



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:46 PM UTC

PDB ID : 4D0M / pdb_00004d0m
Title : Phosphatidylinositol 4-kinase III beta in a complex with Rab11a-GTP-gamma-S and the Rab-binding domain of FIP3
Authors : Burke, J.E.; Inglis, A.J.; Perisic, O.; Masson, G.R.; McLaughlin, S.H.; Rutaganira, F.; Shokat, K.M.; Williams, R.L.
Deposited on : 2014-04-29
Resolution : 6.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

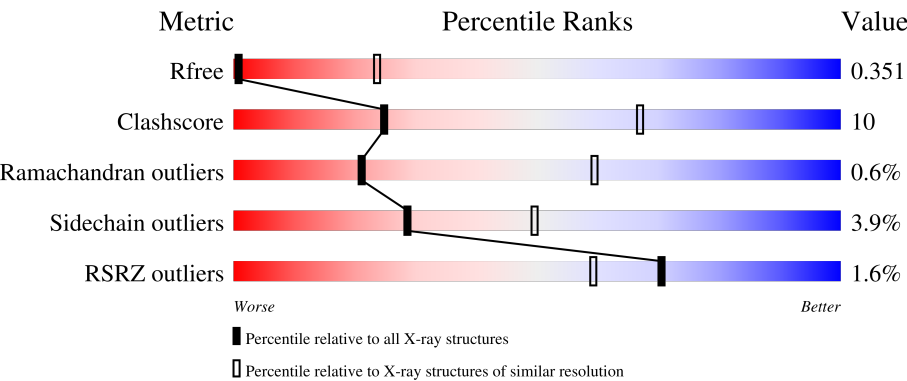
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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.



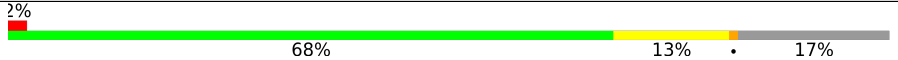
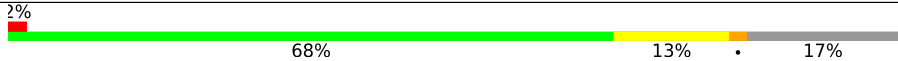
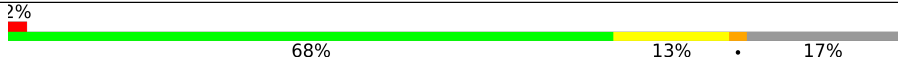
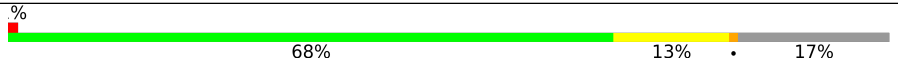
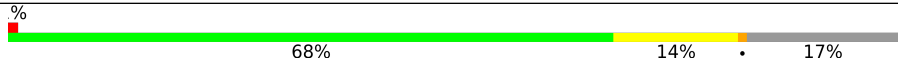
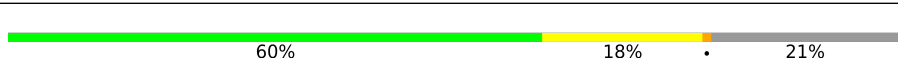
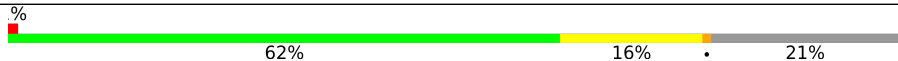
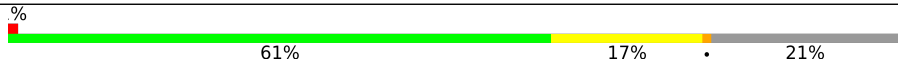
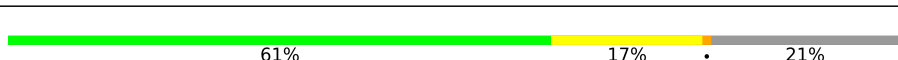
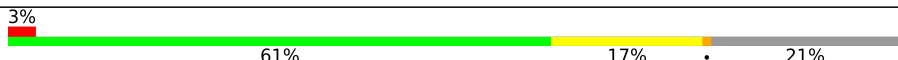
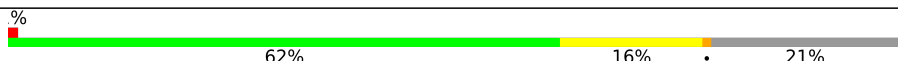
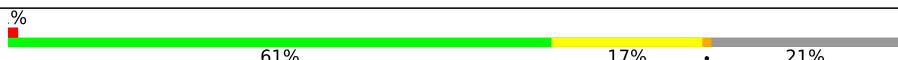
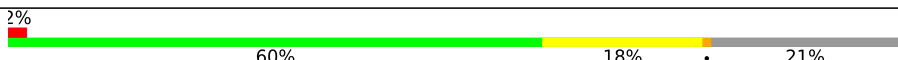
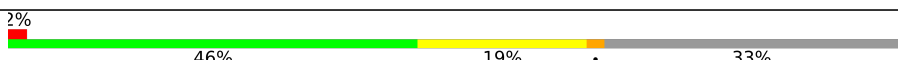
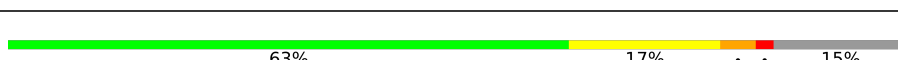
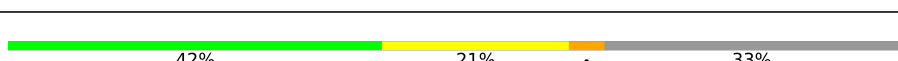
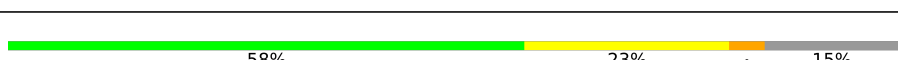
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	566	69%12%17%
1	C	566	3% 68%13%17%
1	G	566	% 69%13%17%
1	I	566	2% 69%13%17%

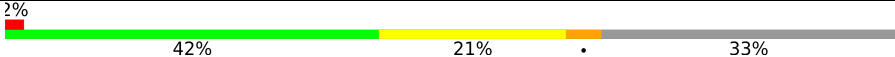
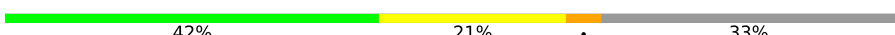
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Mol	Chain	Length	Quality of chain
1	M	566	
1	O	566	
1	Q	566	
1	S	566	
1	W	566	
1	Y	566	
1	c	566	
1	g	566	
2	B	219	
2	D	219	
2	H	219	
2	J	219	
2	N	219	
2	P	219	
2	R	219	
2	T	219	
2	X	219	
2	Z	219	
2	d	219	
2	h	219	
3	E	48	
3	F	48	
3	K	48	
3	L	48	
3	U	48	

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Mol	Chain	Length	Quality of chain
3	V	48	
3	a	48	
3	b	48	
3	e	48	
3	f	48	
3	i	48	
3	j	48	

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
5	GSP	d	2000	-	-	X	-
6	MG	Z	2001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 65970 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 PHOSPHATIDYLINOSITOL 4-KINASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	C	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	G	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	I	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	M	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	O	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Q	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	S	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	W	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	Y	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	c	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			
1	g	470	Total	C	N	O	S	0	0	0
			3788	2430	654	680	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP Q9UBF8
A	120	SER	-	expression tag	UNP Q9UBF8
A	294	ALA	SER	engineered mutation	UNP Q9UBF8
A	507	ARG	LYS	conflict	UNP Q9UBF8
C	119	GLY	-	expression tag	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	120	SER	-	expression tag	UNP Q9UBF8
C	294	ALA	SER	engineered mutation	UNP Q9UBF8
C	507	ARG	LYS	conflict	UNP Q9UBF8
G	119	GLY	-	expression tag	UNP Q9UBF8
G	120	SER	-	expression tag	UNP Q9UBF8
G	294	ALA	SER	engineered mutation	UNP Q9UBF8
G	507	ARG	LYS	conflict	UNP Q9UBF8
I	119	GLY	-	expression tag	UNP Q9UBF8
I	120	SER	-	expression tag	UNP Q9UBF8
I	294	ALA	SER	engineered mutation	UNP Q9UBF8
I	507	ARG	LYS	conflict	UNP Q9UBF8
M	119	GLY	-	expression tag	UNP Q9UBF8
M	120	SER	-	expression tag	UNP Q9UBF8
M	294	ALA	SER	engineered mutation	UNP Q9UBF8
M	507	ARG	LYS	conflict	UNP Q9UBF8
O	119	GLY	-	expression tag	UNP Q9UBF8
O	120	SER	-	expression tag	UNP Q9UBF8
O	294	ALA	SER	engineered mutation	UNP Q9UBF8
O	507	ARG	LYS	conflict	UNP Q9UBF8
Q	119	GLY	-	expression tag	UNP Q9UBF8
Q	120	SER	-	expression tag	UNP Q9UBF8
Q	294	ALA	SER	engineered mutation	UNP Q9UBF8
Q	507	ARG	LYS	conflict	UNP Q9UBF8
S	119	GLY	-	expression tag	UNP Q9UBF8
S	120	SER	-	expression tag	UNP Q9UBF8
S	294	ALA	SER	engineered mutation	UNP Q9UBF8
S	507	ARG	LYS	conflict	UNP Q9UBF8
W	119	GLY	-	expression tag	UNP Q9UBF8
W	120	SER	-	expression tag	UNP Q9UBF8
W	294	ALA	SER	engineered mutation	UNP Q9UBF8
W	507	ARG	LYS	conflict	UNP Q9UBF8
Y	119	GLY	-	expression tag	UNP Q9UBF8
Y	120	SER	-	expression tag	UNP Q9UBF8
Y	294	ALA	SER	engineered mutation	UNP Q9UBF8
Y	507	ARG	LYS	conflict	UNP Q9UBF8
c	119	GLY	-	expression tag	UNP Q9UBF8
c	120	SER	-	expression tag	UNP Q9UBF8
c	294	ALA	SER	engineered mutation	UNP Q9UBF8
c	507	ARG	LYS	conflict	UNP Q9UBF8
g	119	GLY	-	expression tag	UNP Q9UBF8
g	120	SER	-	expression tag	UNP Q9UBF8
g	294	ALA	SER	engineered mutation	UNP Q9UBF8

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Chain	Residue	Modelled	Actual	Comment	Reference
g	507	ARG	LYS	conflict	UNP Q9UBF8

- Molecule 2 is a protein called RAS-RELATED PROTEIN RAB-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	D	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	H	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	J	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	N	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	P	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	R	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	T	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	X	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	Z	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	d	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			
2	h	173	Total	C	N	O	S	0	0	0
			1377	872	238	266	1			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP P62491
B	-1	SER	-	expression tag	UNP P62491
B	0	HIS	-	expression tag	UNP P62491
B	70	LEU	GLN	engineered mutation	UNP P62491
D	-2	GLY	-	expression tag	UNP P62491
D	-1	SER	-	expression tag	UNP P62491
D	0	HIS	-	expression tag	UNP P62491
D	70	LEU	GLN	engineered mutation	UNP P62491
H	-2	GLY	-	expression tag	UNP P62491

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	SER	-	expression tag	UNP P62491
H	0	HIS	-	expression tag	UNP P62491
H	70	LEU	GLN	engineered mutation	UNP P62491
J	-2	GLY	-	expression tag	UNP P62491
J	-1	SER	-	expression tag	UNP P62491
J	0	HIS	-	expression tag	UNP P62491
J	70	LEU	GLN	engineered mutation	UNP P62491
N	-2	GLY	-	expression tag	UNP P62491
N	-1	SER	-	expression tag	UNP P62491
N	0	HIS	-	expression tag	UNP P62491
N	70	LEU	GLN	engineered mutation	UNP P62491
P	-2	GLY	-	expression tag	UNP P62491
P	-1	SER	-	expression tag	UNP P62491
P	0	HIS	-	expression tag	UNP P62491
P	70	LEU	GLN	engineered mutation	UNP P62491
R	-2	GLY	-	expression tag	UNP P62491
R	-1	SER	-	expression tag	UNP P62491
R	0	HIS	-	expression tag	UNP P62491
R	70	LEU	GLN	engineered mutation	UNP P62491
T	-2	GLY	-	expression tag	UNP P62491
T	-1	SER	-	expression tag	UNP P62491
T	0	HIS	-	expression tag	UNP P62491
T	70	LEU	GLN	engineered mutation	UNP P62491
X	-2	GLY	-	expression tag	UNP P62491
X	-1	SER	-	expression tag	UNP P62491
X	0	HIS	-	expression tag	UNP P62491
X	70	LEU	GLN	engineered mutation	UNP P62491
Z	-2	GLY	-	expression tag	UNP P62491
Z	-1	SER	-	expression tag	UNP P62491
Z	0	HIS	-	expression tag	UNP P62491
Z	70	LEU	GLN	engineered mutation	UNP P62491
d	-2	GLY	-	expression tag	UNP P62491
d	-1	SER	-	expression tag	UNP P62491
d	0	HIS	-	expression tag	UNP P62491
d	70	LEU	GLN	engineered mutation	UNP P62491
h	-2	GLY	-	expression tag	UNP P62491
h	-1	SER	-	expression tag	UNP P62491
h	0	HIS	-	expression tag	UNP P62491
h	70	LEU	GLN	engineered mutation	UNP P62491

- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	F	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	K	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	L	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	U	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	V	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	a	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	b	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	e	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	f	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			
3	i	41	Total	C	N	O	S	0	0	0
			314	199	54	60	1			
3	j	32	Total	C	N	O	S	0	0	0
			237	153	41	42	1			

There are 48 discrepancies between the modelled and reference sequences:

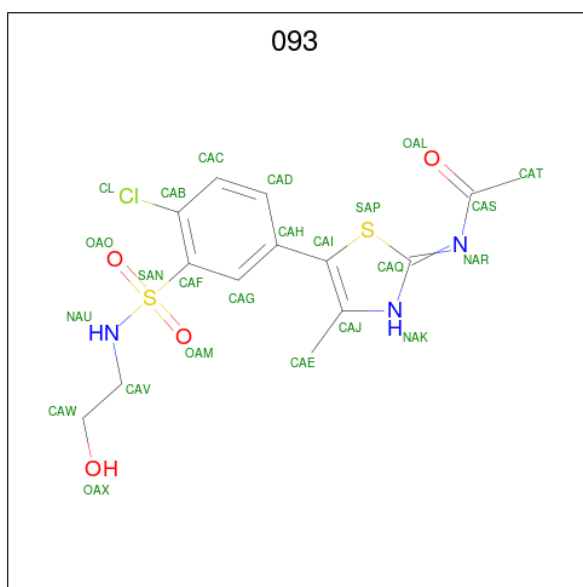
Chain	Residue	Modelled	Actual	Comment	Reference
E	709	GLY	-	expression tag	UNP O75154
E	710	SER	-	expression tag	UNP O75154
E	711	HIS	-	expression tag	UNP O75154
E	712	MET	-	expression tag	UNP O75154
F	709	GLY	-	expression tag	UNP O75154
F	710	SER	-	expression tag	UNP O75154
F	711	HIS	-	expression tag	UNP O75154
F	712	MET	-	expression tag	UNP O75154
K	709	GLY	-	expression tag	UNP O75154
K	710	SER	-	expression tag	UNP O75154
K	711	HIS	-	expression tag	UNP O75154
K	712	MET	-	expression tag	UNP O75154
L	709	GLY	-	expression tag	UNP O75154
L	710	SER	-	expression tag	UNP O75154
L	711	HIS	-	expression tag	UNP O75154
L	712	MET	-	expression tag	UNP O75154

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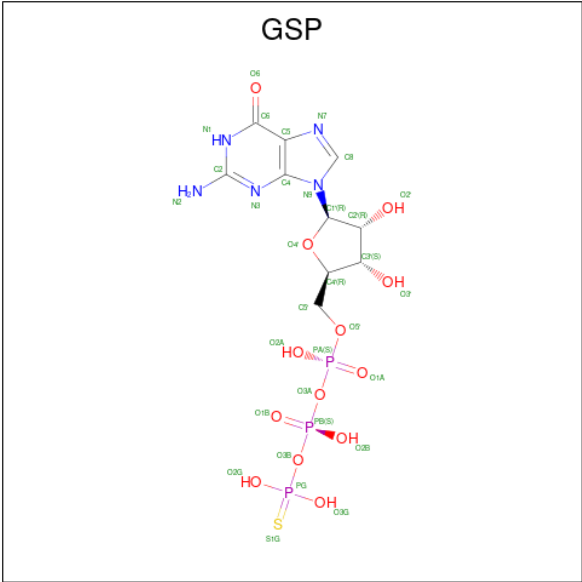
Chain	Residue	Modelled	Actual	Comment	Reference
U	709	GLY	-	expression tag	UNP O75154
U	710	SER	-	expression tag	UNP O75154
U	711	HIS	-	expression tag	UNP O75154
U	712	MET	-	expression tag	UNP O75154
V	709	GLY	-	expression tag	UNP O75154
V	710	SER	-	expression tag	UNP O75154
V	711	HIS	-	expression tag	UNP O75154
V	712	MET	-	expression tag	UNP O75154
a	709	GLY	-	expression tag	UNP O75154
a	710	SER	-	expression tag	UNP O75154
a	711	HIS	-	expression tag	UNP O75154
a	712	MET	-	expression tag	UNP O75154
b	709	GLY	-	expression tag	UNP O75154
b	710	SER	-	expression tag	UNP O75154
b	711	HIS	-	expression tag	UNP O75154
b	712	MET	-	expression tag	UNP O75154
e	709	GLY	-	expression tag	UNP O75154
e	710	SER	-	expression tag	UNP O75154
e	711	HIS	-	expression tag	UNP O75154
e	712	MET	-	expression tag	UNP O75154
f	709	GLY	-	expression tag	UNP O75154
f	710	SER	-	expression tag	UNP O75154
f	711	HIS	-	expression tag	UNP O75154
f	712	MET	-	expression tag	UNP O75154
i	709	GLY	-	expression tag	UNP O75154
i	710	SER	-	expression tag	UNP O75154
i	711	HIS	-	expression tag	UNP O75154
i	712	MET	-	expression tag	UNP O75154
j	709	GLY	-	expression tag	UNP O75154
j	710	SER	-	expression tag	UNP O75154
j	711	HIS	-	expression tag	UNP O75154
j	712	MET	-	expression tag	UNP O75154

- Molecule 4 is N-(5-(4-CHLORO-3-(2-HYDROXY-ETHYLSULFAMOYL)- PHENYLTHIA ZOLE-2-YL)-ACETAMIDE (CCD ID: 093) (formula: C₁₄H₁₆ClN₃O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	C	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	G	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	I	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	M	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	O	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	Q	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	S	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	W	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	Y	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	c	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0
4	g	1	Total 24	C 14	Cl 1	N 3	O 4	S 2	24	0

- Molecule 5 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	H	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	J	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	N	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	P	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	R	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	T	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	X	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	Z	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	d	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		
5	h	1	Total	C	N	O	P	S	0	0
			32	10	5	13	3	1		

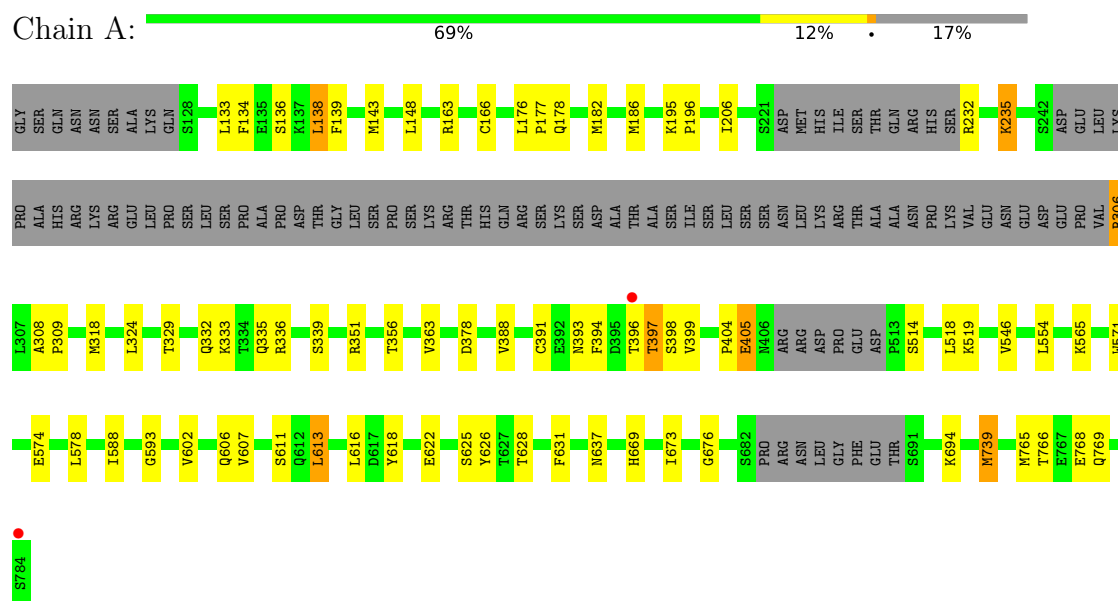
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	H	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		
6	N	1	Total	Mg	0	0
			1	1		
6	P	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	X	1	Total	Mg	0	0
			1	1		
6	Z	1	Total	Mg	0	0
			1	1		
6	d	1	Total	Mg	0	0
			1	1		
6	h	1	Total	Mg	0	0
			1	1		

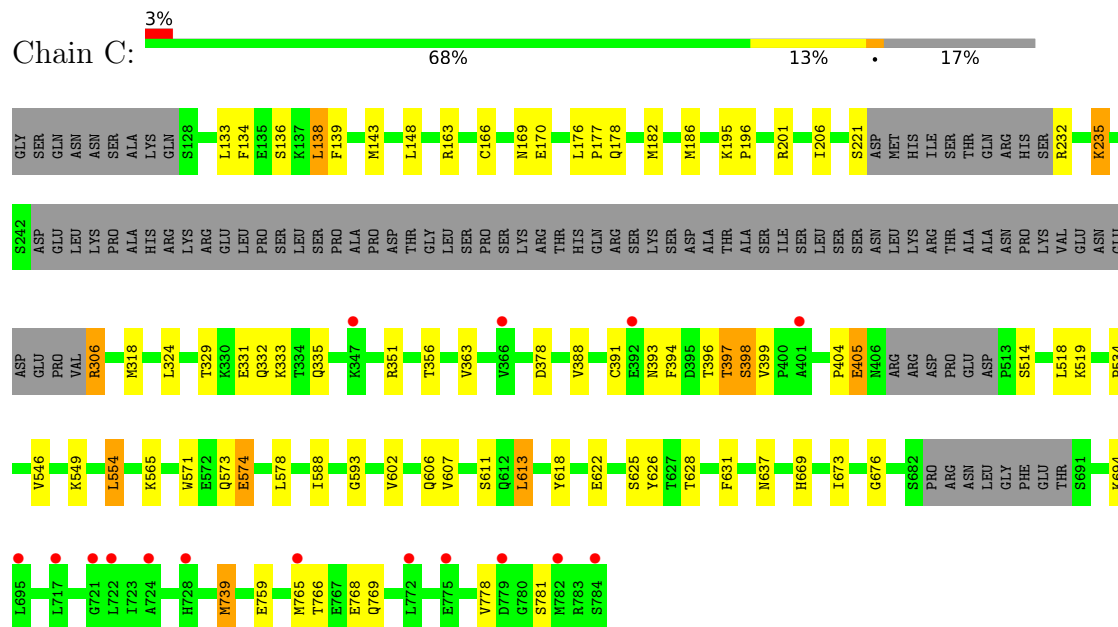
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

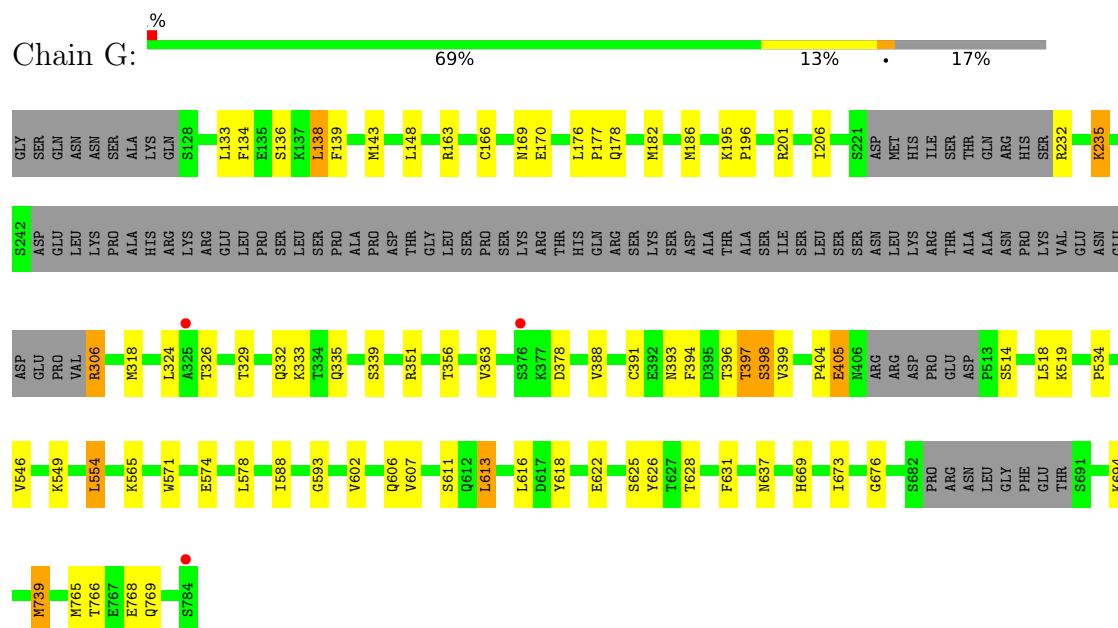
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



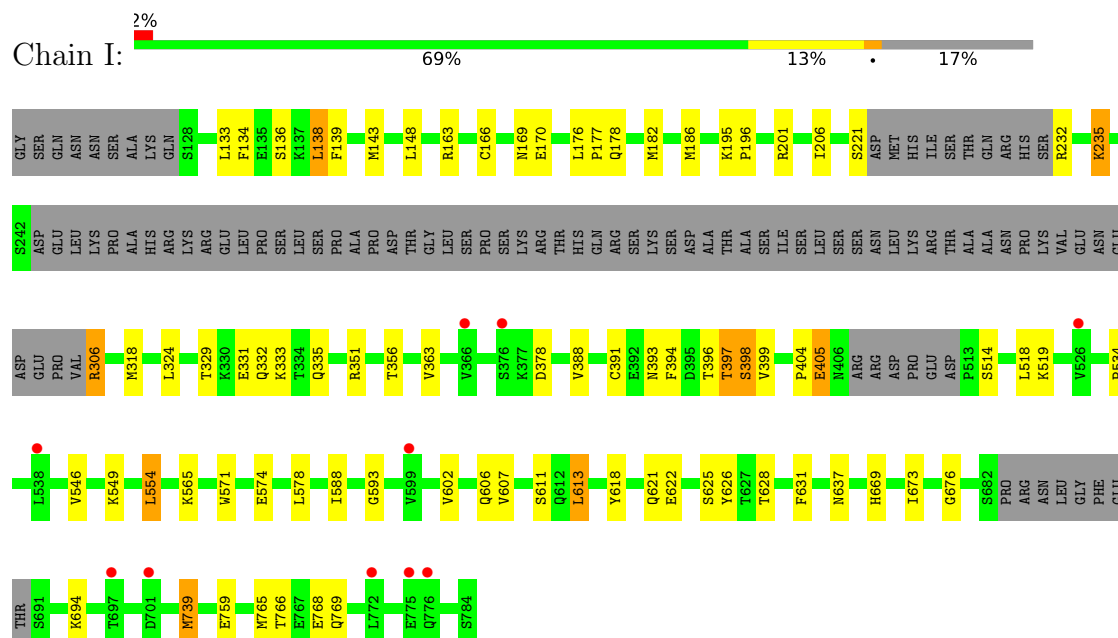
• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



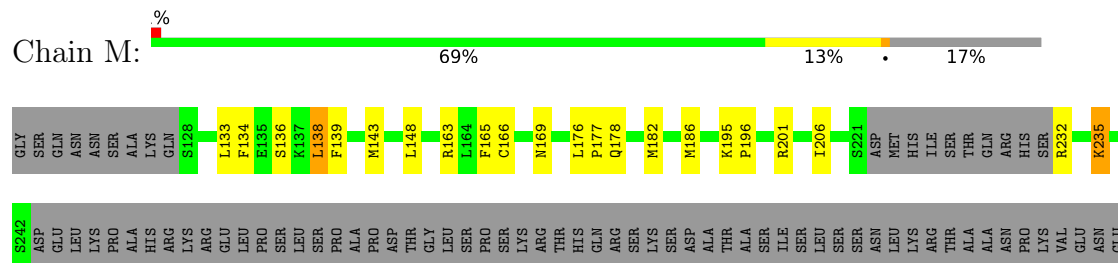
● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

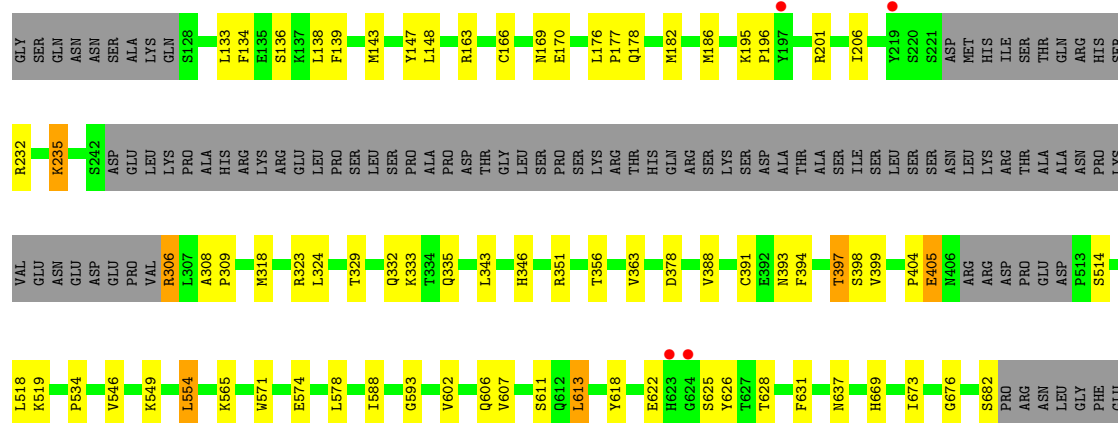


● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



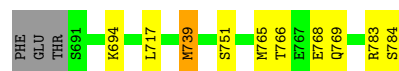
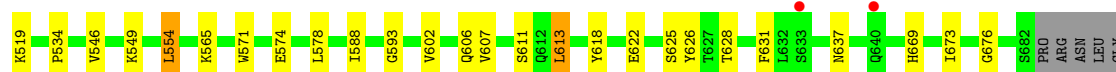
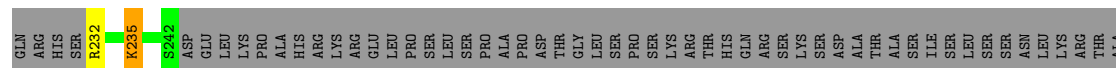
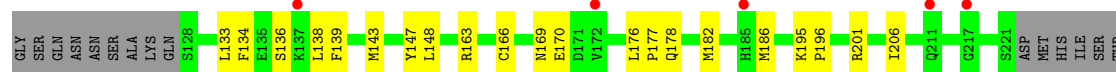
● Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA



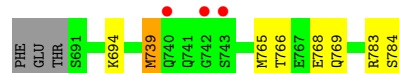
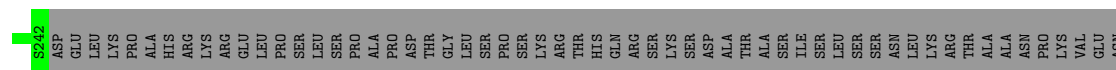
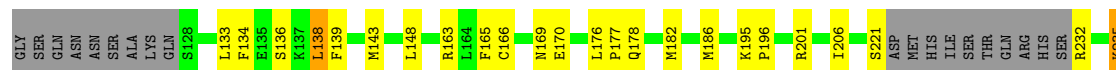




• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

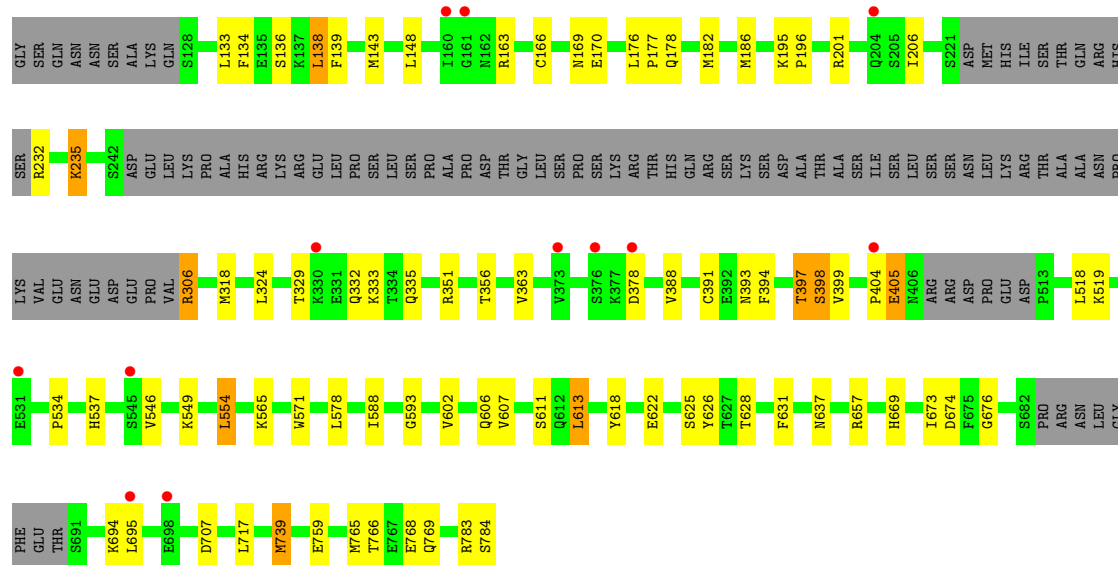


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

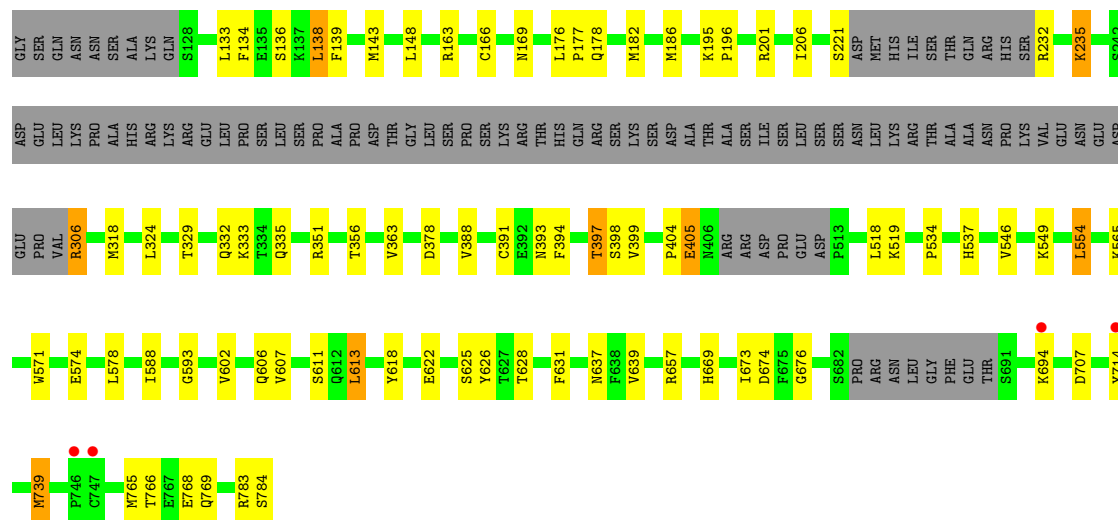


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

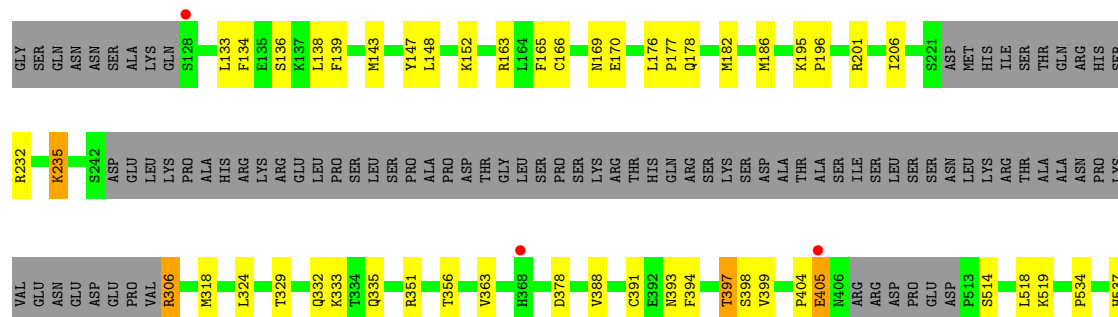


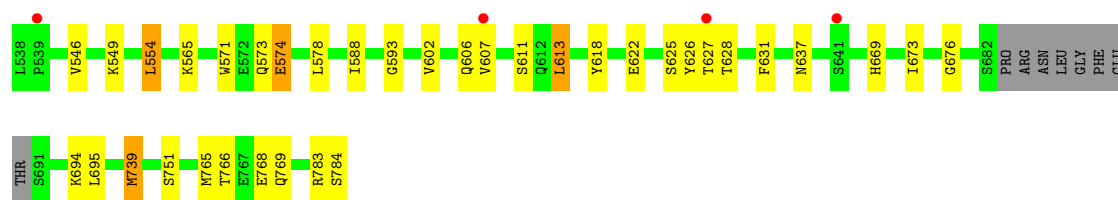


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

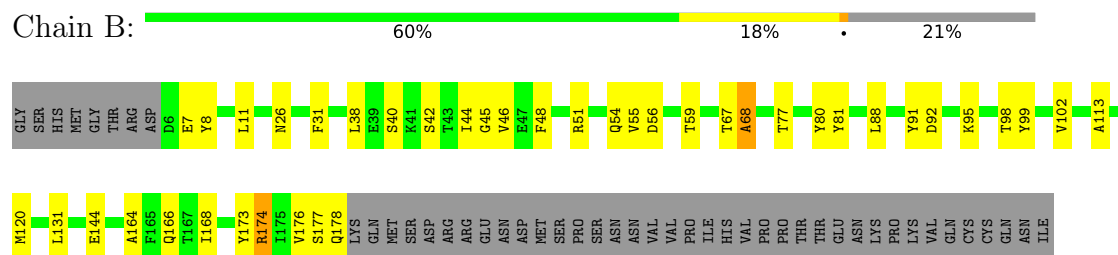


• Molecule 1: PHOSPHATIDYLINOSITOL 4-KINASE BETA

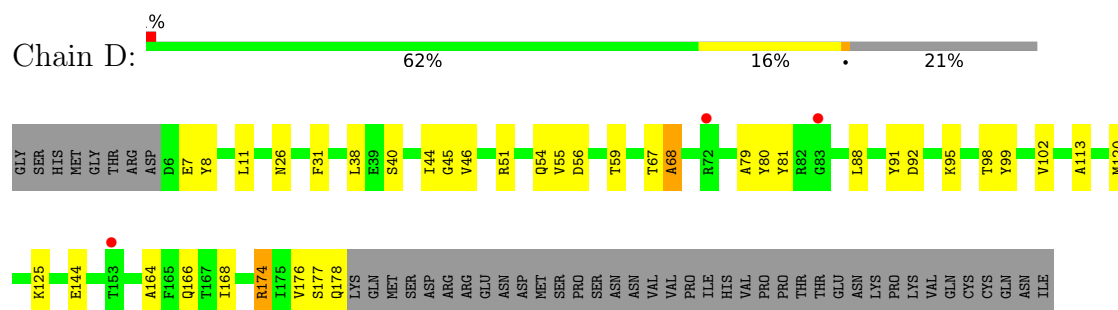




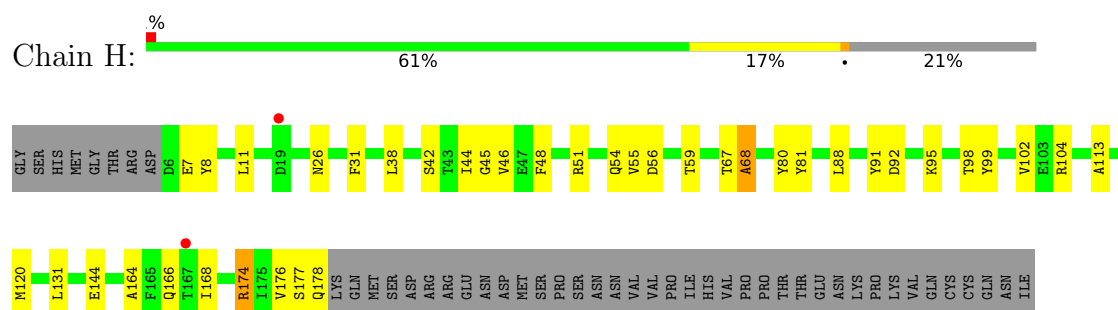
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



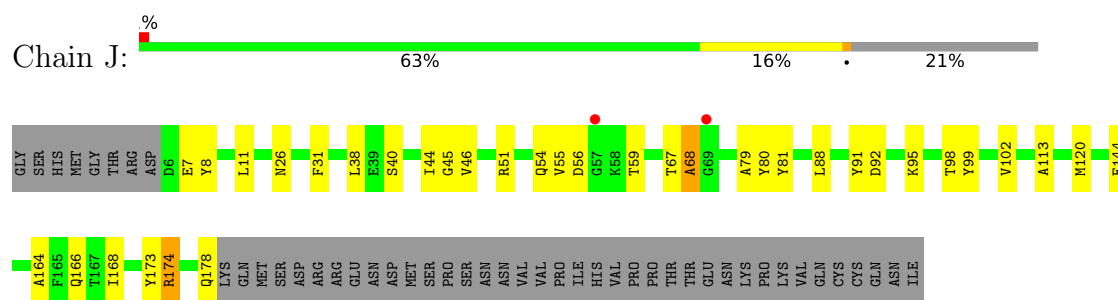
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

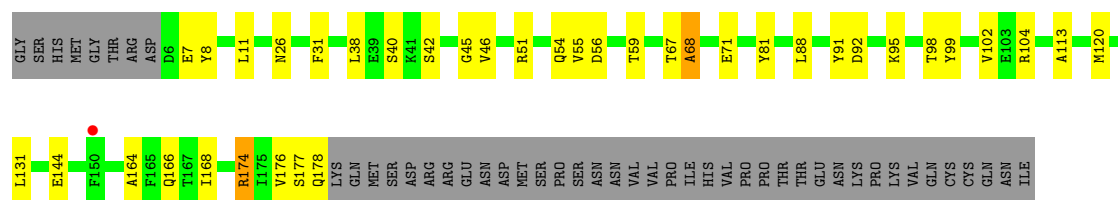


• Molecule 2: RAS-RELATED PROTEIN RAB-11A



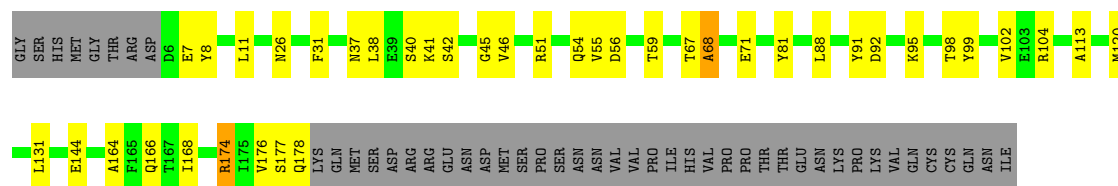
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain N: 



