



wwPDB X-ray Structure Validation Summary Report

Jun 14, 2020 – 04:03 am BST

PDB ID : 1NXK
Title : Crystal structure of staurosporine bound to MAP KAP kinase 2
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Malakian, K.; Telliez, J.B.; Lin, L.L.; Kriz, R.W.; Seehra, J.; Somers, W.S.;
Stahl, M.L.
Deposited on : 2003-02-10
Resolution : 2.70 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  symbol.

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)
Xtrriage (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) : 2.11

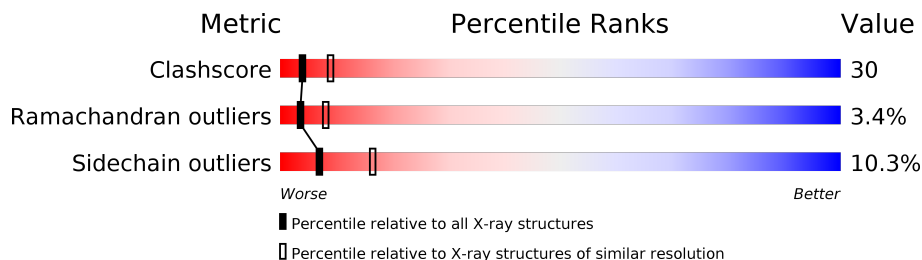
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 ≥ 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	400	
1	B	400	
1	C	400	
1	D	400	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9405 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	290	2289	1471	388	413	6	11	0	0	0
1	B	283	2234	1425	382	410	6	11	0	0	0
1	C	306	2438	1557	421	442	6	12	0	0	0
1	D	288	2252	1452	373	410	6	11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

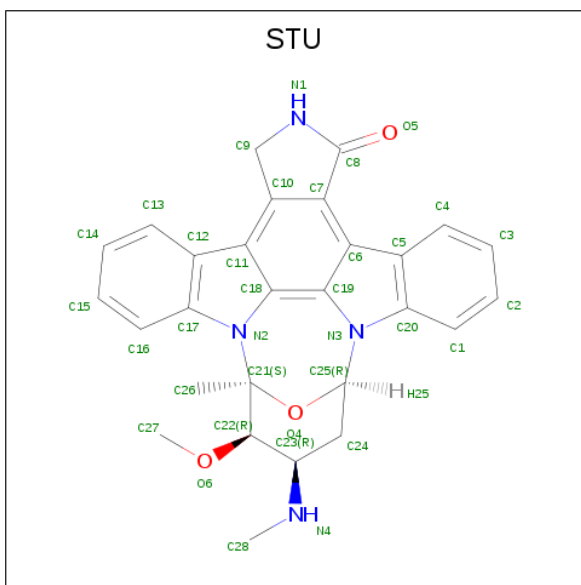
Chain	Residue	Modelled	Actual	Comment	Reference
A	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
A	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	314	MSE	MET	MODIFIED RESIDUE	UNP P49137

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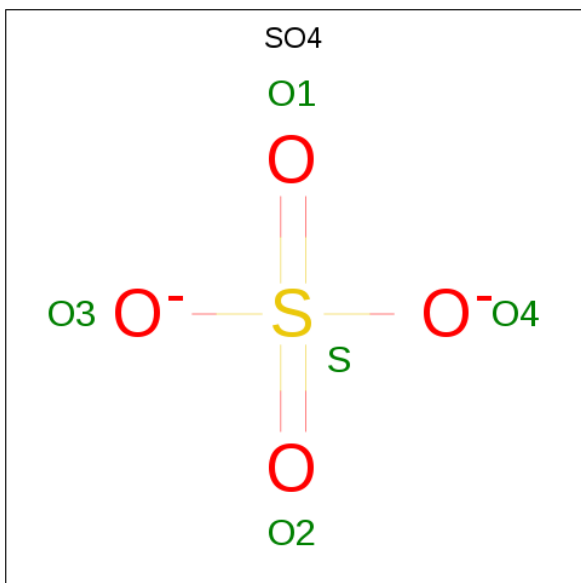
Chain	Residue	Modelled	Actual	Comment	Reference
B	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
B	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
C	356	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	94	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	138	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	167	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	246	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	253	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	275	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	281	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	300	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	314	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	320	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	326	MSE	MET	MODIFIED RESIDUE	UNP P49137
D	356	MSE	MET	MODIFIED RESIDUE	UNP P49137

