



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 4BN5 / pdb_00004bn5
Title : Structure of human SIRT3 in complex with SRT1720 inhibitor
Authors : Nguyen, G.T.T.; Schaefer, S.; Gertz, M.; Weyand, M.; Steegborn, C.
Deposited on : 2013-05-13
Resolution : 3.25 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

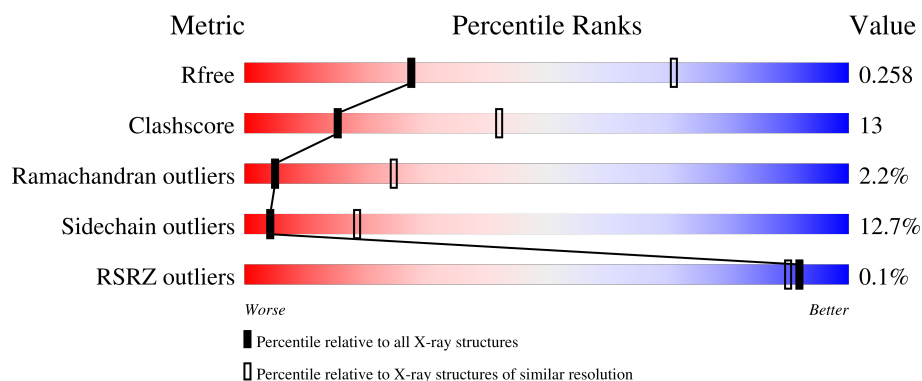
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	281	56% 34% 6% ...
1	B	281	63% 25% 7% ...
1	C	281	57% 32% 8% ...
1	D	281	59% 31% 5% ...
1	E	281	67% 27% ...

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Mol	Chain	Length	Quality of chain
1	F	281	 66% 24% 5% . .
1	G	281	 70% 21% 5% . .
1	H	281	 64% 26% 7% .
1	I	281	 69% 23% 5% .
1	J	281	 71% 22% . . .
1	K	281	 % 62% 29% 5% . .
1	L	281	 69% 24% . .

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
3	SR7	F	1396	-	-	X	-
3	SR7	G	1396	-	-	X	-
3	SR7	H	1396	-	-	X	-
3	SR7	I	1396	-	-	X	-

2 Entry composition

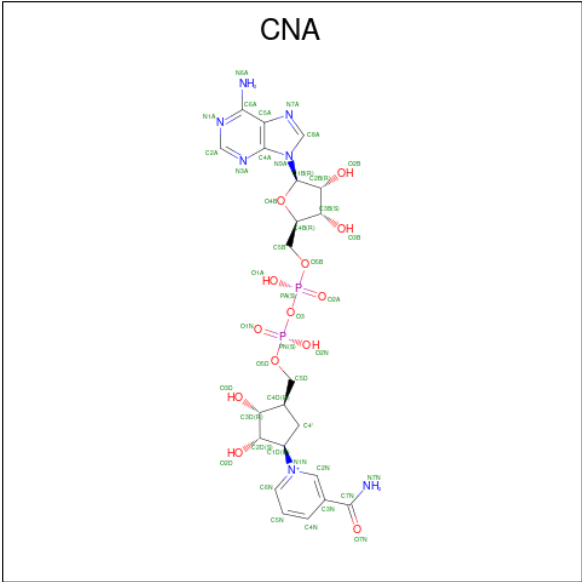
There are 5 unique types of molecules in this entry. The entry contains 26520 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL.

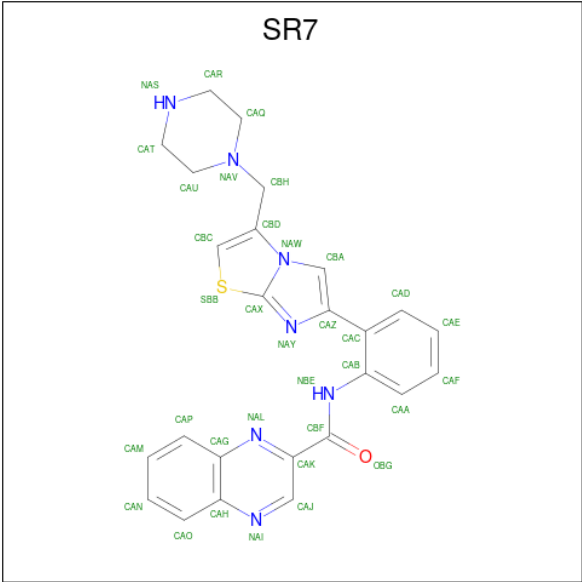
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	B	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	C	273	Total	C	N	O	S	0	0	0
			2131	1372	369	381	9			
1	D	272	Total	C	N	O	S	0	0	0
			2059	1330	346	374	9			
1	E	273	Total	C	N	O	S	0	0	0
			2096	1356	353	378	9			
1	F	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	G	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	H	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	I	273	Total	C	N	O	S	0	0	0
			2120	1369	361	381	9			
1	J	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	K	273	Total	C	N	O	S	0	0	0
			2144	1382	369	384	9			
1	L	273	Total	C	N	O	S	0	0	0
			2134	1377	366	382	9			