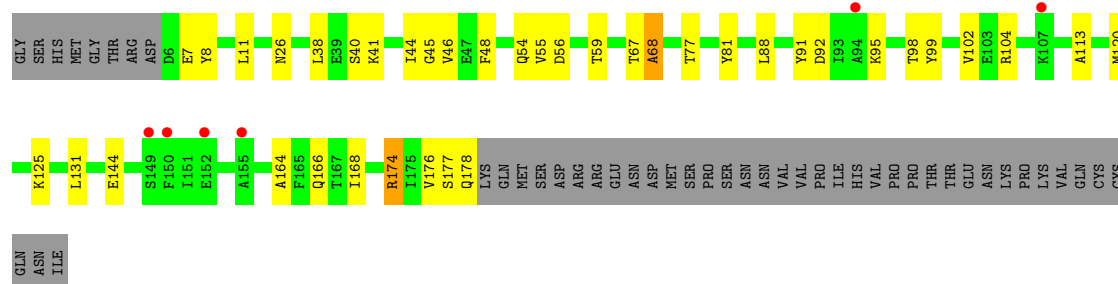
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain P: 



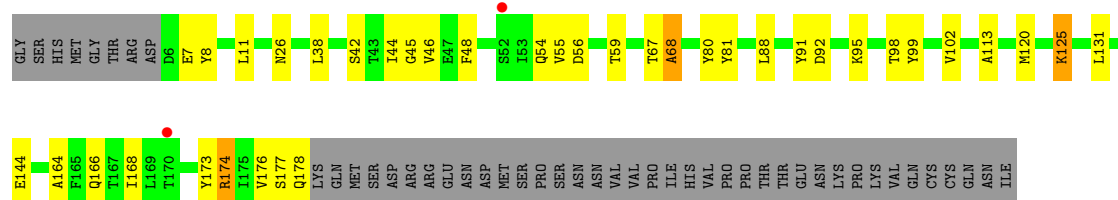
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain R: 



• Molecule 2: RAS-RELATED PROTEIN RAB-11A

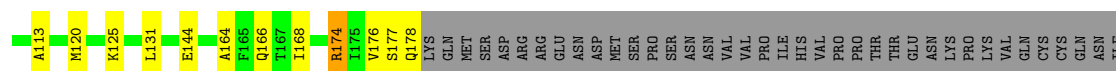
Chain T: 



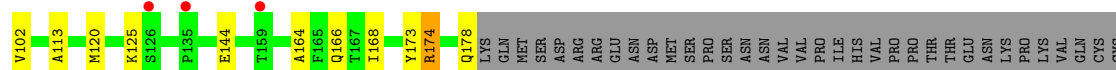
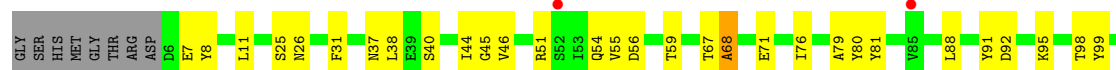
• Molecule 2: RAS-RELATED PROTEIN RAB-11A

Chain X: 

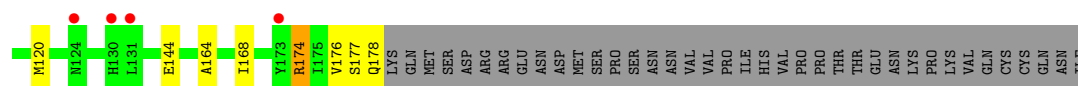




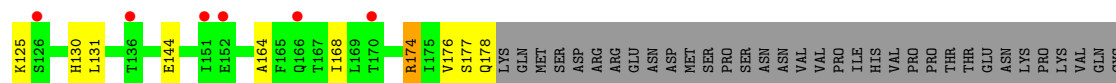
• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 2: RAS-RELATED PROTEIN RAB-11A



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

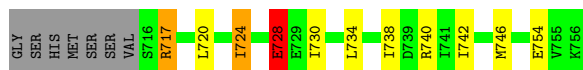


• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

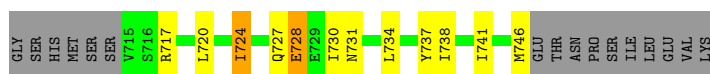




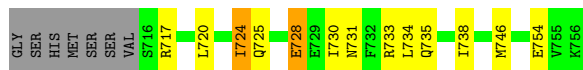
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

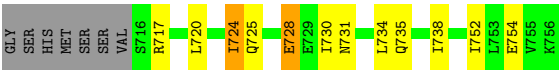


• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3

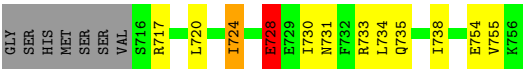




● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



● Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	199.50Å 134.47Å 294.33Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	294.32 – 6.00 294.32 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (294.32-6.00) 92.8 (294.32-6.00)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 6.15Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, R_{free}	0.253 , 0.359 0.252 , 0.351	Depositor DCC
R_{free} test set	2048 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	248.6	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 945.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.389 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	65970	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 093, GSP

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	0.75	0/3866	0.95	6/5219 (0.1%)
1	C	0.73	0/3866	0.94	6/5219 (0.1%)
1	G	0.74	0/3866	0.95	6/5219 (0.1%)
1	I	0.72	0/3866	0.93	5/5219 (0.1%)
1	M	0.74	0/3866	0.95	6/5219 (0.1%)
1	O	0.75	0/3866	0.95	6/5219 (0.1%)
1	Q	0.73	0/3866	0.95	6/5219 (0.1%)
1	S	0.73	0/3866	0.94	6/5219 (0.1%)
1	W	0.75	0/3866	0.94	6/5219 (0.1%)
1	Y	0.74	0/3866	0.94	2/5219 (0.0%)
1	c	0.77	0/3866	0.95	4/5219 (0.1%)
1	g	0.75	0/3866	0.94	6/5219 (0.1%)
2	B	0.82	0/1399	0.98	1/1892 (0.1%)
2	D	0.81	0/1399	0.96	0/1892
2	H	0.80	0/1399	0.97	0/1892
2	J	0.82	0/1399	0.97	0/1892
2	N	0.77	0/1399	0.94	0/1892
2	P	0.77	0/1399	0.94	0/1892
2	R	0.76	0/1399	0.94	1/1892 (0.1%)
2	T	0.75	0/1399	0.94	0/1892
2	X	0.76	0/1399	0.94	0/1892
2	Z	0.77	0/1399	0.93	0/1892
2	d	0.77	0/1399	0.94	1/1892 (0.1%)
2	h	0.78	0/1399	0.93	0/1892
3	E	1.23	2/316 (0.6%)	1.25	1/429 (0.2%)
3	F	1.18	1/238 (0.4%)	1.23	0/323
3	K	1.24	2/316 (0.6%)	1.25	1/429 (0.2%)
3	L	1.20	2/238 (0.8%)	1.24	0/323
3	U	1.11	1/316 (0.3%)	1.13	0/429
3	V	1.26	0/238	1.21	1/323 (0.3%)
3	a	1.25	2/316 (0.6%)	1.24	1/429 (0.2%)
3	b	1.22	0/238	1.21	0/323

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	e	1.15	1/316 (0.3%)	1.15	0/429
3	f	1.24	0/238	1.22	1/323 (0.3%)
3	i	1.16	1/316 (0.3%)	1.15	1/429 (0.2%)
3	j	1.27	0/238	1.19	1/323 (0.3%)
All	All	0.78	12/66504 (0.0%)	0.96	75/89844 (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	1
1	C	0	1
1	G	0	1
1	I	0	1
1	M	0	1
1	O	0	1
1	Q	0	1
1	S	0	1
1	W	0	1
1	Y	0	1
1	c	0	1
1	g	0	1
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	717	ARG	CD-NE	6.71	1.55	1.46
3	E	717	ARG	CD-NE	6.36	1.55	1.46
3	K	724	ILE	C-O	6.33	1.31	1.24
3	K	717	ARG	CD-NE	6.29	1.55	1.46
3	E	724	ILE	C-O	6.17	1.31	1.24
3	a	724	ILE	C-O	6.13	1.30	1.24
3	e	724	ILE	C-O	6.06	1.30	1.24
3	i	724	ILE	C-O	5.55	1.30	1.24
3	U	724	ILE	C-O	5.55	1.30	1.24
3	L	724	ILE	C-O	5.41	1.30	1.24
3	F	728	GLU	C-O	5.24	1.30	1.24
3	L	728	GLU	C-O	5.23	1.30	1.24

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	676	GLY	N-CA-C	-8.07	102.21	112.54
1	W	574	GLU	N-CA-C	-8.00	100.28	110.19
1	O	574	GLU	N-CA-C	-7.71	100.63	110.19
1	g	574	GLU	N-CA-C	-7.53	100.85	110.19
1	G	574	GLU	N-CA-C	-7.52	100.86	110.19
1	S	676	GLY	N-CA-C	-7.47	102.50	112.14
1	c	676	GLY	N-CA-C	-7.46	102.99	112.54
1	W	676	GLY	N-CA-C	-7.45	103.00	112.54
1	M	574	GLU	N-CA-C	-7.42	100.99	110.19
1	A	574	GLU	N-CA-C	-7.38	101.04	110.19
1	M	676	GLY	N-CA-C	-7.33	103.15	112.54
1	C	574	GLU	N-CA-C	-7.33	101.10	110.19
1	G	676	GLY	N-CA-C	-7.15	103.39	112.54
1	A	676	GLY	N-CA-C	-7.11	103.44	112.54
1	C	676	GLY	N-CA-C	-7.05	103.52	112.54
1	S	574	GLU	N-CA-C	-7.03	101.47	110.19
1	Q	574	GLU	N-CA-C	-7.02	101.48	110.19
1	I	676	GLY	N-CA-C	-6.97	103.62	112.54
1	O	676	GLY	N-CA-C	-6.93	103.20	112.14
1	C	673	ILE	N-CA-C	6.91	123.71	109.34
1	A	673	ILE	N-CA-C	6.83	123.54	109.34
1	M	673	ILE	N-CA-C	6.76	123.40	109.34
1	Y	676	GLY	N-CA-C	-6.76	103.42	112.14
1	S	673	ILE	N-CA-C	6.75	123.39	109.34
1	Q	673	ILE	N-CA-C	6.75	123.38	109.34
1	O	673	ILE	N-CA-C	6.74	123.35	109.34
1	I	673	ILE	N-CA-C	6.71	123.30	109.34
1	G	673	ILE	N-CA-C	6.55	122.97	109.34
1	Q	676	GLY	N-CA-C	-6.52	103.72	112.14
1	g	673	ILE	N-CA-C	6.46	122.77	109.34
1	W	673	ILE	N-CA-C	6.39	122.64	109.34
1	Y	673	ILE	N-CA-C	6.33	122.52	109.34
1	c	673	ILE	N-CA-C	6.30	122.44	109.34
1	W	514	SER	N-CA-C	-5.51	105.82	112.54
1	W	574	GLU	CA-C-N	-5.43	115.71	123.20
1	W	574	GLU	C-N-CA	-5.43	115.71	123.20
1	C	514	SER	N-CA-C	-5.41	106.18	112.89
1	O	574	GLU	CA-C-N	-5.41	115.74	123.20
1	O	574	GLU	C-N-CA	-5.41	115.74	123.20
3	i	728	GLU	N-CA-CB	5.38	118.63	110.28
1	Q	514	SER	N-CA-C	-5.38	105.98	112.54
1	G	574	GLU	CA-C-N	-5.37	115.78	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	574	GLU	C-N-CA	-5.37	115.78	123.20
1	g	574	GLU	CA-C-N	-5.31	115.87	123.20
1	g	574	GLU	C-N-CA	-5.31	115.87	123.20
1	G	514	SER	N-CA-C	-5.29	106.08	112.54
3	f	728	GLU	N-CA-C	5.29	117.13	111.36
3	a	728	GLU	N-CA-CB	5.29	118.47	110.28
1	S	514	SER	N-CA-C	-5.29	106.09	112.54
3	j	728	GLU	N-CA-C	5.27	117.10	111.36
3	E	728	GLU	N-CA-CB	5.24	118.37	110.30
3	V	728	GLU	N-CA-C	5.24	117.07	111.36
1	M	514	SER	N-CA-C	-5.22	106.17	112.54
1	A	514	SER	N-CA-C	-5.20	106.19	112.54
1	C	574	GLU	CA-C-N	-5.20	116.03	123.20
1	C	574	GLU	C-N-CA	-5.20	116.03	123.20
3	K	728	GLU	N-CA-CB	5.20	118.31	110.30
1	S	574	GLU	CA-C-N	-5.19	116.04	123.20
1	S	574	GLU	C-N-CA	-5.19	116.04	123.20
1	c	574	GLU	CA-C-N	-5.17	116.07	123.20
1	c	574	GLU	C-N-CA	-5.17	116.07	123.20
1	M	574	GLU	CA-C-N	-5.16	116.08	123.20
1	M	574	GLU	C-N-CA	-5.16	116.08	123.20
1	Q	574	GLU	CA-C-N	-5.16	116.08	123.20
1	Q	574	GLU	C-N-CA	-5.16	116.08	123.20
1	A	574	GLU	CA-C-N	-5.15	116.09	123.20
1	A	574	GLU	C-N-CA	-5.15	116.09	123.20
2	B	77	THR	N-CA-CB	5.14	117.77	110.16
1	I	514	SER	N-CA-C	-5.14	106.27	112.54
1	g	514	SER	N-CA-C	-5.11	106.31	112.54
1	O	514	SER	N-CA-C	-5.10	106.32	112.54
1	I	574	GLU	CA-C-N	-5.06	116.22	123.20
1	I	574	GLU	C-N-CA	-5.06	116.22	123.20
2	R	77	THR	N-CA-CB	5.01	117.58	110.16
2	d	77	THR	N-CA-CB	5.00	117.56	110.16

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	SER	Peptide
1	C	398	SER	Peptide
1	G	398	SER	Peptide
1	I	398	SER	Peptide

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Mol	Chain	Res	Type	Group
1	M	398	SER	Peptide
1	O	398	SER	Peptide
1	Q	398	SER	Peptide
1	S	398	SER	Peptide
1	W	398	SER	Peptide
1	Y	398	SER	Peptide
1	c	398	SER	Peptide
1	g	398	SER	Peptide

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	3788	0	3838	57	8
1	C	3788	0	3839	85	2
1	G	3788	0	3839	54	10
1	I	3788	0	3839	83	2
1	M	3788	0	3839	58	12
1	O	3788	0	3839	59	17
1	Q	3788	0	3839	65	4
1	S	3788	0	3839	67	12
1	W	3788	0	3838	59	4
1	Y	3788	0	3839	60	12
1	c	3788	0	3839	59	7
1	g	3788	0	3839	62	13
2	B	1377	0	1370	47	9
2	D	1377	0	1370	37	4
2	H	1377	0	1370	38	3
2	J	1377	0	1370	36	4
2	N	1377	0	1370	29	0
2	P	1377	0	1371	32	0
2	R	1377	0	1370	32	0
2	T	1377	0	1370	31	0
2	X	1377	0	1370	39	0
2	Z	1377	0	1371	40	0
2	d	1377	0	1370	33	0
2	h	1377	0	1370	39	1
3	E	314	0	298	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	237	0	222	29	0
3	K	314	0	298	53	0
3	L	237	0	222	35	0
3	U	314	0	298	23	0
3	V	237	0	222	47	0
3	a	314	0	298	45	0
3	b	237	0	222	33	0
3	e	314	0	298	30	0
3	f	237	0	222	49	0
3	i	314	0	298	33	0
3	j	237	0	222	59	0
4	A	24	0	16	0	0
4	C	24	0	16	0	0
4	G	24	0	16	0	0
4	I	24	0	16	0	0
4	M	24	0	16	0	0
4	O	24	0	16	0	0
4	Q	24	0	16	0	0
4	S	24	0	16	0	0
4	W	24	0	16	0	0
4	Y	24	0	16	0	0
4	c	24	0	16	0	0
4	g	24	0	16	0	0
5	B	32	0	12	6	0
5	D	32	0	12	6	0
5	H	32	0	12	4	0
5	J	32	0	12	4	0
5	N	32	0	12	6	0
5	P	32	0	12	7	0
5	R	32	0	12	6	0
5	T	32	0	12	6	0
5	X	32	0	12	6	0
5	Z	32	0	12	6	0
5	d	32	0	12	11	0
5	h	32	0	12	7	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	J	1	0	0	0	0
6	N	1	0	0	0	0
6	P	1	0	0	0	0
6	R	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1	0	0	0	0
6	X	1	0	0	0	0
6	Z	1	0	0	2	0
6	d	1	0	0	0	0
6	h	1	0	0	0	0
All	All	65970	0	65964	1287	62

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 10.