- Molecule 2 is STAUROSPORINE (three-letter code: STU) (formula: C₂₈H₂₆N₄O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	35	28	4	3	0	0
2	B	1	35	28	4	3	0	0
2	C	1	35	28	4	3	0	0
2	D	1	35	28	4	3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

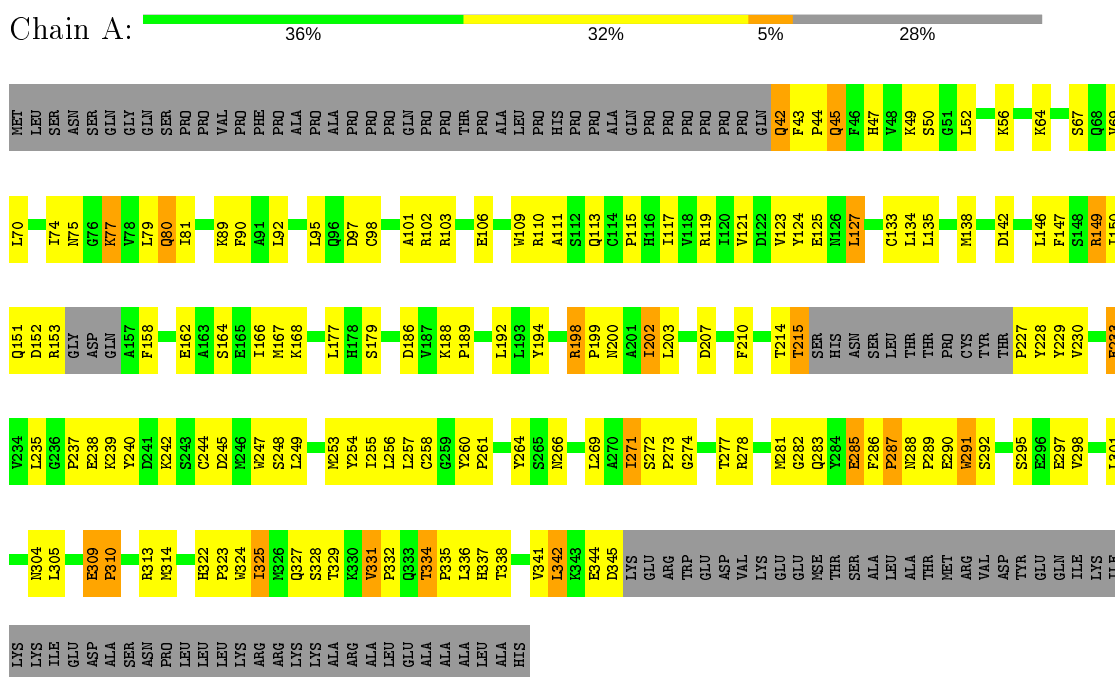
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	16	Total	O	0	0
			16	16		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

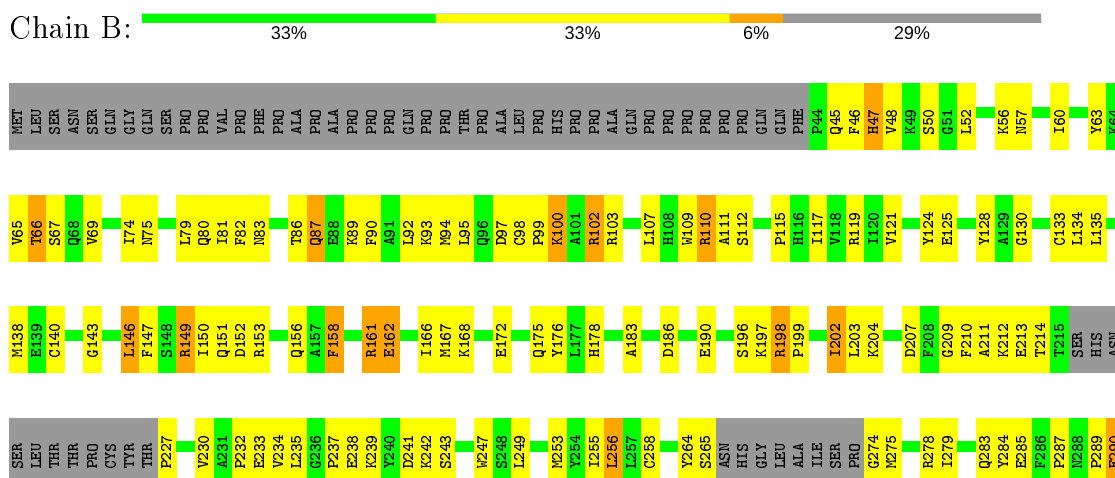
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	160.20Å 160.20Å 133.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	98.0 (20.00-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.239 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: STU, SO4