- Molecule 2 is CARBA-NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: CNA) (formula: $C_{22}H_{30}N_7O_{13}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	B	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	C	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	D	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	E	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	F	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	G	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	H	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	I	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	J	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	K	1	Total	C	N	O	P	0	0
			44	22	7	13	2		
2	L	1	Total	C	N	O	P	0	0
			44	22	7	13	2		

- Molecule 3 is N-{2-[3-(piperazin-1-ylmethyl)imidazo[2,1-b][1,3]thiazol-6-yl]phenyl}quinoxaline-2-carboxamide (CCD ID: SR7) (formula: C₂₅H₂₃N₇OS).

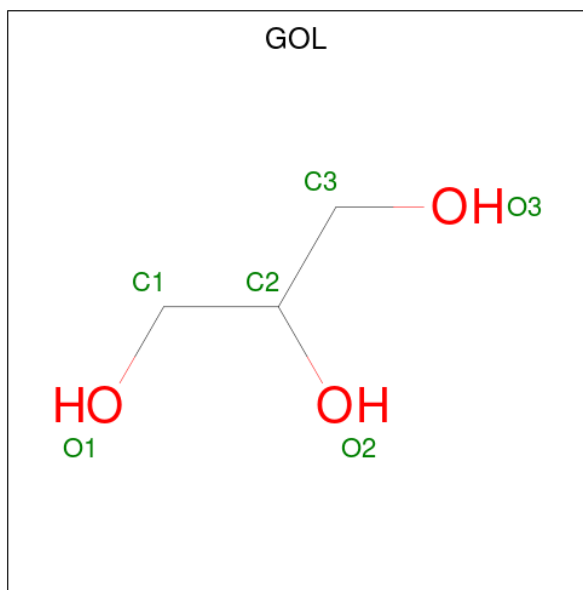


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	B	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	C	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	D	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	E	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	F	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	G	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	H	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	I	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	J	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	K	1	Total	C	N	O	S	0	0
			34	25	7	1	1		
3	L	1	Total	C	N	O	S	0	0
			34	25	7	1	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	E	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0
4	G	1	Total Zn 1 1	0	0
4	H	1	Total Zn 1 1	0	0
4	I	1	Total Zn 1 1	0	0
4	J	1	Total Zn 1 1	0	0
4	K	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

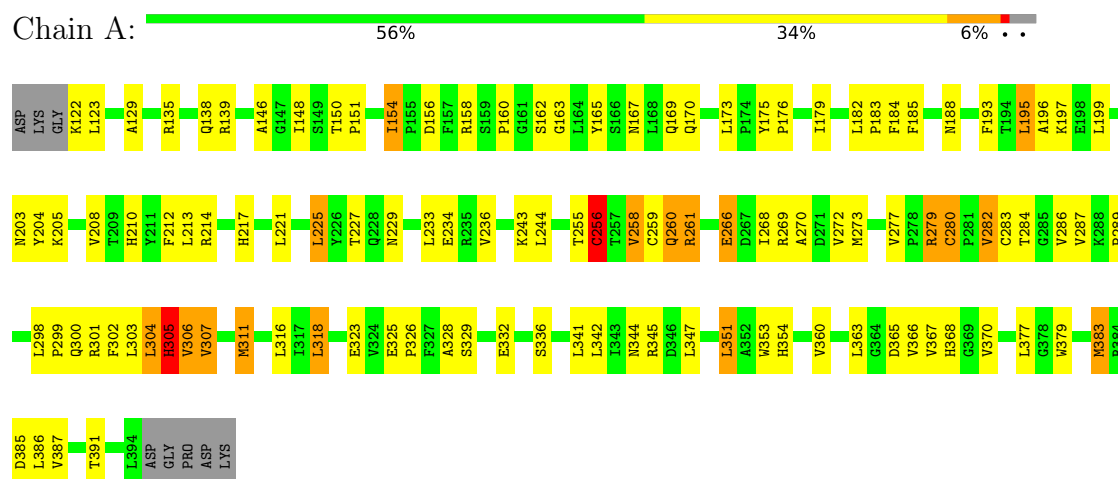


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0
5	K	1	Total 6	C 3	O 3	0	0
5	L	1	Total 6	C 3	O 3	0	0

