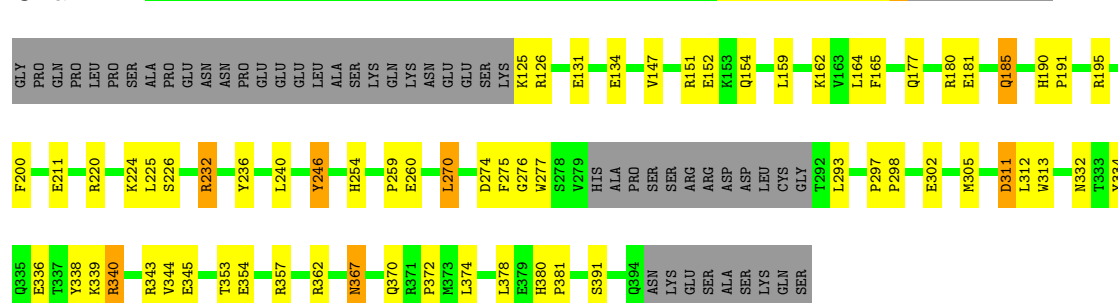
#### • Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

Chain A:



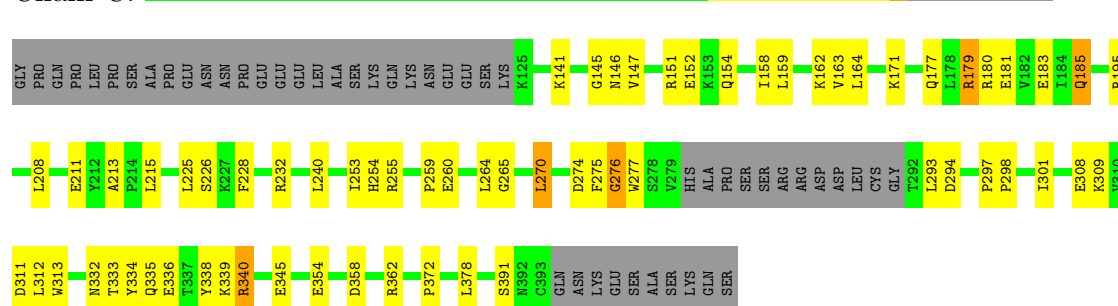
#### • Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

Chain B:



#### • Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

Chain C:



#### • Molecule 1: SERINE THREONINE-PROTEIN KINASE 6

L312	L313	L320	P328	T333	Y334	T337	Y338	R340	R343	V344	E345	D350	R362	N367	P368	S369	Q370	R371	P372	L378	I383	N386	S391	C393	Q394	ASN	LYS	GLU	SER	ALA	LYS	LYS	GLN	LYS	ASN	GLU	GLU	SER	LYS	LYS	ARG	Q127	G145	N146	V147	K153	K156	K162	V163	L164	F165	H176	Q177	R180	E181	V182	E183	I184	Q185	H190	P191	R195	L196	P211
E211	Y212	A213	P214	L215	L225	S226	E230	Q231	R232	Y236	N242	T253	H254	R255	L264	L270	D274	F275	G276	V279	H18	ALA	PRQ	SER	SER	ARG	ARG	ASP	LEU	CYS	GLY	T292	L293	D294	Y295	L296	P297	T298	E299	M300	I301	M305	H306	E307	E308	K309	P310																	
PRO	GLN	PRO	LEU	PRO	SER	ALA	GLU	ASN	ASN	PRO	GLU	GLU	LEU	ALA	SER	LYS	GLN	LYS	LYS	ASN	GLU	GLU	SER	SER	LYS	LYS	ARG	Q127	G145	N146	V147	K153	K156	K162	V163	L164	F165	H176	Q177	R180	E181	V182	E183	I184	Q185	H190	P191	R195	L196	P211														

Chain E:

GLN	D311	Y212	GLY
	L312	A213	PRO
SER	Y320	P214	GLN
	P328	L215	PRO
GLN	N332	R220	LEU
	T337	L225	PRO
SER	Y338	S226	SER
	T339	E230	PRO
GLN	R340	L240	ASN
	P348	A241	ASN
SER	N344	N242	GLU
	E345	T253	LEU
GLN	F346	H254	ALA
	P349	L264	SER
SER	D350	E269	LYS
	T353	L270	GLN
GLN	R357	F275	ASN
	D358	G276	GLU
SER	L359	Y279	SER
	P362	HIS	LYS
GLN	K365	ALA	ARG
	H366	PRO	Q127
SER	N367	SER	L130
	P368	ARG	E131
GLN	S369	ASP	L139
	R371	ASP	V147
SER	P372	LEU	K153
	L378	CYS	Q154
GLN	E379	GLY	S155
	H380	T292	K156
SER	P381	L293	F165
	N386	D294	Q177
GLN	K389	Y295	R180
	P392	T297	E181
SER	C393	P288	V182
	Q394	E299	G183
GLN	ASN	M300	I184
	LYS	T301	Q185
SER	GLU	G303	H190
	ALA	R304	P191
SER	LYS	M305	R195
	GLU	H306	F211
SER	ALA	D307	
	LYS	E308	
SER	GLU	X309	
	LYS	V210	

Chain F:

T333	Q185	GLY
E336	R195	PRO
T337	L209	PRO
Y338	L210	LEU
R339	E211	PRO
R340	L225	SER
R343	S226	ALA
Y344	Q231	PRO
E345	R232	ASN
T353	Y236	PRO
E354	E239	GLU
R357	N242	LEU
D358	I253	ALA
R362	H254	SER
N367	R255	GLN
P368	P259	LYS
S369	L270	ASN
P372	D274	GLU
H380	F275	GLU
P381	W277	SER
N386	S278	SER
N392	V279	GLU
C393	HIS	GLU
Q394	ALA	LYS
ASN	PRO	LYS
LYS	SER	LYS
GLU	SER	LYS
SER	ARG	LYS
ALA	ARG	GLN
ALA	ASP	SER
LYS	ASP	LYS
GLN	LEU	GLN
SER	CYS	SER
	GLY	
	T292	
	L293	
	D294	
	Y295	
	L296	
	P297	
	I301	
	M305	
	H306	
	E181	
	V182	
	E183	
	L212	
	Q177	
	K162	
	V163	
	L159	
	K156	
	S155	
	Q154	
	E152	
	R151	
	A150	
	V147	
	M146	
	G145	
	K141	
	F133	
	D132	
	E131	
	R126	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.02Å 101.22Å 101.49Å 115.73° 92.40° 101.54°	Depositor
Resolution (Å)	29.95 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (29.95-2.60)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX 2000	Depositor
R, $R_{free}$	0.228 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13094	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: MPY

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	0.35	0/2157	0.60	0/2915
1	B	0.34	0/2177	0.61	0/2940
1	C	0.35	0/2168	0.62	0/2928
1	D	0.33	0/2157	0.59	0/2915
1	E	0.32	0/2157	0.60	0/2915
1	F	0.34	0/2168	0.62	0/2929
All	All	0.34	0/12984	0.61	0/17542

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2105	0	2107	51	0
1	B	2125	0	2133	62	0
1	C	2116	0	2125	58	0
1	D	2105	0	2107	70	0
1	E	2105	0	2107	94	0
1	F	2116	0	2120	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	37	0	31	2	0
2	B	37	0	31	2	0
2	C	37	0	31	3	0
2	D	37	0	31	2	0
2	E	37	0	31	1	0
2	F	37	0	31	1	0
3	A	45	0	0	0	0
3	B	37	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	0	0
3	E	29	0	0	2	0
3	F	37	0	0	0	0
All	All	13094	0	12885	369	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 369 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:151:ARG:HD3	1:F:156:LYS:HA	1.50	0.93
1:E:348:PHE:CE2	1:E:357:ARG:HA	2.15	0.81
1:C:253:ILE:HG21	1:C:308:GLU:HG2	1.63	0.80
1:B:367:ASN:HD22	1:B:370:GLN:HG3	1.46	0.80
1:E:333:THR:OG1	1:E:336:GLU:HG3	1.83	0.78

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	252/306 (82%)	244 (97%)	7 (3%)	1 (0%)	43 72
1	B	254/306 (83%)	246 (97%)	7 (3%)	1 (0%)	43 72
1	C	253/306 (83%)	242 (96%)	9 (4%)	2 (1%)	27 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	252/306 (82%)	243 (96%)	7 (3%)	2 (1%)	27	53
1	E	252/306 (82%)	241 (96%)	8 (3%)	3 (1%)	19	39
1	F	253/306 (83%)	241 (95%)	10 (4%)	2 (1%)	27	53
All	All	1516/1836 (83%)	1457 (96%)	48 (3%)	11 (1%)	30	58

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	294	ASP
1	E	294	ASP
1	F	294	ASP
1	C	294	ASP
1	E	154	GLN

### 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	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	B	229/271 (84%)	220 (96%)	9 (4%)	43	74
1	C	228/271 (84%)	223 (98%)	5 (2%)	64	89
1	D	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	E	227/271 (84%)	220 (97%)	7 (3%)	52	81
1	F	228/271 (84%)	219 (96%)	9 (4%)	43	74
All	All	1366/1626 (84%)	1322 (97%)	44 (3%)	51	80

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	340	ARG
1	D	311	ASP
1	F	311	ASP
1	C	354	GLU
1	D	232	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	242	ASN
1	D	386	ASN
1	F	367	ASN
1	D	367	ASN
1	D	392	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

6 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	MPY	A	1395	-	41,41,41	2.71	20 (48%)	55,58,58	4.67	19 (34%)
2	MPY	B	1395	-	41,41,41	2.68	19 (46%)	55,58,58	5.03	18 (32%)
2	MPY	C	1394	-	41,41,41	2.74	19 (46%)	55,58,58	4.93	19 (34%)
2	MPY	D	1395	-	41,41,41	2.79	21 (51%)	55,58,58	5.21	20 (36%)
2	MPY	E	1395	-	41,41,41	2.82	20 (48%)	55,58,58	4.99	18 (32%)
2	MPY	F	1395	-	41,41,41	2.65	17 (41%)	55,58,58	4.81	17 (30%)

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	MPY	A	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	B	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	C	1394	-	-	0/19/43/43	0/3/5/5
2	MPY	D	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	E	1395	-	-	0/19/43/43	0/3/5/5
2	MPY	F	1395	-	-	0/19/43/43	0/3/5/5

The worst 5 of 116 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1395	MPY	C16-N1	6.86	1.50	1.39
2	A	1395	MPY	C15-C14	6.81	1.47	1.38
2	C	1394	MPY	C15-C14	6.59	1.47	1.38
2	B	1395	MPY	C16-N1	6.51	1.49	1.39
2	F	1395	MPY	C16-N1	6.50	1.49	1.39

The worst 5 of 111 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1395	MPY	O26-C25-N1	33.22	122.71	116.25
2	B	1395	MPY	O26-C25-N1	31.85	122.44	116.25
2	E	1395	MPY	O26-C25-N1	31.24	122.33	116.25
2	C	1394	MPY	O26-C25-N1	30.69	122.22	116.25
2	F	1395	MPY	O26-C25-N1	30.06	122.09	116.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.