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	0.76	3/2331 (0.1%)	0.95	3/3140 (0.1%)
1	B	0.79	2/2271 (0.1%)	0.99	3/3057 (0.1%)
1	C	0.75	1/2481 (0.0%)	0.91	2/3337 (0.1%)
1	D	0.66	0/2295	0.86	0/3100
All	All	0.74	6/9378 (0.1%)	0.93	8/12634 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	8

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	291	TRP	NE1-CE2	8.77	1.49	1.37
1	C	324	TRP	NE1-CE2	8.66	1.48	1.37
1	A	109	TRP	NE1-CE2	8.65	1.48	1.37
1	A	291	TRP	NE1-CE2	8.64	1.48	1.37
1	B	247	TRP	NE1-CE2	8.64	1.48	1.37

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	PHE	O-C-N	-7.70	110.39	122.70
1	B	303	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	282	GLY	N-CA-C	-5.54	99.25	113.10
1	B	110	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	183	ALA	N-CA-C	-5.30	96.70	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	103	ARG	Sidechain
1	A	119	ARG	Sidechain
1	B	158	PHE	Mainchain
1	B	176	TYR	Sidechain

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	2289	0	2258	148	0
1	B	2234	0	2197	137	0
1	C	2438	0	2414	152	0
1	D	2252	0	2194	157	0
2	A	35	0	26	3	0
2	B	35	0	26	2	0
2	C	35	0	26	1	0
2	D	35	0	26	7	0
3	B	10	0	0	0	0
4	A	10	0	0	0	0
4	B	16	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
All	All	9405	0	9167	561	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 30.

The worst 5 of 561 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:266:ASN:HD22	1:A:269:LEU:HG	1.30	0.96
1:A:158:PHE:CE1	1:A:162:GLU:HB3	2.00	0.95
1:A:260:TYR:HE2	1:A:290:GLU:HG2	1.30	0.94
1:C:328:SER:O	1:C:331:VAL:HG12	1.66	0.94
1:D:167:MSE:HG3	1:D:253:MSE:HG3	1.47	0.94

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	284/400 (71%)	250 (88%)	25 (9%)	9 (3%)	4	9
1	B	277/400 (69%)	241 (87%)	26 (9%)	10 (4%)	3	7
1	C	302/400 (76%)	261 (86%)	30 (10%)	11 (4%)	3	7
1	D	282/400 (70%)	241 (86%)	32 (11%)	9 (3%)	4	9
All	All	1145/1600 (72%)	993 (87%)	113 (10%)	39 (3%)	3	8

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	ASP
1	B	66	THR
1	B	239	LYS
1	C	42	GLN
1	C	237	PRO

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	246/345 (71%)	224 (91%)	22 (9%)	9	22
1	B	241/345 (70%)	213 (88%)	28 (12%)	5	12
1	C	263/345 (76%)	231 (88%)	32 (12%)	5	11
1	D	241/345 (70%)	221 (92%)	20 (8%)	11	25
All	All	991/1380 (72%)	889 (90%)	102 (10%)	7	16

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	331	VAL
1	C	133	CYS
1	D	264	TYR
1	B	334	THR
1	C	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	337	HIS
1	C	151	GLN
1	D	266	ASN
1	C	42	GLN
1	C	57	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	STU	B	403	-	30,42,42	2.23	10 (33%)	31,68,68	1.55	8 (25%)
3	SO4	B	402	-	4,4,4	0.65	0	6,6,6	0.98	0
2	STU	D	401	-	30,42,42	2.35	11 (36%)	31,68,68	1.77	10 (32%)
3	SO4	B	401	-	4,4,4	0.63	0	6,6,6	0.98	0
2	STU	A	401	-	30,42,42	2.03	12 (40%)	31,68,68	1.65	9 (29%)
2	STU	C	401	-	30,42,42	2.09	9 (30%)	31,68,68	1.69	9 (29%)