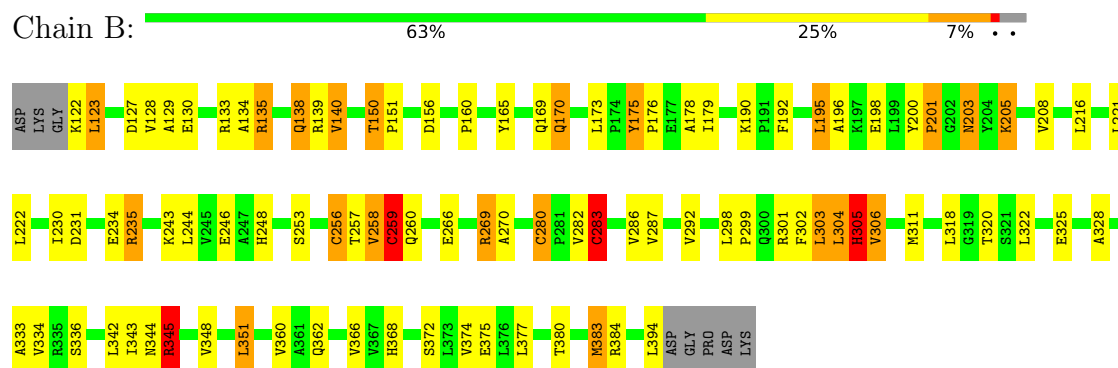
3 Residue-property plots

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.

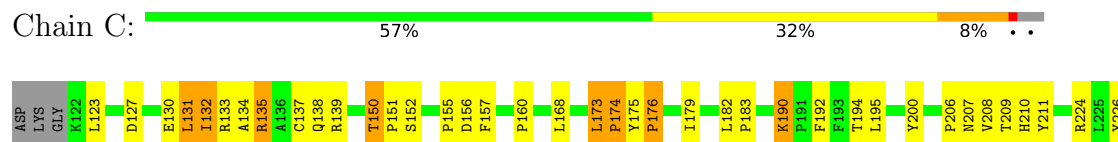
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

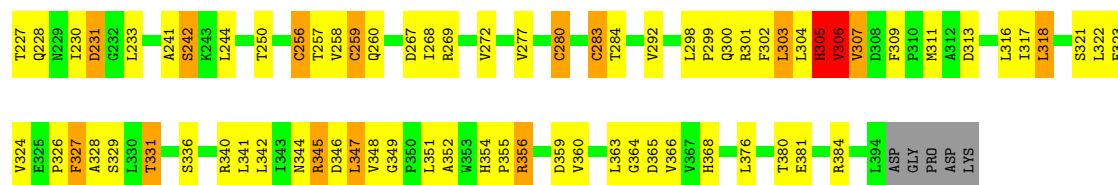


• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL



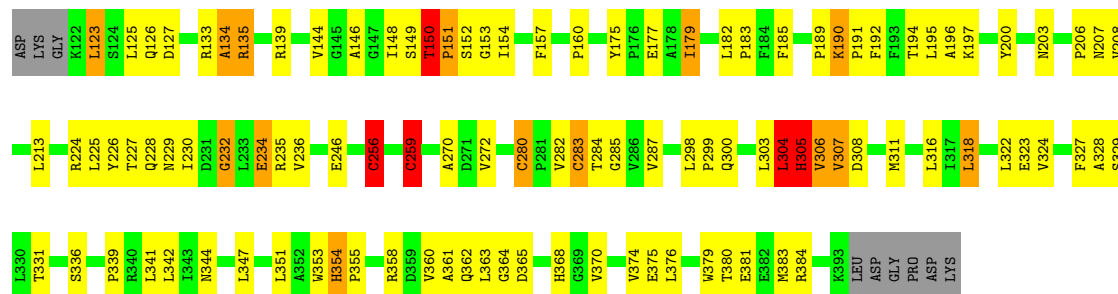
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL





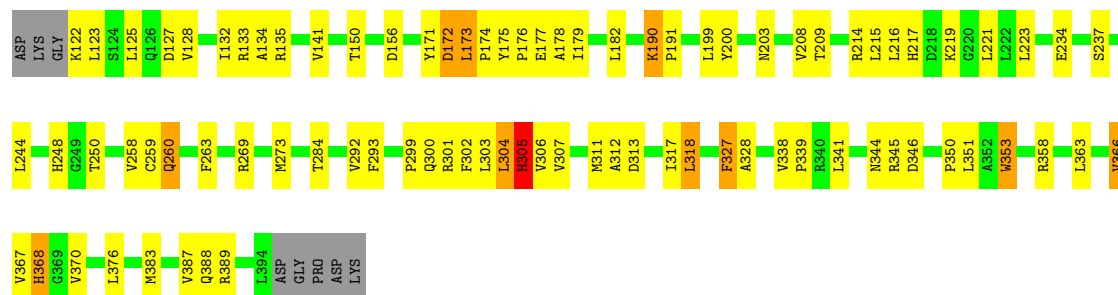
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain D: 59% 31% 5% . .