All (1287) 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:J:44:ILE:HD11	3:K:734:LEU:CD2	1.30	1.59
2:J:44:ILE:CD1	3:K:734:LEU:HD22	1.30	1.59
2:D:44:ILE:HD11	3:E:734:LEU:CD2	1.41	1.50
1:C:138:LEU:HG	1:S:769:GLN:CG	1.41	1.48
2:D:44:ILE:CD1	3:E:734:LEU:HD22	1.44	1.47
1:C:138:LEU:CG	1:S:769:GLN:HG2	1.45	1.42
3:a:717:ARG:CG	3:j:728:GLU:OE2	1.69	1.39
1:I:138:LEU:HG	1:Q:769:GLN:CG	1.52	1.38
1:I:138:LEU:CG	1:Q:769:GLN:HG2	1.53	1.34
3:a:717:ARG:HG3	3:j:728:GLU:OE2	1.18	1.33
1:G:138:LEU:HD21	1:M:765:MET:CE	1.59	1.30
1:A:138:LEU:HD21	1:O:765:MET:CE	1.63	1.27
3:K:717:ARG:HD3	3:f:728:GLU:CD	1.58	1.27
2:Z:44:ILE:HD11	3:a:734:LEU:CD2	1.66	1.25
2:Z:44:ILE:CD1	3:a:734:LEU:HD22	1.66	1.24
3:a:717:ARG:CD	3:j:728:GLU:OE2	1.91	1.18
2:B:80:TYR:OH	3:E:746:MET:CG	1.94	1.15
3:e:731:ASN:HD21	3:f:731:ASN:CG	1.54	1.14
2:B:80:TYR:OH	3:E:746:MET:HG2	1.45	1.14
1:G:138:LEU:CD2	1:M:765:MET:HE2	1.77	1.13
2:H:80:TYR:OH	3:K:746:MET:HG2	1.48	1.12
1:A:138:LEU:HD21	1:O:765:MET:HE2	1.13	1.12
3:i:731:ASN:ND2	3:j:731:ASN:OD1	1.83	1.12
3:K:717:ARG:CD	3:f:728:GLU:CD	2.23	1.11
1:C:138:LEU:HD21	1:S:769:GLN:HB3	1.29	1.09
1:A:138:LEU:CD2	1:O:765:MET:HE2	1.84	1.08
2:Z:79:ALA:HB3	3:b:746:MET:HE3	1.25	1.08
3:E:717:ARG:HD3	3:V:728:GLU:CD	1.80	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:56:ASP:OD2	2:d:174:ARG:NH1	1.90	1.05
2:X:56:ASP:OD2	2:X:174:ARG:NH1	1.89	1.04
2:J:79:ALA:CB	3:L:746:MET:HE3	1.86	1.04
2:R:56:ASP:OD2	2:R:174:ARG:NH1	1.90	1.04
3:U:738:ILE:HD13	3:V:738:ILE:HD13	1.40	1.04
2:D:56:ASP:OD2	2:D:174:ARG:NH1	1.90	1.04
2:D:79:ALA:CB	3:F:746:MET:HE3	1.86	1.04
3:E:717:ARG:CG	3:V:728:GLU:OE2	2.06	1.04
1:I:138:LEU:HD21	1:Q:769:GLN:HB3	1.34	1.04
2:J:56:ASP:OD2	2:J:174:ARG:NH1	1.90	1.04
2:T:56:ASP:OD2	2:T:174:ARG:NH1	1.90	1.04
2:h:56:ASP:OD2	2:h:174:ARG:NH1	1.89	1.04
2:N:56:ASP:OD2	2:N:174:ARG:NH1	1.90	1.03
2:P:56:ASP:OD2	2:P:174:ARG:NH1	1.90	1.03
3:K:717:ARG:CD	3:f:728:GLU:OE1	2.05	1.03
1:W:765:MET:HE2	1:c:138:LEU:HD21	1.39	1.03
1:Y:138:LEU:HG	1:g:769:GLN:HG2	1.39	1.02
2:Z:79:ALA:CB	3:b:746:MET:HE3	1.89	1.02
3:e:738:ILE:HG21	3:f:738:ILE:HD11	1.41	1.02
2:H:56:ASP:OD2	2:H:174:ARG:NH1	1.91	1.02
2:Z:56:ASP:OD2	2:Z:174:ARG:NH1	1.90	1.02
3:K:738:ILE:HD13	3:L:738:ILE:CD1	1.90	1.01
2:B:56:ASP:OD2	2:B:174:ARG:NH1	1.92	1.01
1:W:765:MET:CE	1:c:138:LEU:HD21	1.90	1.01
2:J:44:ILE:HD11	3:K:734:LEU:HD21	1.43	1.00
2:J:79:ALA:HB3	3:L:746:MET:HE3	1.43	1.00
3:e:731:ASN:ND2	3:f:731:ASN:CG	2.18	1.00
2:D:79:ALA:HB3	3:F:746:MET:HE3	1.39	0.99
2:H:48:PHE:HD2	3:K:754:GLU:HA	1.26	0.99
2:J:44:ILE:HD13	3:K:734:LEU:HD22	1.43	0.99
1:C:138:LEU:CG	1:S:769:GLN:CG	2.20	0.99
3:K:717:ARG:CG	3:f:728:GLU:OE2	2.11	0.98
3:K:717:ARG:HD3	3:f:728:GLU:OE2	1.61	0.97
2:D:44:ILE:HD11	3:E:734:LEU:HD21	1.46	0.97
1:G:138:LEU:HD21	1:M:765:MET:HE2	1.00	0.97
2:J:79:ALA:CB	3:L:746:MET:CE	2.43	0.97
3:E:717:ARG:CD	3:V:728:GLU:CD	2.37	0.96
2:B:48:PHE:HD2	3:E:754:GLU:HA	1.29	0.96
1:C:138:LEU:HD23	1:S:769:GLN:CD	1.92	0.95
2:H:80:TYR:OH	3:K:746:MET:CG	2.13	0.95
3:a:717:ARG:HD3	3:j:728:GLU:OE2	1.67	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:138:LEU:HD21	1:c:765:MET:HE3	1.50	0.94
3:i:735:GLN:HE22	3:j:734:LEU:HD13	1.29	0.94
3:i:738:ILE:HD13	3:j:738:ILE:CD1	1.98	0.94
2:d:38:LEU:O	5:d:2000:GSP:O3'	1.85	0.93
2:X:80:TYR:OH	3:a:746:MET:HG2	1.66	0.93
3:U:738:ILE:HG21	3:V:738:ILE:HD11	1.51	0.92
3:i:735:GLN:NE2	3:j:734:LEU:HD13	1.83	0.92
2:Z:71:GLU:OE2	1:c:221:SER:O	1.88	0.92
3:e:738:ILE:HD13	3:f:738:ILE:HD13	1.52	0.92
3:E:717:ARG:HG3	3:V:728:GLU:CD	1.95	0.91
2:D:79:ALA:CB	3:F:746:MET:CE	2.48	0.91
1:C:332:GLN:HE22	1:I:331:GLU:HG3	1.35	0.91
3:E:717:ARG:CD	3:V:724:ILE:HG22	2.01	0.90
2:T:44:ILE:HD11	3:V:734:LEU:CD2	2.01	0.89
1:I:138:LEU:HD23	1:Q:769:GLN:CD	1.98	0.89
1:C:138:LEU:HD21	1:S:765:MET:HG2	1.55	0.89
3:E:738:ILE:HD13	3:F:738:ILE:HG12	1.54	0.88
2:h:44:ILE:HD11	3:j:734:LEU:CD2	2.04	0.88
1:Y:138:LEU:HD21	1:g:765:MET:HG2	1.54	0.88
2:B:48:PHE:CD2	3:E:754:GLU:HA	2.08	0.87
1:Y:759:GLU:OE2	1:g:147:TYR:OH	1.92	0.87
2:H:48:PHE:CD2	3:K:754:GLU:HA	2.09	0.87
2:R:44:ILE:HD11	3:f:734:LEU:CD2	2.05	0.86
3:i:735:GLN:NE2	3:j:734:LEU:CD1	2.38	0.86
3:E:717:ARG:CG	3:V:728:GLU:CD	2.48	0.86
3:E:717:ARG:HG3	3:V:728:GLU:OE2	1.72	0.86
3:K:717:ARG:CD	3:f:728:GLU:OE2	2.17	0.86
3:E:717:ARG:CD	3:V:728:GLU:OE1	2.24	0.86
3:U:731:ASN:HD21	3:V:731:ASN:CG	1.83	0.86
1:C:138:LEU:CD2	1:S:769:GLN:HB3	2.06	0.86
1:Y:138:LEU:HG	1:g:769:GLN:CG	2.05	0.85
1:A:339:SER:OG	1:Y:537:HIS:HB2	1.75	0.85
3:a:717:ARG:CD	3:j:728:GLU:CD	2.48	0.85
2:R:44:ILE:HD11	3:f:734:LEU:HD21	1.56	0.84
1:C:138:LEU:CD2	1:S:769:GLN:CG	2.54	0.84
1:I:138:LEU:CG	1:Q:769:GLN:CG	2.30	0.84
1:C:138:LEU:HD21	1:S:769:GLN:CB	2.05	0.84
3:K:717:ARG:CG	3:f:728:GLU:CD	2.50	0.84
2:H:95:LYS:O	2:H:98:THR:HG22	1.78	0.84
2:X:48:PHE:HD2	3:a:754:GLU:HA	1.39	0.84
1:C:138:LEU:CD2	1:S:769:GLN:CD	2.50	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:95:LYS:O	2:B:98:THR:HG22	1.78	0.83
2:d:37:ASN:O	5:d:2000:GSP:O2'	1.94	0.83
2:R:95:LYS:O	2:R:98:THR:HG22	1.78	0.83
2:N:95:LYS:O	2:N:98:THR:HG22	1.79	0.83
2:T:95:LYS:O	2:T:98:THR:HG22	1.78	0.83
2:P:95:LYS:O	2:P:98:THR:HG22	1.79	0.83
2:B:44:ILE:HB	3:F:737:TYR:CZ	2.14	0.82
2:h:95:LYS:O	2:h:98:THR:HG22	1.78	0.82
3:a:717:ARG:CD	3:j:724:ILE:HG22	2.09	0.82
2:Z:95:LYS:O	2:Z:98:THR:HG22	1.78	0.82
3:a:717:ARG:CD	3:j:724:ILE:CG2	2.58	0.82
3:K:738:ILE:HD13	3:L:738:ILE:CG1	2.09	0.82
2:X:95:LYS:O	2:X:98:THR:HG22	1.79	0.82
3:U:738:ILE:HG21	3:V:738:ILE:CD1	2.09	0.82
2:J:79:ALA:HB3	3:L:746:MET:CE	2.09	0.82
2:D:44:ILE:HD11	3:E:734:LEU:HD22	0.87	0.81
2:J:95:LYS:O	2:J:98:THR:HG22	1.79	0.81
1:M:163:ARG:O	1:M:166:CYS:SG	2.38	0.81
3:i:738:ILE:HD13	3:j:738:ILE:HD11	1.62	0.81
2:D:95:LYS:O	2:D:98:THR:HG22	1.79	0.81
1:A:163:ARG:O	1:A:166:CYS:SG	2.39	0.81
3:a:717:ARG:NE	3:j:724:ILE:HG22	1.94	0.81
2:d:95:LYS:O	2:d:98:THR:HG22	1.79	0.81
3:a:717:ARG:HD2	3:j:724:ILE:CG2	2.11	0.81
2:D:44:ILE:HD13	3:E:734:LEU:HD22	1.59	0.81
1:G:163:ARG:O	1:G:166:CYS:SG	2.39	0.81
3:K:717:ARG:NE	3:f:728:GLU:OE1	2.14	0.81
2:Z:79:ALA:CB	3:b:746:MET:CE	2.58	0.81
1:O:163:ARG:O	1:O:166:CYS:SG	2.39	0.80
3:E:724:ILE:CG2	3:V:717:ARG:CZ	2.59	0.80
1:I:138:LEU:HD21	1:Q:765:MET:HG2	1.61	0.80
1:W:163:ARG:O	1:W:166:CYS:SG	2.39	0.80
3:K:738:ILE:HD13	3:L:738:ILE:HG12	1.61	0.80
1:c:163:ARG:O	1:c:166:CYS:SG	2.39	0.80
1:g:163:ARG:O	1:g:166:CYS:SG	2.39	0.80
3:a:720:LEU:HD13	3:i:724:ILE:HD11	1.64	0.80
2:T:44:ILE:CD1	3:V:734:LEU:HD22	2.11	0.80
3:E:717:ARG:NH2	3:V:725:GLN:CB	2.45	0.79
1:Y:138:LEU:HD21	1:g:769:GLN:HB3	1.65	0.79
1:C:163:ARG:O	1:C:166:CYS:SG	2.39	0.79
3:E:717:ARG:HD3	3:V:728:GLU:OE2	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:717:ARG:CG	3:f:728:GLU:OE1	2.30	0.79
1:Y:138:LEU:CD2	1:g:765:MET:HG2	2.11	0.79
1:I:138:LEU:CD2	1:Q:769:GLN:CG	2.60	0.79
1:I:163:ARG:O	1:I:166:CYS:SG	2.39	0.79
3:a:717:ARG:HD2	3:j:724:ILE:HG21	1.65	0.79
3:i:735:GLN:HE22	3:j:734:LEU:CD1	1.96	0.79
1:Y:163:ARG:O	1:Y:166:CYS:SG	2.39	0.79
3:K:717:ARG:HG3	3:f:728:GLU:CD	2.08	0.79
1:S:163:ARG:O	1:S:166:CYS:SG	2.39	0.79
1:Q:163:ARG:O	1:Q:166:CYS:SG	2.39	0.78
3:a:728:GLU:HB2	3:j:717:ARG:NH1	1.99	0.78
1:I:138:LEU:HD21	1:Q:769:GLN:CB	2.12	0.78
3:e:738:ILE:HG21	3:f:738:ILE:CD1	2.13	0.78
1:A:138:LEU:CD2	1:O:765:MET:CE	2.51	0.78
2:d:42:SER:HA	5:d:2000:GSP:S1G	2.23	0.77
3:E:717:ARG:CG	3:V:728:GLU:OE1	2.32	0.77
1:I:138:LEU:CD2	1:Q:769:GLN:CD	2.57	0.77
1:C:331:GLU:CG	1:I:332:GLN:HE22	1.98	0.77
2:X:48:PHE:CD2	3:a:754:GLU:HA	2.20	0.77
3:K:738:ILE:CD1	3:L:738:ILE:CD1	2.62	0.77
1:W:765:MET:HE2	1:c:138:LEU:CD2	2.14	0.77
3:E:717:ARG:CD	3:V:728:GLU:OE2	2.32	0.77
3:a:724:ILE:HG22	3:j:717:ARG:CZ	2.15	0.76
1:Q:232:ARG:O	1:Q:235:LYS:NZ	2.18	0.76
2:h:48:PHE:HD2	3:i:754:GLU:HA	1.50	0.76
3:i:738:ILE:CD1	3:j:738:ILE:HD13	2.16	0.76
3:E:717:ARG:HG3	3:V:728:GLU:OE1	1.82	0.76
1:S:232:ARG:O	1:S:235:LYS:NZ	2.18	0.75
3:E:724:ILE:HG23	3:V:717:ARG:CZ	2.16	0.75
1:I:138:LEU:CD2	1:Q:769:GLN:HB3	2.13	0.75
2:T:44:ILE:HD11	3:V:734:LEU:HD21	1.67	0.75
1:C:332:GLN:HE22	1:I:331:GLU:CG	2.00	0.75
3:i:738:ILE:HD13	3:j:738:ILE:HD13	1.68	0.75
3:U:731:ASN:ND2	3:V:731:ASN:CG	2.45	0.75
3:i:731:ASN:ND2	3:j:731:ASN:CG	2.45	0.74
2:B:80:TYR:OH	3:E:746:MET:SD	2.45	0.74
2:B:80:TYR:HH	3:E:746:MET:HG2	1.51	0.74
1:G:138:LEU:CD2	1:M:765:MET:CE	2.49	0.74
2:R:44:ILE:CD1	3:f:734:LEU:HD22	2.16	0.74
2:Z:37:ASN:O	5:Z:2000:GSP:O2'	2.05	0.74
2:h:44:ILE:HD11	3:j:734:LEU:HD21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:38:LEU:HA	5:d:2000:GSP:O2'	1.86	0.74
2:B:44:ILE:O	3:F:737:TYR:OH	2.05	0.74
3:E:738:ILE:HD13	3:F:738:ILE:CG1	2.18	0.74
2:X:80:TYR:OH	3:a:746:MET:CG	2.36	0.74
2:D:44:ILE:CD1	3:E:734:LEU:CD2	2.27	0.73
1:S:393:ASN:O	1:S:397:THR:OG1	2.07	0.73
1:W:232:ARG:O	1:W:235:LYS:NZ	2.19	0.73
3:b:717:ARG:NH1	3:i:728:GLU:HB3	2.03	0.73
1:I:232:ARG:O	1:I:235:LYS:NZ	2.19	0.73
3:e:735:GLN:NE2	3:f:734:LEU:CD1	2.51	0.73
1:Q:393:ASN:O	1:Q:397:THR:OG1	2.07	0.73
3:e:735:GLN:NE2	3:f:734:LEU:HD12	2.03	0.73
3:E:717:ARG:HD2	3:V:724:ILE:HG22	1.71	0.73
1:Y:232:ARG:O	1:Y:235:LYS:NZ	2.19	0.73
1:C:232:ARG:O	1:C:235:LYS:NZ	2.19	0.73
1:C:332:GLN:HE21	1:I:332:GLN:HG3	1.53	0.73
2:Z:44:ILE:HD11	3:a:734:LEU:HD22	0.81	0.73
2:J:79:ALA:HB1	3:L:746:MET:HE3	1.71	0.73
1:Y:138:LEU:CD2	1:g:769:GLN:HB3	2.18	0.73
3:a:717:ARG:NE	3:j:728:GLU:OE1	2.22	0.72
2:D:79:ALA:HB3	3:F:746:MET:CE	2.12	0.72
1:g:232:ARG:O	1:g:235:LYS:NZ	2.19	0.72
2:B:44:ILE:HD12	3:F:737:TYR:CD2	2.24	0.72
1:c:393:ASN:O	1:c:397:THR:OG1	2.08	0.72
1:O:393:ASN:O	1:O:397:THR:OG1	2.07	0.72
1:W:393:ASN:O	1:W:397:THR:OG1	2.08	0.72
2:Z:71:GLU:OE2	1:c:221:SER:C	2.33	0.72
1:A:393:ASN:O	1:A:397:THR:OG1	2.07	0.72
1:C:393:ASN:O	1:C:397:THR:OG1	2.07	0.72
1:G:393:ASN:O	1:G:397:THR:OG1	2.07	0.72
1:M:393:ASN:O	1:M:397:THR:OG1	2.07	0.72
3:E:717:ARG:HD2	3:V:724:ILE:CG2	2.20	0.72
1:I:393:ASN:O	1:I:397:THR:OG1	2.07	0.72
1:M:232:ARG:O	1:M:235:LYS:NZ	2.18	0.72
1:g:393:ASN:O	1:g:397:THR:OG1	2.08	0.72
2:d:40:SER:HB3	5:d:2000:GSP:H3'	1.71	0.71
3:a:729:GLU:HG3	1:g:751:SER:OG	1.90	0.71
1:Y:393:ASN:O	1:Y:397:THR:OG1	2.07	0.71
3:K:717:ARG:HG3	3:f:728:GLU:OE1	1.90	0.71
1:O:232:ARG:O	1:O:235:LYS:NZ	2.19	0.71
1:G:232:ARG:O	1:G:235:LYS:NZ	2.19	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:44:ILE:CD1	3:V:734:LEU:CD2	2.69	0.71
1:A:232:ARG:O	1:A:235:LYS:NZ	2.19	0.71
2:J:44:ILE:HD11	3:K:734:LEU:HD22	0.73	0.71
3:E:724:ILE:O	3:V:717:ARG:NH1	2.24	0.70
2:T:44:ILE:HD13	3:V:734:LEU:HD22	1.73	0.70
1:C:138:LEU:CD2	1:S:769:GLN:CB	2.68	0.70
2:H:44:ILE:HB	3:L:737:TYR:CZ	2.26	0.70
3:K:717:ARG:HG3	3:f:728:GLU:OE2	1.92	0.70
1:c:232:ARG:O	1:c:235:LYS:NZ	2.19	0.70
2:h:44:ILE:CD1	3:j:734:LEU:HD22	2.22	0.70
2:P:38:LEU:O	5:P:2000:GSP:O3'	2.10	0.70
3:a:717:ARG:CZ	3:j:724:ILE:HG22	2.21	0.70
2:B:80:TYR:CZ	3:E:746:MET:HE2	2.26	0.70
3:E:738:ILE:HD13	3:F:738:ILE:CD1	2.21	0.70
3:K:738:ILE:CD1	3:L:738:ILE:HD13	2.22	0.69
2:B:80:TYR:OH	3:E:746:MET:CB	2.41	0.69
3:e:738:ILE:HD13	3:f:738:ILE:CD1	2.21	0.69
3:L:731:ASN:HD22	3:e:717:ARG:NH2	1.91	0.69
2:J:44:ILE:CD1	3:K:734:LEU:CD2	2.17	0.69
2:R:44:ILE:CD1	3:f:734:LEU:CD2	2.70	0.68
2:B:38:LEU:HA	5:B:2000:GSP:O2'	1.94	0.68
1:C:332:GLN:HG3	1:I:332:GLN:CG	2.24	0.68
1:c:139:PHE:HA	1:c:143:MET:HE2	1.76	0.68
1:O:139:PHE:HA	1:O:143:MET:HE2	1.75	0.67
2:J:38:LEU:HA	5:J:2000:GSP:O2'	1.94	0.67
2:h:44:ILE:CD1	3:j:734:LEU:CD2	2.72	0.67
3:E:717:ARG:HH21	3:V:725:GLN:CB	2.04	0.67
1:Q:139:PHE:HA	1:Q:143:MET:HE2	1.77	0.67
2:Z:80:TYR:HE1	3:b:746:MET:HG2	1.59	0.67
3:K:724:ILE:O	3:f:717:ARG:NH1	2.28	0.67
3:K:728:GLU:HB2	3:f:717:ARG:NH1	2.09	0.67
1:M:139:PHE:HA	1:M:143:MET:HE2	1.76	0.67
1:Y:139:PHE:HA	1:Y:143:MET:HE2	1.76	0.67
1:C:221:SER:C	2:P:71:GLU:OE2	2.37	0.67
2:Z:79:ALA:HB3	3:b:746:MET:CE	2.14	0.67
1:g:139:PHE:HA	1:g:143:MET:HE2	1.77	0.67
1:S:139:PHE:HA	1:S:143:MET:HE2	1.78	0.66
1:W:138:LEU:HD21	1:c:765:MET:CE	2.24	0.66
2:N:38:LEU:O	5:N:2000:GSP:O3'	2.13	0.66
1:C:138:LEU:CG	1:S:769:GLN:CB	2.73	0.66
3:U:738:ILE:HD13	3:V:738:ILE:CD1	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:HD23	1:S:769:GLN:OE1	1.95	0.66
2:X:44:ILE:HB	3:b:737:TYR:CZ	2.30	0.66
1:W:139:PHE:HA	1:W:143:MET:HE2	1.78	0.66
1:C:139:PHE:HA	1:C:143:MET:HE2	1.78	0.66
3:a:717:ARG:HD3	3:j:728:GLU:CD	2.17	0.66
3:a:738:ILE:HD13	3:b:738:ILE:CD1	2.26	0.66
3:e:752:ILE:HG21	3:f:745:ILE:HD11	1.77	0.65
1:A:139:PHE:HA	1:A:143:MET:HE2	1.77	0.65
3:E:742:ILE:HD11	3:F:741:ILE:HG21	1.79	0.65
1:I:139:PHE:HA	1:I:143:MET:HE2	1.78	0.65
3:K:738:ILE:HD13	3:L:738:ILE:HD11	1.73	0.65
3:a:724:ILE:O	3:j:717:ARG:NH1	2.28	0.65
1:W:221:SER:C	2:h:71:GLU:OE2	2.38	0.65
1:G:139:PHE:HA	1:G:143:MET:HE2	1.77	0.65
2:h:48:PHE:CD2	3:i:754:GLU:HA	2.32	0.65
2:N:38:LEU:HA	5:N:2000:GSP:O2'	1.96	0.65
2:T:26:ASN:ND2	5:T:2000:GSP:O1A	2.29	0.65
1:Y:138:LEU:HG	1:g:769:GLN:CB	2.27	0.64
1:A:138:LEU:HD21	1:O:765:MET:HE3	1.72	0.64
3:K:717:ARG:NH2	3:f:725:GLN:CB	2.60	0.64
3:e:738:ILE:CD1	3:f:738:ILE:HD13	2.25	0.64
2:Z:45:GLY:O	2:Z:67:THR:O	2.16	0.64
3:a:717:ARG:HE	3:j:728:GLU:CD	2.06	0.64
3:b:717:ARG:CZ	3:i:728:GLU:HB3	2.28	0.64
2:h:45:GLY:O	2:h:67:THR:O	2.16	0.64
2:N:45:GLY:O	2:N:67:THR:O	2.16	0.64
2:P:40:SER:HB3	5:P:2000:GSP:H3'	1.79	0.64
2:P:45:GLY:O	2:P:67:THR:O	2.16	0.64
2:T:80:TYR:OH	3:U:746:MET:HB3	1.98	0.64
2:X:45:GLY:O	2:X:67:THR:O	2.16	0.64
1:A:765:MET:HE2	1:O:138:LEU:HD21	1.79	0.63
2:R:45:GLY:O	2:R:67:THR:O	2.16	0.63
2:T:45:GLY:O	2:T:67:THR:O	2.16	0.63
2:H:45:GLY:O	2:H:67:THR:O	2.16	0.63
1:Y:618:TYR:CZ	1:Y:622:GLU:HG3	2.33	0.63
2:d:45:GLY:O	2:d:67:THR:O	2.16	0.63
1:A:138:LEU:CD1	1:O:765:MET:HE2	2.29	0.63
1:G:765:MET:HE2	1:M:138:LEU:HD21	1.79	0.63
2:D:45:GLY:O	2:D:67:THR:O	2.16	0.63
2:Z:25:SER:OG	6:Z:2001:MG:MG	1.40	0.63
2:J:45:GLY:O	2:J:67:THR:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:717:ARG:NE	3:j:728:GLU:CD	2.56	0.63
2:B:45:GLY:O	2:B:67:THR:O	2.16	0.63
3:K:717:ARG:CD	3:f:724:ILE:HG22	2.28	0.63
2:X:44:ILE:HD12	3:b:737:TYR:CD2	2.34	0.63
1:A:138:LEU:HD11	1:O:765:MET:HE2	1.80	0.62
1:C:221:SER:HA	2:P:71:GLU:OE2	1.99	0.62
2:B:81:TYR:HB3	2:B:113:ALA:HB2	1.82	0.62
3:b:717:ARG:CZ	3:i:728:GLU:CB	2.77	0.62
2:H:67:THR:O	2:H:68:ALA:HB3	2.00	0.62
1:Q:618:TYR:CZ	1:Q:622:GLU:HG3	2.35	0.62
1:S:618:TYR:CZ	1:S:622:GLU:HG3	2.35	0.62
2:D:38:LEU:HA	5:D:2000:GSP:O2'	2.00	0.62
1:G:765:MET:HA	1:G:769:GLN:OE1	1.99	0.62
1:I:138:LEU:CD2	1:Q:769:GLN:CB	2.75	0.62
2:Z:67:THR:O	2:Z:68:ALA:HB3	2.00	0.62
3:b:728:GLU:HA	3:i:717:ARG:HH21	1.64	0.62
1:I:221:SER:HA	2:N:71:GLU:OE2	1.99	0.62
2:d:81:TYR:HB3	2:d:113:ALA:HB2	1.82	0.62
2:B:67:THR:O	2:B:68:ALA:HB3	2.00	0.62
3:F:731:ASN:HD22	3:U:717:ARG:NH2	1.98	0.62
1:Q:765:MET:HA	1:Q:769:GLN:OE1	1.99	0.62
2:d:26:ASN:ND2	5:d:2000:GSP:O1A	2.33	0.62
2:H:44:ILE:HD12	3:L:737:TYR:CD2	2.35	0.61
2:P:67:THR:O	2:P:68:ALA:HB3	2.00	0.61
1:O:765:MET:HA	1:O:769:GLN:OE1	1.99	0.61
2:X:81:TYR:HB3	2:X:113:ALA:HB2	1.82	0.61
1:Y:626:TYR:HA	1:Y:631:PHE:CD1	2.35	0.61
2:D:67:THR:O	2:D:68:ALA:HB3	2.01	0.61
2:J:67:THR:O	2:J:68:ALA:HB3	2.01	0.61
3:e:731:ASN:ND2	3:f:731:ASN:ND2	2.47	0.61
2:h:44:ILE:HD13	3:j:734:LEU:HD22	1.82	0.61
2:N:67:THR:O	2:N:68:ALA:HB3	2.00	0.61
1:M:765:MET:HA	1:M:769:GLN:OE1	2.00	0.61
1:W:765:MET:HA	1:W:769:GLN:OE1	2.00	0.61
1:Y:765:MET:HA	1:Y:769:GLN:OE1	2.01	0.61
2:Z:38:LEU:O	5:Z:2000:GSP:O3'	2.16	0.61
3:a:717:ARG:HG3	3:j:728:GLU:CD	2.19	0.61
2:h:120:MET:HE1	2:h:164:ALA:O	2.00	0.61
2:H:81:TYR:HB3	2:H:113:ALA:HB2	1.83	0.61
2:R:44:ILE:HD13	3:f:734:LEU:HD22	1.82	0.61
1:A:626:TYR:HA	1:A:631:PHE:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:618:TYR:CZ	1:G:622:GLU:HG3	2.36	0.61
2:J:81:TYR:HB3	2:J:113:ALA:HB2	1.82	0.61
2:J:120:MET:HE1	2:J:164:ALA:O	2.01	0.61
2:P:38:LEU:HA	5:P:2000:GSP:O2'	2.01	0.61
2:R:81:TYR:HB3	2:R:113:ALA:HB2	1.82	0.61
2:B:80:TYR:CE1	3:E:746:MET:SD	2.94	0.61
2:D:81:TYR:HB3	2:D:113:ALA:HB2	1.82	0.61
2:D:120:MET:HE1	2:D:164:ALA:O	2.01	0.61
1:G:626:TYR:HA	1:G:631:PHE:CD2	2.35	0.61
1:I:134:PHE:O	1:I:163:ARG:NH1	2.34	0.61
2:N:120:MET:HE1	2:N:164:ALA:O	2.01	0.61
2:P:120:MET:HE1	2:P:164:ALA:O	2.01	0.61
1:W:618:TYR:CZ	1:W:622:GLU:HG3	2.35	0.61
1:Y:134:PHE:O	1:Y:163:ARG:NH1	2.34	0.61
2:Z:25:SER:HG	6:Z:2001:MG:MG	1.09	0.61
2:h:81:TYR:HB3	2:h:113:ALA:HB2	1.83	0.61
2:B:120:MET:HE1	2:B:164:ALA:O	2.01	0.61
1:S:765:MET:HA	1:S:769:GLN:OE1	2.00	0.61
2:T:81:TYR:HB3	2:T:113:ALA:HB2	1.82	0.61
1:C:134:PHE:O	1:C:163:ARG:NH1	2.34	0.60
1:G:138:LEU:HD21	1:M:765:MET:HE3	1.75	0.60
1:c:637:ASN:HB3	1:c:669:HIS:CD2	2.36	0.60
2:Z:120:MET:HE1	2:Z:164:ALA:O	2.01	0.60
3:a:724:ILE:CG2	3:j:717:ARG:NH2	2.64	0.60
1:A:765:MET:HA	1:A:769:GLN:OE1	2.01	0.60
2:D:80:TYR:CE1	3:F:746:MET:HG2	2.36	0.60
2:H:120:MET:HE1	2:H:164:ALA:O	2.01	0.60
1:M:637:ASN:HB3	1:M:669:HIS:CD2	2.37	0.60
2:X:120:MET:HE1	2:X:164:ALA:O	2.00	0.60
2:d:67:THR:O	2:d:68:ALA:HB3	2.01	0.60
1:g:765:MET:HA	1:g:769:GLN:OE1	2.01	0.60
1:A:618:TYR:CZ	1:A:622:GLU:HG3	2.36	0.60
1:C:759:GLU:OE2	1:S:147:TYR:OH	2.19	0.60
1:I:637:ASN:HB3	1:I:669:HIS:CD2	2.37	0.60
1:W:637:ASN:HB3	1:W:669:HIS:CD2	2.36	0.60
1:Y:637:ASN:HB3	1:Y:669:HIS:CD2	2.37	0.60
3:b:728:GLU:OE2	3:i:717:ARG:HB3	2.01	0.60
3:E:717:ARG:NE	3:V:728:GLU:OE1	2.35	0.60
2:N:81:TYR:HB3	2:N:113:ALA:HB2	1.82	0.60
2:T:67:THR:O	2:T:68:ALA:HB3	2.00	0.60
2:X:67:THR:O	2:X:68:ALA:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:76:ILE:HB	3:b:746:MET:SD	2.41	0.60
1:c:765:MET:HA	1:c:769:GLN:OE1	2.01	0.60
1:g:618:TYR:CZ	1:g:622:GLU:HG3	2.36	0.60
1:A:134:PHE:O	1:A:163:ARG:NH1	2.35	0.60
1:A:138:LEU:CG	1:O:765:MET:HE2	2.31	0.60
1:A:765:MET:CE	1:O:138:LEU:HD21	2.32	0.60
1:I:765:MET:HA	1:I:769:GLN:OE1	2.01	0.60
2:Z:80:TYR:CE1	3:b:746:MET:HG2	2.36	0.60
2:d:120:MET:HE1	2:d:164:ALA:O	2.01	0.60
2:R:67:THR:O	2:R:68:ALA:HB3	2.00	0.60
1:C:637:ASN:HB3	1:C:669:HIS:CD2	2.37	0.60
1:C:765:MET:HA	1:C:769:GLN:OE1	2.01	0.60
3:K:742:ILE:HD11	3:L:741:ILE:HG21	1.82	0.60
2:Z:81:TYR:HB3	2:Z:113:ALA:HB2	1.82	0.60
1:c:618:TYR:CZ	1:c:622:GLU:HG3	2.36	0.60
3:E:724:ILE:HG22	3:V:717:ARG:CZ	2.31	0.60
1:G:765:MET:CE	1:M:138:LEU:HD21	2.32	0.60
2:H:38:LEU:HA	5:H:2000:GSP:O2'	2.01	0.60
1:Q:637:ASN:HB3	1:Q:669:HIS:CD2	2.37	0.60
2:H:44:ILE:O	3:L:737:TYR:OH	2.15	0.60
1:M:134:PHE:O	1:M:163:ARG:NH1	2.35	0.60
1:g:637:ASN:HB3	1:g:669:HIS:CD2	2.37	0.60
1:G:134:PHE:O	1:G:163:ARG:NH1	2.35	0.59
2:R:120:MET:HE1	2:R:164:ALA:O	2.01	0.59
1:I:178:GLN:HA	1:I:739:MET:HE1	1.84	0.59
2:T:120:MET:HE1	2:T:164:ALA:O	2.01	0.59
3:b:717:ARG:NH2	3:i:728:GLU:HB2	2.17	0.59
1:A:637:ASN:HB3	1:A:669:HIS:CD2	2.36	0.59
2:P:42:SER:HA	5:P:2000:GSP:S1G	2.43	0.59
2:X:40:SER:HB3	5:X:2000:GSP:H3'	1.83	0.59
1:Y:138:LEU:HD21	1:g:765:MET:CG	2.28	0.59
1:C:138:LEU:CD2	1:S:765:MET:HG2	2.27	0.59
1:O:637:ASN:HB3	1:O:669:HIS:CD2	2.38	0.59
2:P:81:TYR:HB3	2:P:113:ALA:HB2	1.83	0.59
1:W:138:LEU:HD11	1:c:765:MET:HE2	1.83	0.59
2:h:67:THR:O	2:h:68:ALA:HB3	2.01	0.59
1:C:332:GLN:NE2	1:I:331:GLU:HG3	2.15	0.59
1:I:618:TYR:CZ	1:I:622:GLU:HG3	2.38	0.59
3:a:724:ILE:CG2	3:j:717:ARG:CZ	2.81	0.59
1:c:134:PHE:O	1:c:163:ARG:NH1	2.36	0.59
2:B:80:TYR:OH	3:E:746:MET:HB3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:ALA:HB1	3:F:746:MET:HE3	1.79	0.58
1:Q:134:PHE:O	1:Q:163:ARG:NH1	2.36	0.58
1:S:637:ASN:HB3	1:S:669:HIS:CD2	2.38	0.58
1:C:332:GLN:CG	1:I:332:GLN:HG2	2.33	0.58
1:O:134:PHE:O	1:O:163:ARG:NH1	2.36	0.58
1:Q:178:GLN:HA	1:Q:739:MET:HE1	1.85	0.58
1:C:178:GLN:HA	1:C:739:MET:HE1	1.85	0.58
2:J:79:ALA:CB	3:L:746:MET:HE1	2.33	0.58
1:A:178:GLN:HA	1:A:739:MET:HE1	1.85	0.58
2:P:88:LEU:HD21	2:P:120:MET:HE2	1.84	0.58
1:Q:626:TYR:HA	1:Q:631:PHE:CD2	2.38	0.58
2:T:38:LEU:HA	5:T:2000:GSP:O2'	2.03	0.58
1:G:637:ASN:HB3	1:G:669:HIS:CD2	2.37	0.58
1:S:178:GLN:HA	1:S:739:MET:HE1	1.86	0.58
2:B:42:SER:HA	5:B:2000:GSP:S1G	2.43	0.58
2:N:40:SER:HB3	5:N:2000:GSP:H3'	1.85	0.58
1:C:332:GLN:CG	1:I:332:GLN:CG	2.82	0.58
1:C:618:TYR:CZ	1:C:622:GLU:HG3	2.39	0.58
1:C:332:GLN:HG3	1:I:332:GLN:HG3	1.85	0.58
1:W:138:LEU:HD11	1:c:765:MET:CE	2.34	0.58
1:S:626:TYR:HA	1:S:631:PHE:CD1	2.38	0.58
1:A:625:SER:O	1:A:628:THR:HG22	2.04	0.58
1:S:134:PHE:O	1:S:163:ARG:NH1	2.37	0.58
1:Y:138:LEU:CG	1:g:769:GLN:HB3	2.34	0.58
1:Y:625:SER:O	1:Y:628:THR:HG22	2.03	0.58
1:c:625:SER:O	1:c:628:THR:HG22	2.04	0.58
1:M:618:TYR:CZ	1:M:622:GLU:HG3	2.40	0.57
1:C:133:LEU:O	1:C:136:SER:OG	2.21	0.57
1:S:625:SER:O	1:S:628:THR:HG22	2.04	0.57
1:W:134:PHE:O	1:W:163:ARG:NH1	2.37	0.57
1:G:625:SER:O	1:G:628:THR:HG22	2.04	0.57
1:I:133:LEU:O	1:I:136:SER:OG	2.21	0.57
1:O:618:TYR:CZ	1:O:622:GLU:HG3	2.40	0.57
2:X:44:ILE:HD13	3:b:737:TYR:CD1	2.40	0.57
2:B:88:LEU:HD21	2:B:120:MET:HE2	1.86	0.57
2:D:26:ASN:ND2	5:D:2000:GSP:O1A	2.36	0.57
1:G:178:GLN:HA	1:G:739:MET:HE1	1.86	0.57
2:J:26:ASN:ND2	5:J:2000:GSP:O1A	2.37	0.57
1:Q:625:SER:O	1:Q:628:THR:HG22	2.04	0.57
1:C:138:LEU:HG	1:S:769:GLN:CB	2.28	0.57
1:g:134:PHE:O	1:g:163:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:626:TYR:HA	1:g:631:PHE:CD1	2.40	0.57
3:i:735:GLN:NE2	3:j:734:LEU:HD12	2.18	0.57
1:M:626:TYR:HA	1:M:631:PHE:CD1	2.40	0.57
2:N:42:SER:HA	5:N:2000:GSP:S1G	2.45	0.57
2:h:40:SER:HB3	5:h:2000:GSP:H3'	1.85	0.57
1:G:611:SER:HB2	1:G:613:LEU:HD22	1.87	0.57
1:M:625:SER:O	1:M:628:THR:HG22	2.04	0.57
1:W:626:TYR:HA	1:W:631:PHE:CD1	2.40	0.57
1:W:765:MET:HE2	1:c:138:LEU:HD11	1.86	0.57
1:W:625:SER:O	1:W:628:THR:HG22	2.04	0.57
2:X:88:LEU:HD21	2:X:120:MET:HE2	1.87	0.57
1:g:178:GLN:HA	1:g:739:MET:HE1	1.86	0.57
2:h:42:SER:HA	5:h:2000:GSP:S1G	2.45	0.57
1:C:329:THR:HG21	1:I:329:THR:HG21	1.86	0.56
2:N:88:LEU:HD21	2:N:120:MET:HE2	1.86	0.56
1:Y:178:GLN:HA	1:Y:739:MET:HE1	1.85	0.56
1:C:138:LEU:CG	1:S:769:GLN:CD	2.79	0.56
1:C:221:SER:CA	2:P:71:GLU:OE2	2.53	0.56
1:W:178:GLN:HA	1:W:739:MET:HE1	1.86	0.56
3:e:735:GLN:NE2	3:f:734:LEU:HD13	2.19	0.56
1:C:332:GLN:HG2	1:I:332:GLN:HG2	1.87	0.56
2:H:88:LEU:HD21	2:H:120:MET:HE2	1.87	0.56
1:I:625:SER:O	1:I:628:THR:HG22	2.05	0.56
1:O:625:SER:O	1:O:628:THR:HG22	2.04	0.56
2:Z:88:LEU:HD21	2:Z:120:MET:HE2	1.88	0.56
1:c:178:GLN:HA	1:c:739:MET:HE1	1.86	0.56
1:I:138:LEU:CG	1:Q:769:GLN:CB	2.84	0.56
1:I:611:SER:HB2	1:I:613:LEU:HD22	1.88	0.56
1:g:625:SER:O	1:g:628:THR:HG22	2.04	0.56
1:C:625:SER:O	1:C:628:THR:HG22	2.05	0.56
2:J:88:LEU:HD21	2:J:120:MET:HE2	1.87	0.56
1:C:611:SER:HB2	1:C:613:LEU:HD22	1.88	0.56
1:M:178:GLN:HA	1:M:739:MET:HE1	1.86	0.56
1:O:626:TYR:HA	1:O:631:PHE:CD1	2.41	0.56
3:a:717:ARG:NH1	3:j:724:ILE:CG2	2.68	0.56
2:d:88:LEU:HD21	2:d:120:MET:HE2	1.87	0.56
2:h:88:LEU:HD21	2:h:120:MET:HE2	1.87	0.56
1:A:611:SER:HB2	1:A:613:LEU:HD22	1.88	0.56
2:H:80:TYR:CZ	3:K:746:MET:HE2	2.41	0.56
1:M:611:SER:HB2	1:M:613:LEU:HD22	1.88	0.56
1:O:178:GLN:HA	1:O:739:MET:HE1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:38:LEU:HA	5:X:2000:GSP:O2'	2.05	0.56
2:J:80:TYR:CE1	3:L:746:MET:HG2	2.40	0.56
2:h:38:LEU:O	5:h:2000:GSP:O3'	2.19	0.56
2:d:144:GLU:HA	2:d:144:GLU:OE1	2.06	0.56
2:P:144:GLU:HA	2:P:144:GLU:OE1	2.06	0.56
2:D:88:LEU:HD21	2:D:120:MET:HE2	1.87	0.55
1:Y:611:SER:HB2	1:Y:613:LEU:HD22	1.88	0.55
2:d:25:SER:OG	5:d:2000:GSP:O2B	2.24	0.55
3:e:731:ASN:ND2	3:f:731:ASN:OD1	2.31	0.55
1:I:626:TYR:HA	1:I:631:PHE:CD1	2.40	0.55
3:L:717:ARG:NH2	3:e:725:GLN:HA	2.22	0.55
1:c:611:SER:HB2	1:c:613:LEU:HD22	1.88	0.55
1:A:178:GLN:CD	1:A:739:MET:CE	2.79	0.55
1:G:138:LEU:CG	1:M:765:MET:HE2	2.35	0.55
2:J:144:GLU:OE1	2:J:144:GLU:HA	2.06	0.55
2:N:144:GLU:HA	2:N:144:GLU:OE1	2.06	0.55
2:X:144:GLU:HA	2:X:144:GLU:OE1	2.07	0.55
2:Z:40:SER:HB3	5:Z:2000:GSP:H3'	1.87	0.55
2:B:144:GLU:HA	2:B:144:GLU:OE1	2.07	0.55
1:W:611:SER:HB2	1:W:613:LEU:HD22	1.87	0.55
2:X:38:LEU:O	5:X:2000:GSP:O3'	2.18	0.55
3:a:724:ILE:HG23	3:j:717:ARG:NH2	2.22	0.55
1:M:607:VAL:O	1:M:611:SER:OG	2.20	0.55
1:O:607:VAL:O	1:O:611:SER:OG	2.20	0.55
1:O:611:SER:HB2	1:O:613:LEU:HD22	1.89	0.55
2:R:88:LEU:HD21	2:R:120:MET:HE2	1.88	0.55
1:g:611:SER:HB2	1:g:613:LEU:HD22	1.88	0.55
2:B:80:TYR:HE1	3:E:746:MET:SD	2.30	0.55
3:E:717:ARG:HD3	3:V:724:ILE:HG22	1.85	0.55
2:h:144:GLU:OE1	2:h:144:GLU:HA	2.07	0.55
1:S:611:SER:HB2	1:S:613:LEU:HD22	1.88	0.55
3:b:717:ARG:NH1	3:i:728:GLU:CB	2.68	0.55
2:T:88:LEU:HD21	2:T:120:MET:HE2	1.88	0.55
1:Q:611:SER:HB2	1:Q:613:LEU:HD22	1.88	0.55
1:c:607:VAL:O	1:c:611:SER:OG	2.20	0.55
3:E:717:ARG:CD	3:V:724:ILE:CG2	2.77	0.54
2:H:144:GLU:OE1	2:H:144:GLU:HA	2.07	0.54
2:T:38:LEU:O	5:T:2000:GSP:O3'	2.22	0.54
1:O:196:PRO:HG2	2:P:131:LEU:HD22	1.89	0.54
2:T:144:GLU:OE1	2:T:144:GLU:HA	2.07	0.54
2:Z:144:GLU:HA	2:Z:144:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:144:GLU:HA	2:D:144:GLU:OE1	2.07	0.54
3:E:717:ARG:NH2	3:V:725:GLN:CA	2.71	0.54
3:L:728:GLU:CG	3:e:717:ARG:NH2	2.70	0.54
1:O:133:LEU:O	1:O:136:SER:OG	2.21	0.54
2:B:38:LEU:O	5:B:2000:GSP:O3'	2.14	0.54
2:R:125:LYS:HG2	5:R:2000:GSP:C6	2.42	0.54
1:c:133:LEU:O	1:c:136:SER:OG	2.21	0.54
2:B:40:SER:HB3	5:B:2000:GSP:H3'	1.89	0.54
2:h:125:LYS:HG2	5:h:2000:GSP:C6	2.43	0.54
1:M:133:LEU:O	1:M:136:SER:OG	2.21	0.54
2:R:144:GLU:OE1	2:R:144:GLU:HA	2.07	0.54
1:c:626:TYR:HA	1:c:631:PHE:CD1	2.43	0.54
1:c:768:GLU:CD	1:c:768:GLU:H	2.16	0.54
3:K:724:ILE:CG2	3:f:717:ARG:CZ	2.85	0.53
3:L:728:GLU:HG2	3:e:717:ARG:NH2	2.22	0.53
1:W:607:VAL:O	1:W:611:SER:OG	2.20	0.53
1:M:178:GLN:CD	1:M:739:MET:CE	2.81	0.53
1:M:196:PRO:HG2	2:N:131:LEU:HD22	1.89	0.53
2:X:80:TYR:CE1	3:a:746:MET:HE2	2.43	0.53
2:H:80:TYR:OH	3:K:746:MET:CB	2.56	0.53
1:M:306:ARG:O	1:M:351:ARG:NH1	2.41	0.53
1:O:306:ARG:O	1:O:351:ARG:NH1	2.41	0.53
1:A:178:GLN:CD	1:A:739:MET:HE3	2.34	0.53
2:P:88:LEU:CD2	2:P:120:MET:HE2	2.38	0.53
1:Q:602:VAL:HG23	1:Q:607:VAL:HG23	1.90	0.53
2:X:8:TYR:HA	2:X:59:THR:OG1	2.08	0.53
2:h:8:TYR:HA	2:h:59:THR:OG1	2.08	0.53
3:b:728:GLU:HG3	3:i:717:ARG:NH2	2.24	0.53
3:E:724:ILE:HG23	3:V:717:ARG:NH2	2.23	0.53
1:c:602:VAL:HG23	1:c:607:VAL:HG23	1.91	0.53
1:C:331:GLU:HG3	1:I:332:GLN:HE22	1.73	0.53
1:I:602:VAL:HG23	1:I:607:VAL:HG23	1.91	0.53
1:M:768:GLU:CD	1:M:768:GLU:H	2.17	0.53
2:Z:67:THR:O	2:Z:68:ALA:CB	2.57	0.53
2:d:8:TYR:CE2	2:d:11:LEU:HB2	2.43	0.53
1:C:626:TYR:HA	1:C:631:PHE:CD1	2.43	0.53
2:H:80:TYR:CE1	3:K:746:MET:HE2	2.44	0.53
1:I:138:LEU:HD23	1:Q:769:GLN:OE1	2.06	0.53
1:M:602:VAL:HG23	1:M:607:VAL:HG23	1.91	0.53
2:R:8:TYR:HA	2:R:59:THR:OG1	2.09	0.53
1:S:306:ARG:O	1:S:351:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:h:67:THR:O	2:h:68:ALA:CB	2.57	0.53
1:C:602:VAL:HG23	1:C:607:VAL:HG23	1.92	0.52
1:O:768:GLU:CD	1:O:768:GLU:H	2.17	0.52
2:R:40:SER:HB3	5:R:2000:GSP:H3'	1.91	0.52
1:S:602:VAL:HG23	1:S:607:VAL:HG23	1.90	0.52
5:X:2000:GSP:O3G	5:X:2000:GSP:O2B	2.27	0.52
1:Y:133:LEU:O	1:Y:136:SER:OG	2.21	0.52
1:W:768:GLU:CD	1:W:768:GLU:H	2.17	0.52
5:d:2000:GSP:O2B	5:d:2000:GSP:O3G	2.27	0.52
1:A:306:ARG:O	1:A:351:ARG:NH1	2.42	0.52
2:N:8:TYR:CE2	2:N:11:LEU:HB2	2.44	0.52
2:P:8:TYR:CE2	2:P:11:LEU:HB2	2.44	0.52
2:R:92:ASP:H	2:R:98:THR:HG21	1.74	0.52
1:S:768:GLU:H	1:S:768:GLU:CD	2.17	0.52
5:T:2000:GSP:O2B	5:T:2000:GSP:O3G	2.27	0.52
1:g:768:GLU:H	1:g:768:GLU:CD	2.16	0.52
2:D:92:ASP:H	2:D:98:THR:HG21	1.74	0.52
2:H:26:ASN:ND2	5:H:2000:GSP:O1A	2.40	0.52
1:O:602:VAL:HG23	1:O:607:VAL:HG23	1.92	0.52
2:T:8:TYR:HA	2:T:59:THR:OG1	2.10	0.52
2:X:67:THR:O	2:X:68:ALA:CB	2.58	0.52
1:g:306:ARG:O	1:g:351:ARG:NH1	2.43	0.52
1:g:607:VAL:O	1:g:611:SER:OG	2.20	0.52
3:i:738:ILE:CD1	3:j:738:ILE:CD1	2.74	0.52
1:G:133:LEU:O	1:G:136:SER:OG	2.21	0.52
3:U:735:GLN:NE2	3:V:734:LEU:CD1	2.72	0.52
1:W:306:ARG:O	1:W:351:ARG:NH1	2.43	0.52
2:Z:8:TYR:CE2	2:Z:11:LEU:HB2	2.45	0.52
1:A:602:VAL:HG23	1:A:607:VAL:HG23	1.92	0.52
2:D:67:THR:O	2:D:68:ALA:CB	2.57	0.52
3:b:717:ARG:CZ	3:i:728:GLU:HB2	2.40	0.52
2:d:67:THR:O	2:d:68:ALA:CB	2.57	0.52
2:H:67:THR:O	2:H:68:ALA:CB	2.57	0.52
2:P:26:ASN:ND2	5:P:2000:GSP:O1A	2.39	0.52
1:Q:306:ARG:O	1:Q:351:ARG:NH1	2.42	0.52
1:Q:628:THR:HG23	1:Q:631:PHE:H	1.75	0.52
1:Q:768:GLU:H	1:Q:768:GLU:CD	2.17	0.52
2:h:41:LYS:CD	3:j:733:ARG:HD2	2.39	0.52
2:h:41:LYS:HD2	3:j:733:ARG:HD2	1.91	0.52
1:A:133:LEU:O	1:A:136:SER:OG	2.21	0.52
2:R:67:THR:O	2:R:68:ALA:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Z:2000:GSP:O3G	5:Z:2000:GSP:O2B	2.27	0.52
3:a:717:ARG:NH1	3:j:724:ILE:HB	2.25	0.52
2:H:92:ASP:H	2:H:98:THR:HG21	1.75	0.52
1:I:138:LEU:CD2	1:Q:765:MET:HG2	2.35	0.52
2:N:8:TYR:HA	2:N:59:THR:OG1	2.09	0.52
2:N:88:LEU:CD2	2:N:120:MET:HE2	2.39	0.52
1:Y:306:ARG:O	1:Y:351:ARG:NH1	2.43	0.52
1:C:306:ARG:O	1:C:351:ARG:NH1	2.43	0.52
1:I:306:ARG:O	1:I:351:ARG:NH1	2.43	0.52
1:I:607:VAL:O	1:I:611:SER:OG	2.20	0.52
2:T:67:THR:O	2:T:68:ALA:CB	2.57	0.52
3:U:738:ILE:CD1	3:V:738:ILE:HD13	2.26	0.52
1:Y:602:VAL:HG23	1:Y:607:VAL:HG23	1.92	0.52
2:d:8:TYR:HA	2:d:59:THR:OG1	2.10	0.52
5:h:2000:GSP:O2B	5:h:2000:GSP:O3G	2.28	0.52
2:B:67:THR:O	2:B:68:ALA:CB	2.57	0.51
3:E:738:ILE:CD1	3:F:738:ILE:CD1	2.88	0.51
1:G:178:GLN:CD	1:G:739:MET:CE	2.83	0.51
1:G:306:ARG:O	1:G:351:ARG:NH1	2.42	0.51
2:J:8:TYR:HA	2:J:59:THR:OG1	2.09	0.51
2:N:26:ASN:ND2	5:N:2000:GSP:O1A	2.41	0.51
2:P:8:TYR:HA	2:P:59:THR:OG1	2.09	0.51
1:S:196:PRO:HG2	2:T:131:LEU:HD22	1.92	0.51
3:b:728:GLU:OE2	3:i:717:ARG:CB	2.58	0.51
1:c:306:ARG:O	1:c:351:ARG:NH1	2.43	0.51
5:D:2000:GSP:O3G	5:D:2000:GSP:O2B	2.29	0.51
1:S:628:THR:HG23	1:S:631:PHE:H	1.75	0.51
1:g:602:VAL:HG23	1:g:607:VAL:HG23	1.92	0.51
2:h:8:TYR:CE2	2:h:11:LEU:HB2	2.45	0.51
2:B:88:LEU:CD2	2:B:120:MET:HE2	2.40	0.51
1:W:602:VAL:HG23	1:W:607:VAL:HG23	1.91	0.51
2:Z:92:ASP:H	2:Z:98:THR:HG21	1.75	0.51
3:a:720:LEU:HD13	3:i:724:ILE:CD1	2.37	0.51
1:G:602:VAL:HG23	1:G:607:VAL:HG23	1.93	0.51
2:H:8:TYR:HA	2:H:59:THR:OG1	2.10	0.51
2:J:67:THR:O	2:J:68:ALA:CB	2.58	0.51
2:X:88:LEU:CD2	2:X:120:MET:HE2	2.41	0.51
1:I:206:ILE:HD11	1:I:394:PHE:HE2	1.75	0.51
2:P:67:THR:O	2:P:68:ALA:CB	2.57	0.51
1:W:628:THR:HG23	1:W:631:PHE:H	1.75	0.51
1:A:768:GLU:CD	1:A:768:GLU:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:LEU:CG	1:S:769:GLN:HB3	2.40	0.51
1:Y:178:GLN:CD	1:Y:739:MET:CE	2.84	0.51
2:Z:8:TYR:HA	2:Z:59:THR:OG1	2.10	0.51
2:Z:26:ASN:ND2	5:Z:2000:GSP:O1A	2.43	0.51
2:Z:79:ALA:HB2	3:b:746:MET:CE	2.39	0.51
2:d:79:ALA:HB3	3:j:746:MET:HE3	1.92	0.51
2:d:88:LEU:CD2	2:d:120:MET:HE2	2.40	0.51
2:h:88:LEU:CD2	2:h:120:MET:HE2	2.40	0.51
3:E:738:ILE:CD1	3:F:738:ILE:HG12	2.33	0.51
2:J:88:LEU:CD2	2:J:120:MET:HE2	2.40	0.51
1:O:178:GLN:CD	1:O:739:MET:CE	2.83	0.51
2:P:92:ASP:H	2:P:98:THR:HG21	1.76	0.51
2:X:8:TYR:CE2	2:X:11:LEU:HB2	2.46	0.51
2:X:92:ASP:H	2:X:98:THR:HG21	1.74	0.51
1:g:178:GLN:CD	1:g:739:MET:CE	2.84	0.51
2:B:8:TYR:HA	2:B:59:THR:OG1	2.10	0.51
1:G:628:THR:HG23	1:G:631:PHE:H	1.75	0.51
2:B:92:ASP:H	2:B:98:THR:HG21	1.76	0.51
1:C:178:GLN:CD	1:C:739:MET:CE	2.84	0.51
1:C:331:GLU:CB	1:I:332:GLN:HE22	2.23	0.51
3:K:738:ILE:CD1	3:L:738:ILE:HG12	2.35	0.51
3:L:728:GLU:HG2	3:e:717:ARG:HH21	1.76	0.51
2:N:67:THR:O	2:N:68:ALA:CB	2.57	0.51
2:N:92:ASP:H	2:N:98:THR:HG21	1.76	0.51
2:X:125:LYS:HG2	5:X:2000:GSP:C6	2.46	0.51
1:Y:768:GLU:CD	1:Y:768:GLU:H	2.18	0.51
1:g:133:LEU:O	1:g:136:SER:OG	2.21	0.51
2:X:42:SER:HA	5:X:2000:GSP:S1G	2.51	0.51
1:Y:628:THR:HG23	1:Y:631:PHE:H	1.77	0.51
2:D:88:LEU:CD2	2:D:120:MET:HE2	2.41	0.50
2:T:8:TYR:CE2	2:T:11:LEU:HB2	2.45	0.50
1:W:133:LEU:O	1:W:136:SER:OG	2.21	0.50
2:Z:76:ILE:HA	3:b:746:MET:HE1	1.92	0.50
1:A:628:THR:HG23	1:A:631:PHE:H	1.76	0.50
1:C:768:GLU:CD	1:C:768:GLU:H	2.19	0.50
1:G:138:LEU:CD1	1:M:765:MET:HE2	2.42	0.50
2:H:88:LEU:CD2	2:H:120:MET:HE2	2.40	0.50
3:K:724:ILE:HG22	3:f:717:ARG:CZ	2.41	0.50
5:N:2000:GSP:O3G	5:N:2000:GSP:O2B	2.28	0.50
1:W:356:THR:HG21	1:W:546:VAL:HG12	1.93	0.50
1:C:206:ILE:HD11	1:C:394:PHE:HE2	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:768:GLU:H	1:G:768:GLU:CD	2.19	0.50
1:M:178:GLN:CD	1:M:739:MET:HE3	2.36	0.50
1:Q:178:GLN:CD	1:Q:739:MET:CE	2.84	0.50
1:S:133:LEU:O	1:S:136:SER:OG	2.21	0.50
1:g:628:THR:HG23	1:g:631:PHE:H	1.75	0.50
2:D:91:TYR:HB2	2:D:98:THR:HG23	1.94	0.50
3:L:728:GLU:HA	3:e:717:ARG:NH2	2.27	0.50
1:I:178:GLN:CD	1:I:739:MET:CE	2.84	0.50
2:R:8:TYR:CE2	2:R:11:LEU:HB2	2.46	0.50
2:T:92:ASP:H	2:T:98:THR:HG21	1.76	0.50
2:Z:88:LEU:CD2	2:Z:120:MET:HE2	2.41	0.50
2:h:92:ASP:H	2:h:98:THR:HG21	1.76	0.50
2:D:8:TYR:HA	2:D:59:THR:OG1	2.11	0.50
2:H:8:TYR:CE2	2:H:11:LEU:HB2	2.47	0.50
1:I:768:GLU:CD	1:I:768:GLU:H	2.19	0.50
1:Q:356:THR:HG21	1:Q:546:VAL:HG12	1.93	0.50
1:g:196:PRO:HG2	2:h:131:LEU:HD22	1.94	0.50
1:Q:133:LEU:O	1:Q:136:SER:OG	2.21	0.50
2:R:88:LEU:CD2	2:R:120:MET:HE2	2.42	0.50
5:B:2000:GSP:O3G	5:B:2000:GSP:O2B	2.29	0.49
3:K:720:LEU:O	3:K:724:ILE:HG12	2.11	0.49
3:a:717:ARG:CZ	3:j:724:ILE:CG2	2.90	0.49
1:O:628:THR:HG23	1:O:631:PHE:H	1.77	0.49
5:P:2000:GSP:O3G	5:P:2000:GSP:O2B	2.29	0.49
5:R:2000:GSP:O2B	5:R:2000:GSP:O3G	2.30	0.49
1:I:628:THR:HG23	1:I:631:PHE:H	1.76	0.49
2:H:38:LEU:O	5:H:2000:GSP:O3'	2.20	0.49
3:L:717:ARG:NH2	3:e:728:GLU:CB	2.75	0.49
1:S:356:THR:HG21	1:S:546:VAL:HG12	1.94	0.49
1:c:178:GLN:CD	1:c:739:MET:CE	2.85	0.49
1:A:765:MET:HE2	1:O:138:LEU:HD11	1.93	0.49
1:G:178:GLN:CD	1:G:739:MET:HE3	2.37	0.49
1:M:518:LEU:HG	1:M:519:LYS:H	1.77	0.49
1:M:628:THR:HG23	1:M:631:PHE:H	1.78	0.49
2:d:92:ASP:H	2:d:98:THR:HG21	1.76	0.49
3:K:717:ARG:HD2	3:f:724:ILE:HG22	1.94	0.49
3:L:728:GLU:HA	3:e:717:ARG:HH21	1.77	0.49
1:O:356:THR:HG21	1:O:546:VAL:HG12	1.95	0.49
2:T:88:LEU:CD2	2:T:120:MET:HE2	2.42	0.49
2:B:80:TYR:OH	3:E:746:MET:HE2	2.12	0.49
2:B:91:TYR:HB2	2:B:98:THR:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:628:THR:HG23	1:C:631:PHE:H	1.76	0.49
2:J:91:TYR:HB2	2:J:98:THR:HG23	1.95	0.49
1:W:611:SER:HB2	1:W:613:LEU:CD2	2.43	0.49
1:g:356:THR:HG21	1:g:546:VAL:HG12	1.95	0.49
1:g:518:LEU:HG	1:g:519:LYS:H	1.77	0.49
2:h:38:LEU:HA	5:h:2000:GSP:O2'	2.13	0.49
1:A:138:LEU:HD21	1:O:765:MET:SD	2.50	0.49
1:I:356:THR:HG21	1:I:546:VAL:HG12	1.95	0.49
1:W:178:GLN:CD	1:W:739:MET:CE	2.85	0.49
3:a:720:LEU:O	3:a:724:ILE:HG12	2.13	0.49
2:H:91:TYR:HB2	2:H:98:THR:HG23	1.95	0.49
1:S:178:GLN:CD	1:S:739:MET:CE	2.85	0.49
1:Y:138:LEU:HG	1:g:769:GLN:HB3	1.93	0.49
3:a:738:ILE:HD13	3:b:738:ILE:HG12	1.95	0.49
1:G:356:THR:HG21	1:G:546:VAL:HG12	1.95	0.48
3:K:717:ARG:HH21	3:f:725:GLN:CB	2.25	0.48
1:Q:607:VAL:O	1:Q:611:SER:OG	2.20	0.48
3:a:717:ARG:HH11	3:j:724:ILE:HG21	1.78	0.48
2:d:120:MET:HB2	2:d:168:ILE:HD12	1.95	0.48
2:D:8:TYR:CE2	2:D:11:LEU:HB2	2.47	0.48
3:E:717:ARG:HD2	3:V:724:ILE:HG21	1.94	0.48
1:I:611:SER:HB2	1:I:613:LEU:CD2	2.43	0.48
2:J:92:ASP:H	2:J:98:THR:HG21	1.78	0.48
1:S:766:THR:HG22	1:S:769:GLN:HG3	1.95	0.48
3:U:735:GLN:NE2	3:V:734:LEU:HD12	2.27	0.48
1:M:206:ILE:HD11	1:M:394:PHE:HE2	1.77	0.48
1:g:152:LYS:CD	3:j:722:GLU:CB	2.91	0.48
1:g:611:SER:HB2	1:g:613:LEU:CD2	2.43	0.48
3:i:720:LEU:O	3:i:724:ILE:HG12	2.13	0.48
1:A:356:THR:HG21	1:A:546:VAL:HG12	1.95	0.48
2:B:8:TYR:CE2	2:B:11:LEU:HB2	2.48	0.48
1:C:611:SER:HB2	1:C:613:LEU:CD2	2.44	0.48
3:E:729:GLU:HG3	1:S:751:SER:OG	2.13	0.48
1:I:221:SER:CA	2:N:71:GLU:OE2	2.61	0.48
1:I:518:LEU:HG	1:I:519:LYS:H	1.79	0.48
1:M:518:LEU:HG	1:M:519:LYS:N	2.29	0.48
1:Q:766:THR:HG22	1:Q:769:GLN:HG3	1.95	0.48
2:T:42:SER:HA	5:T:2000:GSP:S1G	2.53	0.48
3:e:752:ILE:HG21	3:f:745:ILE:CD1	2.43	0.48
2:P:91:TYR:HB2	2:P:98:THR:HG23	1.95	0.48
2:R:91:TYR:HB2	2:R:98:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:720:LEU:O	3:e:724:ILE:HG12	2.13	0.48
1:g:178:GLN:CD	1:g:739:MET:HE3	2.38	0.48
3:E:720:LEU:O	3:E:724:ILE:HG12	2.12	0.48
2:N:91:TYR:HB2	2:N:98:THR:HG23	1.95	0.48
1:Q:178:GLN:CD	1:Q:739:MET:HE3	2.39	0.48
1:W:206:ILE:HD11	1:W:394:PHE:HE2	1.79	0.48
1:c:206:ILE:HD11	1:c:394:PHE:HE1	1.78	0.48
1:G:611:SER:HB2	1:G:613:LEU:CD2	2.43	0.48
3:L:731:ASN:ND2	3:e:717:ARG:NH2	2.61	0.48
1:S:607:VAL:O	1:S:611:SER:OG	2.20	0.48
1:S:611:SER:HB2	1:S:613:LEU:CD2	2.43	0.48
2:X:91:TYR:HB2	2:X:98:THR:HG23	1.95	0.48
1:Y:206:ILE:HD11	1:Y:394:PHE:HE1	1.79	0.48
2:B:120:MET:HB2	2:B:168:ILE:HD12	1.96	0.48
1:C:178:GLN:CD	1:C:739:MET:HE3	2.39	0.48
3:L:720:LEU:O	3:L:724:ILE:HG13	2.14	0.48
1:M:356:THR:HG21	1:M:546:VAL:HG12	1.96	0.48
1:S:588:ILE:HD12	1:S:593:GLY:HA2	1.95	0.48
1:Y:356:THR:HG21	1:Y:546:VAL:HG12	1.96	0.48
1:C:518:LEU:HG	1:C:519:LYS:H	1.79	0.48
1:I:221:SER:C	2:N:71:GLU:OE2	2.56	0.48
2:J:8:TYR:CE2	2:J:11:LEU:HB2	2.48	0.48
2:P:41:LYS:HD2	3:U:733:ARG:NH2	2.29	0.48
3:U:720:LEU:O	3:U:724:ILE:HG12	2.14	0.48
1:g:182:MET:HA	1:g:186:MET:HG3	1.96	0.48
2:h:91:TYR:HB2	2:h:98:THR:HG23	1.95	0.48
1:C:356:THR:HG21	1:C:546:VAL:HG12	1.96	0.48
2:J:79:ALA:HB1	3:L:746:MET:CE	2.33	0.48
1:O:178:GLN:CD	1:O:739:MET:HE3	2.38	0.48
2:R:41:LYS:HD2	3:f:733:ARG:HD2	1.96	0.48
2:X:80:TYR:CZ	3:a:746:MET:HE2	2.49	0.48
1:c:628:THR:HG23	1:c:631:PHE:H	1.79	0.48
2:J:120:MET:HB2	2:J:168:ILE:HD12	1.95	0.47
1:c:356:THR:HG21	1:c:546:VAL:HG12	1.96	0.47
1:g:206:ILE:HD11	1:g:394:PHE:HE1	1.79	0.47
3:F:717:ARG:NH2	3:U:728:GLU:HB3	2.29	0.47
2:X:31:PHE:O	2:X:51:ARG:NH1	2.46	0.47
1:Y:178:GLN:CD	1:Y:739:MET:HE3	2.38	0.47
3:F:720:LEU:O	3:F:724:ILE:HG13	2.15	0.47
1:I:178:GLN:CD	1:I:739:MET:HE3	2.39	0.47
1:A:611:SER:HB2	1:A:613:LEU:CD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:766:THR:HG22	1:O:769:GLN:HG3	1.97	0.47
1:Q:611:SER:HB2	1:Q:613:LEU:CD2	2.44	0.47
1:S:518:LEU:HG	1:S:519:LYS:H	1.78	0.47
2:T:91:TYR:HB2	2:T:98:THR:HG23	1.95	0.47
1:Y:611:SER:HB2	1:Y:613:LEU:CD2	2.43	0.47
2:D:31:PHE:O	2:D:51:ARG:NH1	2.45	0.47
1:G:182:MET:HA	1:G:186:MET:HG3	1.97	0.47
1:Q:206:ILE:HD11	1:Q:394:PHE:HE2	1.79	0.47
2:Z:120:MET:HB2	2:Z:168:ILE:HD12	1.96	0.47
1:c:178:GLN:CD	1:c:739:MET:HE3	2.39	0.47
2:d:91:TYR:HB2	2:d:98:THR:HG23	1.96	0.47
2:h:120:MET:HB2	2:h:168:ILE:HD12	1.95	0.47
3:F:717:ARG:NH2	3:U:725:GLN:HA	2.29	0.47
1:A:324:LEU:O	1:A:333:LYS:HE3	2.15	0.47
1:I:138:LEU:HG	1:Q:769:GLN:CB	2.37	0.47
2:J:31:PHE:O	2:J:51:ARG:NH1	2.46	0.47
1:O:518:LEU:HG	1:O:519:LYS:H	1.80	0.47
2:P:120:MET:HB2	2:P:168:ILE:HD12	1.96	0.47
1:W:518:LEU:HG	1:W:519:LYS:H	1.80	0.47
1:W:765:MET:HE2	1:c:138:LEU:CD1	2.44	0.47
2:Z:91:TYR:HB2	2:Z:98:THR:HG23	1.95	0.47
1:g:152:LYS:HZ3	3:j:722:GLU:HA	1.80	0.47
1:C:331:GLU:HB3	1:I:332:GLN:HE22	1.79	0.47
2:D:120:MET:HB2	2:D:168:ILE:HD12	1.95	0.47
1:S:178:GLN:CD	1:S:739:MET:HE3	2.40	0.47
3:V:720:LEU:O	3:V:724:ILE:HG13	2.15	0.47
1:g:324:LEU:O	1:g:333:LYS:HE3	2.14	0.47
2:B:80:TYR:CE1	3:E:746:MET:CE	2.98	0.47
1:G:518:LEU:HG	1:G:519:LYS:H	1.80	0.47
1:Q:195:LYS:HB3	1:Q:196:PRO:HD3	1.97	0.47
1:Q:602:VAL:HG23	1:Q:607:VAL:CG2	2.45	0.47
3:F:728:GLU:HG2	3:U:717:ARG:HH21	1.80	0.47
1:G:324:LEU:O	1:G:333:LYS:HE3	2.15	0.47
2:H:120:MET:HB2	2:H:168:ILE:HD12	1.97	0.47
1:M:611:SER:HB2	1:M:613:LEU:CD2	2.44	0.47
1:Q:329:THR:HG23	1:Q:332:GLN:H	1.80	0.47
1:O:206:ILE:HD11	1:O:394:PHE:HE2	1.79	0.46
2:R:120:MET:HB2	2:R:168:ILE:HD12	1.97	0.46
1:g:363:VAL:HA	1:g:388:VAL:HG12	1.97	0.46
1:C:766:THR:HG22	1:C:769:GLN:HG3	1.98	0.46
2:N:120:MET:HB2	2:N:168:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:120:MET:HB2	2:T:168:ILE:HD12	1.97	0.46
1:c:324:LEU:O	1:c:333:LYS:HE3	2.15	0.46
1:g:152:LYS:NZ	3:j:722:GLU:HA	2.30	0.46
1:S:602:VAL:HG23	1:S:607:VAL:CG2	2.45	0.46
1:A:182:MET:HA	1:A:186:MET:HG3	1.98	0.46
1:I:138:LEU:CG	1:Q:769:GLN:CD	2.89	0.46
1:M:324:LEU:O	1:M:333:LYS:HE3	2.15	0.46
1:O:324:LEU:O	1:O:333:LYS:HE3	2.15	0.46
2:P:31:PHE:O	2:P:51:ARG:NH1	2.45	0.46
1:W:178:GLN:CD	1:W:739:MET:HE3	2.40	0.46
1:Y:324:LEU:O	1:Y:333:LYS:HE3	2.15	0.46
1:A:195:LYS:HB3	1:A:196:PRO:HD3	1.98	0.46
3:E:717:ARG:NH1	3:V:724:ILE:HB	2.31	0.46
1:G:766:THR:HG22	1:G:769:GLN:HG3	1.98	0.46
1:I:766:THR:HG22	1:I:769:GLN:HG3	1.98	0.46
1:M:404:PRO:O	1:M:405:GLU:CB	2.64	0.46
1:W:324:LEU:O	1:W:333:LYS:HE3	2.16	0.46
3:b:720:LEU:O	3:b:724:ILE:HG13	2.15	0.46
3:j:720:LEU:O	3:j:724:ILE:HG13	2.15	0.46
1:A:176:LEU:N	1:A:177:PRO:CD	2.78	0.46
2:D:99:TYR:O	2:D:102:VAL:HG22	2.16	0.46
1:G:138:LEU:HD11	1:M:765:MET:HE2	1.97	0.46
2:P:99:TYR:O	2:P:102:VAL:HG22	2.16	0.46
1:Q:518:LEU:HG	1:Q:519:LYS:H	1.79	0.46
2:X:120:MET:HB2	2:X:168:ILE:HD12	1.96	0.46
1:c:611:SER:HB2	1:c:613:LEU:CD2	2.44	0.46
3:f:720:LEU:O	3:f:724:ILE:HG13	2.15	0.46
1:g:518:LEU:HG	1:g:519:LYS:N	2.30	0.46
1:G:138:LEU:HD21	1:M:765:MET:SD	2.53	0.46
2:H:80:TYR:HE1	3:K:746:MET:SD	2.39	0.46
2:N:99:TYR:O	2:N:102:VAL:HG22	2.16	0.46
1:S:329:THR:HG23	1:S:332:GLN:H	1.81	0.46
1:c:182:MET:HA	1:c:186:MET:HG3	1.97	0.46
1:c:602:VAL:HG23	1:c:607:VAL:CG2	2.45	0.46
2:H:176:VAL:HG23	2:H:177:SER:N	2.31	0.46
3:K:717:ARG:NH2	3:f:725:GLN:CA	2.79	0.46
1:M:182:MET:HA	1:M:186:MET:HG3	1.98	0.46
1:O:404:PRO:O	1:O:405:GLU:CB	2.64	0.46
1:O:611:SER:HB2	1:O:613:LEU:CD2	2.45	0.46
1:S:182:MET:HA	1:S:186:MET:HG3	1.98	0.46
1:S:206:ILE:HD11	1:S:394:PHE:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:182:MET:HA	1:W:186:MET:HG3	1.98	0.46
1:Y:182:MET:HA	1:Y:186:MET:HG3	1.98	0.46
2:B:99:TYR:O	2:B:102:VAL:HG22	2.16	0.46
2:H:99:TYR:O	2:H:102:VAL:HG22	2.16	0.46
2:R:38:LEU:O	5:R:2000:GSP:O3'	2.30	0.46
1:g:766:THR:HG22	1:g:769:GLN:HG3	1.97	0.46
2:B:176:VAL:HG23	2:B:177:SER:N	2.31	0.46
3:E:724:ILE:HG22	3:V:717:ARG:NE	2.31	0.46
1:G:195:LYS:HB3	1:G:196:PRO:HD3	1.98	0.46
1:M:766:THR:HG22	1:M:769:GLN:HG3	1.98	0.46
1:A:518:LEU:HG	1:A:519:LYS:H	1.81	0.45
2:B:80:TYR:OH	3:E:746:MET:CE	2.64	0.45
3:E:724:ILE:CG2	3:V:717:ARG:NE	2.78	0.45
2:H:42:SER:HA	5:H:2000:GSP:S1G	2.56	0.45
2:N:31:PHE:O	2:N:51:ARG:NH1	2.46	0.45
2:B:80:TYR:CZ	3:E:746:MET:SD	3.09	0.45
3:F:728:GLU:CG	3:U:717:ARG:NH2	2.78	0.45
1:G:196:PRO:HG2	2:H:131:LEU:HD22	1.98	0.45
2:J:99:TYR:O	2:J:102:VAL:HG22	2.17	0.45
1:M:329:THR:HG23	1:M:332:GLN:H	1.81	0.45
1:Q:324:LEU:O	1:Q:333:LYS:HE3	2.17	0.45
1:A:363:VAL:HA	1:A:388:VAL:HG12	1.98	0.45
1:C:138:LEU:CD2	1:S:769:GLN:OE1	2.61	0.45
1:M:588:ILE:HD12	1:M:593:GLY:HA2	1.98	0.45
1:O:195:LYS:HB3	1:O:196:PRO:HD3	1.97	0.45
1:O:518:LEU:HG	1:O:519:LYS:N	2.32	0.45
1:Q:363:VAL:HA	1:Q:388:VAL:HG12	1.98	0.45
1:Y:602:VAL:HG23	1:Y:607:VAL:CG2	2.47	0.45
3:F:728:GLU:HG2	3:U:717:ARG:NH2	2.31	0.45
1:I:404:PRO:O	1:I:405:GLU:CB	2.65	0.45
1:O:329:THR:HG23	1:O:332:GLN:H	1.81	0.45
1:C:404:PRO:O	1:C:405:GLU:CB	2.65	0.45
1:I:182:MET:HA	1:I:186:MET:HG3	1.97	0.45
1:Q:404:PRO:O	1:Q:405:GLU:CB	2.64	0.45
1:S:195:LYS:HB3	1:S:196:PRO:HD3	1.99	0.45
1:S:518:LEU:HG	1:S:519:LYS:N	2.31	0.45
1:W:602:VAL:HG23	1:W:607:VAL:CG2	2.46	0.45
2:X:99:TYR:O	2:X:102:VAL:HG22	2.16	0.45
1:I:206:ILE:HD11	1:I:394:PHE:CE2	2.51	0.45
2:R:38:LEU:HA	5:R:2000:GSP:O2'	2.16	0.45
2:R:99:TYR:O	2:R:102:VAL:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:404:PRO:O	1:S:405:GLU:CB	2.64	0.45
1:Y:607:VAL:O	1:Y:611:SER:OG	2.20	0.45
2:Z:38:LEU:HA	5:Z:2000:GSP:O2'	2.16	0.45
3:a:717:ARG:HH11	3:j:724:ILE:CG2	2.29	0.45
1:c:195:LYS:HB3	1:c:196:PRO:HD3	1.99	0.45
2:h:99:TYR:O	2:h:102:VAL:HG22	2.16	0.45
1:C:182:MET:HA	1:C:186:MET:HG3	1.97	0.45
1:C:206:ILE:HD11	1:C:394:PHE:CE2	2.51	0.45
2:D:80:TYR:HE1	3:F:746:MET:HG2	1.82	0.45
1:I:602:VAL:HG23	1:I:607:VAL:CG2	2.47	0.45
3:K:717:ARG:HD2	3:f:724:ILE:CG2	2.47	0.45
1:M:602:VAL:HG23	1:M:607:VAL:CG2	2.46	0.45
1:S:324:LEU:O	1:S:333:LYS:HE3	2.17	0.45
1:Y:363:VAL:HA	1:Y:388:VAL:HG12	1.99	0.45
1:g:602:VAL:HG23	1:g:607:VAL:CG2	2.47	0.45
1:C:602:VAL:HG23	1:C:607:VAL:CG2	2.46	0.45
1:C:607:VAL:O	1:C:611:SER:OG	2.20	0.45
1:G:765:MET:HE2	1:M:138:LEU:HD11	1.98	0.45
1:O:588:ILE:HD12	1:O:593:GLY:HA2	1.99	0.45
1:Q:588:ILE:HD12	1:Q:593:GLY:HA2	1.98	0.45
1:W:404:PRO:O	1:W:405:GLU:CB	2.65	0.45
2:d:99:TYR:O	2:d:102:VAL:HG22	2.16	0.45
1:g:404:PRO:O	1:g:405:GLU:CB	2.65	0.45
2:B:80:TYR:CE1	3:E:746:MET:HE2	2.52	0.45
1:G:329:THR:HG23	1:G:332:GLN:H	1.82	0.45
1:I:329:THR:HG23	1:I:332:GLN:H	1.82	0.45
1:I:518:LEU:HG	1:I:519:LYS:N	2.31	0.45
2:J:38:LEU:O	5:J:2000:GSP:O3'	2.22	0.45
1:M:176:LEU:N	1:M:177:PRO:CD	2.80	0.45
1:M:363:VAL:HA	1:M:388:VAL:HG12	1.99	0.45
1:Q:182:MET:HA	1:Q:186:MET:HG3	1.99	0.45
1:Q:196:PRO:HG2	2:R:131:LEU:HD22	1.98	0.45
2:T:99:TYR:O	2:T:102:VAL:HG22	2.16	0.45
1:A:329:THR:HG23	1:A:332:GLN:H	1.82	0.45
1:C:324:LEU:O	1:C:333:LYS:HE3	2.16	0.45
1:C:518:LEU:HG	1:C:519:LYS:N	2.31	0.45
2:D:38:LEU:O	5:D:2000:GSP:O3'	2.20	0.45
1:G:363:VAL:HA	1:G:388:VAL:HG12	1.99	0.45
1:Y:588:ILE:HD12	1:Y:593:GLY:HA2	1.99	0.45
1:Y:766:THR:HG22	1:Y:769:GLN:HG3	1.99	0.45
1:c:363:VAL:HA	1:c:388:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:d:31:PHE:O	2:d:51:ARG:NH1	2.46	0.45
3:E:717:ARG:HG2	3:V:728:GLU:OE2	2.12	0.44
1:S:363:VAL:HA	1:S:388:VAL:HG12	1.99	0.44
1:S:405:GLU:HA	1:S:534:PRO:HG3	1.99	0.44
1:Y:195:LYS:HB3	1:Y:196:PRO:HD3	1.99	0.44
1:Y:518:LEU:HG	1:Y:519:LYS:H	1.83	0.44
2:d:38:LEU:CA	5:d:2000:GSP:O2'	2.63	0.44
3:a:717:ARG:CG	3:j:728:GLU:CD	2.71	0.44
3:b:728:GLU:HG2	3:i:717:ARG:HE	1.82	0.44
1:A:766:THR:HG22	1:A:769:GLN:HG3	2.00	0.44
1:C:588:ILE:HD12	1:C:593:GLY:HA2	1.98	0.44
1:I:178:GLN:CA	1:I:739:MET:HE1	2.47	0.44
1:I:324:LEU:O	1:I:333:LYS:HE3	2.16	0.44
1:M:195:LYS:HB3	1:M:196:PRO:HD3	1.98	0.44
1:O:602:VAL:HG23	1:O:607:VAL:CG2	2.47	0.44
1:Q:518:LEU:HG	1:Q:519:LYS:N	2.31	0.44
2:h:48:PHE:O	3:i:755:VAL:HG23	2.18	0.44
1:A:336:ARG:HA	1:Y:537:HIS:CD2	2.53	0.44
1:I:195:LYS:HB3	1:I:196:PRO:HD3	1.99	0.44
2:P:120:MET:HE1	2:P:164:ALA:C	2.43	0.44
2:T:125:LYS:HG2	5:T:2000:GSP:C6	2.53	0.44
1:W:518:LEU:HG	1:W:519:LYS:N	2.32	0.44
1:g:176:LEU:N	1:g:177:PRO:CD	2.80	0.44
1:A:206:ILE:HD11	1:A:394:PHE:HE1	1.81	0.44
1:G:206:ILE:HD11	1:G:394:PHE:HE2	1.81	0.44
1:G:518:LEU:HG	1:G:519:LYS:N	2.32	0.44
1:I:759:GLU:OE2	1:Q:147:TYR:OH	2.33	0.44
2:R:26:ASN:ND2	5:R:2000:GSP:O1A	2.50	0.44
2:Z:99:TYR:O	2:Z:102:VAL:HG22	2.17	0.44
1:c:176:LEU:N	1:c:177:PRO:CD	2.81	0.44
1:c:404:PRO:O	1:c:405:GLU:CB	2.64	0.44
2:B:44:ILE:HD12	3:F:737:TYR:CE2	2.51	0.44
1:C:329:THR:HG23	1:C:332:GLN:H	1.83	0.44
1:G:176:LEU:N	1:G:177:PRO:CD	2.80	0.44
3:K:740:ARG:HH22	1:Q:682:SER:HB3	1.83	0.44
2:h:104:ARG:HD2	2:h:104:ARG:HA	1.79	0.44
1:C:176:LEU:N	1:C:177:PRO:CD	2.81	0.44
2:R:41:LYS:HB3	3:f:733:ARG:CZ	2.46	0.44
2:T:176:VAL:HG23	2:T:177:SER:N	2.33	0.44
1:W:765:MET:CE	1:c:138:LEU:CD2	2.78	0.44
1:W:766:THR:HG22	1:W:769:GLN:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:329:THR:HG23	1:Y:332:GLN:H	1.83	0.44
1:Y:404:PRO:O	1:Y:405:GLU:CB	2.65	0.44
1:c:518:LEU:HG	1:c:519:LYS:H	1.83	0.44
1:g:195:LYS:HB3	1:g:196:PRO:HD3	1.98	0.44
1:I:588:ILE:HD12	1:I:593:GLY:HA2	1.98	0.44
3:K:728:GLU:HB2	3:f:717:ARG:HH11	1.81	0.44
3:K:738:ILE:HD11	3:L:738:ILE:HD13	1.99	0.44
2:N:120:MET:HE1	2:N:164:ALA:C	2.43	0.44
1:Y:178:GLN:CA	1:Y:739:MET:HE1	2.48	0.44
1:c:329:THR:HG23	1:c:332:GLN:H	1.83	0.44
1:g:329:THR:HG23	1:g:332:GLN:H	1.81	0.44
1:A:178:GLN:CA	1:A:739:MET:HE1	2.47	0.44
1:A:588:ILE:HD12	1:A:593:GLY:HA2	1.99	0.44
2:B:26:ASN:ND2	5:B:2000:GSP:O1A	2.48	0.44
2:D:40:SER:HB3	5:D:2000:GSP:H3'	1.99	0.44
1:M:206:ILE:HD11	1:M:394:PHE:CE2	2.53	0.44
1:O:363:VAL:HA	1:O:388:VAL:HG12	2.00	0.44
2:X:44:ILE:HD12	3:b:737:TYR:CG	2.53	0.44
1:c:206:ILE:HD11	1:c:394:PHE:CE1	2.53	0.44
3:e:735:GLN:HE22	3:f:734:LEU:CD1	2.30	0.44
1:g:178:GLN:CA	1:g:739:MET:HE1	2.48	0.44
1:G:588:ILE:HD12	1:G:593:GLY:HA2	1.99	0.43
1:O:169:ASN:OD1	1:O:201:ARG:CZ	2.66	0.43
2:R:176:VAL:HG23	2:R:177:SER:N	2.34	0.43
1:W:176:LEU:N	1:W:177:PRO:CD	2.81	0.43
1:W:363:VAL:HA	1:W:388:VAL:HG12	2.00	0.43
2:X:120:MET:HE1	2:X:164:ALA:C	2.43	0.43
1:C:195:LYS:HB3	1:C:196:PRO:HD3	1.99	0.43
1:G:404:PRO:O	1:G:405:GLU:CB	2.65	0.43
1:I:405:GLU:HA	1:I:534:PRO:HG3	2.00	0.43
2:R:104:ARG:HD2	2:R:104:ARG:HA	1.79	0.43
1:c:571:TRP:CE2	1:c:578:LEU:HD12	2.52	0.43
2:d:79:ALA:CB	3:j:746:MET:HE3	2.48	0.43
1:A:404:PRO:O	1:A:405:GLU:CB	2.65	0.43
1:W:138:LEU:CD1	1:c:765:MET:HE2	2.49	0.43
2:X:44:ILE:CD1	3:b:737:TYR:CG	3.02	0.43
1:C:405:GLU:HA	1:C:534:PRO:HG3	2.00	0.43
2:J:40:SER:HB3	5:J:2000:GSP:H3'	2.00	0.43
2:d:37:ASN:C	5:d:2000:GSP:HO2'	2.09	0.43
3:e:752:ILE:HD13	3:f:745:ILE:CD1	2.48	0.43
1:A:571:TRP:CE2	1:A:578:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:GLU:HG3	1:I:332:GLN:NE2	2.32	0.43
2:D:79:ALA:CB	3:F:746:MET:HE1	2.44	0.43
2:N:104:ARG:HD2	2:N:104:ARG:HA	1.77	0.43
2:X:44:ILE:CD1	3:b:737:TYR:CD1	3.02	0.43
1:Y:518:LEU:HG	1:Y:519:LYS:N	2.34	0.43
1:c:588:ILE:HD12	1:c:593:GLY:HA2	2.00	0.43
1:c:766:THR:HG22	1:c:769:GLN:HG3	1.98	0.43
1:C:178:GLN:CA	1:C:739:MET:HE1	2.48	0.43
3:F:731:ASN:ND2	3:U:717:ARG:NH2	2.64	0.43
1:W:178:GLN:CA	1:W:739:MET:HE1	2.49	0.43
1:Y:206:ILE:HD11	1:Y:394:PHE:CE1	2.54	0.43
3:j:724:ILE:HA	3:j:727:GLN:HE21	1.83	0.43
1:A:518:LEU:HG	1:A:519:LYS:N	2.33	0.43
1:O:176:LEU:N	1:O:177:PRO:CD	2.82	0.43
1:W:195:LYS:HB3	1:W:196:PRO:HD3	1.99	0.43
1:Y:176:LEU:N	1:Y:177:PRO:CD	2.81	0.43
1:g:152:LYS:HD3	3:j:722:GLU:CB	2.49	0.43
1:C:138:LEU:HA	1:S:769:GLN:HE21	1.84	0.43
1:W:573:GLN:C	1:W:574:GLU:O	2.60	0.43
1:c:178:GLN:CA	1:c:739:MET:HE1	2.49	0.43
1:g:206:ILE:HD11	1:g:394:PHE:CE1	2.53	0.43
1:G:139:PHE:HD1	1:G:143:MET:HE2	1.84	0.43
1:G:178:GLN:CA	1:G:739:MET:HE1	2.48	0.43
1:M:169:ASN:OD1	1:M:201:ARG:CZ	2.67	0.43
1:c:549:LYS:HD3	1:c:554:LEU:HD21	2.01	0.43
3:f:730:ILE:O	3:f:734:LEU:HG	2.19	0.43
2:h:120:MET:HE1	2:h:164:ALA:C	2.44	0.43
1:O:405:GLU:HA	1:O:534:PRO:HG3	1.99	0.43
1:Q:206:ILE:HD11	1:Q:394:PHE:CE2	2.54	0.43
1:Q:405:GLU:HA	1:Q:534:PRO:HG3	2.01	0.43
1:W:588:ILE:HD12	1:W:593:GLY:HA2	1.99	0.43
1:c:518:LEU:HG	1:c:519:LYS:N	2.34	0.43
1:G:571:TRP:CE2	1:G:578:LEU:HD12	2.54	0.42
2:H:80:TYR:CE1	3:K:746:MET:SD	3.12	0.42
1:M:571:TRP:CE2	1:M:578:LEU:HD12	2.54	0.42
2:P:37:ASN:O	5:P:2000:GSP:O2'	2.21	0.42
1:Q:308:ALA:N	1:Q:309:PRO:CD	2.81	0.42
1:W:329:THR:HG23	1:W:332:GLN:H	1.82	0.42
3:b:728:GLU:CG	3:i:717:ARG:NH2	2.82	0.42
1:A:602:VAL:HG23	1:A:607:VAL:CG2	2.48	0.42
2:B:80:TYR:CZ	3:E:746:MET:CE	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:LYS:HG2	5:D:2000:GSP:C6	2.55	0.42
1:I:363:VAL:HA	1:I:388:VAL:HG12	2.01	0.42
3:V:730:ILE:O	3:V:734:LEU:HG	2.20	0.42
3:F:717:ARG:NH2	3:U:728:GLU:CB	2.82	0.42
1:I:138:LEU:CG	1:Q:769:GLN:HB3	2.49	0.42
1:I:176:LEU:N	1:I:177:PRO:CD	2.82	0.42
3:L:717:ARG:CZ	3:e:728:GLU:HB3	2.50	0.42
1:O:178:GLN:CA	1:O:739:MET:HE1	2.48	0.42
1:O:182:MET:HA	1:O:186:MET:HG3	2.02	0.42
2:P:176:VAL:HG23	2:P:177:SER:N	2.34	0.42
1:W:206:ILE:HD11	1:W:394:PHE:CE2	2.53	0.42
2:X:44:ILE:HD12	3:b:737:TYR:CE2	2.53	0.42
2:d:40:SER:HB3	5:d:2000:GSP:C3'	2.46	0.42
1:g:588:ILE:HD12	1:g:593:GLY:HA2	2.00	0.42
3:E:730:ILE:O	3:E:734:LEU:HG	2.20	0.42
1:G:602:VAL:HG23	1:G:607:VAL:CG2	2.48	0.42
1:I:139:PHE:HD1	1:I:143:MET:HE2	1.84	0.42
1:I:571:TRP:CE2	1:I:578:LEU:HD12	2.54	0.42
1:M:178:GLN:CA	1:M:739:MET:HE1	2.48	0.42
1:M:405:GLU:HA	1:M:534:PRO:HG3	2.00	0.42
2:N:176:VAL:HG23	2:N:177:SER:N	2.34	0.42
2:X:176:VAL:HG23	2:X:177:SER:N	2.34	0.42
1:C:571:TRP:CE2	1:C:578:LEU:HD12	2.55	0.42
1:S:206:ILE:HD11	1:S:394:PHE:CE2	2.55	0.42
3:a:738:ILE:HD13	3:b:738:ILE:CG1	2.50	0.42
1:c:405:GLU:HA	1:c:534:PRO:HG3	2.02	0.42
1:A:139:PHE:HD1	1:A:143:MET:HE2	1.84	0.42
1:A:178:GLN:NE2	1:A:739:MET:HE3	2.34	0.42
1:C:363:VAL:HA	1:C:388:VAL:HG12	2.01	0.42
1:O:206:ILE:HD11	1:O:394:PHE:CE2	2.54	0.42
1:Q:178:GLN:CA	1:Q:739:MET:HE1	2.48	0.42
1:g:152:LYS:HD2	3:j:722:GLU:CB	2.49	0.42
3:L:717:ARG:NH2	3:e:728:GLU:HB3	2.34	0.42
1:Q:139:PHE:HD1	1:Q:143:MET:HE2	1.85	0.42
1:c:657:ARG:NH2	1:c:674:ASP:O	2.53	0.42
2:d:41:LYS:HB3	3:i:733:ARG:HH22	1.84	0.42
1:S:178:GLN:CA	1:S:739:MET:HE1	2.48	0.42
1:Y:405:GLU:HA	1:Y:534:PRO:HG3	2.02	0.42
2:d:80:TYR:HE1	3:j:746:MET:HG2	1.85	0.42
2:d:176:VAL:HG23	2:d:177:SER:N	2.34	0.42
1:A:206:ILE:HD11	1:A:394:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:730:ILE:O	3:K:734:LEU:HG	2.20	0.42
1:Q:176:LEU:N	1:Q:177:PRO:CD	2.83	0.42
2:R:48:PHE:HD2	3:e:754:GLU:HA	1.84	0.42
1:Y:571:TRP:CE2	1:Y:578:LEU:HD12	2.55	0.42
2:Z:173:TYR:O	2:Z:173:TYR:CG	2.73	0.42
2:d:120:MET:HE1	2:d:164:ALA:C	2.45	0.42
1:S:169:ASN:OD1	1:S:201:ARG:CZ	2.68	0.41
1:W:196:PRO:HG2	2:X:131:LEU:HD22	2.02	0.41
1:W:405:GLU:HA	1:W:534:PRO:HG3	2.02	0.41
1:g:549:LYS:HD3	1:g:554:LEU:HD21	2.02	0.41
2:B:173:TYR:O	2:B:173:TYR:CG	2.72	0.41
1:C:139:PHE:HD1	1:C:143:MET:HE2	1.85	0.41
1:I:169:ASN:OD1	1:I:201:ARG:CZ	2.68	0.41
2:J:173:TYR:O	2:J:173:TYR:CG	2.73	0.41
2:P:41:LYS:HB3	3:U:733:ARG:HH22	1.83	0.41
1:S:176:LEU:N	1:S:177:PRO:CD	2.83	0.41
1:c:571:TRP:CD2	1:c:578:LEU:HD12	2.54	0.41
3:f:724:ILE:HA	3:f:727:GLN:HE21	1.85	0.41
2:h:41:LYS:HB3	3:j:733:ARG:CZ	2.50	0.41
2:H:80:TYR:OH	3:K:746:MET:HB3	2.19	0.41
1:M:308:ALA:N	1:M:309:PRO:CD	2.83	0.41
3:b:724:ILE:HA	3:b:727:GLN:HE21	1.85	0.41
1:g:169:ASN:OD1	1:g:201:ARG:CZ	2.68	0.41
1:g:573:GLN:C	1:g:574:GLU:O	2.62	0.41
2:h:26:ASN:ND2	5:h:2000:GSP:O1A	2.51	0.41
2:h:176:VAL:HG23	2:h:177:SER:N	2.36	0.41
2:B:44:ILE:HD13	3:F:737:TYR:CD1	2.56	0.41
2:P:104:ARG:HD2	2:P:104:ARG:HA	1.79	0.41
1:g:405:GLU:HA	1:g:534:PRO:HG3	2.02	0.41
3:j:730:ILE:O	3:j:734:LEU:HG	2.21	0.41
1:A:308:ALA:N	1:A:309:PRO:CD	2.83	0.41
1:C:169:ASN:OD1	1:C:201:ARG:CZ	2.68	0.41
1:G:169:ASN:OD1	1:G:201:ARG:CZ	2.68	0.41
1:G:206:ILE:HD11	1:G:394:PHE:CE2	2.55	0.41
1:S:139:PHE:HD1	1:S:143:MET:HE2	1.86	0.41
1:W:169:ASN:OD1	1:W:201:ARG:CZ	2.68	0.41
1:Y:139:PHE:HD1	1:Y:143:MET:HE2	1.86	0.41
1:A:571:TRP:CD2	1:A:578:LEU:HD12	2.56	0.41
2:H:80:TYR:CE1	3:K:746:MET:CE	3.04	0.41
1:I:549:LYS:HD3	1:I:554:LEU:HD21	2.02	0.41
1:Q:169:ASN:OD1	1:Q:201:ARG:CZ	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:31:PHE:O	2:Z:51:ARG:NH1	2.46	0.41
1:C:332:GLN:NE2	1:I:332:GLN:HG3	2.30	0.41
1:C:778:VAL:O	1:C:781:SER:OG	2.37	0.41
1:G:405:GLU:HA	1:G:534:PRO:HG3	2.02	0.41
3:V:724:ILE:HA	3:V:727:GLN:HE21	1.85	0.41
2:h:48:PHE:O	3:i:755:VAL:CG2	2.68	0.41
1:A:336:ARG:HE	1:Y:537:HIS:CE1	2.37	0.41
2:H:31:PHE:O	2:H:51:ARG:NH1	2.46	0.41
1:S:549:LYS:HD3	1:S:554:LEU:HD21	2.02	0.41
1:S:578:LEU:CD2	1:S:717:LEU:HB3	2.51	0.41
1:Y:549:LYS:HD3	1:Y:554:LEU:HD21	2.02	0.41
1:Y:578:LEU:CD2	1:Y:717:LEU:HB3	2.50	0.41
1:g:695:LEU:HD12	1:g:695:LEU:HA	1.94	0.41
1:A:196:PRO:HG2	2:B:131:LEU:HD22	2.01	0.41
2:B:31:PHE:O	2:B:51:ARG:NH1	2.46	0.41
3:F:724:ILE:HA	3:F:727:GLN:HE21	1.85	0.41
3:L:730:ILE:O	3:L:734:LEU:HG	2.19	0.41
1:O:139:PHE:HD1	1:O:143:MET:HE2	1.86	0.41
1:O:571:TRP:CE2	1:O:578:LEU:HD12	2.56	0.41
1:Q:571:TRP:CE2	1:Q:578:LEU:HD12	2.55	0.41
1:S:766:THR:O	1:S:769:GLN:HB2	2.21	0.41
1:W:308:ALA:N	1:W:309:PRO:CD	2.84	0.41
1:Y:695:LEU:HD12	1:Y:695:LEU:HA	1.96	0.41
1:C:332:GLN:HG3	1:I:332:GLN:HE21	1.85	0.41
1:C:549:LYS:HD3	1:C:554:LEU:HD21	2.02	0.41
1:I:133:LEU:HD11	1:I:138:LEU:HD22	2.03	0.41
1:M:139:PHE:HD1	1:M:143:MET:HE2	1.86	0.41
1:O:573:GLN:C	1:O:574:GLU:O	2.61	0.41
1:Q:578:LEU:CD2	1:Q:717:LEU:HB3	2.52	0.41
3:U:730:ILE:O	3:U:734:LEU:HG	2.21	0.41
1:W:571:TRP:CE2	1:W:578:LEU:HD12	2.56	0.41
1:W:783:ARG:O	1:W:784:SER:CB	2.69	0.41
1:Y:657:ARG:NH2	1:Y:674:ASP:O	2.54	0.41
2:Z:120:MET:HE1	2:Z:164:ALA:C	2.46	0.41
2:H:104:ARG:HA	2:H:104:ARG:HD2	1.79	0.40
1:I:621:GLN:NE2	1:I:622:GLU:OE2	2.53	0.40
1:O:578:LEU:HD21	1:O:717:LEU:HB3	2.03	0.40
1:O:639:VAL:HG13	1:O:714:TYR:HB2	2.03	0.40
1:Q:549:LYS:HD3	1:Q:554:LEU:HD21	2.03	0.40
1:W:138:LEU:CG	1:c:765:MET:HE2	2.51	0.40
1:c:639:VAL:HG13	1:c:714:TYR:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:783:ARG:O	1:c:784:SER:CB	2.69	0.40
3:i:730:ILE:O	3:i:734:LEU:HG	2.21	0.40
1:M:571:TRP:CD2	1:M:578:LEU:HD12	2.55	0.40
1:S:571:TRP:CE2	1:S:578:LEU:HD12	2.55	0.40
2:T:48:PHE:HD2	3:U:754:GLU:HA	1.86	0.40
2:T:173:TYR:O	2:T:173:TYR:CG	2.74	0.40
1:W:549:LYS:HD3	1:W:554:LEU:HD21	2.03	0.40
2:X:104:ARG:HA	2:X:104:ARG:HD2	1.78	0.40
1:Y:783:ARG:O	1:Y:784:SER:CB	2.70	0.40
1:c:169:ASN:OD1	1:c:201:ARG:CZ	2.69	0.40
3:e:730:ILE:O	3:e:734:LEU:HG	2.21	0.40
1:g:571:TRP:CD2	1:g:578:LEU:HD12	2.57	0.40
1:G:549:LYS:HD3	1:G:554:LEU:HD21	2.03	0.40
1:Q:766:THR:O	1:Q:769:GLN:HB2	2.22	0.40
1:S:783:ARG:O	1:S:784:SER:CB	2.69	0.40
3:a:730:ILE:O	3:a:734:LEU:HG	2.21	0.40
1:g:783:ARG:O	1:g:784:SER:CB	2.69	0.40
2:D:176:VAL:HG23	2:D:177:SER:N	2.36	0.40
3:K:742:ILE:HD11	3:L:741:ILE:HD13	2.04	0.40
3:L:724:ILE:HA	3:L:727:GLN:HE21	1.86	0.40
1:M:178:GLN:NE2	1:M:739:MET:HE3	2.37	0.40
1:O:578:LEU:CD2	1:O:717:LEU:HB3	2.51	0.40
1:O:783:ARG:O	1:O:784:SER:CB	2.69	0.40
1:W:657:ARG:NH2	1:W:674:ASP:O	2.54	0.40
1:Y:169:ASN:OD1	1:Y:201:ARG:CZ	2.69	0.40
1:C:133:LEU:HD11	1:C:138:LEU:HD22	2.04	0.40
1:C:573:GLN:C	1:C:574:GLU:O	2.63	0.40
1:I:139:PHE:HD1	1:I:143:MET:CE	2.34	0.40
1:M:783:ARG:O	1:M:784:SER:CB	2.70	0.40