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	STU	B	403	-	-	0/4/42/42	-
2	STU	A	401	-	-	2/4/42/42	-
2	STU	D	401	-	-	2/4/42/42	-
2	STU	C	401	-	-	1/4/42/42	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	STU	C22-C23	6.85	1.59	1.52
2	B	403	STU	C9-C10	6.28	1.55	1.50
2	D	401	STU	C9-C10	4.94	1.54	1.50
2	C	401	STU	C22-C23	4.80	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	STU	C7-C6	4.47	1.50	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	STU	C9-N1-C8	3.74	117.45	113.85
2	C	401	STU	C9-N1-C8	3.69	117.40	113.85
2	D	401	STU	C24-C23-N4	-3.46	104.48	112.17
2	D	401	STU	C7-C8-N1	-3.43	102.90	106.37
2	A	401	STU	C9-N1-C8	3.39	117.11	113.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	STU	C24-C23-N4-C28
2	D	401	STU	C22-C23-N4-C28
2	A	401	STU	C22-C23-N4-C28
2	D	401	STU	C24-C23-N4-C28
2	C	401	STU	C24-C23-N4-C28

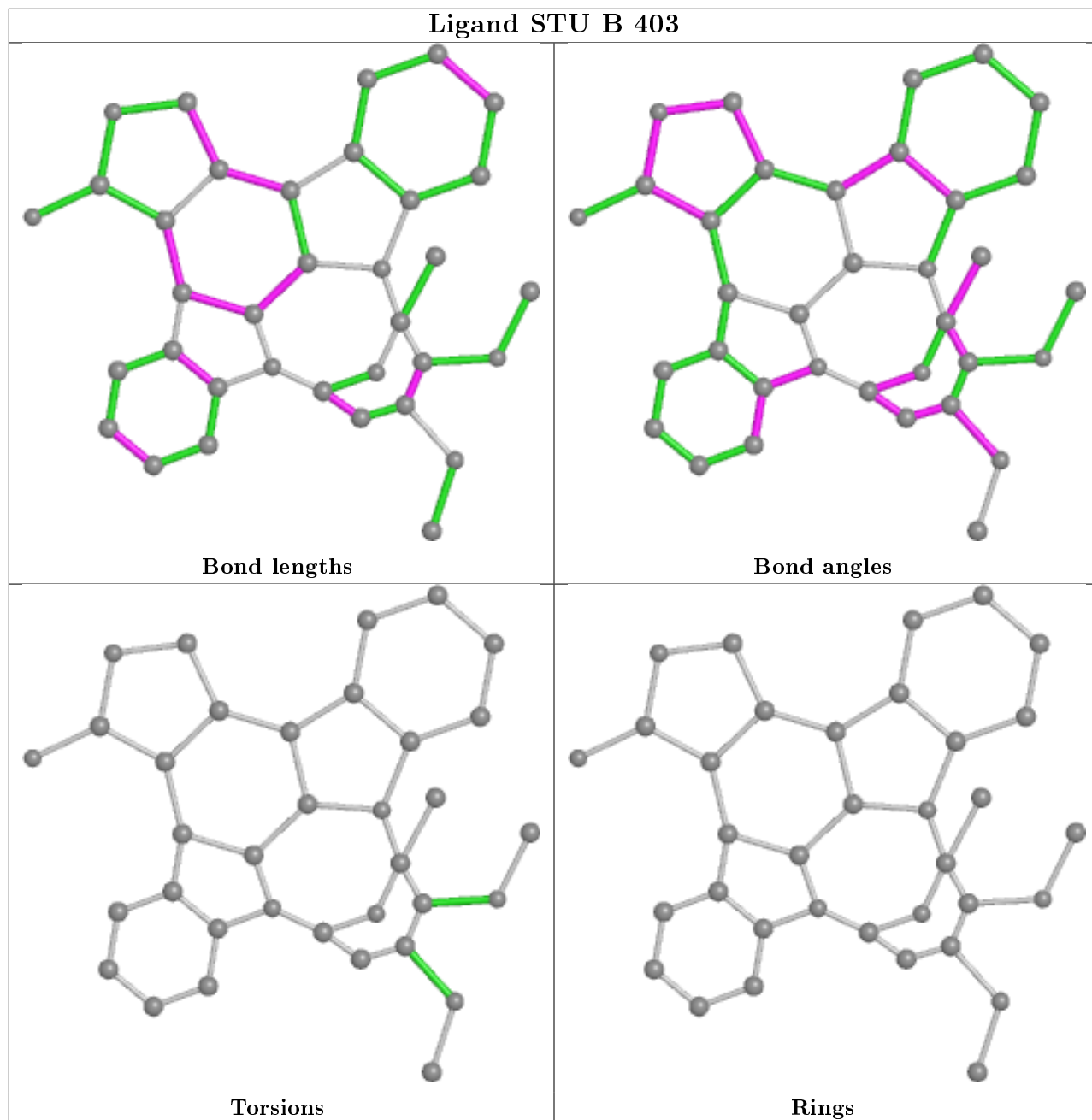
There are no ring outliers.