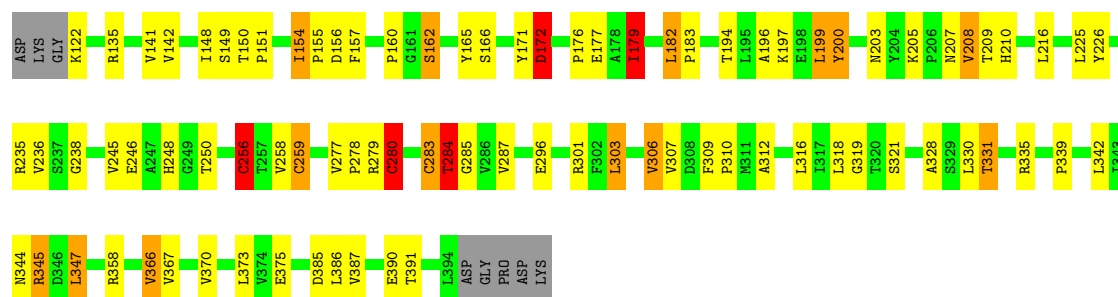
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain E: 67% 27% . .



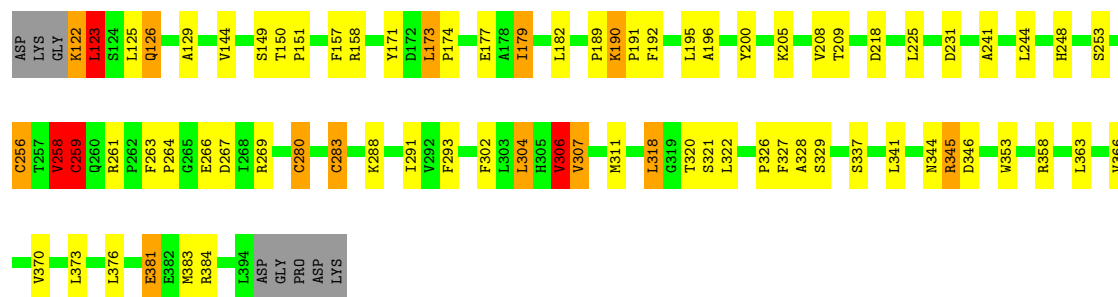
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain F: 66% 24% 5% . .



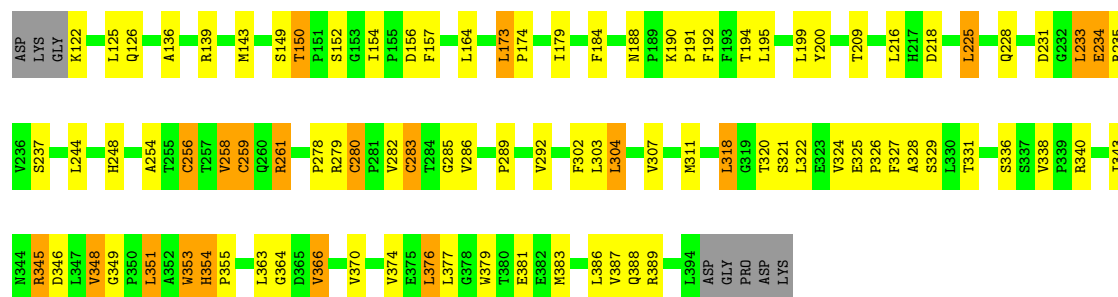
• Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain G: 70% 21% 5% . .



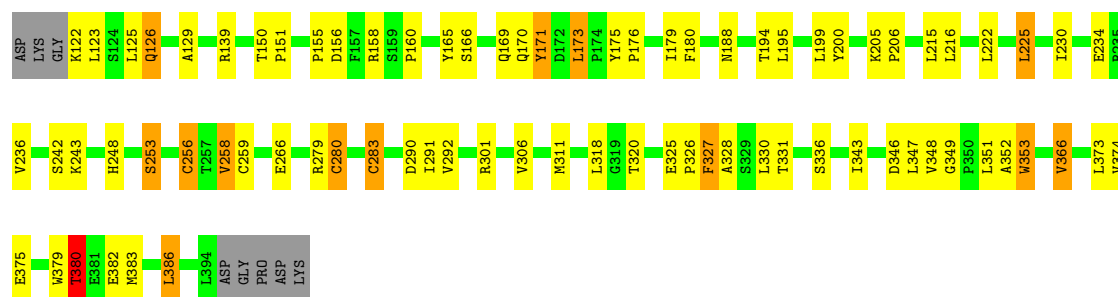
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain H: 64% 26% 7% .