All (62) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:174:ARG:NH2	1:M:166:CYS:O[2_545]	0.72	1.48
2:D:174:ARG:NH2	1:O:166:CYS:O[2_556]	0.76	1.44
2:B:174:ARG:NH2	1:g:166:CYS:O[2_656]	0.78	1.42
1:I:396:THR:OG1	1:M:627:THR:OG1[2_545]	0.85	1.35
1:C:396:THR:OG1	1:O:627:THR:OG1[2_556]	1.08	1.12
2:H:174:ARG:NH2	1:W:166:CYS:O[2_655]	1.08	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:346:HIS:O	1:Y:626:TYR:CE1[2_656]	1.08	1.12
1:S:346:HIS:CA	1:Y:626:TYR:OH[2_656]	1.20	1.00
1:Q:343:LEU:O	1:c:626:TYR:OH[2_655]	1.29	0.91
1:O:779:ASP:OD2	1:g:537:HIS:CD2[2_656]	1.37	0.83
2:D:174:ARG:CZ	1:O:166:CYS:O[2_556]	1.41	0.79
2:J:56:ASP:OD1	1:M:165:PHE:O[2_545]	1.44	0.76
2:B:56:ASP:OD1	1:g:165:PHE:O[2_656]	1.47	0.73
2:D:56:ASP:OD1	1:O:165:PHE:O[2_556]	1.47	0.73
2:J:174:ARG:CZ	1:M:166:CYS:O[2_545]	1.51	0.69
1:A:626:TYR:CD2	1:O:346:HIS:O[2_546]	1.53	0.67
1:G:626:TYR:OH	1:M:348:LEU:N[2_555]	1.55	0.65
1:G:339:SER:OG	1:c:537:HIS:CB[1_565]	1.56	0.64
1:G:626:TYR:CD2	1:M:346:HIS:O[2_555]	1.56	0.64
1:S:346:HIS:C	1:Y:626:TYR:OH[2_656]	1.61	0.59
1:S:346:HIS:O	1:Y:626:TYR:CZ[2_656]	1.61	0.59
1:A:626:TYR:OH	1:O:348:LEU:N[2_546]	1.63	0.57
1:G:626:TYR:CE2	1:M:346:HIS:O[2_555]	1.69	0.51
1:A:626:TYR:OH	1:O:348:LEU:O[2_546]	1.72	0.48
1:S:346:HIS:CA	1:Y:626:TYR:CZ[2_656]	1.75	0.45
1:A:626:TYR:CE2	1:O:346:HIS:O[2_546]	1.76	0.44
1:G:626:TYR:OH	1:M:348:LEU:O[2_555]	1.80	0.40
1:A:396:THR:OG1	1:g:627:THR:OG1[2_656]	1.81	0.39
1:S:323:ARG:NH1	1:Y:707:ASP:OD2[2_656]	1.81	0.39
2:B:174:ARG:CZ	1:g:166:CYS:O[2_656]	1.84	0.36
1:Q:346:HIS:CB	1:c:626:TYR:CZ[2_655]	1.84	0.36
2:B:174:ARG:NH2	1:g:166:CYS:C[2_656]	1.87	0.33
2:H:56:ASP:OD1	1:W:165:PHE:O[2_655]	1.87	0.33
1:I:396:THR:CB	1:M:627:THR:OG1[2_545]	1.87	0.33
2:H:174:ARG:CZ	1:W:166:CYS:O[2_655]	1.88	0.32
1:S:346:HIS:C	1:Y:626:TYR:CZ[2_656]	1.88	0.32
2:B:56:ASP:OD2	1:g:166:CYS:CA[2_656]	1.89	0.31
2:J:174:ARG:NH2	1:M:166:CYS:C[2_545]	1.93	0.27
1:G:339:SER:OG	1:c:537:HIS:CG[1_565]	1.94	0.26
2:D:174:ARG:NH2	1:O:166:CYS:C[2_556]	1.97	0.23
1:S:346:HIS:O	1:Y:626:TYR:OH[2_656]	1.98	0.22
1:S:346:HIS:CB	1:Y:626:TYR:CE2[2_656]	2.00	0.20
2:B:56:ASP:CG	1:g:166:CYS:CA[2_656]	2.01	0.19
1:A:616:LEU:CD2	1:O:346:HIS:CD2[2_546]	2.03	0.17
1:Q:346:HIS:CB	1:c:626:TYR:OH[2_655]	2.03	0.17
1:G:616:LEU:CD2	1:M:346:HIS:CD2[2_555]	2.07	0.13
1:S:346:HIS:C	1:Y:626:TYR:CE1[2_656]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:THR:CB	1:O:627:THR:OG1[2_556]	2.08	0.12
2:B:56:ASP:O	2:h:130:HIS:CE1[2_656]	2.09	0.11
1:Q:323:ARG:NH1	1:c:707:ASP:OD2[2_655]	2.09	0.11
2:B:56:ASP:OD1	1:g:166:CYS:C[2_656]	2.10	0.10
2:B:56:ASP:OD1	1:g:166:CYS:CA[2_656]	2.10	0.10
1:G:326:THR:O	1:c:404:PRO:CD[1_565]	2.10	0.10
1:O:779:ASP:OD2	1:g:537:HIS:NE2[2_656]	2.10	0.10
1:G:396:THR:OG1	1:W:627:THR:OG1[2_655]	2.11	0.09
1:O:779:ASP:CG	1:g:537:HIS:CD2[2_656]	2.14	0.06
1:O:779:ASP:OD2	1:g:537:HIS:CG[2_656]	2.15	0.05
1:S:346:HIS:CB	1:Y:626:TYR:CZ[2_656]	2.17	0.03
1:A:626:TYR:CG	1:O:346:HIS:O[2_546]	2.18	0.02
1:S:346:HIS:N	1:Y:626:TYR:OH[2_656]	2.18	0.02
1:A:626:TYR:OH	1:O:348:LEU:C[2_546]	2.19	0.01
1:G:626:TYR:OH	1:M:348:LEU:CA[2_555]	2.19	0.01

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	460/566 (81%)	442 (96%)	16 (4%)	2 (0%)	30	67
1	C	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	G	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	I	460/566 (81%)	440 (96%)	17 (4%)	3 (1%)	18	56
1	M	460/566 (81%)	441 (96%)	16 (4%)	3 (1%)	18	56
1	O	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	18	56
1	Q	460/566 (81%)	439 (95%)	19 (4%)	2 (0%)	30	67
1	S	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56
1	W	460/566 (81%)	442 (96%)	15 (3%)	3 (1%)	18	56
1	Y	460/566 (81%)	439 (95%)	18 (4%)	3 (1%)	18	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	30	67
1	g	460/566 (81%)	440 (96%)	18 (4%)	2 (0%)	30	67
2	B	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	D	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	H	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	J	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	N	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	P	171/219 (78%)	162 (95%)	8 (5%)	1 (1%)	21	59
2	R	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	T	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	10	44
2	X	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	Z	171/219 (78%)	163 (95%)	6 (4%)	2 (1%)	10	44
2	d	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
2	h	171/219 (78%)	163 (95%)	7 (4%)	1 (1%)	21	59
3	E	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	F	30/48 (62%)	30 (100%)	0	0	100	100
3	K	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	L	30/48 (62%)	30 (100%)	0	0	100	100
3	U	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	V	30/48 (62%)	30 (100%)	0	0	100	100
3	a	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	b	30/48 (62%)	30 (100%)	0	0	100	100
3	e	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	f	30/48 (62%)	30 (100%)	0	0	100	100
3	i	39/48 (81%)	38 (97%)	1 (3%)	0	100	100
3	j	30/48 (62%)	30 (100%)	0	0	100	100
All	All	7986/9996 (80%)	7645 (96%)	295 (4%)	46 (1%)	21	59

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	GLU
2	B	68	ALA

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Mol	Chain	Res	Type
1	C	405	GLU
2	D	68	ALA
1	G	405	GLU
2	H	68	ALA
1	I	405	GLU
2	J	68	ALA
1	M	405	GLU
2	N	68	ALA
1	O	405	GLU
2	P	68	ALA
1	Q	405	GLU
2	R	68	ALA
1	S	405	GLU
2	T	68	ALA
1	W	405	GLU
2	X	68	ALA
1	Y	405	GLU
2	Z	68	ALA
1	c	405	GLU
2	d	68	ALA
1	g	405	GLU
2	h	68	ALA
1	W	398	SER
1	C	398	SER
1	G	398	SER
1	I	398	SER
1	M	398	SER
1	O	398	SER
1	S	398	SER
2	T	125	LYS
1	Y	398	SER
2	Z	125	LYS
1	A	399	VAL
1	O	399	VAL
1	W	399	VAL
1	g	399	VAL
1	C	399	VAL
1	G	399	VAL
1	I	399	VAL
1	M	399	VAL
1	Q	399	VAL
1	Y	399	VAL

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Mol	Chain	Res	Type
1	c	399	VAL
1	S	399	VAL

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	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	C	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	G	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	I	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	M	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	O	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	Q	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	S	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	W	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	Y	422/508 (83%)	406 (96%)	16 (4%)	29	50
1	c	422/508 (83%)	407 (96%)	15 (4%)	31	52
1	g	422/508 (83%)	406 (96%)	16 (4%)	29	50
2	B	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	D	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	H	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	J	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	N	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	P	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	R	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	T	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	X	147/191 (77%)	140 (95%)	7 (5%)	23	44
2	Z	147/191 (77%)	140 (95%)	7 (5%)	23	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	147/191 (77%)	141 (96%)	6 (4%)	27	48
2	h	147/191 (77%)	141 (96%)	6 (4%)	27	48
3	E	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	F	21/45 (47%)	21 (100%)	0	100	100
3	K	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	L	21/45 (47%)	21 (100%)	0	100	100
3	U	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	V	21/45 (47%)	20 (95%)	1 (5%)	23	44
3	a	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	b	21/45 (47%)	21 (100%)	0	100	100
3	e	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	f	21/45 (47%)	20 (95%)	1 (5%)	23	44
3	i	31/45 (69%)	30 (97%)	1 (3%)	34	56
3	j	21/45 (47%)	20 (95%)	1 (5%)	23	44
All	All	7140/8928 (80%)	6861 (96%)	279 (4%)	28	49