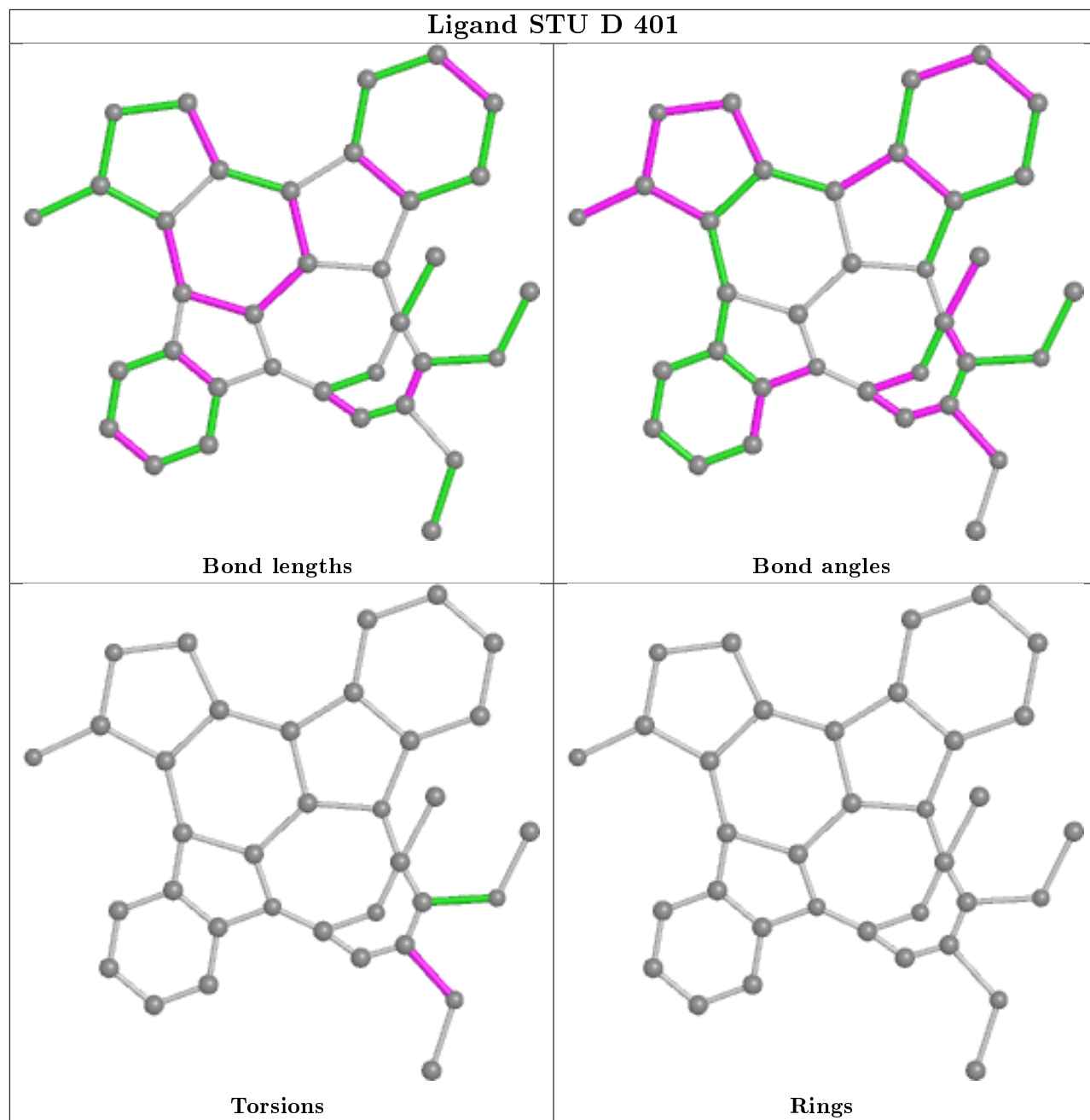
4 monomers are involved in 13 short contacts:

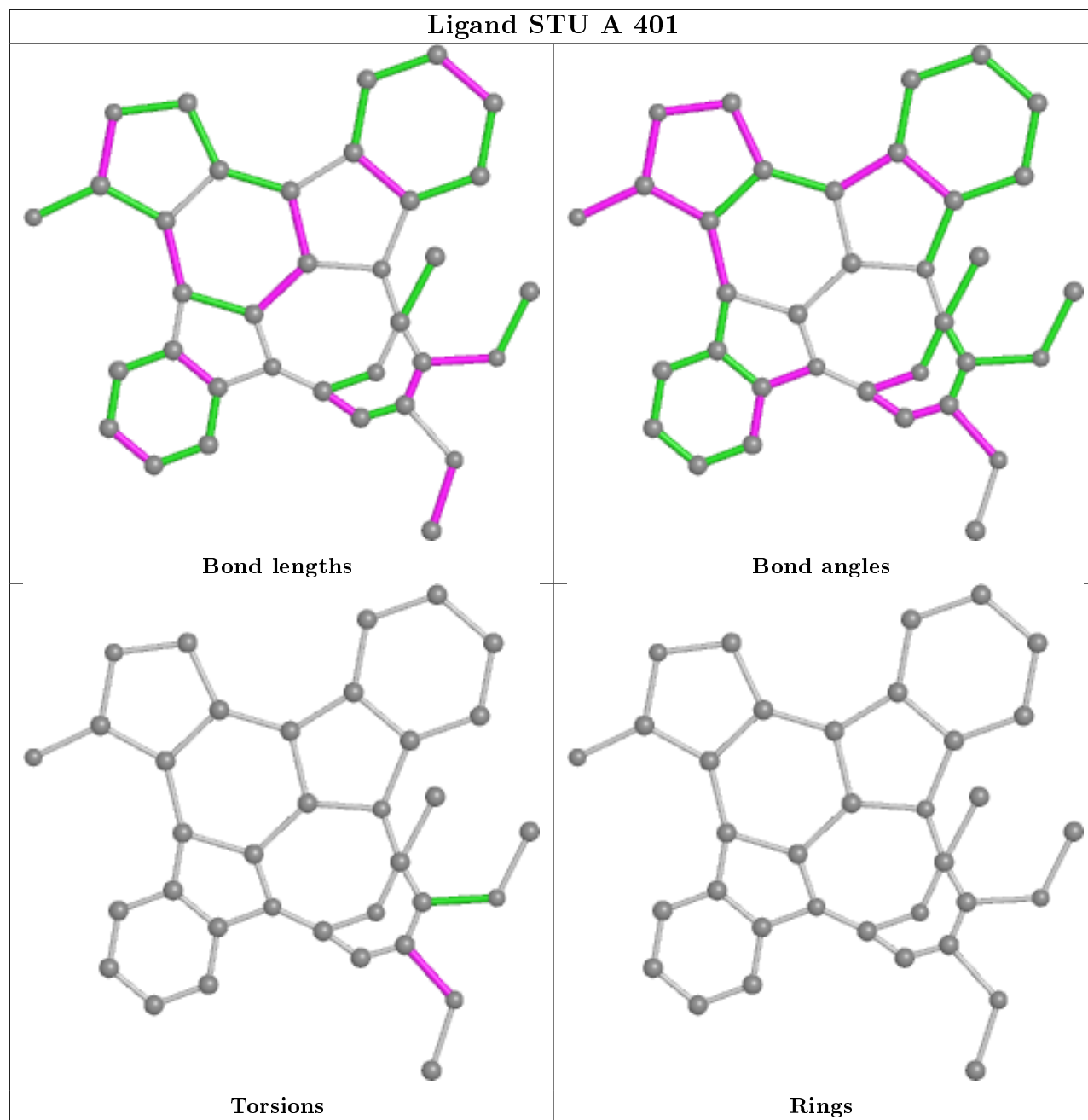
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	403	STU	2	0
2	D	401	STU	7	0
2	A	401	STU	3	0
2	C	401	STU	1	0