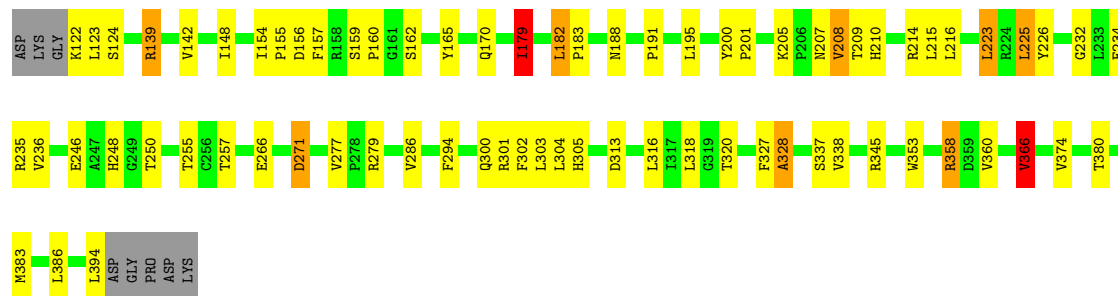
- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

Chain I: 69% 23% 5% .

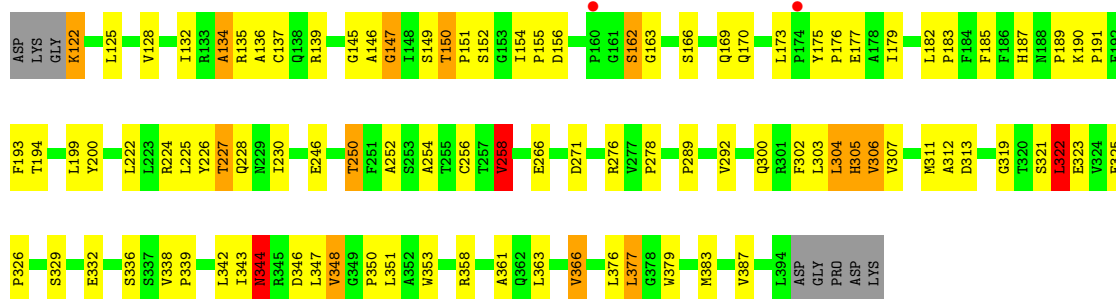


- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL

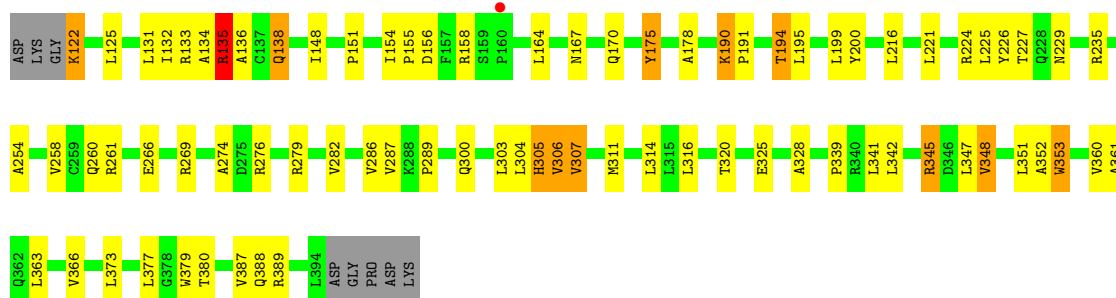
Chain J: 71% 22% . . .



- Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL



● Molecule 1: NAD-DEPENDENT PROTEIN DEACETYLASE SIRTUIN-3, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.82Å 246.06Å 127.34Å 90.00° 123.88° 90.00°	Depositor
Resolution (Å)	48.57 – 3.25 48.57 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.57-3.25) 99.4 (48.57-3.25)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.208 , 0.265 0.203 , 0.258	Depositor DCC
R_{free} test set	4558 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.428 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26520	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CNA, ZN, SR7, GOL

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	0.99	2/2199 (0.1%)	1.15	10/2996 (0.3%)
1	B	0.95	2/2199 (0.1%)	1.14	8/2996 (0.3%)
1	C	0.93	3/2184 (0.1%)	1.16	17/2975 (0.6%)
1	D	0.97	6/2110 (0.3%)	1.13	10/2883 (0.3%)
1	E	0.77	0/2150	1.05	7/2938 (0.2%)
1	F	0.77	1/2199 (0.0%)	1.06	11/2996 (0.4%)
1	G	0.78	1/2199 (0.0%)	1.06	4/2996 (0.1%)
1	H	0.75	0/2199	1.08	12/2996 (0.4%)
1	I	0.76	1/2175 (0.0%)	1.02	9/2968 (0.3%)
1	J	0.73	0/2199	0.99	4/2996 (0.1%)
1	K	0.68	0/2199	0.93	1/2996 (0.0%)
1	L	0.67	0/2189	0.93	3/2984 (0.1%)
All	All	0.82	16/26201 (0.1%)	1.06	96/35720 (0.3%)