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	LEU
1	A	148	LEU
1	A	235	LYS
1	A	306	ARG
1	A	318	MET
1	A	335	GLN
1	A	378	ASP
1	A	391	CYS
1	A	397	THR
1	A	554	LEU
1	A	565	LYS
1	A	606	GLN
1	A	613	LEU
1	A	694	LYS
1	A	739	MET
2	B	7	GLU
2	B	46	VAL
2	B	54	GLN

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Mol	Chain	Res	Type
2	B	55	VAL
2	B	166	GLN
2	B	174	ARG
2	B	178	GLN
1	C	138	LEU
1	C	148	LEU
1	C	170	GLU
1	C	235	LYS
1	C	306	ARG
1	C	318	MET
1	C	335	GLN
1	C	378	ASP
1	C	391	CYS
1	C	397	THR
1	C	554	LEU
1	C	565	LYS
1	C	606	GLN
1	C	613	LEU
1	C	694	LYS
1	C	739	MET
2	D	7	GLU
2	D	46	VAL
2	D	54	GLN
2	D	55	VAL
2	D	166	GLN
2	D	174	ARG
2	D	178	GLN
3	E	728	GLU
1	G	138	LEU
1	G	148	LEU
1	G	170	GLU
1	G	235	LYS
1	G	306	ARG
1	G	318	MET
1	G	335	GLN
1	G	378	ASP
1	G	391	CYS
1	G	397	THR
1	G	554	LEU
1	G	565	LYS
1	G	606	GLN
1	G	613	LEU

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Mol	Chain	Res	Type
1	G	694	LYS
1	G	739	MET
2	H	7	GLU
2	H	46	VAL
2	H	54	GLN
2	H	55	VAL
2	H	166	GLN
2	H	174	ARG
2	H	178	GLN
1	I	138	LEU
1	I	148	LEU
1	I	170	GLU
1	I	235	LYS
1	I	306	ARG
1	I	318	MET
1	I	335	GLN
1	I	378	ASP
1	I	391	CYS
1	I	397	THR
1	I	554	LEU
1	I	565	LYS
1	I	606	GLN
1	I	613	LEU
1	I	694	LYS
1	I	739	MET
2	J	7	GLU
2	J	46	VAL
2	J	54	GLN
2	J	55	VAL
2	J	166	GLN
2	J	174	ARG
2	J	178	GLN
3	K	728	GLU
1	M	138	LEU
1	M	148	LEU
1	M	235	LYS
1	M	306	ARG
1	M	318	MET
1	M	335	GLN
1	M	378	ASP
1	M	391	CYS
1	M	397	THR

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Mol	Chain	Res	Type
1	M	554	LEU
1	M	565	LYS
1	M	606	GLN
1	M	613	LEU
1	M	694	LYS
1	M	739	MET
2	N	7	GLU
2	N	46	VAL
2	N	54	GLN
2	N	55	VAL
2	N	166	GLN
2	N	174	ARG
2	N	178	GLN
1	O	138	LEU
1	O	148	LEU
1	O	235	LYS
1	O	306	ARG
1	O	318	MET
1	O	335	GLN
1	O	378	ASP
1	O	391	CYS
1	O	397	THR
1	O	554	LEU
1	O	565	LYS
1	O	606	GLN
1	O	613	LEU
1	O	694	LYS
1	O	739	MET
2	P	7	GLU
2	P	46	VAL
2	P	54	GLN
2	P	55	VAL
2	P	166	GLN
2	P	174	ARG
2	P	178	GLN
1	Q	138	LEU
1	Q	148	LEU
1	Q	170	GLU
1	Q	235	LYS
1	Q	306	ARG
1	Q	318	MET
1	Q	335	GLN

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Mol	Chain	Res	Type
1	Q	378	ASP
1	Q	391	CYS
1	Q	397	THR
1	Q	554	LEU
1	Q	565	LYS
1	Q	606	GLN
1	Q	613	LEU
1	Q	694	LYS
1	Q	739	MET
2	R	7	GLU
2	R	46	VAL
2	R	54	GLN
2	R	55	VAL
2	R	166	GLN
2	R	174	ARG
2	R	178	GLN
1	S	138	LEU
1	S	148	LEU
1	S	170	GLU
1	S	235	LYS
1	S	306	ARG
1	S	318	MET
1	S	335	GLN
1	S	378	ASP
1	S	391	CYS
1	S	397	THR
1	S	554	LEU
1	S	565	LYS
1	S	606	GLN
1	S	613	LEU
1	S	694	LYS
1	S	739	MET
2	T	7	GLU
2	T	46	VAL
2	T	54	GLN
2	T	55	VAL
2	T	166	GLN
2	T	174	ARG
2	T	178	GLN
3	U	728	GLU
3	V	717	ARG
1	W	138	LEU

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Mol	Chain	Res	Type
1	W	148	LEU
1	W	170	GLU
1	W	235	LYS
1	W	306	ARG
1	W	318	MET
1	W	335	GLN
1	W	378	ASP
1	W	391	CYS
1	W	397	THR
1	W	554	LEU
1	W	565	LYS
1	W	606	GLN
1	W	613	LEU
1	W	694	LYS
1	W	739	MET
2	X	7	GLU
2	X	46	VAL
2	X	54	GLN
2	X	55	VAL
2	X	166	GLN
2	X	174	ARG
2	X	178	GLN
1	Y	138	LEU
1	Y	148	LEU
1	Y	170	GLU
1	Y	235	LYS
1	Y	306	ARG
1	Y	318	MET
1	Y	335	GLN
1	Y	378	ASP
1	Y	391	CYS
1	Y	397	THR
1	Y	554	LEU
1	Y	565	LYS
1	Y	606	GLN
1	Y	613	LEU
1	Y	694	LYS
1	Y	739	MET
2	Z	7	GLU
2	Z	46	VAL
2	Z	54	GLN
2	Z	55	VAL

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Mol	Chain	Res	Type
2	Z	166	GLN
2	Z	174	ARG
2	Z	178	GLN
3	a	728	GLU
1	c	138	LEU
1	c	148	LEU
1	c	235	LYS
1	c	306	ARG
1	c	318	MET
1	c	335	GLN
1	c	378	ASP
1	c	391	CYS
1	c	397	THR
1	c	554	LEU
1	c	565	LYS
1	c	606	GLN
1	c	613	LEU
1	c	694	LYS
1	c	739	MET
2	d	7	GLU
2	d	46	VAL
2	d	54	GLN
2	d	55	VAL
2	d	174	ARG
2	d	178	GLN
3	e	728	GLU
3	f	717	ARG
1	g	138	LEU
1	g	148	LEU
1	g	170	GLU
1	g	235	LYS
1	g	306	ARG
1	g	318	MET
1	g	335	GLN
1	g	378	ASP
1	g	391	CYS
1	g	397	THR
1	g	554	LEU
1	g	565	LYS
1	g	606	GLN
1	g	613	LEU
1	g	694	LYS

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Mol	Chain	Res	Type
1	g	739	MET
2	h	7	GLU
2	h	46	VAL
2	h	54	GLN
2	h	55	VAL
2	h	174	ARG
2	h	178	GLN
3	i	728	GLU
3	j	717	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	185	HIS
1	A	335	GLN
1	A	362	HIS
1	A	393	ASN
1	A	540	ASN
1	A	566	GLN
1	A	606	GLN
1	A	621	GLN
1	A	776	GLN
1	C	162	ASN
1	C	185	HIS
1	C	332	GLN
1	C	362	HIS
1	C	393	ASN
1	C	566	GLN
1	C	606	GLN
1	C	621	GLN
1	C	776	GLN
3	F	727	GLN
3	F	731	ASN
1	G	162	ASN
1	G	362	HIS
1	G	393	ASN
1	G	540	ASN
1	G	566	GLN
1	G	606	GLN
1	G	621	GLN
1	G	776	GLN

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Mol	Chain	Res	Type
2	H	130	HIS
1	I	162	ASN
1	I	185	HIS
1	I	332	GLN
1	I	362	HIS
1	I	540	ASN
1	I	566	GLN
1	I	606	GLN
1	I	621	GLN
1	I	776	GLN
3	K	731	ASN
3	K	735	GLN
3	L	727	GLN
3	L	731	ASN
1	M	162	ASN
1	M	185	HIS
1	M	362	HIS
1	M	393	ASN
1	M	566	GLN
1	M	606	GLN
1	M	621	GLN
1	M	728	HIS
1	M	776	GLN
2	N	130	HIS
1	O	162	ASN
1	O	185	HIS
1	O	207	ASN
1	O	362	HIS
1	O	393	ASN
1	O	540	ASN
1	O	566	GLN
1	O	606	GLN
1	O	621	GLN
1	O	776	GLN
1	Q	162	ASN
1	Q	362	HIS
1	Q	393	ASN
1	Q	540	ASN
1	Q	566	GLN
1	Q	606	GLN
1	Q	621	GLN
1	Q	776	GLN

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Mol	Chain	Res	Type
1	S	162	ASN
1	S	362	HIS
1	S	393	ASN
1	S	540	ASN
1	S	566	GLN
1	S	606	GLN
1	S	621	GLN
1	S	776	GLN
3	U	731	ASN
3	U	735	GLN
3	V	727	GLN
1	W	162	ASN
1	W	362	HIS
1	W	540	ASN
1	W	566	GLN
1	W	606	GLN
1	W	621	GLN
1	W	659	ASN
1	W	776	GLN
1	Y	185	HIS
1	Y	362	HIS
1	Y	393	ASN
1	Y	540	ASN
1	Y	566	GLN
1	Y	606	GLN
1	Y	621	GLN
1	Y	659	ASN
1	Y	776	GLN
3	a	731	ASN
3	b	727	GLN
3	b	731	ASN
1	c	185	HIS
1	c	362	HIS
1	c	393	ASN
1	c	540	ASN
1	c	566	GLN
1	c	606	GLN
1	c	621	GLN
1	c	776	GLN
3	e	731	ASN
3	e	735	GLN
3	f	727	GLN

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Mol	Chain	Res	Type
1	g	162	ASN
1	g	362	HIS
1	g	540	ASN
1	g	566	GLN
1	g	606	GLN
1	g	621	GLN
1	g	776	GLN
3	i	735	GLN
3	j	727	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 12 are monoatomic - leaving 24 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	$\# Z > 2$
4	093	S	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	14 (42%)
4	093	c	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	15 (45%)
5	GSP	T	2000	6	33,34,34	1.26	3 (9%)	47,54,54	1.99	10 (21%)
4	093	Y	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.43	14 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GSP	R	2000	6	33,34,34	1.44	6 (18%)	47,54,54	1.95	9 (19%)
5	GSP	J	2000	6	33,34,34	1.48	6 (18%)	47,54,54	1.97	11 (23%)
5	GSP	H	2000	6	33,34,34	1.37	4 (12%)	47,54,54	2.06	10 (21%)
5	GSP	X	2000	6	33,34,34	1.42	6 (18%)	47,54,54	2.03	13 (27%)
4	093	C	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.44	14 (42%)
5	GSP	P	2000	6	33,34,34	1.38	6 (18%)	47,54,54	1.95	13 (27%)
4	093	O	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	15 (45%)
4	093	W	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.45	15 (45%)
4	093	M	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	15 (45%)
5	GSP	D	2000	6	33,34,34	1.44	6 (18%)	47,54,54	2.01	10 (21%)
4	093	A	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.45	14 (42%)
5	GSP	B	2000	6	33,34,34	1.44	5 (15%)	47,54,54	2.01	9 (19%)
5	GSP	Z	2000	6	33,34,34	1.40	6 (18%)	47,54,54	1.87	12 (25%)
4	093	Q	2002	-	25,25,25	3.35	9 (36%)	33,36,36	5.43	14 (42%)
5	GSP	d	2000	6	33,34,34	1.42	6 (18%)	47,54,54	1.93	9 (19%)
4	093	g	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	13 (39%)
5	GSP	h	2000	6	33,34,34	1.44	5 (15%)	47,54,54	2.10	12 (25%)
5	GSP	N	2000	6	33,34,34	1.33	7 (21%)	47,54,54	1.91	11 (23%)
4	093	I	2002	-	25,25,25	3.34	9 (36%)	33,36,36	5.44	14 (42%)
4	093	G	2002	-	25,25,25	3.33	9 (36%)	33,36,36	5.44	14 (42%)

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
4	093	S	2002	-	-	8/19/19/19	0/2/2/2
4	093	c	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	T	2000	6	-	3/21/38/38	0/3/3/3
4	093	Y	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	R	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	J	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	H	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	X	2000	6	-	3/21/38/38	0/3/3/3
4	093	C	2002	-	-	8/19/19/19	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GSP	P	2000	6	-	3/21/38/38	0/3/3/3
4	093	O	2002	-	-	8/19/19/19	0/2/2/2
4	093	W	2002	-	-	8/19/19/19	0/2/2/2
4	093	M	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	D	2000	6	-	3/21/38/38	0/3/3/3
4	093	A	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	B	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	Z	2000	6	-	3/21/38/38	0/3/3/3
4	093	Q	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	d	2000	6	-	3/21/38/38	0/3/3/3
4	093	g	2002	-	-	8/19/19/19	0/2/2/2
5	GSP	h	2000	6	-	3/21/38/38	0/3/3/3
5	GSP	N	2000	6	-	3/21/38/38	0/3/3/3
4	093	I	2002	-	-	8/19/19/19	0/2/2/2
4	093	G	2002	-	-	8/19/19/19	0/2/2/2

All (174) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	2002	093	CAQ-SAP	-8.79	1.59	1.73
4	Q	2002	093	CAQ-SAP	-8.78	1.59	1.73
4	S	2002	093	CAQ-SAP	-8.76	1.59	1.73
4	A	2002	093	CAQ-SAP	-8.75	1.59	1.73
4	W	2002	093	CAQ-SAP	-8.74	1.59	1.73
4	M	2002	093	CAQ-SAP	-8.73	1.59	1.73
4	O	2002	093	CAQ-SAP	-8.73	1.59	1.73
4	c	2002	093	CAQ-SAP	-8.73	1.59	1.73
4	g	2002	093	CAQ-SAP	-8.73	1.59	1.73
4	C	2002	093	CAQ-SAP	-8.69	1.59	1.73
4	Y	2002	093	CAQ-SAP	-8.67	1.59	1.73
4	G	2002	093	CAQ-SAP	-8.66	1.59	1.73
4	Q	2002	093	CAQ-NAR	8.34	1.45	1.32
4	S	2002	093	CAQ-NAR	8.32	1.45	1.32
4	W	2002	093	CAQ-NAR	8.31	1.45	1.32
4	O	2002	093	CAQ-NAR	8.30	1.45	1.32
4	g	2002	093	CAQ-NAR	8.28	1.45	1.32
4	M	2002	093	CAQ-NAR	8.28	1.45	1.32
4	c	2002	093	CAQ-NAR	8.28	1.45	1.32
4	G	2002	093	CAQ-NAR	8.27	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Y	2002	093	CAQ-NAR	8.26	1.45	1.32
4	A	2002	093	CAQ-NAR	8.24	1.45	1.32
4	I	2002	093	CAQ-NAR	8.23	1.45	1.32
4	C	2002	093	CAQ-NAR	8.19	1.45	1.32
4	C	2002	093	CAI-SAP	-7.61	1.55	1.74
4	Y	2002	093	CAI-SAP	-7.59	1.55	1.74
4	O	2002	093	CAI-SAP	-7.57	1.55	1.74
4	g	2002	093	CAI-SAP	-7.57	1.55	1.74
4	c	2002	093	CAI-SAP	-7.56	1.55	1.74
4	S	2002	093	CAI-SAP	-7.56	1.55	1.74
4	I	2002	093	CAI-SAP	-7.56	1.55	1.74
4	W	2002	093	CAI-SAP	-7.55	1.55	1.74
4	A	2002	093	CAI-SAP	-7.55	1.55	1.74
4	Q	2002	093	CAI-SAP	-7.54	1.55	1.74
4	M	2002	093	CAI-SAP	-7.54	1.55	1.74
4	G	2002	093	CAI-SAP	-7.54	1.55	1.74
4	c	2002	093	SAN-NAU	4.20	1.67	1.61
4	G	2002	093	SAN-NAU	4.18	1.67	1.61
4	M	2002	093	SAN-NAU	4.17	1.67	1.61
4	Y	2002	093	SAN-NAU	4.17	1.67	1.61
4	O	2002	093	SAN-NAU	4.17	1.67	1.61
4	W	2002	093	SAN-NAU	4.17	1.67	1.61
4	Q	2002	093	SAN-NAU	4.16	1.67	1.61
4	C	2002	093	SAN-NAU	4.15	1.67	1.61
4	I	2002	093	SAN-NAU	4.12	1.67	1.61
4	S	2002	093	SAN-NAU	4.12	1.67	1.61
4	A	2002	093	SAN-NAU	4.10	1.67	1.61
4	g	2002	093	SAN-NAU	4.07	1.67	1.61
4	W	2002	093	CAJ-NAK	3.67	1.47	1.37
4	G	2002	093	CAJ-NAK	3.67	1.47	1.37
4	I	2002	093	CAJ-NAK	3.66	1.47	1.37
4	g	2002	093	CAJ-NAK	3.66	1.47	1.37
4	S	2002	093	CAJ-NAK	3.65	1.47	1.37
4	Y	2002	093	CAJ-NAK	3.64	1.47	1.37
4	A	2002	093	CAJ-NAK	3.64	1.47	1.37
4	Q	2002	093	CAJ-NAK	3.64	1.47	1.37
4	M	2002	093	CAJ-NAK	3.63	1.47	1.37
4	O	2002	093	CAJ-NAK	3.62	1.47	1.37
4	C	2002	093	CAJ-NAK	3.62	1.47	1.37
4	c	2002	093	CAJ-NAK	3.62	1.47	1.37
5	D	2000	GSP	C5-C4	3.42	1.48	1.38
5	J	2000	GSP	C5-C4	3.38	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2000	GSP	PG-O2G	3.36	1.65	1.54
5	B	2000	GSP	C6-N1	-3.33	1.32	1.38
5	Z	2000	GSP	PG-O2G	3.27	1.65	1.54
5	R	2000	GSP	C5-C4	3.26	1.47	1.38
5	T	2000	GSP	C5-C4	3.22	1.47	1.38
5	h	2000	GSP	C5-C4	3.19	1.47	1.38
5	J	2000	GSP	PG-O2G	3.16	1.65	1.54
5	h	2000	GSP	PG-O2G	3.15	1.65	1.54
5	d	2000	GSP	PG-O2G	3.13	1.64	1.54
5	Z	2000	GSP	C5-C4	3.11	1.47	1.38
5	X	2000	GSP	C5-C4	3.11	1.47	1.38
4	c	2002	093	OAM-SAN	-3.08	1.40	1.43
5	d	2000	GSP	C5-C4	3.08	1.47	1.38
5	N	2000	GSP	PG-O2G	3.07	1.64	1.54
5	B	2000	GSP	C5-C4	3.06	1.47	1.38
5	J	2000	GSP	PG-S1G	3.05	1.97	1.90
4	O	2002	093	OAM-SAN	-3.05	1.40	1.43
4	M	2002	093	OAM-SAN	-3.03	1.40	1.43
4	g	2002	093	OAM-SAN	-3.01	1.40	1.43
5	R	2000	GSP	PG-O2G	3.01	1.64	1.54
5	H	2000	GSP	C6-N1	-3.00	1.33	1.38
5	H	2000	GSP	C5-C4	3.00	1.47	1.38
5	B	2000	GSP	PG-S1G	3.00	1.97	1.90
4	W	2002	093	OAM-SAN	-2.99	1.40	1.43
4	C	2002	093	OAM-SAN	-2.96	1.40	1.43
4	S	2002	093	OAM-SAN	-2.96	1.40	1.43
4	A	2002	093	OAM-SAN	-2.95	1.40	1.43
5	H	2000	GSP	PG-O2G	2.94	1.64	1.54
4	Q	2002	093	OAM-SAN	-2.94	1.40	1.43
5	R	2000	GSP	PA-O3A	2.93	1.62	1.59
4	I	2002	093	OAM-SAN	-2.91	1.40	1.43
4	G	2002	093	OAM-SAN	-2.90	1.40	1.43
5	P	2000	GSP	C6-N1	-2.90	1.33	1.38
5	D	2000	GSP	PG-O2G	2.88	1.64	1.54
4	Y	2002	093	OAM-SAN	-2.88	1.40	1.43
5	T	2000	GSP	C6-N1	-2.83	1.33	1.38
4	G	2002	093	CAS-NAR	2.82	1.44	1.38
5	D	2000	GSP	PG-S1G	2.80	1.96	1.90
5	X	2000	GSP	C6-N1	-2.80	1.33	1.38
4	C	2002	093	CAS-NAR	2.80	1.44	1.38
4	M	2002	093	CAS-NAR	2.80	1.44	1.38
4	c	2002	093	CAS-NAR	2.80	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	O	2002	093	CAS-NAR	2.77	1.44	1.38
4	A	2002	093	CAS-NAR	2.76	1.44	1.38
5	h	2000	GSP	PG-S1G	2.76	1.96	1.90
5	h	2000	GSP	C6-N1	-2.76	1.33	1.38
4	I	2002	093	CAS-NAR	2.75	1.44	1.38
4	S	2002	093	CAS-NAR	2.74	1.44	1.38
4	g	2002	093	CAS-NAR	2.74	1.44	1.38
5	P	2000	GSP	PG-O2G	2.74	1.63	1.54
4	Q	2002	093	CAS-NAR	2.73	1.44	1.38
4	W	2002	093	CAS-NAR	2.73	1.44	1.38
4	Y	2002	093	CAS-NAR	2.73	1.44	1.38
5	N	2000	GSP	C4-N9	-2.73	1.31	1.38
5	P	2000	GSP	C5-C4	2.70	1.46	1.38
5	N	2000	GSP	C5-C4	2.70	1.46	1.38
5	Z	2000	GSP	C6-N1	-2.68	1.33	1.38
5	P	2000	GSP	PG-S1G	2.64	1.96	1.90
5	N	2000	GSP	C6-N1	-2.64	1.33	1.38
5	P	2000	GSP	C4-N9	-2.64	1.31	1.38
4	I	2002	093	CAV-CAW	-2.62	1.41	1.50
5	J	2000	GSP	C6-N1	-2.61	1.34	1.38
4	G	2002	093	CAV-CAW	-2.61	1.42	1.50
4	C	2002	093	CAV-CAW	-2.60	1.42	1.50
4	Y	2002	093	CAV-CAW	-2.60	1.42	1.50
4	g	2002	093	CAV-CAW	-2.60	1.42	1.50
4	Q	2002	093	CAV-CAW	-2.59	1.42	1.50
4	S	2002	093	CAV-CAW	-2.59	1.42	1.50
4	W	2002	093	CAV-CAW	-2.59	1.42	1.50
4	c	2002	093	CAV-CAW	-2.59	1.42	1.50
4	A	2002	093	CAV-CAW	-2.57	1.42	1.50
4	M	2002	093	CAV-CAW	-2.57	1.42	1.50
4	I	2002	093	CAT-CAS	2.57	1.53	1.49
4	Y	2002	093	CAT-CAS	2.57	1.53	1.49
4	O	2002	093	CAV-CAW	-2.55	1.42	1.50
4	C	2002	093	CAT-CAS	2.55	1.53	1.49
5	d	2000	GSP	PG-O3G	2.54	1.63	1.54
5	d	2000	GSP	C6-N1	-2.53	1.34	1.38
5	X	2000	GSP	PG-O2G	2.53	1.62	1.54
4	O	2002	093	CAT-CAS	2.52	1.53	1.49
4	Q	2002	093	CAT-CAS	2.52	1.53	1.49
4	A	2002	093	CAT-CAS	2.49	1.53	1.49
4	M	2002	093	CAT-CAS	2.49	1.53	1.49
4	g	2002	093	CAT-CAS	2.49	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	T	2000	GSP	PG-O2G	2.48	1.62	1.54
4	G	2002	093	CAT-CAS	2.47	1.53	1.49
4	c	2002	093	CAT-CAS	2.44	1.53	1.49
4	W	2002	093	CAT-CAS	2.44	1.53	1.49
4	S	2002	093	CAT-CAS	2.44	1.53	1.49
5	P	2000	GSP	PG-O3G	2.44	1.62	1.54
5	D	2000	GSP	C6-N1	-2.43	1.34	1.38
5	Z	2000	GSP	C4-N9	-2.39	1.32	1.38
5	d	2000	GSP	C4-N9	-2.38	1.32	1.38
5	h	2000	GSP	PG-O3G	2.34	1.62	1.54
5	d	2000	GSP	PG-S1G	2.32	1.95	1.90
5	Z	2000	GSP	PG-O3G	2.28	1.62	1.54
5	Z	2000	GSP	PG-S1G	2.26	1.95	1.90
5	J	2000	GSP	C4-N9	-2.25	1.32	1.38
5	J	2000	GSP	C5-N7	-2.24	1.34	1.39
5	H	2000	GSP	PG-S1G	2.18	1.95	1.90
5	X	2000	GSP	PG-O3G	2.16	1.61	1.54
5	N	2000	GSP	PG-O3G	2.15	1.61	1.54
5	N	2000	GSP	PG-S1G	2.15	1.95	1.90
5	X	2000	GSP	PB-O3B	2.12	1.61	1.59
5	D	2000	GSP	PG-O3G	2.11	1.61	1.54
5	R	2000	GSP	PG-S1G	2.09	1.95	1.90
5	R	2000	GSP	C6-N1	-2.06	1.35	1.38
5	X	2000	GSP	PG-S1G	2.06	1.95	1.90
5	B	2000	GSP	C5-N7	-2.06	1.35	1.39
5	N	2000	GSP	C5-N7	-2.05	1.35	1.39
5	D	2000	GSP	C5-N7	-2.03	1.35	1.39
5	R	2000	GSP	PG-O3G	2.00	1.61	1.54

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	OAO-SAN-OAM	-20.60	94.51	119.52
4	g	2002	093	OAO-SAN-OAM	-20.57	94.53	119.52
4	Q	2002	093	OAO-SAN-OAM	-20.56	94.55	119.52
4	G	2002	093	OAO-SAN-OAM	-20.55	94.56	119.52
4	C	2002	093	OAO-SAN-OAM	-20.55	94.56	119.52
4	A	2002	093	OAO-SAN-OAM	-20.55	94.57	119.52
4	I	2002	093	OAO-SAN-OAM	-20.54	94.57	119.52
4	Y	2002	093	OAO-SAN-OAM	-20.54	94.58	119.52
4	M	2002	093	OAO-SAN-OAM	-20.53	94.58	119.52
4	W	2002	093	OAO-SAN-OAM	-20.53	94.59	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	O	2002	093	OAO-SAN-OAM	-20.52	94.60	119.52
4	c	2002	093	OAO-SAN-OAM	-20.51	94.61	119.52
4	A	2002	093	CAQ-SAP-CAI	19.60	100.56	88.35
4	W	2002	093	CAQ-SAP-CAI	19.59	100.55	88.35
4	I	2002	093	CAQ-SAP-CAI	19.54	100.52	88.35
4	C	2002	093	CAQ-SAP-CAI	19.53	100.51	88.35
4	G	2002	093	CAQ-SAP-CAI	19.51	100.50	88.35
4	M	2002	093	CAQ-SAP-CAI	19.48	100.48	88.35
4	Y	2002	093	CAQ-SAP-CAI	19.47	100.47	88.35
4	O	2002	093	CAQ-SAP-CAI	19.47	100.47	88.35
4	g	2002	093	CAQ-SAP-CAI	19.45	100.46	88.35
4	c	2002	093	CAQ-SAP-CAI	19.44	100.45	88.35
4	S	2002	093	CAQ-SAP-CAI	19.43	100.45	88.35
4	Q	2002	093	CAQ-SAP-CAI	19.43	100.45	88.35
5	H	2000	GSP	C5-C4-N3	-6.66	117.80	128.39
5	h	2000	GSP	C5-C4-N3	-6.59	117.90	128.39
5	B	2000	GSP	C5-C4-N3	-6.56	117.94	128.39
5	T	2000	GSP	C5-C4-N3	-6.18	118.56	128.39
5	X	2000	GSP	C5-C4-N3	-6.10	118.67	128.39
5	D	2000	GSP	C5-C4-N3	-6.03	118.80	128.39
5	R	2000	GSP	C5-C4-N3	-5.95	118.92	128.39
5	J	2000	GSP	C5-C4-N3	-5.78	119.19	128.39
5	Z	2000	GSP	C5-C4-N3	-5.49	119.65	128.39
5	T	2000	GSP	PB-O3B-PG	-5.43	113.31	133.17
5	h	2000	GSP	C2-N3-C4	5.43	121.65	112.30
5	d	2000	GSP	C5-C4-N3	-5.42	119.76	128.39
5	P	2000	GSP	C5-C4-N3	-5.30	119.96	128.39
4	S	2002	093	OAO-SAN-NAU	5.23	115.18	107.03
4	Q	2002	093	OAO-SAN-NAU	5.22	115.15	107.03
4	Y	2002	093	OAO-SAN-NAU	5.21	115.15	107.03
4	O	2002	093	OAO-SAN-NAU	5.20	115.13	107.03
4	A	2002	093	OAO-SAN-NAU	5.20	115.12	107.03
4	W	2002	093	OAO-SAN-NAU	5.19	115.11	107.03
4	G	2002	093	OAO-SAN-NAU	5.19	115.11	107.03
4	c	2002	093	OAO-SAN-NAU	5.18	115.10	107.03
5	H	2000	GSP	PB-O3B-PG	-5.17	114.24	133.17
4	g	2002	093	OAO-SAN-NAU	5.17	115.08	107.03
4	M	2002	093	OAO-SAN-NAU	5.17	115.08	107.03
4	C	2002	093	OAO-SAN-NAU	5.17	115.07	107.03
4	I	2002	093	OAO-SAN-NAU	5.17	115.07	107.03
5	N	2000	GSP	PB-O3B-PG	-5.14	114.37	133.17
5	d	2000	GSP	PB-O3B-PG	-5.11	114.48	133.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	2000	GSP	PB-O3B-PG	-5.10	114.50	133.17
5	J	2000	GSP	PB-O3B-PG	-5.04	114.73	133.17
5	R	2000	GSP	N9-C4-N3	5.01	135.96	125.95
5	Z	2000	GSP	PB-O3B-PG	-4.98	114.93	133.17
5	H	2000	GSP	C2-N3-C4	4.97	120.85	112.30
5	D	2000	GSP	PB-O3B-PG	-4.92	115.17	133.17
5	B	2000	GSP	PB-O3B-PG	-4.90	115.24	133.17
5	N	2000	GSP	C5-C4-N3	-4.87	120.63	128.39
5	X	2000	GSP	C2-N3-C4	4.87	120.68	112.30
5	B	2000	GSP	C2-N3-C4	4.86	120.67	112.30
5	X	2000	GSP	PB-O3B-PG	-4.80	115.60	133.17
5	H	2000	GSP	N9-C4-N3	4.79	135.52	125.95
5	P	2000	GSP	PB-O3B-PG	-4.76	115.73	133.17
5	R	2000	GSP	C2-N3-C4	4.75	120.48	112.30
4	g	2002	093	OAM-SAN-NAU	4.68	114.32	107.03
5	h	2000	GSP	N9-C4-N3	4.67	135.29	125.95
4	S	2002	093	OAM-SAN-NAU	4.66	114.28	107.03
4	Q	2002	093	OAM-SAN-NAU	4.65	114.27	107.03
4	A	2002	093	OAM-SAN-NAU	4.64	114.26	107.03
4	I	2002	093	OAM-SAN-NAU	4.64	114.26	107.03
4	W	2002	093	OAM-SAN-NAU	4.63	114.25	107.03
4	G	2002	093	OAM-SAN-NAU	4.63	114.24	107.03
4	M	2002	093	OAM-SAN-NAU	4.61	114.21	107.03
4	c	2002	093	OAM-SAN-NAU	4.61	114.20	107.03
4	C	2002	093	OAM-SAN-NAU	4.61	114.20	107.03
5	h	2000	GSP	PB-O3B-PG	-4.60	116.34	133.17
4	Y	2002	093	OAM-SAN-NAU	4.59	114.18	107.03
4	O	2002	093	OAM-SAN-NAU	4.59	114.18	107.03
4	c	2002	093	CAE-CAJ-CAI	-4.55	125.62	130.98
5	d	2000	GSP	C2-N3-C4	4.55	120.14	112.30
4	Y	2002	093	CAE-CAJ-CAI	-4.55	125.63	130.98
4	A	2002	093	CAE-CAJ-CAI	-4.54	125.64	130.98
4	W	2002	093	CAE-CAJ-CAI	-4.54	125.64	130.98
5	T	2000	GSP	N9-C4-N3	4.53	135.02	125.95
4	G	2002	093	CAE-CAJ-CAI	-4.53	125.65	130.98
5	D	2000	GSP	C2-N3-C4	4.53	120.10	112.30
4	M	2002	093	CAE-CAJ-CAI	-4.53	125.66	130.98
4	O	2002	093	CAE-CAJ-CAI	-4.52	125.66	130.98
4	C	2002	093	CAE-CAJ-CAI	-4.51	125.68	130.98
4	I	2002	093	CAE-CAJ-CAI	-4.49	125.70	130.98
4	g	2002	093	CAE-CAJ-CAI	-4.47	125.72	130.98
4	Q	2002	093	CAE-CAJ-CAI	-4.47	125.73	130.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	CAE-CAJ-CAI	-4.45	125.74	130.98
5	T	2000	GSP	C2-N3-C4	4.45	119.96	112.30
5	X	2000	GSP	N9-C4-N3	4.43	134.82	125.95
5	B	2000	GSP	N9-C4-N3	4.30	134.54	125.95
5	D	2000	GSP	N9-C4-N3	4.29	134.53	125.95
5	J	2000	GSP	C2-N3-C4	4.26	119.64	112.30
5	N	2000	GSP	N9-C4-N3	4.23	134.42	125.95
5	P	2000	GSP	N9-C4-N3	4.22	134.39	125.95
4	C	2002	093	CAT-CAS-NAR	4.16	121.00	114.84
4	G	2002	093	CAT-CAS-NAR	4.16	121.00	114.84
4	A	2002	093	CAT-CAS-NAR	4.15	120.98	114.84
4	W	2002	093	CAT-CAS-NAR	4.15	120.98	114.84
4	I	2002	093	CAT-CAS-NAR	4.14	120.98	114.84
4	Y	2002	093	CAT-CAS-NAR	4.13	120.96	114.84
5	Z	2000	GSP	N9-C4-N3	4.12	134.20	125.95
4	g	2002	093	CAT-CAS-NAR	4.12	120.95	114.84
4	S	2002	093	CAT-CAS-NAR	4.12	120.94	114.84
4	c	2002	093	CAT-CAS-NAR	4.12	120.94	114.84
4	Q	2002	093	CAT-CAS-NAR	4.10	120.91	114.84
5	Z	2000	GSP	C2-N3-C4	4.09	119.34	112.30
4	M	2002	093	CAT-CAS-NAR	4.09	120.90	114.84
4	O	2002	093	CAT-CAS-NAR	4.09	120.90	114.84
5	P	2000	GSP	C2-N3-C4	4.05	119.27	112.30
4	C	2002	093	OAM-SAN-CAF	3.91	114.14	107.68
4	c	2002	093	OAM-SAN-CAF	3.91	114.13	107.68
4	M	2002	093	OAM-SAN-CAF	3.88	114.09	107.68
4	I	2002	093	OAM-SAN-CAF	3.88	114.08	107.68
4	Y	2002	093	OAM-SAN-CAF	3.87	114.07	107.68
4	G	2002	093	OAM-SAN-CAF	3.86	114.06	107.68
4	Q	2002	093	OAO-SAN-CAF	3.86	114.05	107.68
4	O	2002	093	OAO-SAN-CAF	3.86	114.05	107.68
4	S	2002	093	OAO-SAN-CAF	3.86	114.05	107.68
4	Y	2002	093	OAO-SAN-CAF	3.86	114.05	107.68
4	O	2002	093	OAM-SAN-CAF	3.86	114.05	107.68
4	C	2002	093	OAO-SAN-CAF	3.86	114.05	107.68
5	d	2000	GSP	N9-C4-N3	3.86	133.66	125.95
4	W	2002	093	OAM-SAN-CAF	3.85	114.04	107.68
4	g	2002	093	OAM-SAN-CAF	3.85	114.04	107.68
4	A	2002	093	OAM-SAN-CAF	3.85	114.03	107.68
4	M	2002	093	OAO-SAN-CAF	3.85	114.03	107.68
4	W	2002	093	OAO-SAN-CAF	3.84	114.02	107.68
4	Q	2002	093	OAM-SAN-CAF	3.84	114.02	107.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	2002	093	OAM-SAN-CAF	3.83	114.01	107.68
4	G	2002	093	OAO-SAN-CAF	3.83	114.01	107.68
4	g	2002	093	OAO-SAN-CAF	3.83	114.00	107.68
4	I	2002	093	OAO-SAN-CAF	3.82	113.99	107.68
4	c	2002	093	OAO-SAN-CAF	3.82	113.98	107.68
4	A	2002	093	OAO-SAN-CAF	3.81	113.98	107.68
5	J	2000	GSP	N9-C4-N3	3.79	133.53	125.95
5	B	2000	GSP	C6-C5-N7	3.79	137.18	130.29
5	N	2000	GSP	C2-N3-C4	3.78	118.81	112.30
5	h	2000	GSP	C6-C5-N7	3.76	137.12	130.29
5	d	2000	GSP	C6-C5-N7	3.69	137.01	130.29
5	X	2000	GSP	C6-C5-N7	3.64	136.91	130.29
5	J	2000	GSP	C4-C5-N7	-3.62	104.93	110.67
5	J	2000	GSP	C6-C5-N7	3.59	136.82	130.29
5	D	2000	GSP	C6-C5-N7	3.57	136.80	130.29
5	H	2000	GSP	C6-C5-N7	3.47	136.60	130.29
5	P	2000	GSP	C6-C5-N7	3.46	136.58	130.29
5	D	2000	GSP	C4-C5-N7	-3.44	105.22	110.67
5	B	2000	GSP	C4-C5-N7	-3.41	105.26	110.67
5	Z	2000	GSP	C6-C5-N7	3.33	136.34	130.29
4	g	2002	093	OAX-CAW-CAV	-3.28	99.44	111.50
4	A	2002	093	OAX-CAW-CAV	-3.28	99.45	111.50
4	G	2002	093	OAX-CAW-CAV	-3.28	99.46	111.50
4	W	2002	093	OAX-CAW-CAV	-3.28	99.47	111.50
4	c	2002	093	OAX-CAW-CAV	-3.27	99.47	111.50
4	O	2002	093	OAX-CAW-CAV	-3.27	99.49	111.50
4	Q	2002	093	OAX-CAW-CAV	-3.27	99.49	111.50
4	M	2002	093	OAX-CAW-CAV	-3.27	99.49	111.50
4	S	2002	093	OAX-CAW-CAV	-3.26	99.51	111.50
4	C	2002	093	OAX-CAW-CAV	-3.26	99.52	111.50
4	Y	2002	093	OAX-CAW-CAV	-3.26	99.53	111.50
4	I	2002	093	OAX-CAW-CAV	-3.24	99.60	111.50
5	H	2000	GSP	C4-C5-N7	-3.22	105.57	110.67
5	N	2000	GSP	C6-C5-N7	3.20	136.12	130.29
5	X	2000	GSP	C2'-C3'-C4'	3.12	108.63	102.61
5	T	2000	GSP	C6-C5-N7	3.04	135.82	130.29
5	h	2000	GSP	C4-C5-N7	-3.00	105.92	110.67
5	h	2000	GSP	C2'-C3'-C4'	2.89	108.19	102.61
5	N	2000	GSP	C8-N9-C4	2.87	111.41	106.03
5	T	2000	GSP	O2G-PG-O3B	2.85	114.15	104.64
5	R	2000	GSP	C6-C5-N7	2.84	135.45	130.29
4	c	2002	093	OAL-CAS-NAR	-2.82	118.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2002	093	OAL-CAS-NAR	-2.82	118.25	123.63
4	S	2002	093	OAL-CAS-NAR	-2.82	118.25	123.63
4	O	2002	093	OAL-CAS-NAR	-2.81	118.26	123.63
5	Z	2000	GSP	C4-C5-N7	-2.81	106.22	110.67
4	g	2002	093	OAL-CAS-NAR	-2.80	118.27	123.63
4	C	2002	093	OAL-CAS-NAR	-2.80	118.28	123.63
4	A	2002	093	OAL-CAS-NAR	-2.80	118.28	123.63
4	W	2002	093	OAL-CAS-NAR	-2.79	118.29	123.63
4	I	2002	093	OAL-CAS-NAR	-2.79	118.30	123.63
4	M	2002	093	OAL-CAS-NAR	-2.79	118.30	123.63
4	Q	2002	093	OAL-CAS-NAR	-2.77	118.33	123.63
4	Y	2002	093	OAL-CAS-NAR	-2.77	118.33	123.63
5	T	2000	GSP	C4-C5-N7	-2.73	106.35	110.67
5	X	2000	GSP	C4-C5-N7	-2.72	106.35	110.67
5	R	2000	GSP	O2G-PG-O3B	2.67	113.56	104.64
5	P	2000	GSP	C4-C5-N7	-2.65	106.47	110.67
5	P	2000	GSP	C8-N9-C4	2.64	110.97	106.03
5	d	2000	GSP	C4-C5-N7	-2.63	106.51	110.67
5	D	2000	GSP	C8-N7-C5	2.60	108.89	104.26
4	M	2002	093	CAD-CAH-CAG	2.60	122.25	119.25
4	c	2002	093	CAD-CAH-CAG	2.57	122.23	119.25
4	g	2002	093	CAD-CAH-CAG	2.57	122.22	119.25
4	C	2002	093	CAD-CAH-CAG	2.56	122.21	119.25
5	J	2000	GSP	C8-N7-C5	2.56	108.82	104.26
4	O	2002	093	CAD-CAH-CAG	2.56	122.21	119.25
5	P	2000	GSP	N9-C8-N7	-2.55	108.67	113.40
4	I	2002	093	CAD-CAH-CAG	2.55	122.20	119.25
4	Y	2002	093	CAD-CAH-CAG	2.55	122.20	119.25
4	S	2002	093	CAD-CAH-CAG	2.55	122.19	119.25
4	W	2002	093	CAD-CAH-CAG	2.53	122.18	119.25
5	N	2000	GSP	N9-C8-N7	-2.52	108.73	113.40
4	Q	2002	093	CAD-CAH-CAG	2.51	122.16	119.25
5	B	2000	GSP	C2-N1-C6	-2.50	120.58	125.11
4	G	2002	093	CAD-CAH-CAG	2.50	122.14	119.25
4	A	2002	093	CAD-CAH-CAG	2.49	122.13	119.25
5	P	2000	GSP	O3B-PB-O1B	-2.45	103.32	110.70
5	N	2000	GSP	O2B-PB-O1B	2.45	123.86	112.44
5	N	2000	GSP	O2G-PG-O3B	2.44	112.79	104.64
5	H	2000	GSP	C8-N7-C5	2.44	108.60	104.26
5	J	2000	GSP	O2B-PB-O1B	2.44	123.78	112.44
5	P	2000	GSP	O2B-PB-O1B	2.42	123.72	112.44
5	X	2000	GSP	O2B-PB-O1B	2.41	123.67	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2000	GSP	O2B-PB-O1B	2.41	123.64	112.44
5	h	2000	GSP	O2B-PB-O1B	2.38	123.50	112.44
5	N	2000	GSP	C4-C5-N7	-2.38	106.91	110.67
5	D	2000	GSP	C2'-C3'-C4'	2.36	107.17	102.61
5	D	2000	GSP	O2G-PG-O3B	2.35	112.50	104.64
5	d	2000	GSP	C2'-C3'-C4'	2.35	107.15	102.61
5	R	2000	GSP	O6-C6-C5	-2.35	120.34	126.53
5	B	2000	GSP	C8-N7-C5	2.34	108.43	104.26
5	d	2000	GSP	O2G-PG-O3B	2.29	112.29	104.64
5	h	2000	GSP	C5-C6-N1	2.27	119.02	113.25
5	h	2000	GSP	C8-N7-C5	2.26	108.28	104.26
5	J	2000	GSP	O2G-PG-O3B	2.25	112.16	104.64
5	P	2000	GSP	C8-N7-C5	2.23	108.24	104.26
5	X	2000	GSP	C5-C6-N1	2.23	118.92	113.25
5	R	2000	GSP	C4-C5-N7	-2.19	107.19	110.67
5	Z	2000	GSP	O2B-PB-O1B	2.19	122.61	112.44
5	Z	2000	GSP	C8-N7-C5	2.17	108.13	104.26
5	Z	2000	GSP	C2'-C3'-C4'	2.17	106.79	102.61
5	T	2000	GSP	O2B-PB-O1B	2.15	122.44	112.44
5	H	2000	GSP	C2-N1-C6	-2.15	121.22	125.11
5	h	2000	GSP	O3B-PB-O1B	-2.15	104.25	110.70
5	T	2000	GSP	C2'-C3'-C4'	2.14	106.75	102.61
4	C	2002	093	CAE-CAJ-NAK	2.13	125.70	121.36
4	I	2002	093	CAE-CAJ-NAK	2.13	125.69	121.36
4	Y	2002	093	CAE-CAJ-NAK	2.13	125.69	121.36
5	H	2000	GSP	O2G-PG-O3B	2.13	111.74	104.64
5	B	2000	GSP	C5-C6-N1	2.12	118.65	113.25
5	N	2000	GSP	C8-N7-C5	2.11	108.01	104.26
4	G	2002	093	CAE-CAJ-NAK	2.11	125.64	121.36
5	h	2000	GSP	O6-C6-C5	-2.10	120.99	126.53
4	g	2002	093	CAE-CAJ-NAK	2.10	125.63	121.36
4	W	2002	093	CAE-CAJ-NAK	2.09	125.62	121.36
5	Z	2000	GSP	C8-N9-C4	2.09	109.95	106.03
5	R	2000	GSP	C8-N9-C4	2.09	109.95	106.03
4	A	2002	093	CAE-CAJ-NAK	2.09	125.62	121.36
4	c	2002	093	CAE-CAJ-NAK	2.09	125.62	121.36
4	Q	2002	093	CAE-CAJ-NAK	2.09	125.61	121.36
5	X	2000	GSP	O3B-PB-O1B	-2.09	104.42	110.70
4	M	2002	093	CAE-CAJ-NAK	2.09	125.61	121.36
4	O	2002	093	CAE-CAJ-NAK	2.08	125.60	121.36
5	X	2000	GSP	C2-N1-C6	-2.08	121.33	125.11
5	H	2000	GSP	O2B-PB-O1B	2.08	122.13	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	2000	GSP	N9-C8-N7	-2.08	109.55	113.40
5	P	2000	GSP	C2-N1-C6	-2.08	121.35	125.11
4	S	2002	093	CAE-CAJ-NAK	2.07	125.58	121.36
5	J	2000	GSP	O3A-PA-O1A	2.07	116.92	110.70
4	A	2002	093	CAH-CAI-SAP	2.06	122.57	117.32
5	d	2000	GSP	C5-C6-N1	2.06	118.49	113.25
4	G	2002	093	CAH-CAI-SAP	2.05	122.54	117.32
4	Q	2002	093	CAF-SAN-NAU	-2.05	105.07	107.86
4	W	2002	093	CAH-CAI-SAP	2.04	122.52	117.32
4	S	2002	093	CAF-SAN-NAU	-2.04	105.08	107.86
4	c	2002	093	CAF-SAN-NAU	-2.04	105.08	107.86
4	Y	2002	093	CAF-SAN-NAU	-2.04	105.08	107.86
4	C	2002	093	CAF-SAN-NAU	-2.03	105.09	107.86
5	J	2000	GSP	O3B-PB-O1B	-2.03	104.60	110.70
4	S	2002	093	CAH-CAI-SAP	2.03	122.48	117.32
4	I	2002	093	CAH-CAI-SAP	2.03	122.48	117.32
4	O	2002	093	CAF-SAN-NAU	-2.03	105.10	107.86
5	P	2000	GSP	O2G-PG-O3B	2.02	111.40	104.64
5	X	2000	GSP	C8-N7-C5	2.02	107.87	104.26
4	c	2002	093	CAI-CAJ-NAK	2.02	108.76	105.70
4	W	2002	093	CAF-SAN-NAU	-2.02	105.10	107.86
4	C	2002	093	CAH-CAI-SAP	2.02	122.47	117.32
5	T	2000	GSP	C8-N7-C5	2.02	107.86	104.26
4	Y	2002	093	CAH-CAI-SAP	2.02	122.47	117.32
4	M	2002	093	CAH-CAI-SAP	2.02	122.47	117.32
4	O	2002	093	CAH-CAI-SAP	2.02	122.46	117.32
4	M	2002	093	CAF-SAN-NAU	-2.02	105.11	107.86
4	A	2002	093	CAI-CAJ-NAK	2.02	108.75	105.70
4	Q	2002	093	CAH-CAI-SAP	2.01	122.44	117.32
4	M	2002	093	CAI-CAJ-NAK	2.01	108.74	105.70
4	W	2002	093	CAI-CAJ-NAK	2.01	108.74	105.70
5	X	2000	GSP	O6-C6-C5	-2.01	121.23	126.53
4	G	2002	093	CAF-SAN-NAU	-2.01	105.12	107.86
4	g	2002	093	CAF-SAN-NAU	-2.01	105.13	107.86
4	O	2002	093	CAI-CAJ-NAK	2.01	108.73	105.70
4	c	2002	093	CAH-CAI-SAP	2.00	122.42	117.32
4	I	2002	093	CAF-SAN-NAU	-2.00	105.13	107.86
5	Z	2000	GSP	C2-N1-C6	-2.00	121.48	125.11