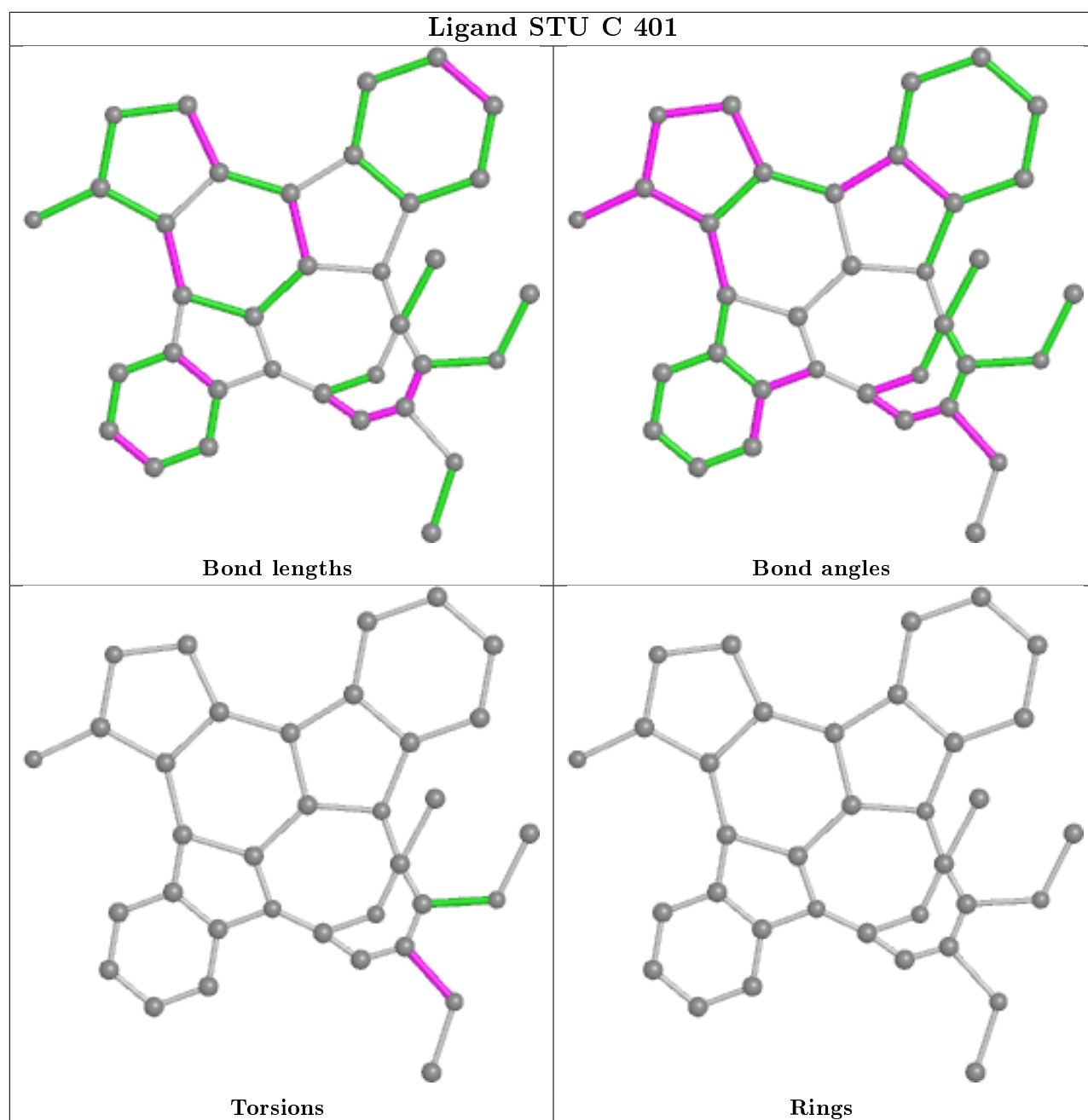
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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.