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	B	0	2
1	D	0	2
1	E	0	2
1	K	0	2
1	L	0	1
All	All	0	10

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	CYS	CA-CB	6.55	1.64	1.53
1	D	160	PRO	C-O	6.50	1.31	1.23
1	D	365	ASP	CB-CG	6.15	1.67	1.52
1	D	305	HIS	CA-CB	5.61	1.62	1.53
1	D	259	CYS	CA-CB	5.57	1.62	1.53
1	I	259	CYS	CA-CB	5.57	1.62	1.53
1	C	174	PRO	CA-C	5.47	1.60	1.52
1	C	160	PRO	C-O	5.47	1.30	1.23
1	G	259	CYS	CA-CB	5.39	1.62	1.53
1	D	305	HIS	N-CA	5.35	1.53	1.46
1	B	259	CYS	CA-CB	5.29	1.62	1.53
1	B	222	LEU	CA-C	-5.27	1.46	1.52
1	F	259	CYS	N-CA	5.21	1.52	1.46
1	A	365	ASP	CA-C	-5.21	1.46	1.52
1	D	304	LEU	CA-C	5.16	1.59	1.52
1	A	305	HIS	CA-CB	5.15	1.62	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	307	VAL	CB-CA-C	-8.90	103.22	111.06
1	F	366	VAL	CB-CA-C	-8.89	100.13	112.14
1	J	366	VAL	CB-CA-C	-8.04	100.31	112.05
1	H	354	HIS	CA-C-N	7.72	127.76	119.89
1	H	354	HIS	C-N-CA	7.72	127.76	119.89
1	D	234	GLU	N-CA-C	-7.71	102.81	111.14
1	F	345	ARG	N-CA-CB	7.52	120.89	109.91
1	F	277	VAL	CA-C-N	7.35	127.33	119.76
1	F	277	VAL	C-N-CA	7.35	127.33	119.76
1	C	309	PHE	CA-C-N	-7.13	111.63	119.19
1	C	309	PHE	C-N-CA	-7.13	111.63	119.19
1	I	348	VAL	N-CA-C	7.07	120.26	108.81
1	A	305	HIS	N-CA-C	-6.99	95.91	110.80
1	C	176	PRO	N-CA-CB	6.97	110.57	103.25
1	A	280	CYS	CA-CB-SG	6.82	130.08	114.40
1	H	348	VAL	N-CA-C	6.68	119.99	108.90
1	I	366	VAL	CB-CA-C	-6.64	103.38	111.88
1	L	348	VAL	N-CA-C	6.61	116.52	108.06
1	C	348	VAL	N-CA-C	6.57	116.95	107.88
1	J	353	TRP	N-CA-C	6.54	118.10	110.97
1	F	179	ILE	N-CA-CB	6.53	118.63	110.47
1	A	306	VAL	N-CA-C	6.45	118.03	111.00
1	F	345	ARG	N-CA-C	-6.43	103.96	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	287	VAL	N-CA-C	6.40	116.61	106.88
1	C	280	CYS	CA-CB-SG	6.38	129.07	114.40
1	D	280	CYS	CA-CB-SG	6.34	128.98	114.40
1	A	260	GLN	N-CA-C	6.32	124.26	110.80
1	D	203	ASN	N-CA-C	6.25	118.64	111.02
1	D	323	GLU	N-CA-C	-6.19	103.85	112.45
1	D	305	HIS	N-CA-C	-6.16	97.67	110.80
1	B	280	CYS	CA-CB-SG	5.99	128.17	114.40
1	C	345	ARG	N-CA-C	-5.97	104.69	111.14
1	A	256	CYS	CA-CB-SG	5.90	127.97	114.40
1	H	338	VAL	N-CA-C	5.85	114.68	108.95
1	G	280	CYS	CA-CB-SG	5.84	127.83	114.40
1	E	366	VAL	CB-CA-C	-5.82	104.29	112.14
1	E	368	HIS	N-CA-C	-5.80	104.31	111.33
1	F	207	ASN	N-CA-C	5.79	116.19	108.38
1	E	338	VAL	N-CA-C	5.77	113.59	108.63
1	I	175	TYR	CA-C-N	5.75	127.02	119.84
1	I	175	TYR	C-N-CA	5.75	127.02	119.84
1	B	280	CYS	N-CA-CB	5.71	117.66	109.78
1	B	305	HIS	CA-CB-CG	5.68	119.48	113.80
1	I	259	CYS	CA-CB-SG	5.67	127.44	114.40
1	A	305	HIS	CA-CB-CG	5.65	119.45	113.80
1	G	179	ILE	CB-CA-C	-5.64	104.53	112.14
1	D	280	CYS	N-CA-CB	5.62	118.32	110.11
1	D	307	VAL	CB-CA-C	-5.62	106.11	111.06
1	H	234	GLU	N-CA-C	-5.61	105.07	111.07
1	E	179	ILE	N-CA-C	-5.60	104.05	111.05
1	C	259	CYS	CA-CB-SG	5.54	127.15	114.40
1	H	366	VAL	CB-CA-C	-5.54	104.89	111.81
1	H	307	VAL	CB-CA-C	-5.51	104.87	110.88
1	A	205	LYS	CA-C-N	-5.50	115.07	120.52
1	A	205	LYS	C-N-CA	-5.50	115.07	120.52
1	C	327	PHE	N-CA-C	5.50	117.99	111.33
1	F	280	CYS	CA-CB-SG	5.50	127.05	114.40
1	B	280	CYS	CA-C-N	5.46	125.17	119.82
1	B	280	CYS	C-N-CA	5.46	125.17	119.82
1	L	132	ILE	CB-CA-C	-5.40	104.84	111.92
1	D	368	HIS	N-CA-C	-5.37	105.42	111.28
1	C	326	PRO	CA-C-N	5.37	127.74	120.38
1	C	326	PRO	C-N-CA	5.37	127.74	120.38
1	C	173	LEU	CA-C-N	5.32	126.48	119.84
1	C	173	LEU	C-N-CA	5.32	126.48	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	364	GLY	N-CA-C	-5.31	106.71	112.08
1	E	305	HIS	CA-CB-CG	5.27	119.07	113.80
1	H	304	LEU	N-CA-C	-5.27	106.90	113.38
1	A	280	CYS	N-CA-CB	5.26	118.34	110.02
1	H	136	ALA	N-CA-C	-5.26	106.36	112.89
1	J	179	ILE	N-CA-CB	5.25	117.68	110.54
1	H	259	CYS	CA-CB-SG	5.22	126.42	114.40
1	J	234	GLU	N-CA-C	-5.22	105.48	111.07
1	I	256	CYS	CA-CB-SG	5.21	126.39	114.40
1	C	190	LYS	CA-C-N	5.20	124.65	119.24
1	C	190	LYS	C-N-CA	5.20	124.65	119.24
1	G	123	LEU	N-CA-C	5.20	118.17	110.48
1	C	305	HIS	CB-CA-C	5.18	120.74	110.42
1	K	344	ASN	N-CA-C	5.18	116.71	108.79
1	H	280	CYS	CA-CB-SG	5.17	126.30	114.40
1	A	306	VAL	CB-CA-C	-5.16	105.33	112.24
1	F	296	GLU	N-CA-C	-5.14	103.71	110.39
1	F	256	CYS	N-CA-CB	5.14	117.57	110.17
1	E	263	PHE	CA-C-N	-5.11	114.97	120.03
1	E	263	PHE	C-N-CA	-5.11	114.97	120.03
1	C	331	THR	N-CA-C	-5.11	106.56	112.89
1	B	123	LEU	N-CA-C	5.08	117.36	110.35
1	I	234	GLU	N-CA-C	-5.08	105.64	111.07
1	D	256	CYS	N-CA-CB	5.08	117.48	110.17
1	B	345	ARG	N-CA-CB	5.05	117.64	110.06
1	B	259	CYS	CA-CB-SG	5.04	126.00	114.40
1	C	306	VAL	CB-CA-C	-5.04	103.94	112.16
1	I	188	ASN	CA-C-N	5.02	124.51	119.19
1	I	188	ASN	C-N-CA	5.02	124.51	119.19
1	D	305	HIS	CA-CB-CG	5.02	118.82	113.80
1	F	179	ILE	CB-CA-C	-5.01	105.47	112.04