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2002	093	NAK-CAQ-NAR-CAS
4	A	2002	093	SAP-CAQ-NAR-CAS
4	C	2002	093	NAK-CAQ-NAR-CAS
4	C	2002	093	SAP-CAQ-NAR-CAS
4	G	2002	093	NAK-CAQ-NAR-CAS
4	G	2002	093	SAP-CAQ-NAR-CAS
4	I	2002	093	NAK-CAQ-NAR-CAS
4	I	2002	093	SAP-CAQ-NAR-CAS
4	M	2002	093	NAK-CAQ-NAR-CAS
4	M	2002	093	SAP-CAQ-NAR-CAS
4	O	2002	093	NAK-CAQ-NAR-CAS
4	O	2002	093	SAP-CAQ-NAR-CAS
4	Q	2002	093	NAK-CAQ-NAR-CAS
4	Q	2002	093	SAP-CAQ-NAR-CAS
4	S	2002	093	NAK-CAQ-NAR-CAS
4	S	2002	093	SAP-CAQ-NAR-CAS
4	W	2002	093	NAK-CAQ-NAR-CAS
4	W	2002	093	SAP-CAQ-NAR-CAS
4	Y	2002	093	NAK-CAQ-NAR-CAS
4	Y	2002	093	SAP-CAQ-NAR-CAS
4	c	2002	093	NAK-CAQ-NAR-CAS
4	c	2002	093	SAP-CAQ-NAR-CAS
4	g	2002	093	NAK-CAQ-NAR-CAS
4	g	2002	093	SAP-CAQ-NAR-CAS
5	B	2000	GSP	C5'-O5'-PA-O2A
5	B	2000	GSP	C5'-O5'-PA-O3A
5	D	2000	GSP	C5'-O5'-PA-O2A
5	H	2000	GSP	C5'-O5'-PA-O2A
5	H	2000	GSP	C5'-O5'-PA-O3A
5	J	2000	GSP	C5'-O5'-PA-O2A
5	N	2000	GSP	C5'-O5'-PA-O2A
5	P	2000	GSP	C5'-O5'-PA-O2A
5	R	2000	GSP	C5'-O5'-PA-O2A
5	T	2000	GSP	C5'-O5'-PA-O2A
5	X	2000	GSP	C5'-O5'-PA-O2A
5	X	2000	GSP	C5'-O5'-PA-O3A
5	Z	2000	GSP	C5'-O5'-PA-O2A
5	Z	2000	GSP	C5'-O5'-PA-O3A
5	d	2000	GSP	C5'-O5'-PA-O2A
5	h	2000	GSP	C5'-O5'-PA-O2A
5	h	2000	GSP	C5'-O5'-PA-O3A
4	A	2002	093	CAV-NAU-SAN-OAO
4	C	2002	093	CAV-NAU-SAN-OAO

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Mol	Chain	Res	Type	Atoms
4	G	2002	093	CAV-NAU-SAN-OAO
4	I	2002	093	CAV-NAU-SAN-OAO
4	M	2002	093	CAV-NAU-SAN-OAO
4	O	2002	093	CAV-NAU-SAN-OAO
4	Q	2002	093	CAV-NAU-SAN-OAO
4	S	2002	093	CAV-NAU-SAN-OAO
4	W	2002	093	CAV-NAU-SAN-OAO
4	Y	2002	093	CAV-NAU-SAN-OAO
4	c	2002	093	CAV-NAU-SAN-OAO
4	g	2002	093	CAV-NAU-SAN-OAO
4	A	2002	093	NAU-CAV-CAW-OAX
4	C	2002	093	NAU-CAV-CAW-OAX
4	G	2002	093	NAU-CAV-CAW-OAX
4	I	2002	093	NAU-CAV-CAW-OAX
4	M	2002	093	NAU-CAV-CAW-OAX
4	O	2002	093	NAU-CAV-CAW-OAX
4	Q	2002	093	NAU-CAV-CAW-OAX
4	S	2002	093	NAU-CAV-CAW-OAX
4	W	2002	093	NAU-CAV-CAW-OAX
4	Y	2002	093	NAU-CAV-CAW-OAX
4	c	2002	093	NAU-CAV-CAW-OAX
4	g	2002	093	NAU-CAV-CAW-OAX
4	A	2002	093	CAV-NAU-SAN-CAF
4	C	2002	093	CAV-NAU-SAN-CAF
4	G	2002	093	CAV-NAU-SAN-CAF
4	I	2002	093	CAV-NAU-SAN-CAF
4	M	2002	093	CAV-NAU-SAN-CAF
4	O	2002	093	CAV-NAU-SAN-CAF
4	Q	2002	093	CAV-NAU-SAN-CAF
4	S	2002	093	CAV-NAU-SAN-CAF
4	W	2002	093	CAV-NAU-SAN-CAF
4	Y	2002	093	CAV-NAU-SAN-CAF
4	c	2002	093	CAV-NAU-SAN-CAF
4	g	2002	093	CAV-NAU-SAN-CAF
4	A	2002	093	CAV-NAU-SAN-OAM
4	C	2002	093	CAV-NAU-SAN-OAM
4	G	2002	093	CAV-NAU-SAN-OAM
4	I	2002	093	CAV-NAU-SAN-OAM
4	M	2002	093	CAV-NAU-SAN-OAM
4	O	2002	093	CAV-NAU-SAN-OAM
4	Q	2002	093	CAV-NAU-SAN-OAM
4	S	2002	093	CAV-NAU-SAN-OAM

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Mol	Chain	Res	Type	Atoms
4	W	2002	093	CAV-NAU-SAN-OAM
4	Y	2002	093	CAV-NAU-SAN-OAM
4	c	2002	093	CAV-NAU-SAN-OAM
4	g	2002	093	CAV-NAU-SAN-OAM
4	A	2002	093	CAB-CAF-SAN-OAO
4	C	2002	093	CAB-CAF-SAN-OAO
4	G	2002	093	CAB-CAF-SAN-OAO
4	I	2002	093	CAB-CAF-SAN-OAO
4	M	2002	093	CAB-CAF-SAN-OAO
4	O	2002	093	CAB-CAF-SAN-OAO
4	Q	2002	093	CAB-CAF-SAN-OAO
4	S	2002	093	CAB-CAF-SAN-OAO
4	W	2002	093	CAB-CAF-SAN-OAO
4	Y	2002	093	CAB-CAF-SAN-OAO
4	c	2002	093	CAB-CAF-SAN-OAO
4	g	2002	093	CAB-CAF-SAN-OAO
5	B	2000	GSP	C5'-O5'-PA-O1A
5	D	2000	GSP	C5'-O5'-PA-O1A
5	D	2000	GSP	C5'-O5'-PA-O3A
5	H	2000	GSP	C5'-O5'-PA-O1A
5	J	2000	GSP	C5'-O5'-PA-O1A
5	J	2000	GSP	C5'-O5'-PA-O3A
5	N	2000	GSP	C5'-O5'-PA-O1A
5	N	2000	GSP	C5'-O5'-PA-O3A
5	P	2000	GSP	C5'-O5'-PA-O1A
5	P	2000	GSP	C5'-O5'-PA-O3A
5	R	2000	GSP	C5'-O5'-PA-O1A
5	R	2000	GSP	C5'-O5'-PA-O3A
5	T	2000	GSP	C5'-O5'-PA-O1A
5	T	2000	GSP	C5'-O5'-PA-O3A
5	X	2000	GSP	C5'-O5'-PA-O1A
5	Z	2000	GSP	C5'-O5'-PA-O1A
5	d	2000	GSP	C5'-O5'-PA-O1A
5	d	2000	GSP	C5'-O5'-PA-O3A
5	h	2000	GSP	C5'-O5'-PA-O1A
4	Q	2002	093	CAG-CAF-SAN-OAO
4	S	2002	093	CAG-CAF-SAN-OAO
4	g	2002	093	CAG-CAF-SAN-OAO
4	A	2002	093	CAG-CAF-SAN-OAO
4	I	2002	093	CAG-CAF-SAN-OAO
4	M	2002	093	CAG-CAF-SAN-OAO
4	O	2002	093	CAG-CAF-SAN-OAO

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Mol	Chain	Res	Type	Atoms
4	W	2002	093	CAG-CAF-SAN-OAO
4	Y	2002	093	CAG-CAF-SAN-OAO
4	G	2002	093	CAG-CAF-SAN-OAO
4	c	2002	093	CAG-CAF-SAN-OAO
4	C	2002	093	CAG-CAF-SAN-OAO

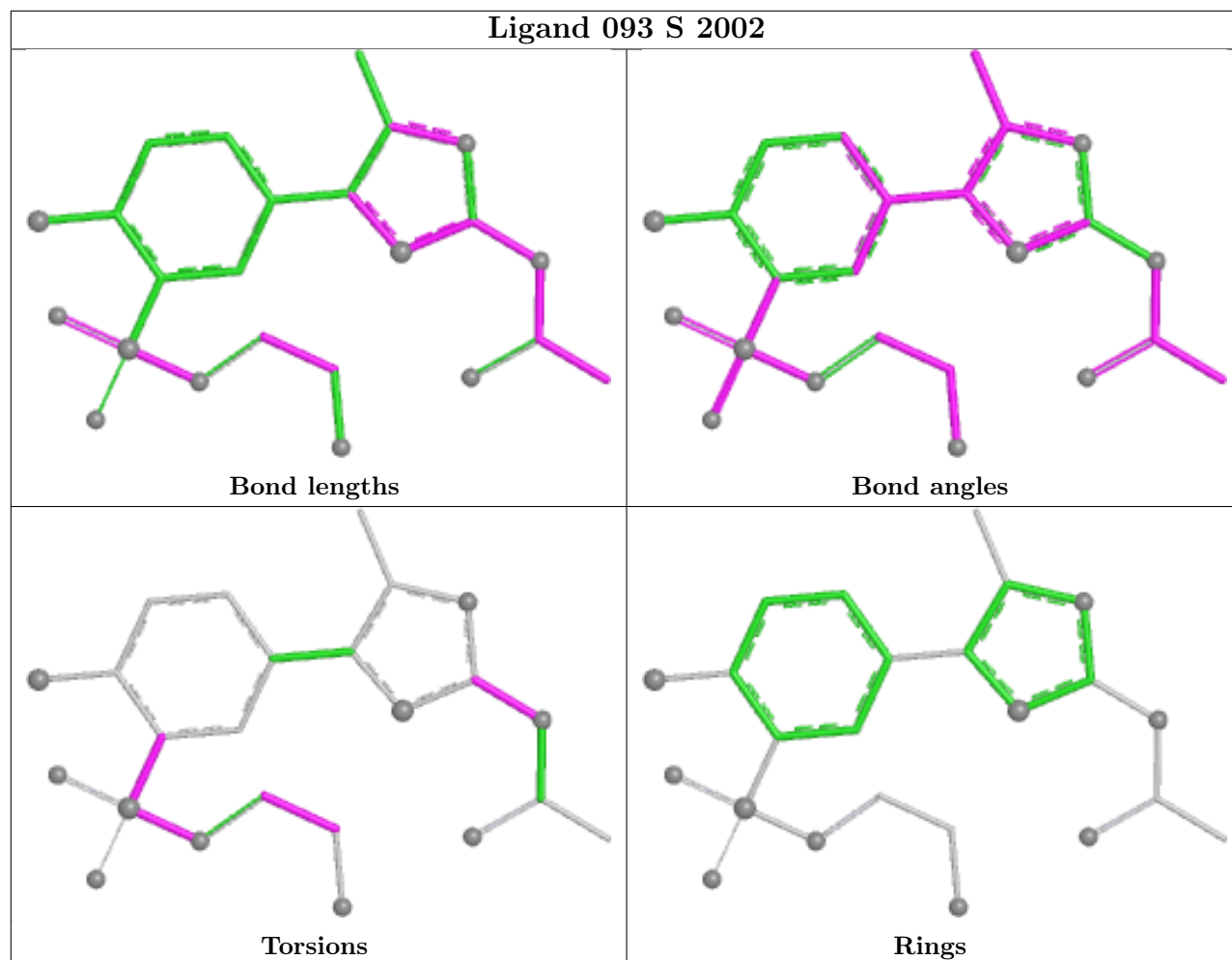
There are no ring outliers.

12 monomers are involved in 75 short contacts:

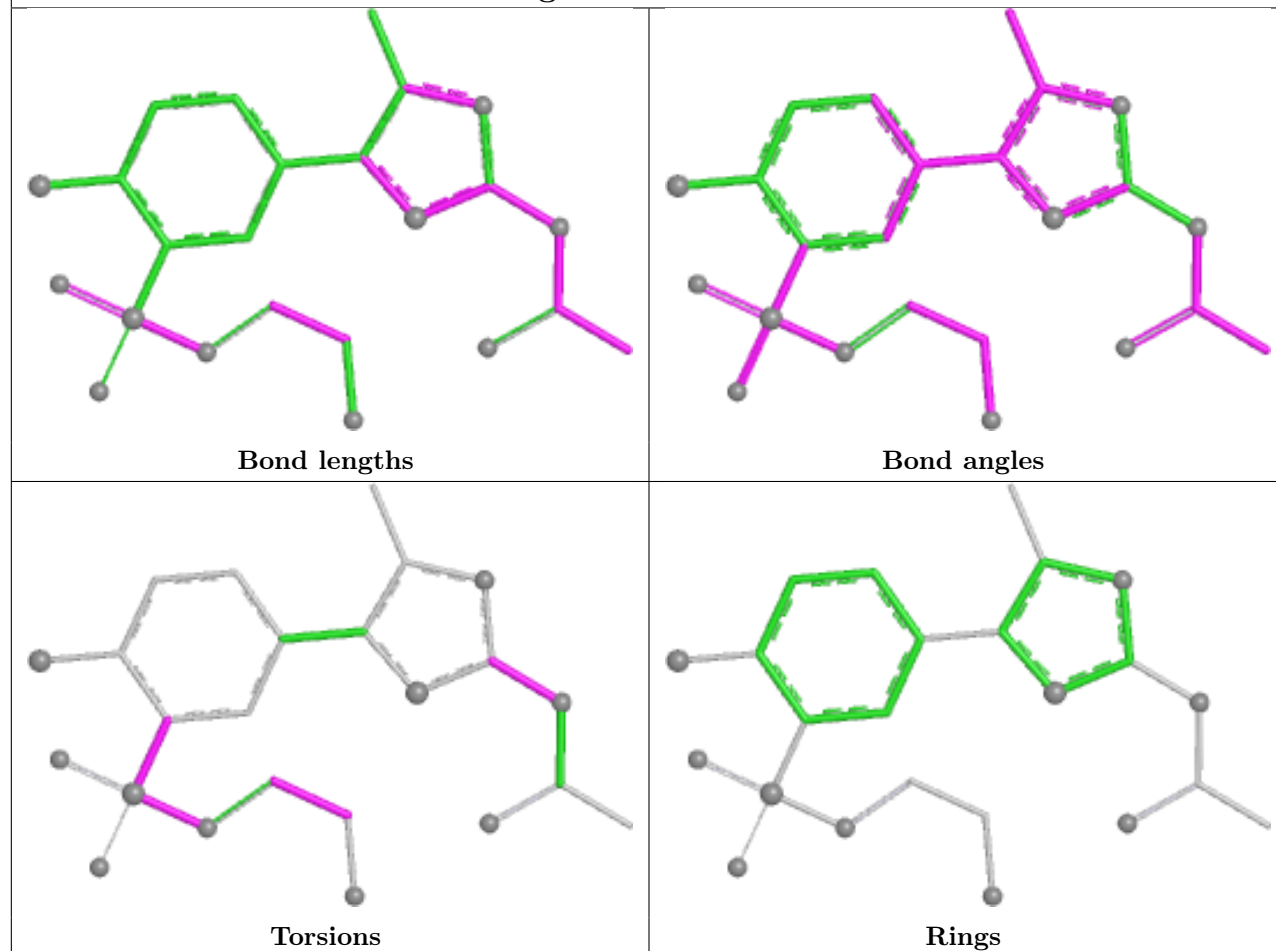
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	2000	GSP	6	0
5	R	2000	GSP	6	0
5	J	2000	GSP	4	0
5	H	2000	GSP	4	0
5	X	2000	GSP	6	0
5	P	2000	GSP	7	0
5	D	2000	GSP	6	0
5	B	2000	GSP	6	0
5	Z	2000	GSP	6	0
5	d	2000	GSP	11	0
5	h	2000	GSP	7	0
5	N	2000	GSP	6	0

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

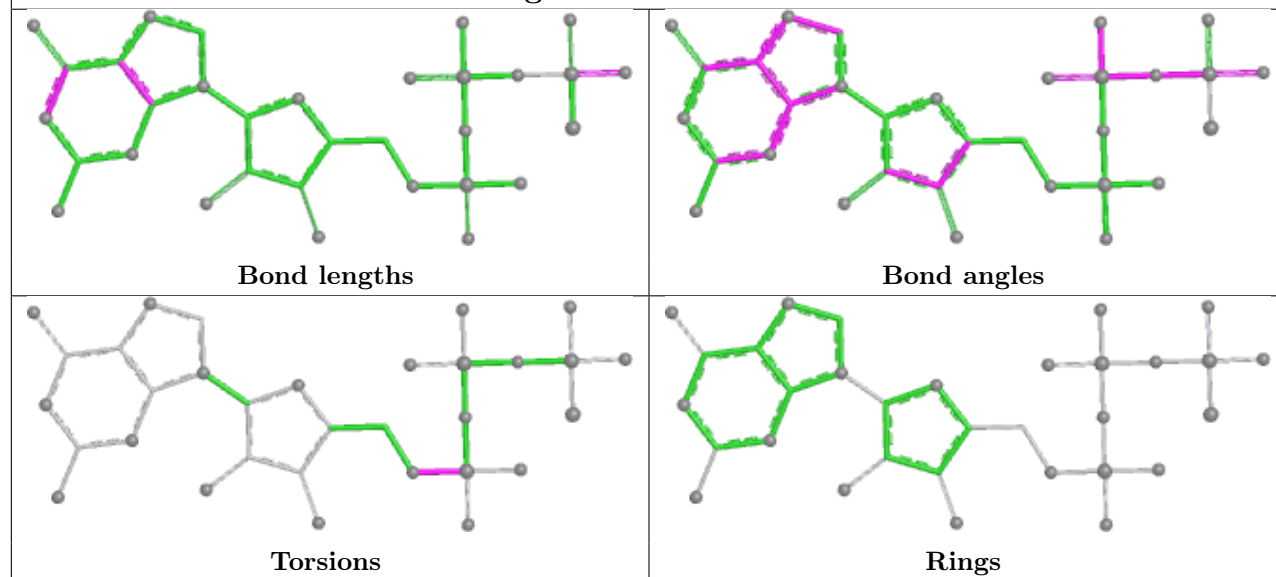
Ligand 093 S 2002



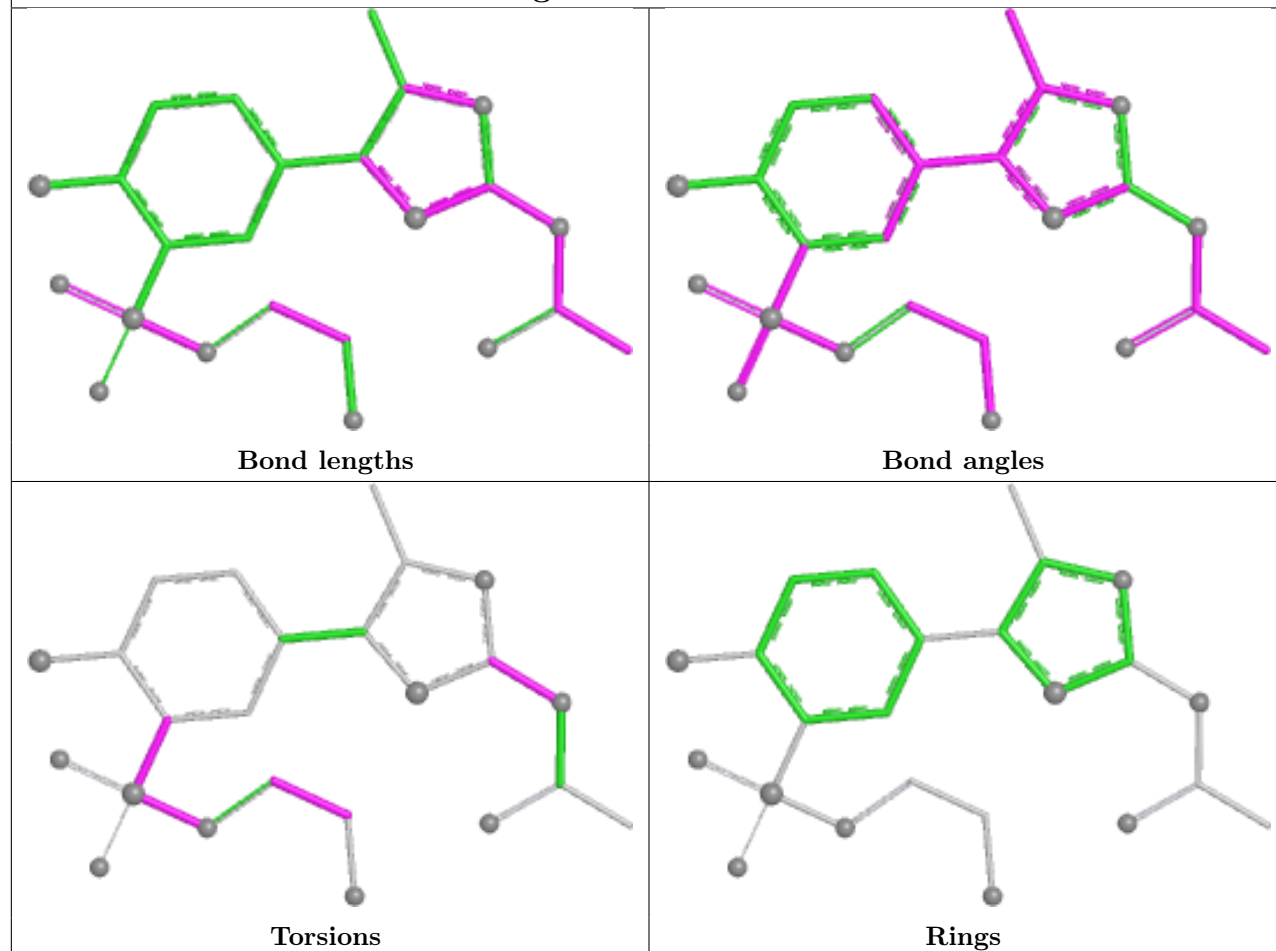
Ligand 093 c 2002



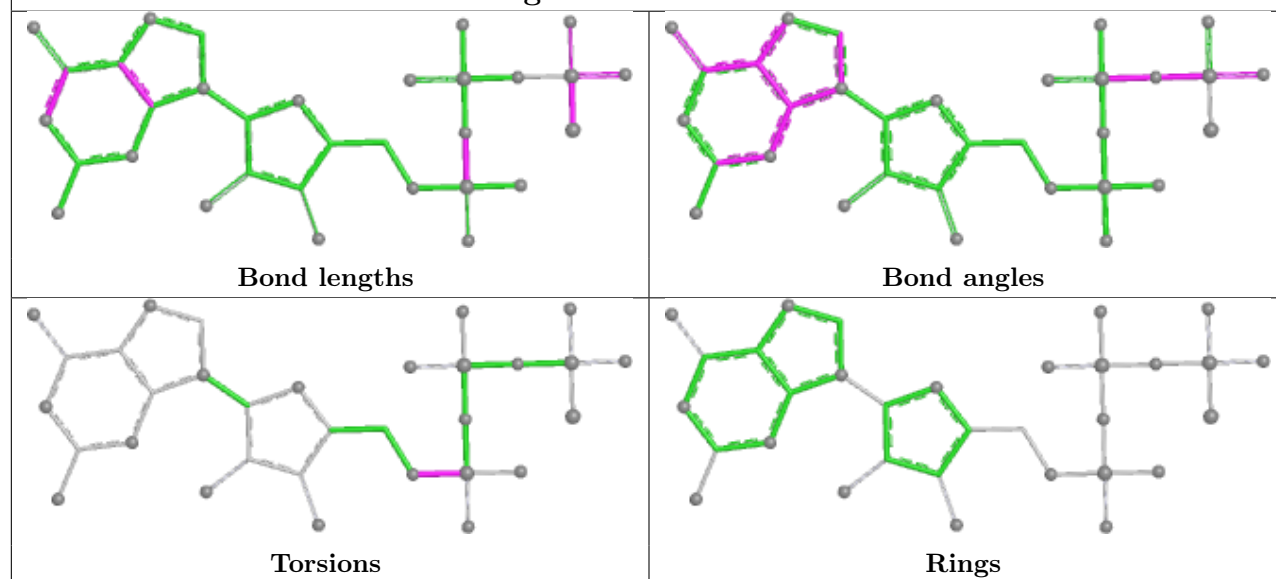
Ligand GSP T 2000

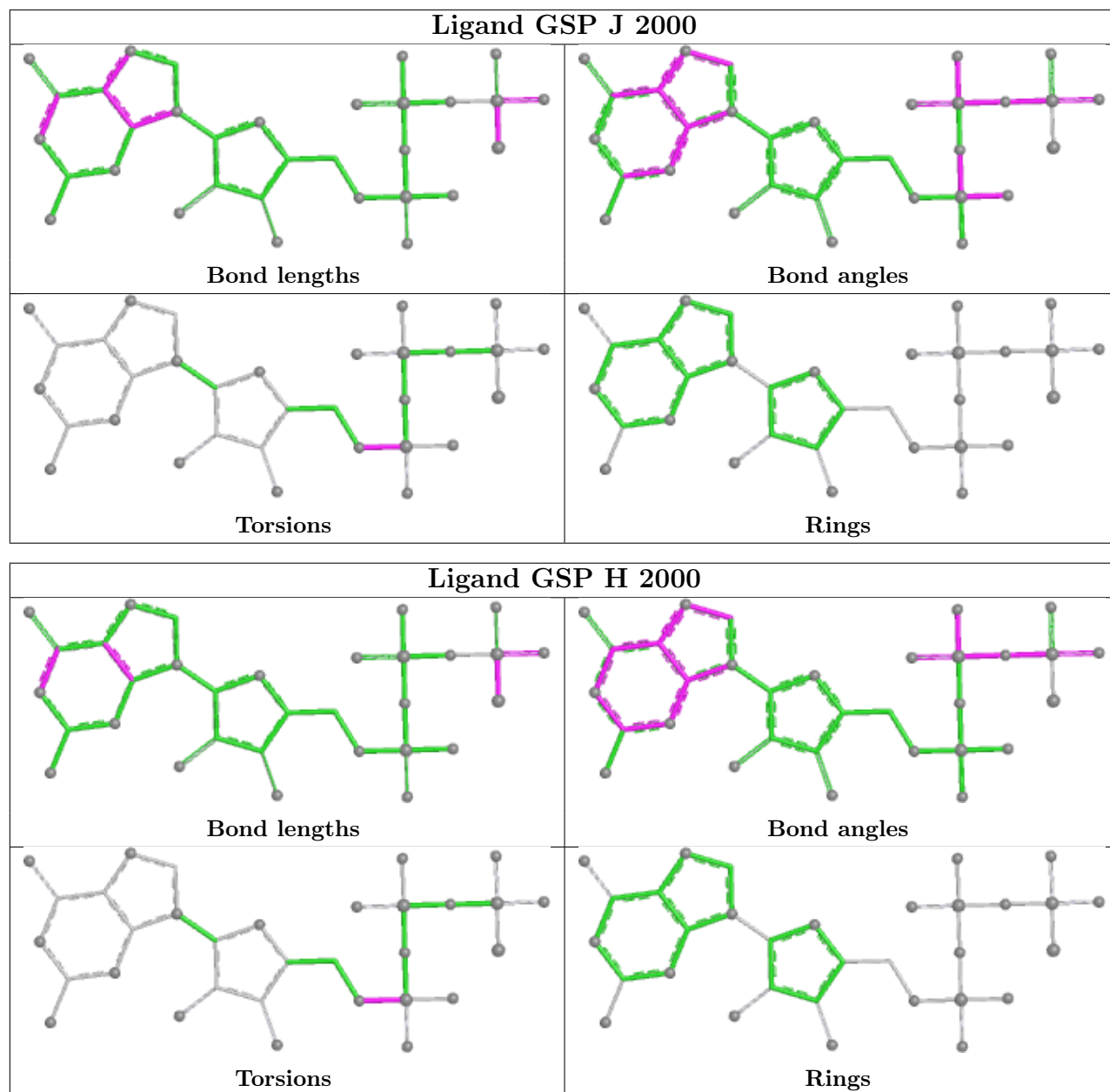


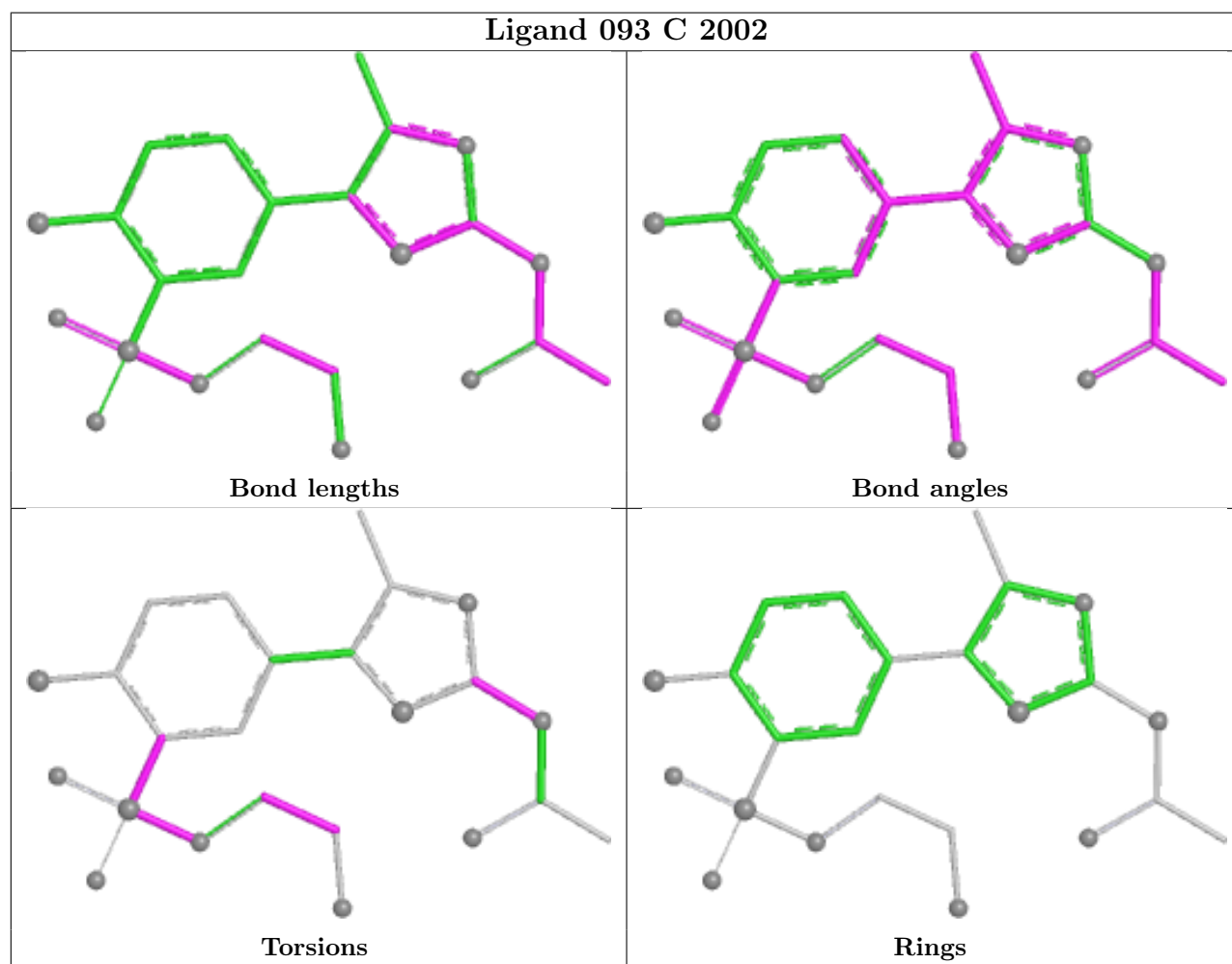
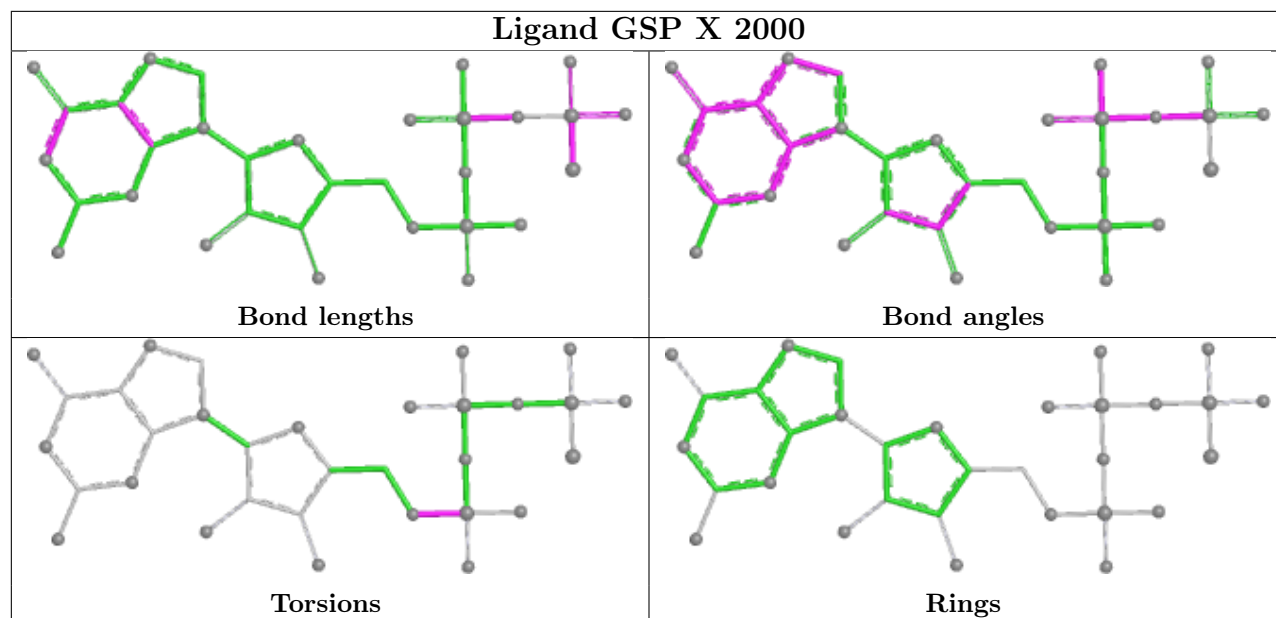
Ligand 093 Y 2002

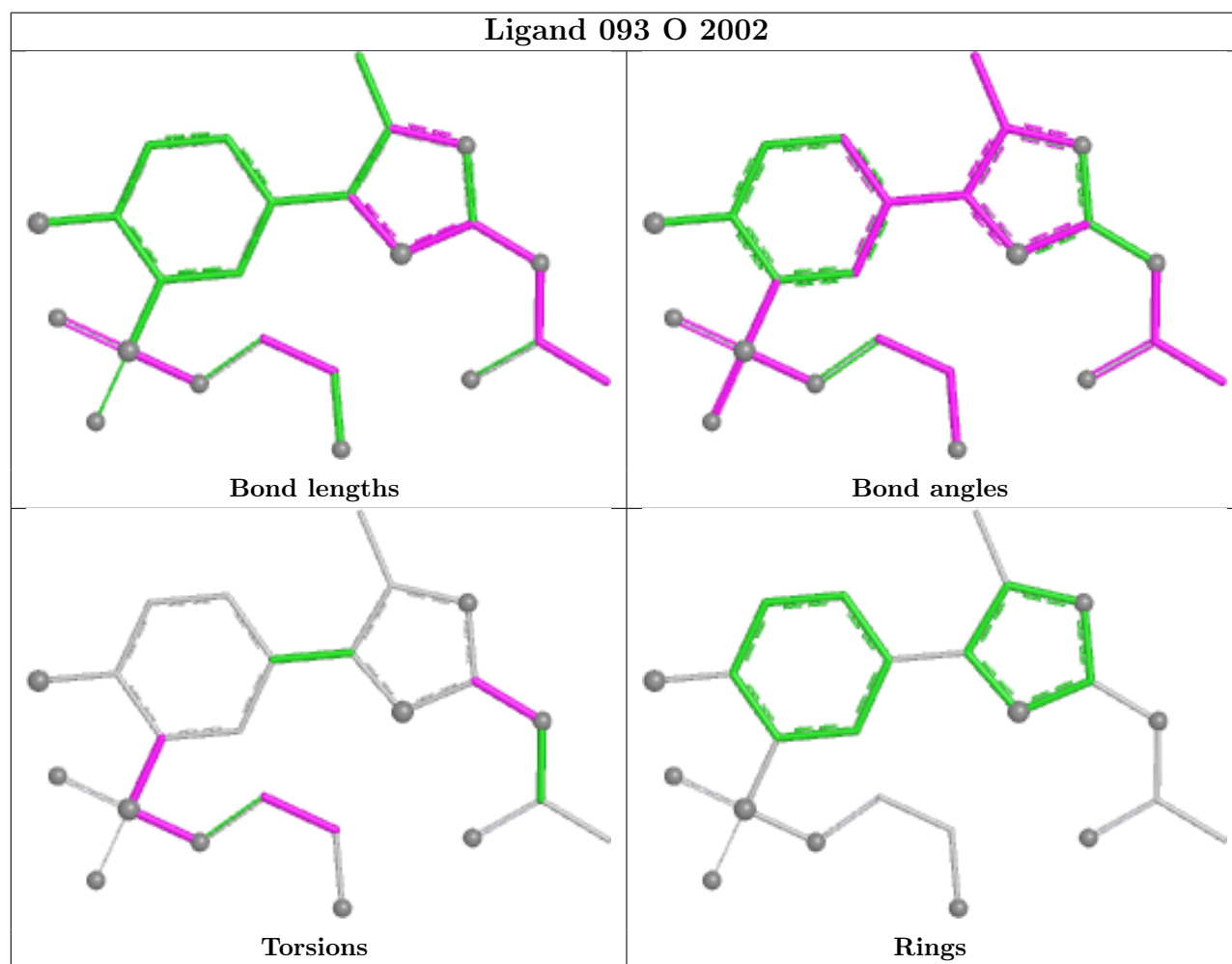
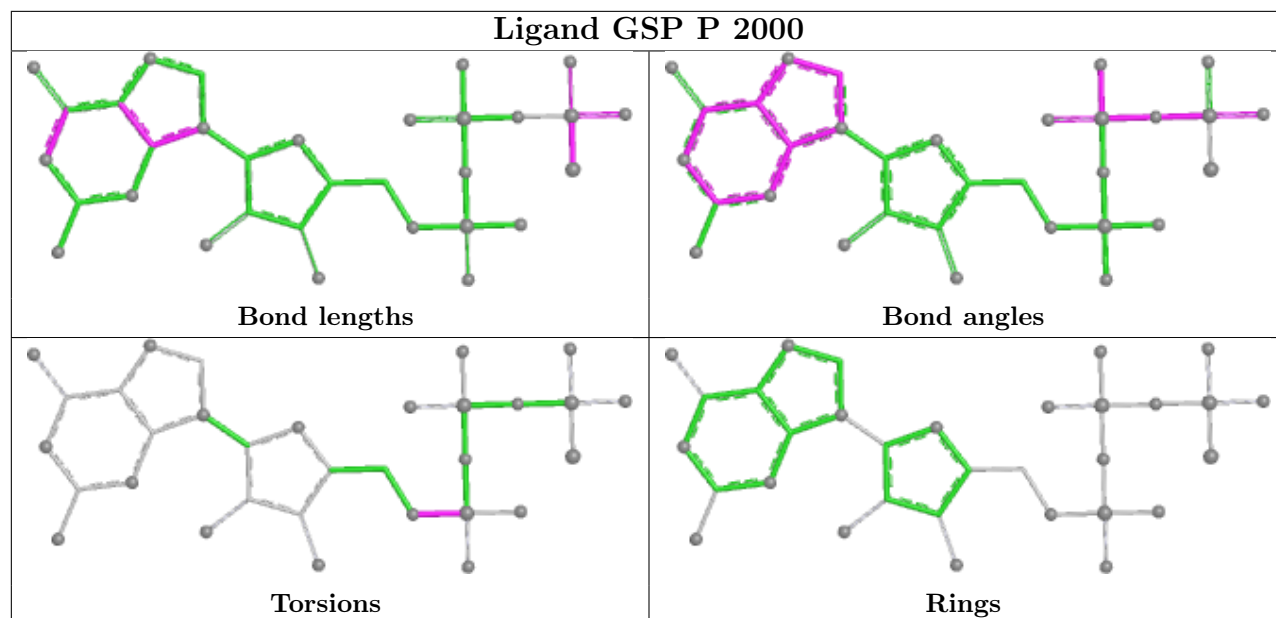


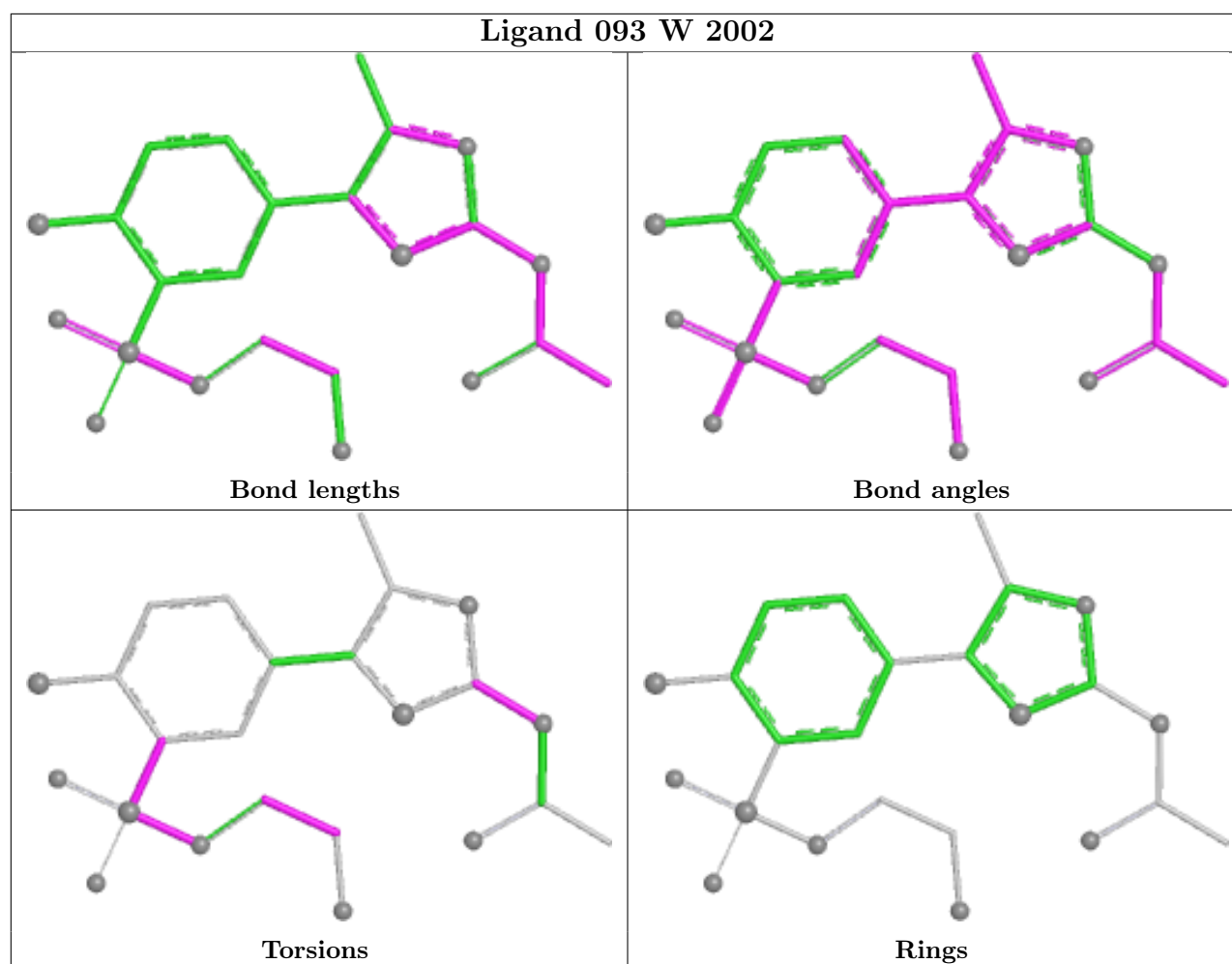
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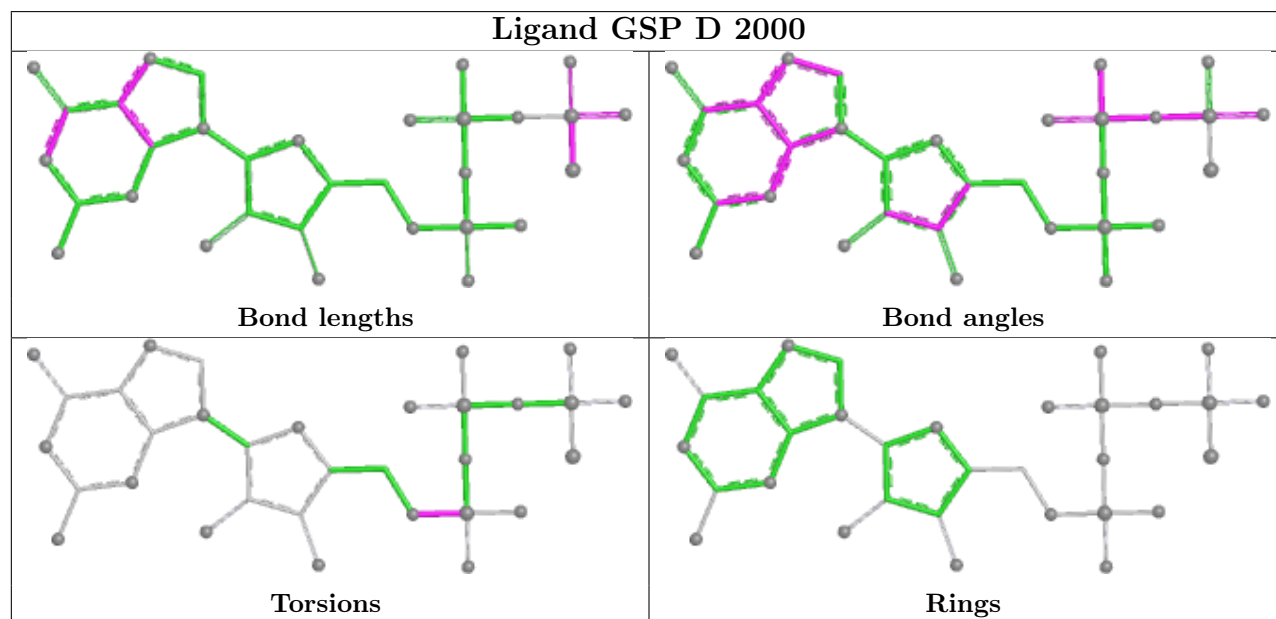
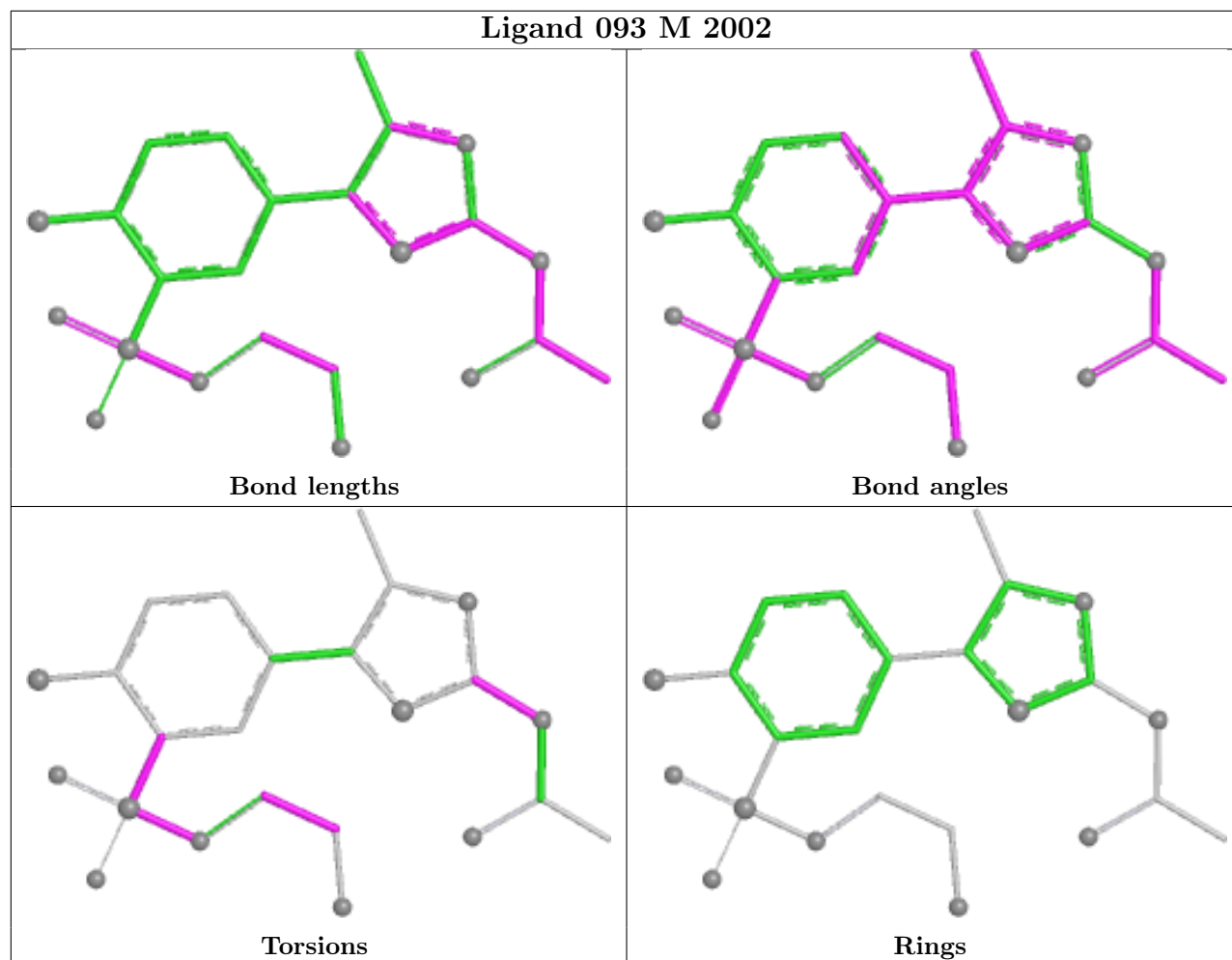




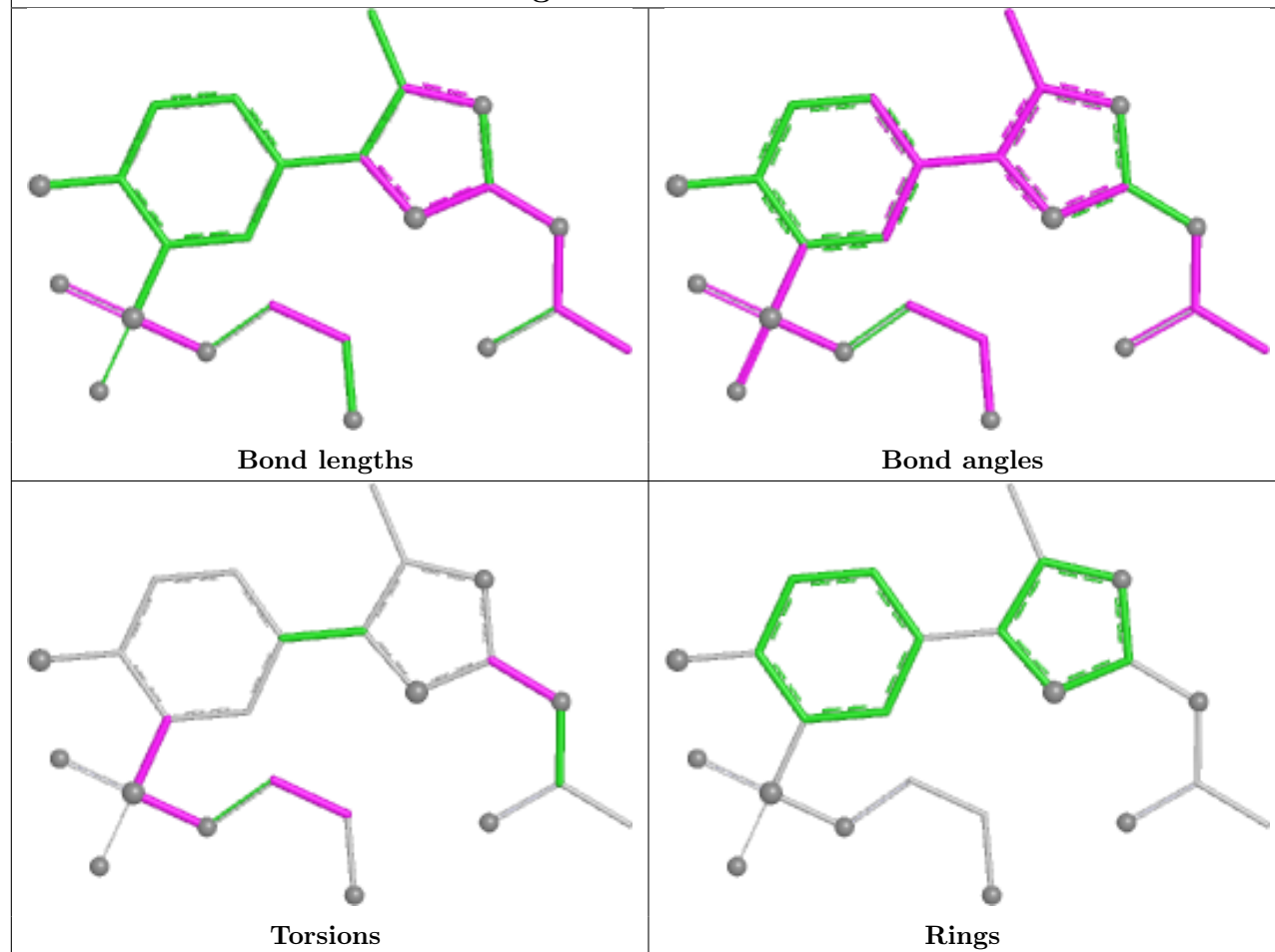




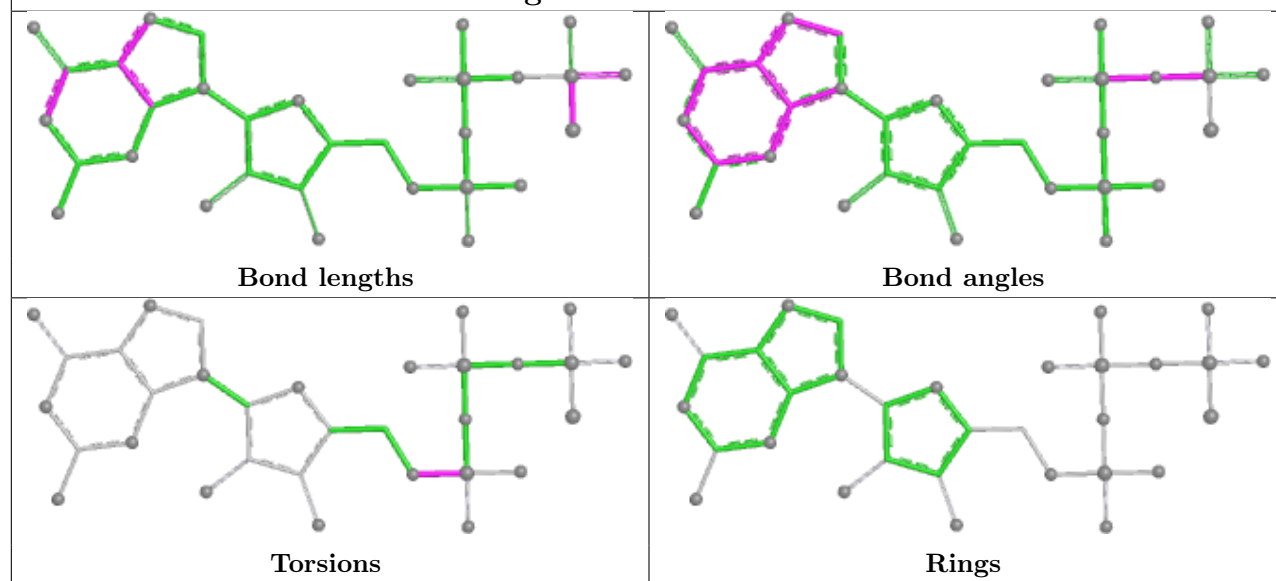


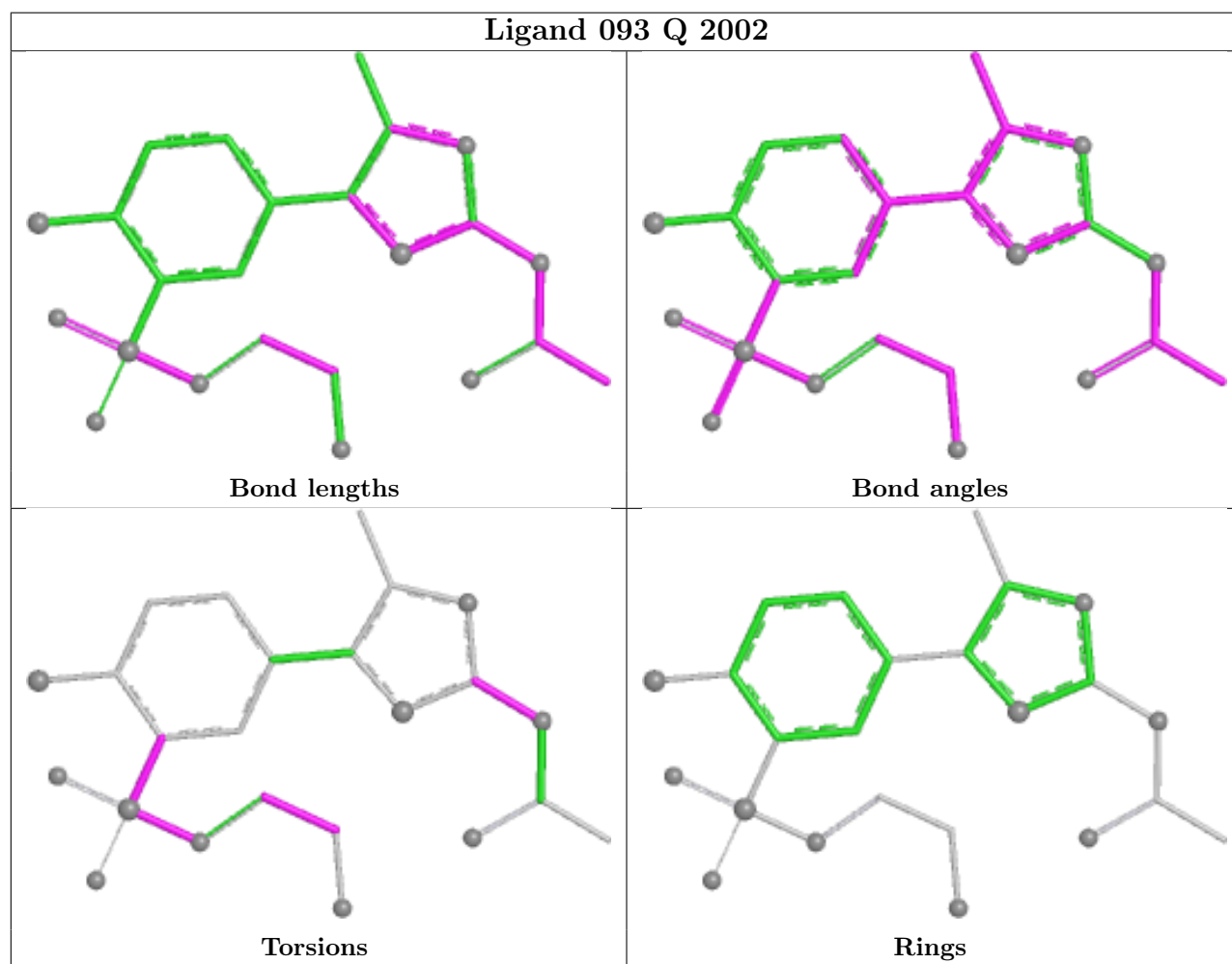
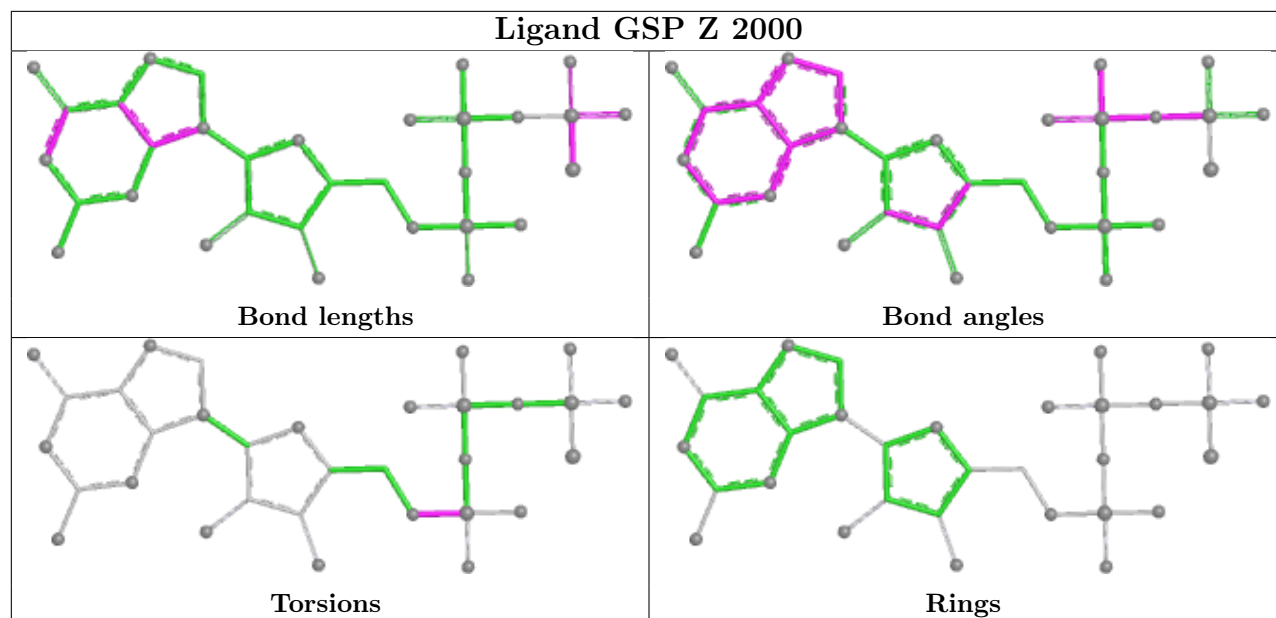


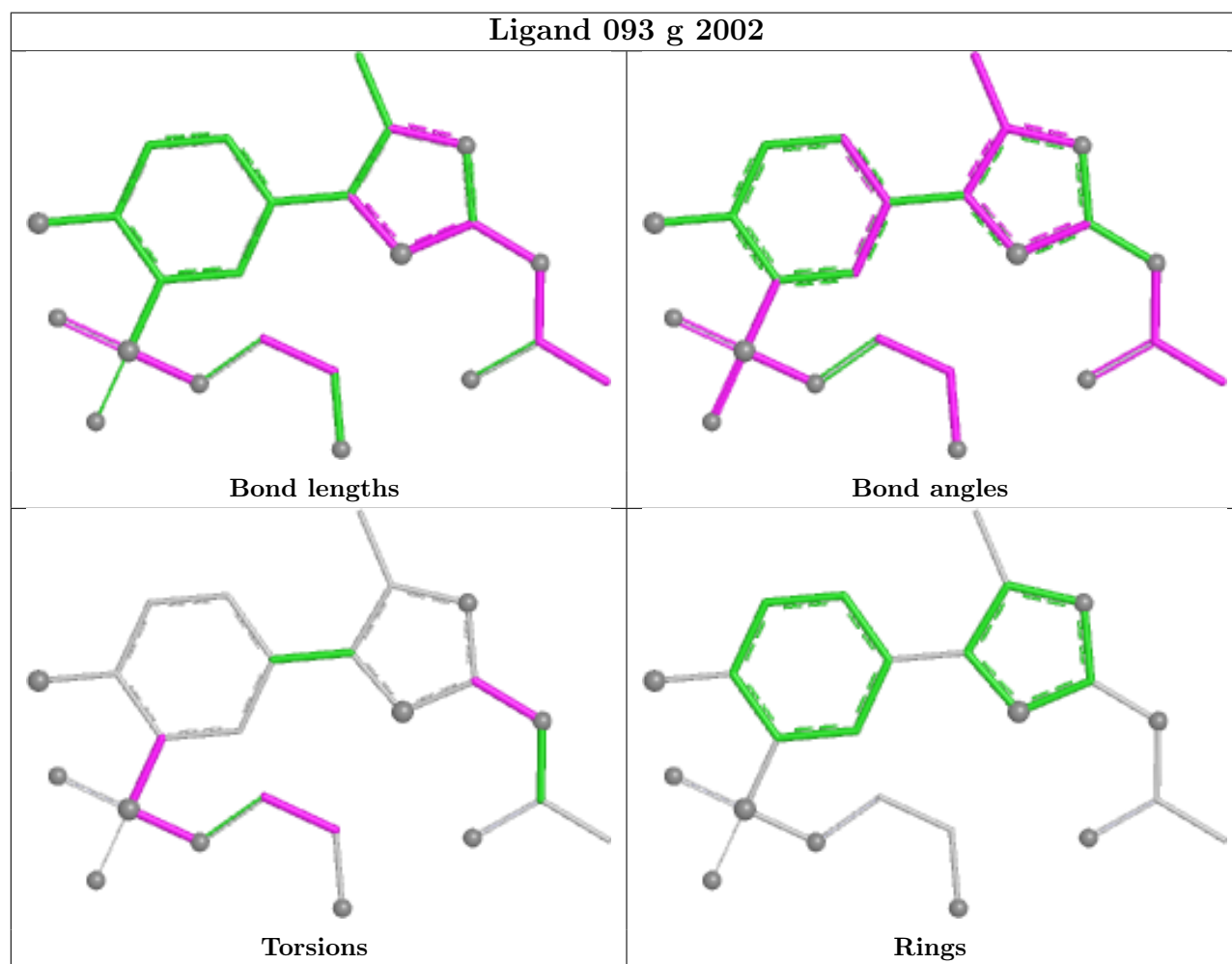
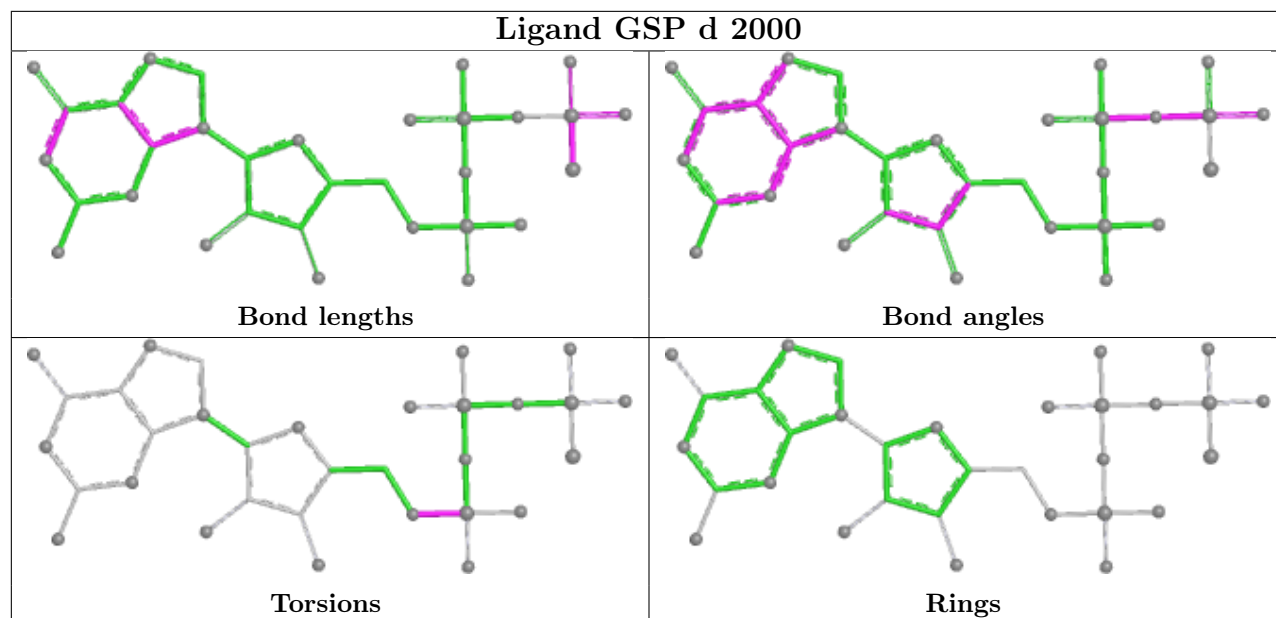
Ligand 093 A 2002

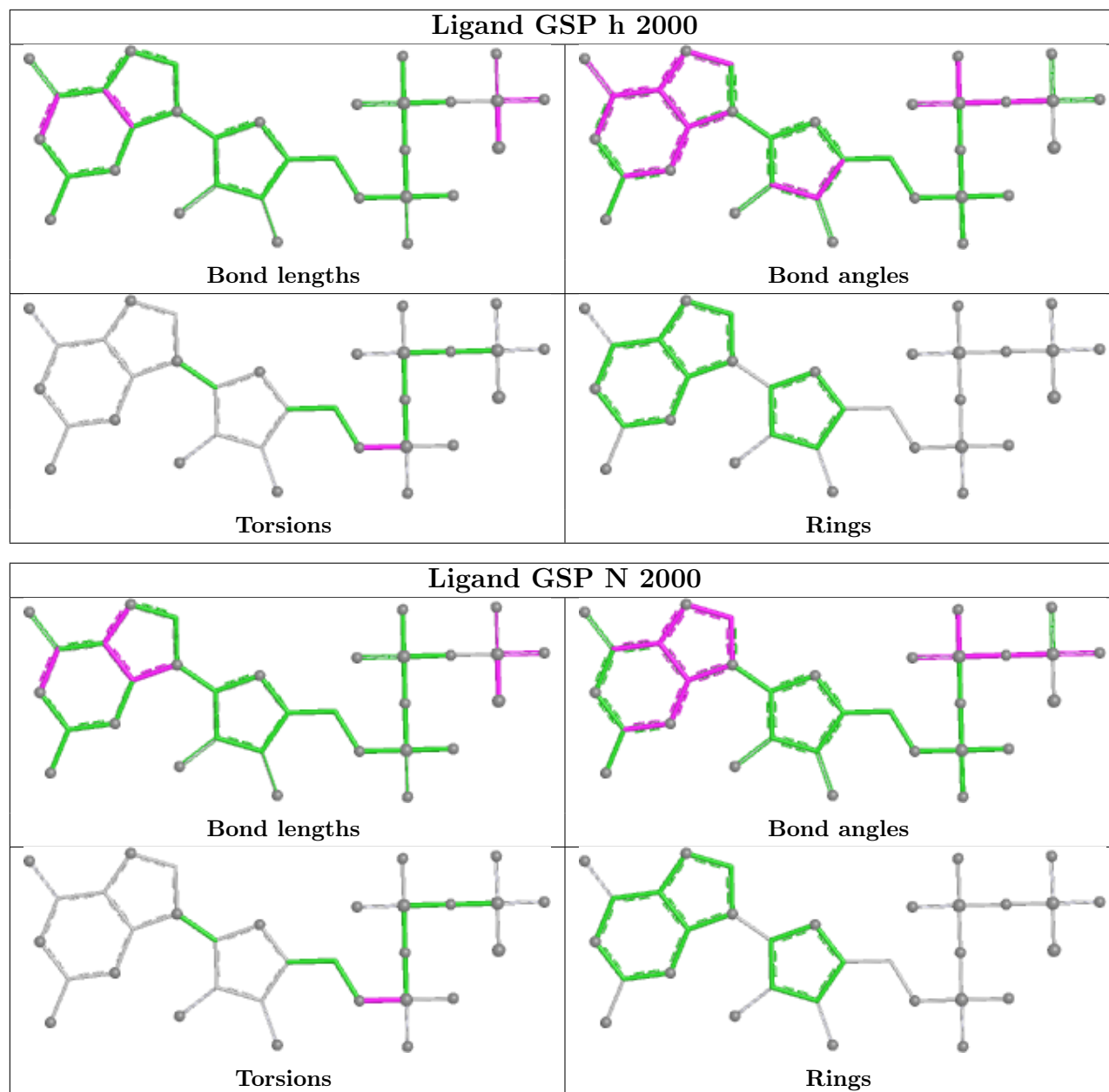


Ligand GSP B 2000

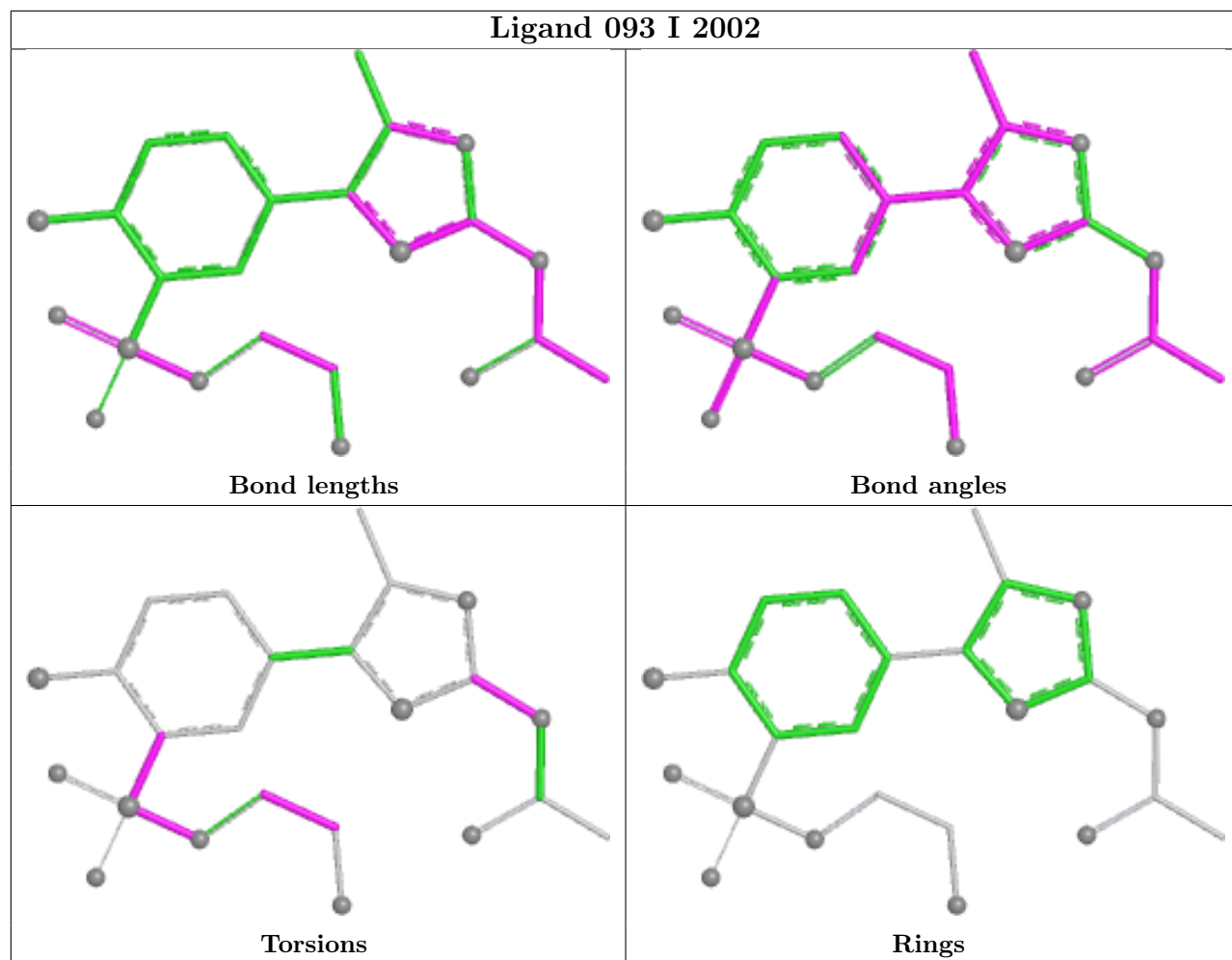


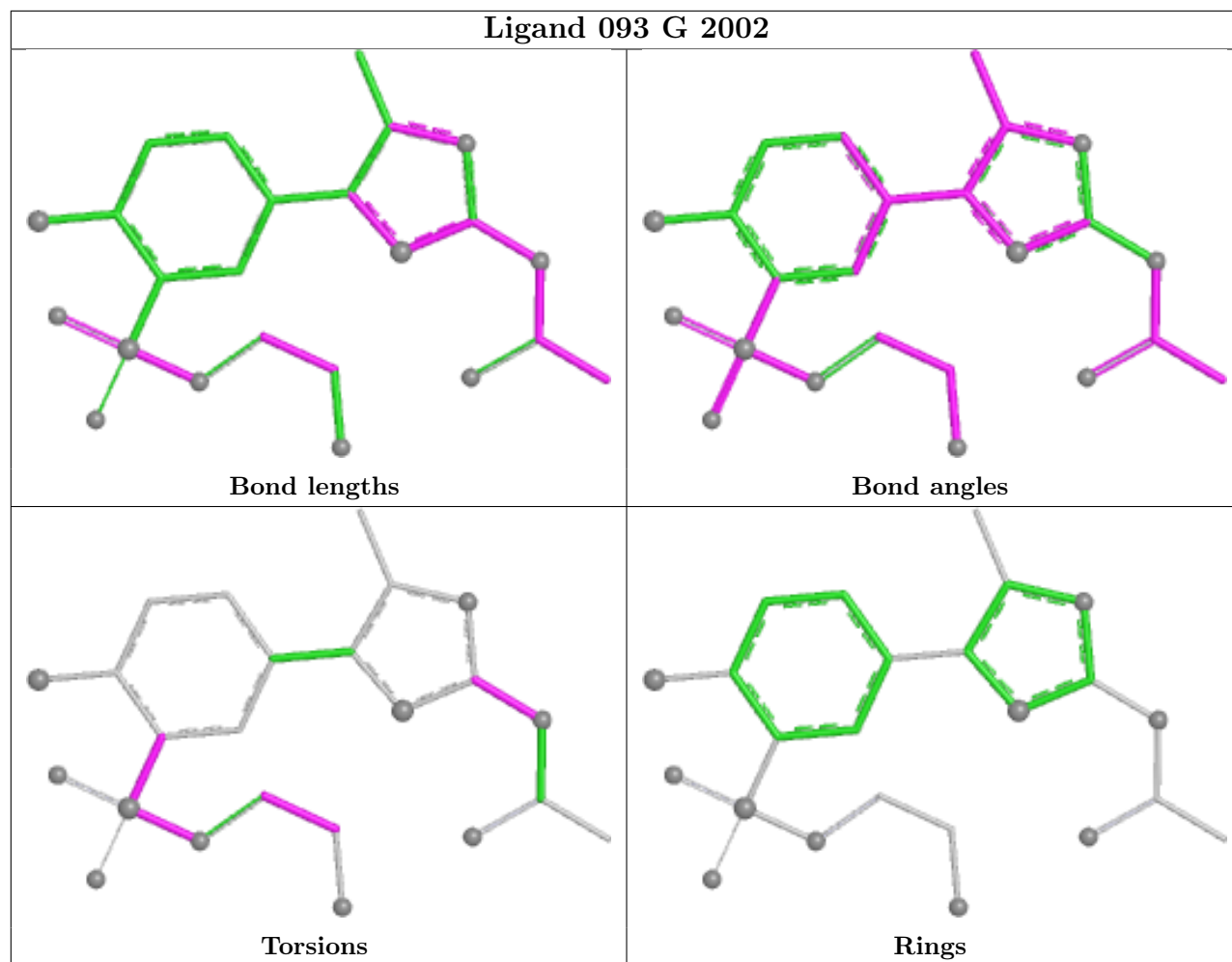






Ligand 093 I 2002





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, 95th 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 ²)	Q<0.9
1	A	470/566 (83%)	-0.33	2 (0%) 88 79	95, 212, 331, 500	0
1	C	470/566 (83%)	-0.09	16 (3%) 48 43	126, 300, 456, 500	0
1	G	470/566 (83%)	-0.32	3 (0%) 85 75	98, 214, 342, 500	0
1	I	470/566 (83%)	-0.01	10 (2%) 63 54	124, 306, 474, 500	0
1	M	470/566 (83%)	-0.27	4 (0%) 81 70	95, 217, 341, 500	0
1	O	470/566 (83%)	-0.25	9 (1%) 66 56	102, 208, 335, 500	0
1	Q	470/566 (83%)	-0.19	4 (0%) 81 70	102, 247, 364, 498	0
1	S	470/566 (83%)	-0.14	9 (1%) 66 56	114, 251, 389, 500	0
1	W	470/566 (83%)	-0.13	12 (2%) 57 49	99, 253, 387, 500	0
1	Y	470/566 (83%)	-0.05	12 (2%) 57 49	115, 250, 364, 474	0
1	c	470/566 (83%)	-0.17	4 (0%) 81 70	119, 305, 478, 500	0
1	g	470/566 (83%)	-0.11	7 (1%) 72 60	126, 268, 416, 500	0
2	B	173/219 (78%)	-0.33	0 100 100	94, 201, 375, 493	0
2	D	173/219 (78%)	-0.10	3 (1%) 69 58	95, 220, 341, 488	0
2	H	173/219 (78%)	-0.21	2 (1%) 76 65	94, 207, 382, 499	0
2	J	173/219 (78%)	-0.28	2 (1%) 76 65	92, 198, 338, 500	0
2	N	173/219 (78%)	-0.19	1 (0%) 85 75	137, 282, 424, 496	0
2	P	173/219 (78%)	0.01	0 100 100	132, 277, 432, 496	0
2	R	173/219 (78%)	-0.02	6 (3%) 47 43	139, 269, 415, 496	0
2	T	173/219 (78%)	-0.11	2 (1%) 76 65	136, 266, 407, 493	0
2	X	173/219 (78%)	-0.02	3 (1%) 69 58	146, 282, 453, 500	0
2	Z	173/219 (78%)	0.12	5 (2%) 53 46	165, 262, 362, 494	0
2	d	173/219 (78%)	0.13	6 (3%) 47 43	146, 308, 447, 500	0
2	h	173/219 (78%)	0.06	7 (4%) 42 40	158, 294, 440, 500	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	E	41/48 (85%)	-0.35	0 100 100	153, 251, 365, 489	0
3	F	32/48 (66%)	-0.10	1 (3%) 51 45	169, 285, 399, 466	0
3	K	41/48 (85%)	-0.27	0 100 100	131, 240, 410, 465	0
3	L	32/48 (66%)	-0.21	0 100 100	170, 263, 384, 436	0
3	U	41/48 (85%)	0.11	0 100 100	175, 284, 408, 494	0
3	V	32/48 (66%)	-0.47	0 100 100	170, 260, 403, 435	0
3	a	41/48 (85%)	-0.22	1 (2%) 59 51	195, 318, 423, 476	0
3	b	32/48 (66%)	-0.10	0 100 100	213, 309, 428, 479	0
3	e	41/48 (85%)	-0.16	0 100 100	175, 255, 384, 478	0
3	f	32/48 (66%)	-0.13	1 (3%) 51 45	194, 288, 337, 363	0
3	i	41/48 (85%)	-0.21	0 100 100	202, 325, 441, 500	0
3	j	32/48 (66%)	-0.02	0 100 100	194, 282, 404, 462	0
All	All	8154/9996 (81%)	-0.15	132 (1%) 70 59	92, 255, 416, 500	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	775	GLU	6.0
1	M	707	ASP	4.8
2	X	84	ALA	4.8
1	Q	624	GLY	4.4
1	C	721	GLY	4.2
1	Y	698	GLU	4.2
2	h	151	ILE	4.2
1	g	405	GLU	4.1
2	D	83	GLY	4.1
1	W	514	SER	4.1
1	C	784	SER	4.0
1	S	633	SER	3.8
1	W	743	SER	3.8
1	S	514	SER	3.7
1	G	376	SER	3.7
1	W	577	PRO	3.7
1	I	776	GLN	3.7
1	C	772	LEU	3.6
1	Y	404	PRO	3.5
2	X	12	PHE	3.5
1	c	746	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	g	539	PRO	3.4
2	T	52	SER	3.4
1	C	775	GLU	3.4
2	h	12	PHE	3.4
1	O	395	ASP	3.3
1	Y	161	GLY	3.2
2	d	130	HIS	3.2
1	S	513	PRO	3.2
1	S	185	HIS	3.2
3	f	739	ASP	3.2
1	W	335	GLN	3.1
1	C	392	GLU	3.1
1	A	396	THR	3.1
1	Y	545	SER	3.1
1	I	538	LEU	3.0
1	g	627	THR	3.0
2	Z	159	THR	2.9
1	Q	623	HIS	2.9
1	W	740	GLN	2.9
1	S	137	LYS	2.9
2	Z	85	VAL	2.9
1	O	514	SER	2.8
2	Z	52	SER	2.8
1	C	695	LEU	2.8
1	I	701	ASP	2.8
2	d	124	ASN	2.8
2	D	72	ARG	2.8
1	W	742	GLY	2.8
1	G	784	SER	2.8
1	g	607	VAL	2.7
1	O	574	GLU	2.7
1	O	707	ASP	2.7
1	g	128	SER	2.7
2	R	155	ALA	2.7
2	h	152	GLU	2.7
1	C	782	MET	2.7
1	Y	378	ASP	2.7
1	C	366	VAL	2.6
1	W	406	ASN	2.6
2	H	167	THR	2.6
1	c	694	LYS	2.6
1	I	772	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	h	170	THR	2.6
1	G	325	ALA	2.6
1	I	366	VAL	2.5
2	R	150	PHE	2.5
2	R	107	LYS	2.5
1	Y	695	LEU	2.5
1	C	347	LYS	2.4
1	M	334	THR	2.4
2	d	173	TYR	2.4
1	Q	219	TYR	2.4
2	h	166	GLN	2.4
2	J	57	GLY	2.4
1	C	779	ASP	2.4
1	I	526	VAL	2.4
1	W	575	ARG	2.4
1	W	640	GLN	2.4
2	J	69	GLY	2.3
1	A	784	SER	2.3
2	R	149	SER	2.3
1	O	154	PRO	2.3
1	I	599	VAL	2.3
1	I	376	SER	2.3
2	d	103	GLU	2.3
1	W	404	PRO	2.3
1	O	360	ASP	2.3
1	Y	204	GLN	2.3
1	c	714	TYR	2.2
1	Y	376	SER	2.2
1	C	717	LEU	2.2
1	Y	330	LYS	2.2
2	R	94	ALA	2.2
2	T	170	THR	2.2
1	c	747	CYS	2.2
2	d	131	LEU	2.2
2	D	153	THR	2.2
1	g	641	SER	2.2
1	Y	531	GLU	2.2
2	N	150	PHE	2.2
1	S	217	GLY	2.2
1	C	728	HIS	2.2
1	Q	197	TYR	2.2
1	W	667	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	19	ASP	2.1
1	W	605	HIS	2.1
2	h	126	SER	2.1
1	M	371	ALA	2.1
1	S	172	VAL	2.1
1	M	519	LYS	2.1
1	I	697	THR	2.1
1	S	640	GLN	2.1
1	O	371	ALA	2.1
2	d	45	GLY	2.1
1	g	368	HIS	2.1
1	C	722	LEU	2.1
2	h	136	THR	2.1
1	Y	160	ILE	2.1
3	a	735	GLN	2.1
2	Z	126	SER	2.1
1	S	211	GLN	2.1
2	Z	135	PRO	2.1
1	O	372	VAL	2.1
1	C	765	MET	2.0
1	C	401	ALA	2.0
2	X	63	GLN	2.0
1	Y	373	VAL	2.0
3	F	736	ASP	2.0
1	O	393	ASN	2.0
2	R	152	GLU	2.0
1	C	724	ALA	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 oligosaccharides 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,