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	304	LEU	Peptide
1	B	283	CYS	Peptide
1	B	304	LEU	Peptide
1	D	304	LEU	Peptide
1	D	305	HIS	Peptide
1	E	303	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	E	305	HIS	Peptide
1	K	170	GLN	Peptide
1	K	304	LEU	Peptide
1	L	170	GLN	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	2144	0	2160	89	0
1	B	2144	0	2160	80	0
1	C	2131	0	2143	73	0
1	D	2059	0	2025	75	0
1	E	2096	0	2079	46	1
1	F	2144	0	2160	53	0
1	G	2144	0	2160	46	0
1	H	2144	0	2160	57	0
1	I	2120	0	2117	37	0
1	J	2144	0	2160	36	0
1	K	2144	0	2160	61	0
1	L	2134	0	2145	46	0
2	A	44	0	29	5	0
2	B	44	0	29	4	0
2	C	44	0	29	1	0
2	D	44	0	29	5	0
2	E	44	0	29	1	0
2	F	44	0	29	3	0
2	G	44	0	29	12	0
2	H	44	0	29	10	0
2	I	44	0	29	5	0
2	J	44	0	29	4	0
2	K	44	0	29	6	0
2	L	44	0	29	5	0
3	A	34	0	23	4	0
3	B	34	0	23	5	0
3	C	34	0	23	4	0
3	D	34	0	23	2	0
3	E	34	0	23	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	34	0	23	11	0
3	G	34	0	23	18	0
3	H	34	0	23	11	0
3	I	34	0	23	10	0
3	J	34	0	23	7	0
3	K	34	0	23	8	0
3	L	34	0	23	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	C	6	0	8	2	0
5	D	6	0	8	3	0
5	K	6	0	8	1	0
5	L	6	0	8	0	0
All	All	26520	0	26285	711	1

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 13.