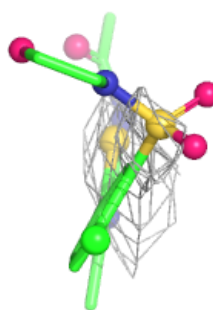
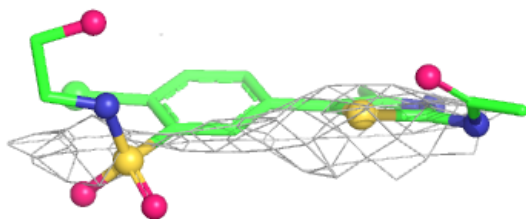
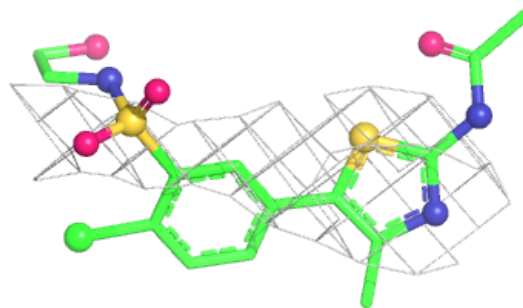
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	093	A	2002	24/24	-	-	60,76,105,130	24
4	093	C	2002	24/24	-	-	60,76,105,130	24
4	093	G	2002	24/24	-	-	60,76,105,130	24
4	093	I	2002	24/24	-	-	60,76,105,130	24
4	093	M	2002	24/24	-	-	60,76,105,130	24
4	093	O	2002	24/24	-	-	60,76,105,130	24
4	093	Q	2002	24/24	-	-	60,76,105,130	24
4	093	S	2002	24/24	-	-	60,76,105,130	24
4	093	W	2002	24/24	-	-	60,76,105,130	24
4	093	Y	2002	24/24	-	-	60,76,105,130	24
4	093	c	2002	24/24	-	-	60,76,105,130	24
4	093	g	2002	24/24	-	-	60,76,105,130	24
5	GSP	J	2000	32/32	0.95	0.09	94,165,285,323	0
6	MG	X	2001	1/1	0.95	0.06	255,255,255,255	0
5	GSP	X	2000	32/32	0.97	0.07	134,226,322,330	0
5	GSP	R	2000	32/32	0.97	0.07	108,197,262,274	0
5	GSP	P	2000	32/32	0.98	0.07	111,168,247,275	0
5	GSP	D	2000	32/32	0.98	0.07	110,193,250,272	0
5	GSP	T	2000	32/32	0.98	0.07	123,205,238,264	0
5	GSP	H	2000	32/32	0.98	0.05	141,183,247,282	0
5	GSP	d	2000	32/32	0.98	0.07	174,212,349,391	0
5	GSP	h	2000	32/32	0.98	0.07	123,249,350,363	0
6	MG	H	2001	1/1	0.98	0.04	139,139,139,139	0
6	MG	N	2001	1/1	0.98	0.07	240,240,240,240	0
5	GSP	B	2000	32/32	0.98	0.05	141,197,232,249	0
6	MG	h	2001	1/1	0.98	0.04	190,190,190,190	0
6	MG	J	2001	1/1	0.99	0.06	142,142,142,142	0
5	GSP	Z	2000	32/32	0.99	0.07	176,212,274,298	0
6	MG	R	2001	1/1	0.99	0.03	106,106,106,106	0
6	MG	T	2001	1/1	0.99	0.03	127,127,127,127	0
6	MG	B	2001	1/1	0.99	0.03	159,159,159,159	0
6	MG	Z	2001	1/1	0.99	0.05	178,178,178,178	0
6	MG	d	2001	1/1	0.99	0.05	167,167,167,167	0
5	GSP	N	2000	32/32	0.99	0.05	97,151,255,301	0
6	MG	D	2001	1/1	1.00	0.04	64,64,64,64	0
6	MG	P	2001	1/1	1.00	0.10	244,244,244,244	0

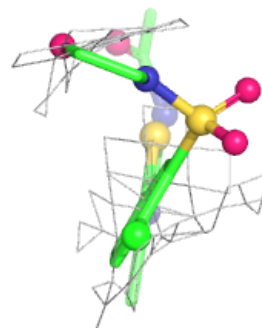
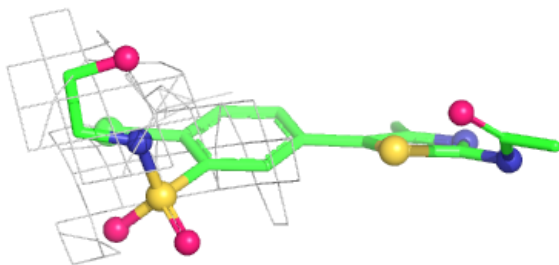
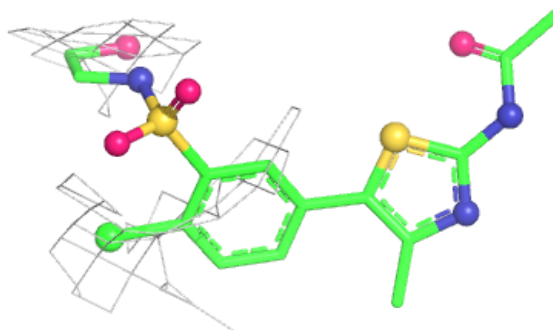
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 093 A 2002:

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

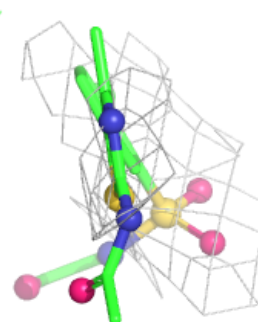
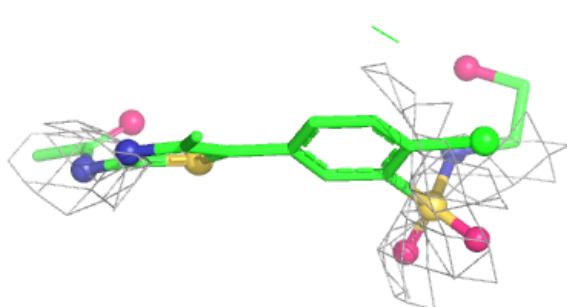
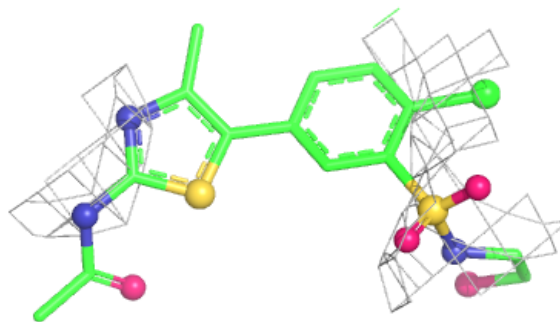
**Electron density around 093 C 2002:**

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

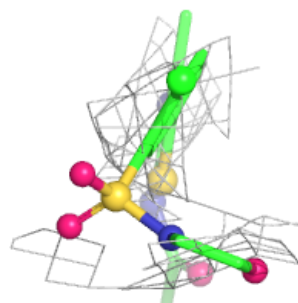
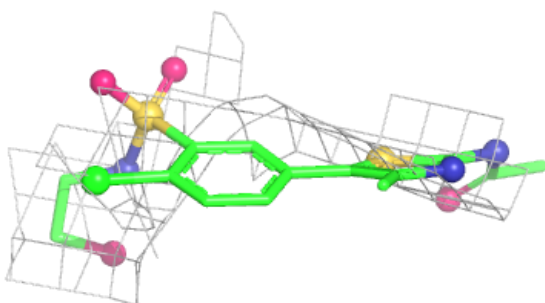
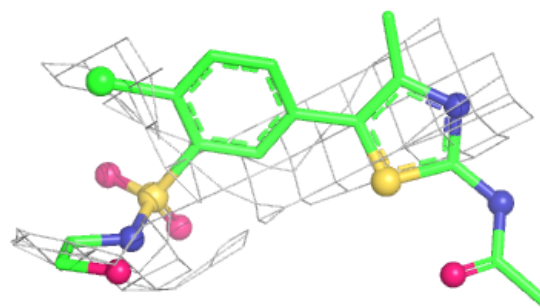


Electron density around 093 G 2002:

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

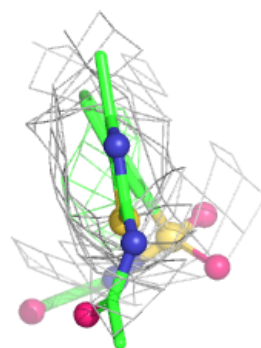
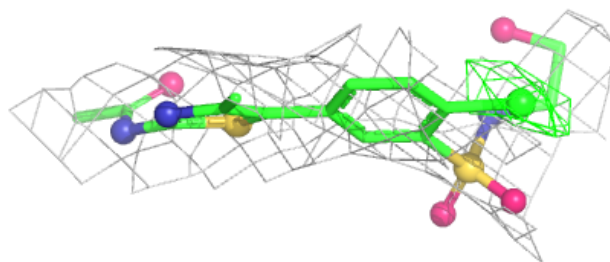
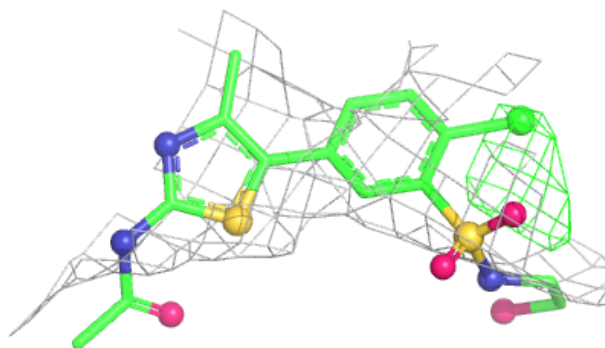
**Electron density around 093 I 2002:**

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

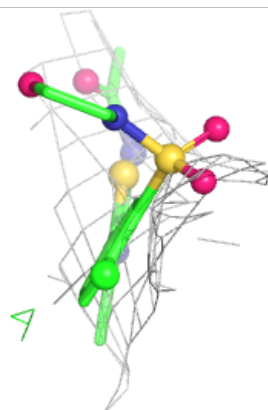
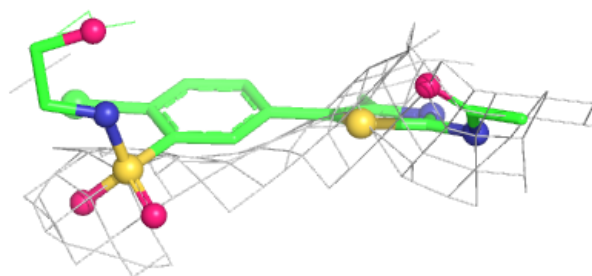
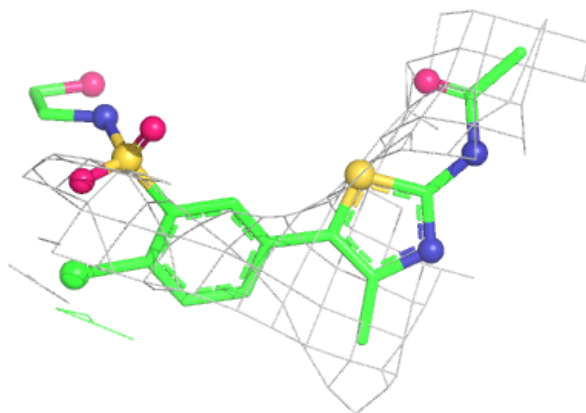


Electron density around 093 M 2002:

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

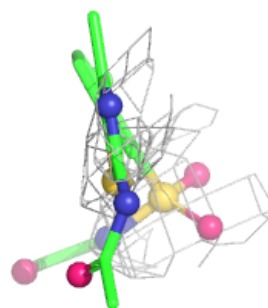
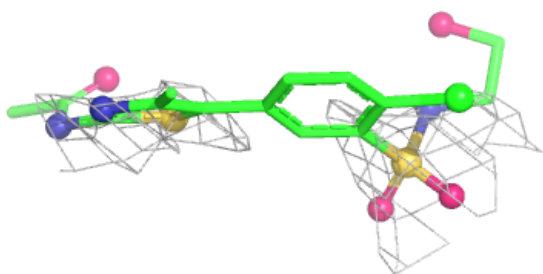
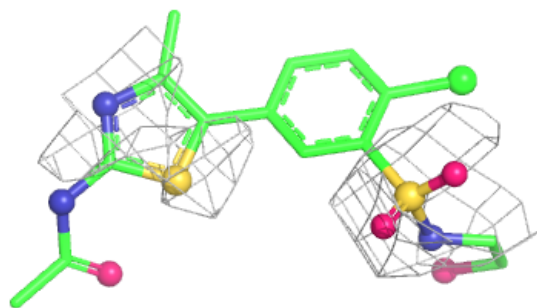
**Electron density around 093 O 2002:**

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

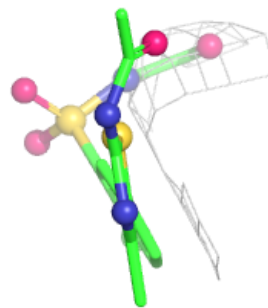
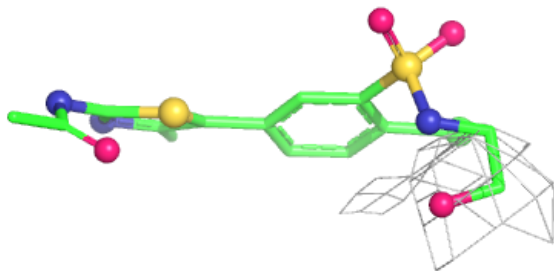
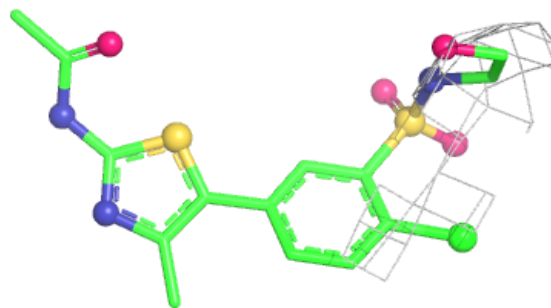


Electron density around 093 Q 2002:

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

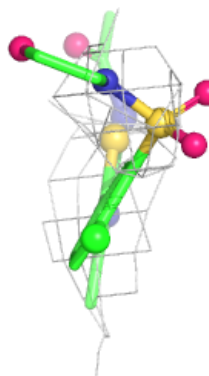
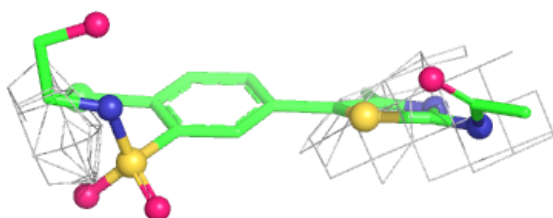
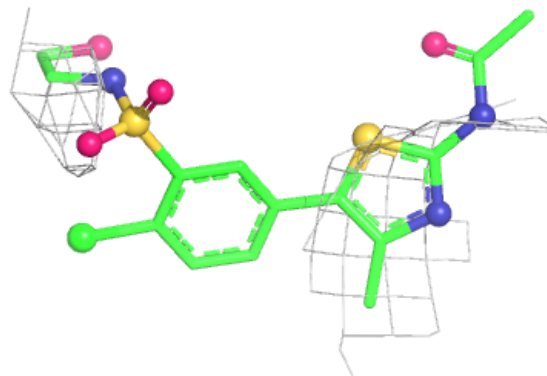
**Electron density around 093 S 2002:**

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

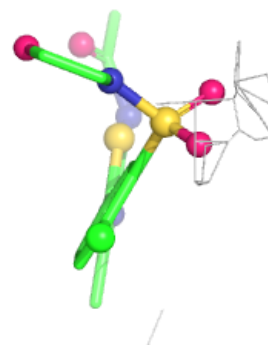
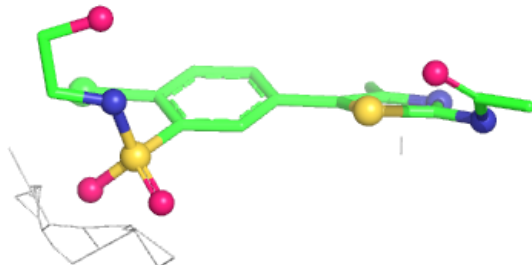
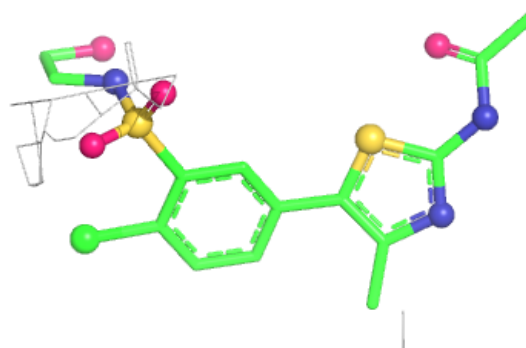


Electron density around 093 W 2002:

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

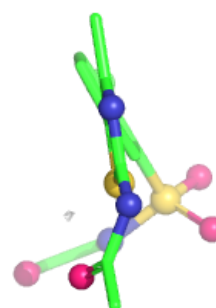
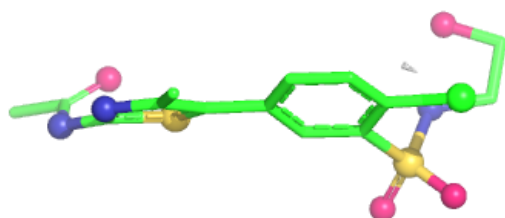
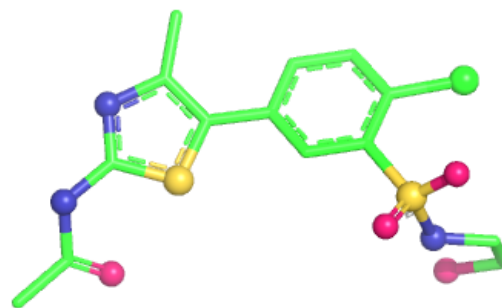
**Electron density around 093 Y 2002:**

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

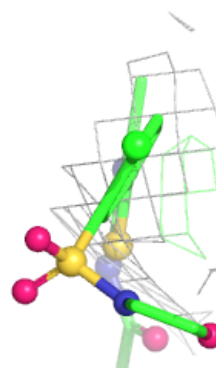
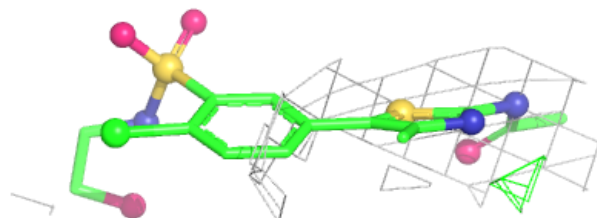
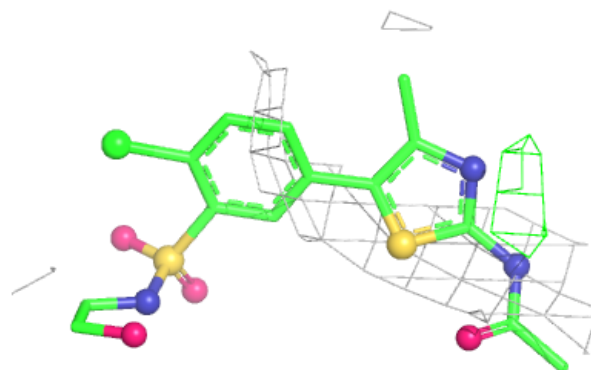


Electron density around 093 c 2002:

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

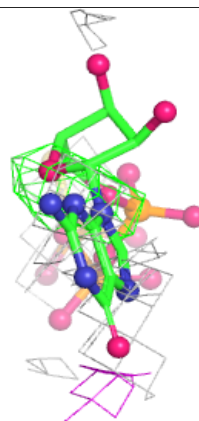
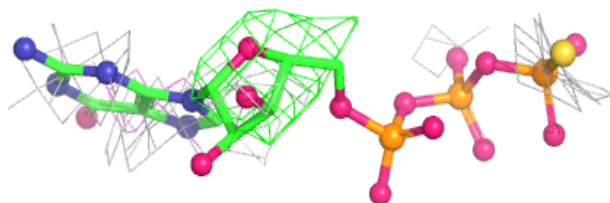
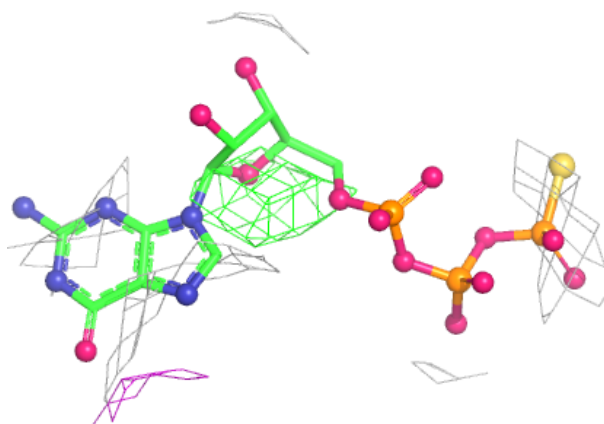
**Electron density around 093 g 2002:**

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

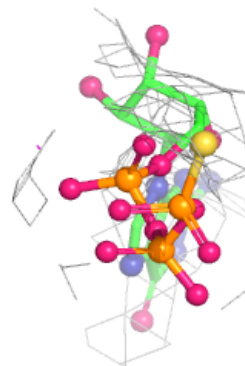
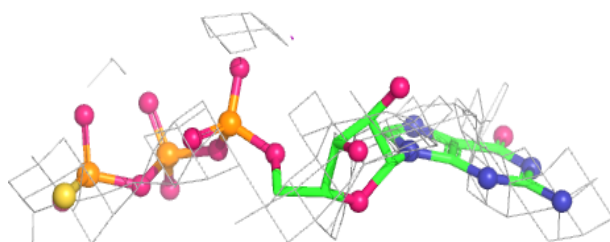
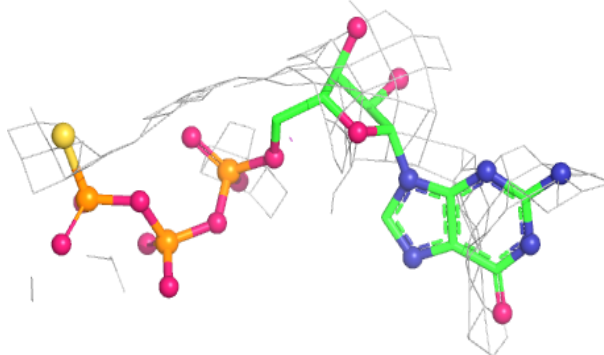


Electron density around GSP J 2000:

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

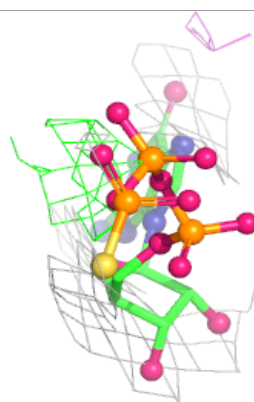
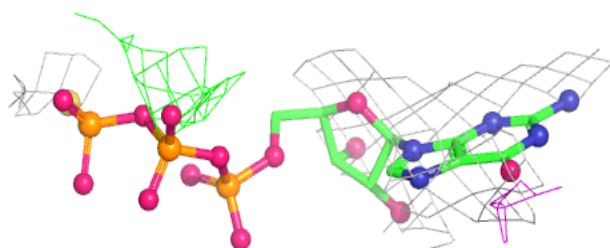
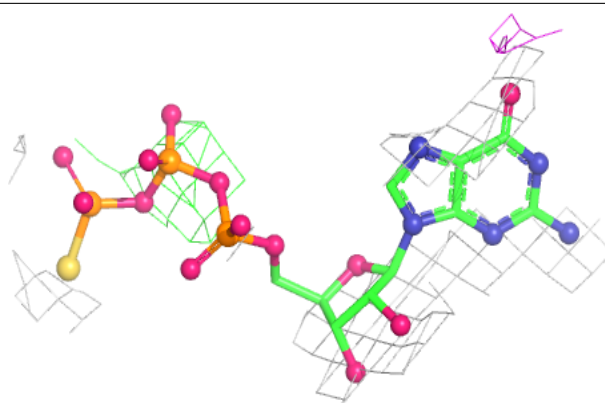
**Electron density around GSP X 2000:**

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

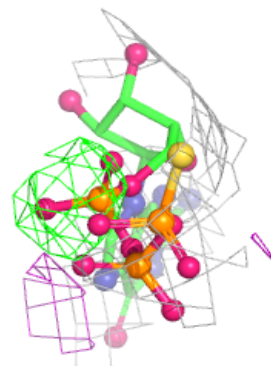
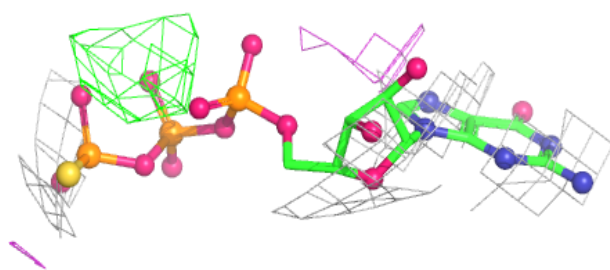
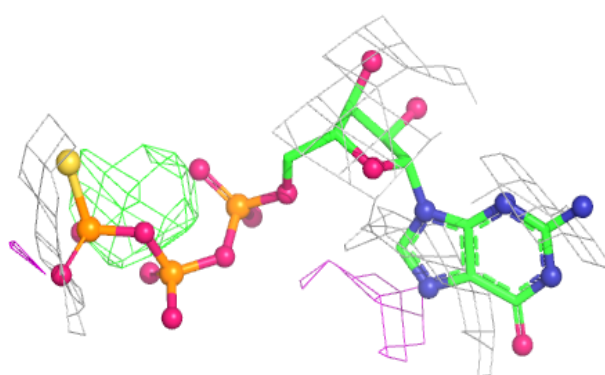


Electron density around GSP R 2000:

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

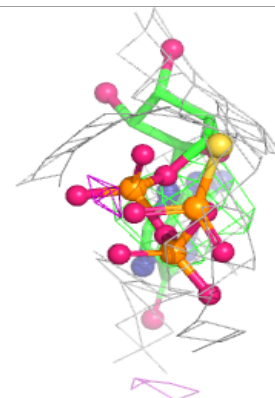
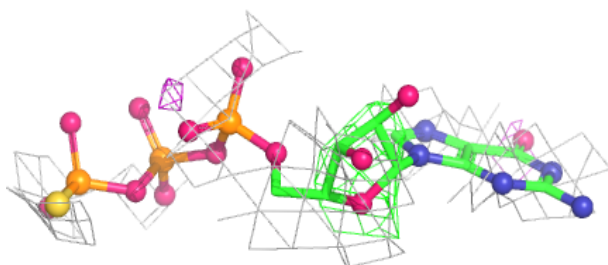
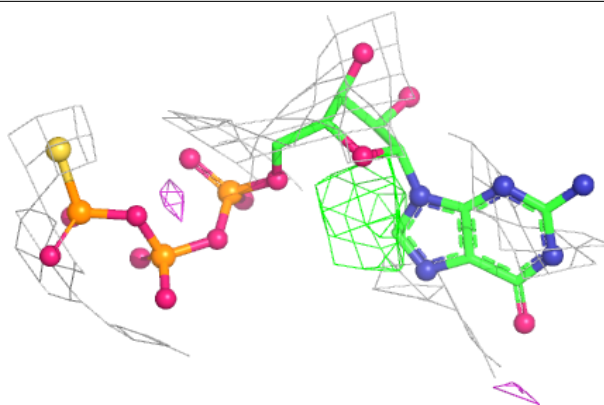
**Electron density around GSP P 2000:**

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

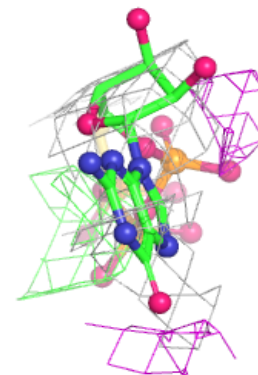
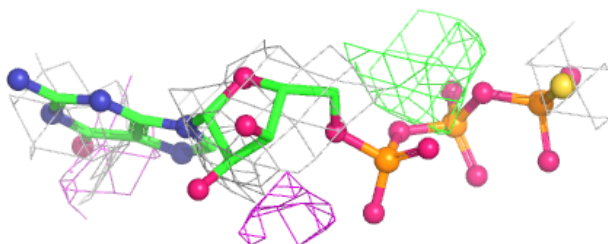
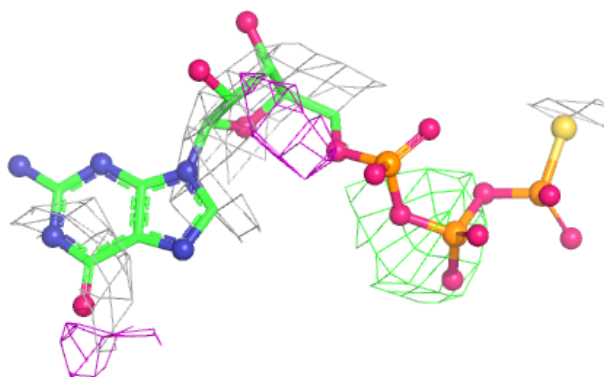


Electron density around GSP D 2000:

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

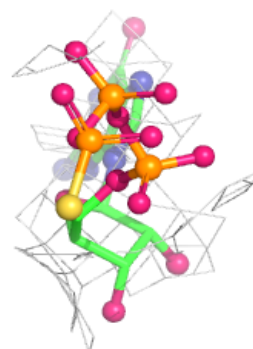
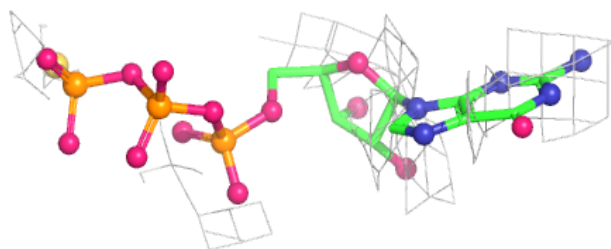
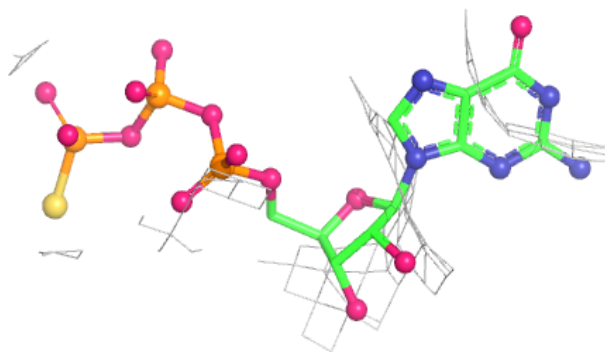
**Electron density around GSP T 2000:**

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

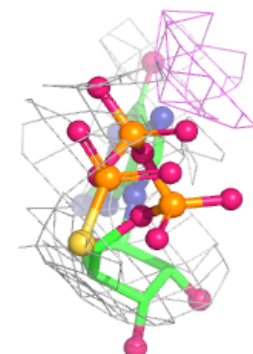
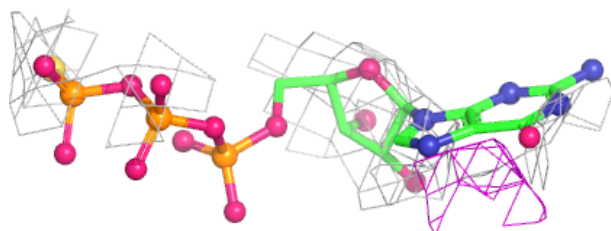
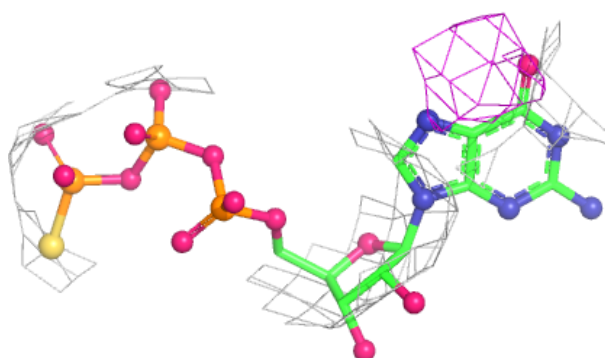


Electron density around GSP H 2000:

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

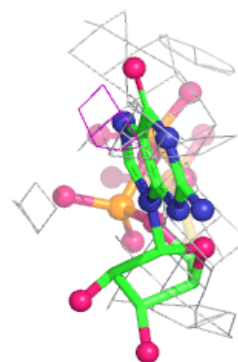
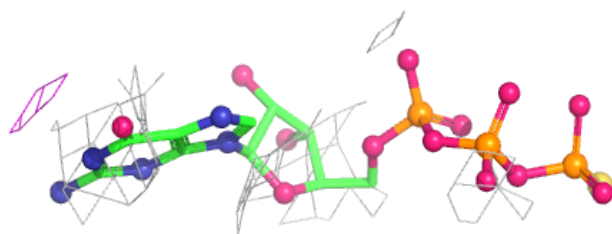
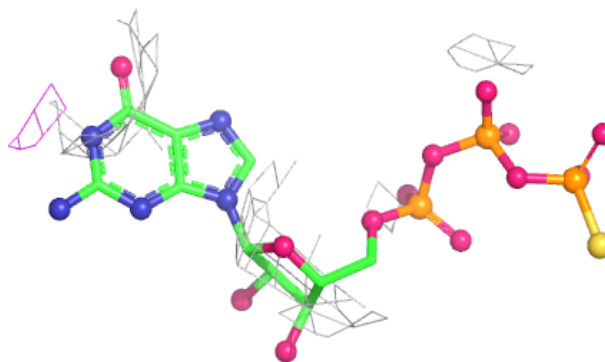
**Electron density around GSP d 2000:**

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

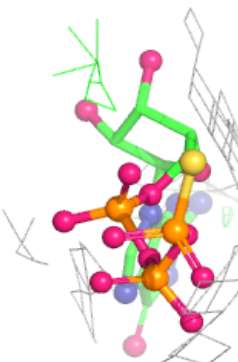
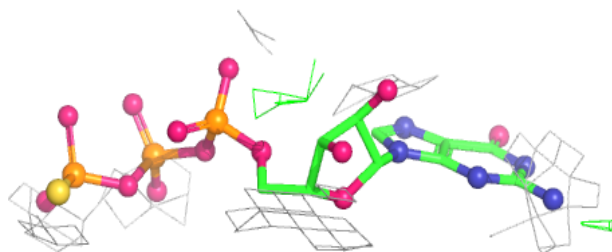
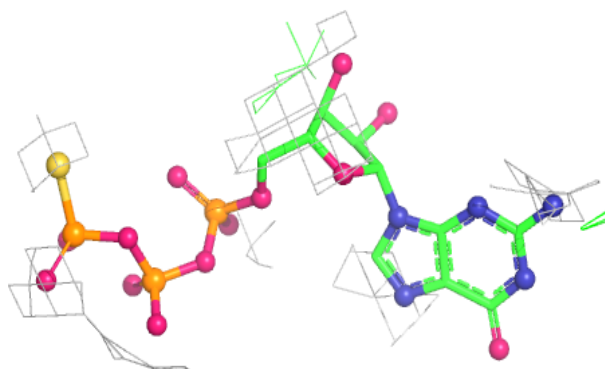


Electron density around GSP h 2000:

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

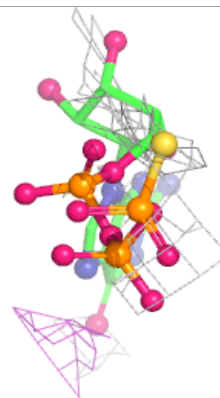
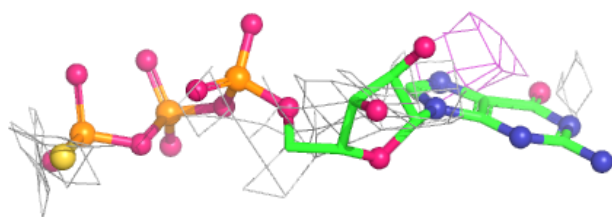
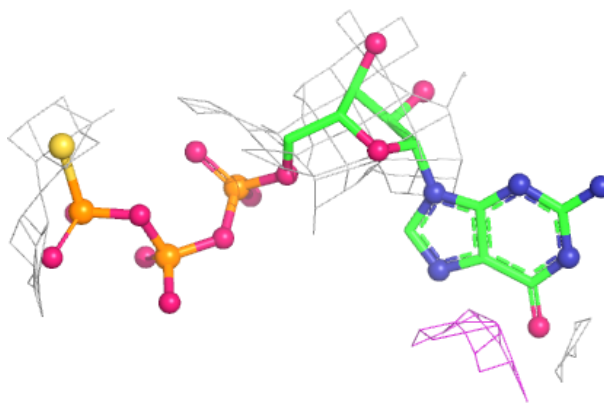
**Electron density around GSP B 2000:**

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

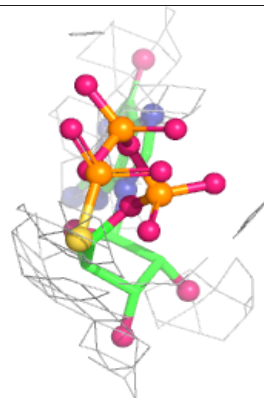
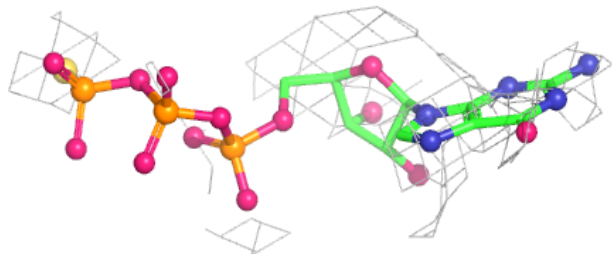
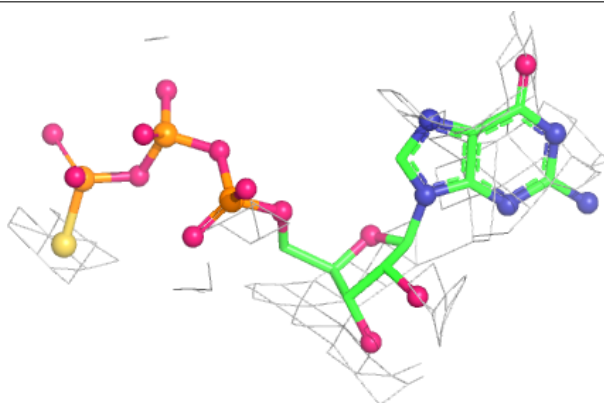


Electron density around GSP Z 2000:

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

**Electron density around GSP N 2000:**

$2mF_o-DF_c$ (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.