All (711) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:HIS:CE1	1:D:305:HIS:CE1	1.88	1.58
1:A:305:HIS:CE1	1:B:305:HIS:NE2	1.85	1.43
1:A:305:HIS:NE2	1:B:305:HIS:NE2	1.68	1.36
1:C:305:HIS:NE2	1:D:305:HIS:CE1	1.84	1.35
1:A:305:HIS:NE2	1:B:305:HIS:CE1	1.96	1.31
1:C:305:HIS:NE2	1:D:305:HIS:NE2	1.91	1.18
2:A:1395:CNA:O2N	2:A:1395:CNA:H17	1.50	1.09
2:G:1395:CNA:C6N	3:G:1396:SR7:NAI	2.18	1.07
1:H:349:GLY:O	1:H:353:TRP:CD1	2.10	1.04
1:C:305:HIS:HE1	1:D:305:HIS:CE1	1.72	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1395:CNA:C6N	3:H:1396:SR7:HAP	1.94	0.97
2:H:1395:CNA:C5N	3:H:1396:SR7:HAP	1.95	0.95
1:H:157:PHE:CE1	1:H:179:ILE:HD13	2.03	0.94
1:G:157:PHE:HE1	3:G:1396:SR7:NAL	1.67	0.93
1:K:305:HIS:CE1	1:L:305:HIS:NE2	2.36	0.93
1:A:280:CYS:SG	1:A:283:CYS:N	2.41	0.92
1:G:157:PHE:CE1	3:G:1396:SR7:NAL	2.38	0.92
2:G:1395:CNA:C3N	3:G:1396:SR7:HAO	2.03	0.88
1:C:305:HIS:CE1	1:D:305:HIS:HE1	1.70	0.88
2:J:1395:CNA:H17	2:J:1395:CNA:O2N	1.73	0.87
1:K:305:HIS:NE2	1:L:305:HIS:NE2	2.22	0.87
1:C:155:PRO:O	3:C:1397:SR7:HAM	1.72	0.86
1:D:342:LEU:HD22	1:D:351:LEU:HD12	1.58	0.85
1:J:142:VAL:HG12	1:J:316:LEU:HB3	1.59	0.85
1:C:305:HIS:CE1	1:D:305:HIS:ND1	2.44	0.84
1:A:306:VAL:HG21	1:B:306:VAL:HG21	1.60	0.83
1:A:279:ARG:HG3	1:A:284:THR:C	2.07	0.80
1:G:261:ARG:HG3	1:H:218:ASP:O	1.81	0.79
1:C:302:PHE:O	1:C:305:HIS:HB3	1.84	0.78
1:D:342:LEU:HD11	1:D:344:ASN:HB2	1.66	0.78
1:H:325:GLU:OE1	1:H:326:PRO:HA	1.84	0.77
1:A:138:GLN:HA	1:A:221:LEU:HD23	1.65	0.77
1:I:156:ASP:HA	3:I:1396:SR7:HAP	1.67	0.75
1:H:280:CYS:SG	1:H:283:CYS:N	2.58	0.75
2:G:1395:CNA:N1N	3:G:1396:SR7:NAI	2.35	0.74
1:K:305:HIS:NE2	1:L:305:HIS:CE1	2.56	0.74
1:F:256:CYS:HA	1:F:287:VAL:HA	1.69	0.74
1:F:208:VAL:HG11	1:F:367:VAL:HG13	1.69	0.74
2:I:1395:CNA:O3D	3:I:1396:SR7:NAY	2.18	0.74
1:E:156:ASP:HA	3:E:1396:SR7:HAP	1.69	0.73
2:G:1395:CNA:C4N	3:G:1396:SR7:HAO	2.18	0.73
1:C:322:LEU:HD13	1:C:331:THR:HG21	1.68	0.73
1:K:122:LYS:HE3	1:K:122:LYS:HA	1.71	0.73
1:B:156:ASP:HA	3:B:1396:SR7:HAP	1.69	0.72
1:F:171:TYR:O	1:F:172:ASP:C	2.32	0.72
1:F:256:CYS:SG	1:F:259:CYS:N	2.61	0.72
1:D:280:CYS:SG	1:D:283:CYS:N	2.62	0.72
1:H:349:GLY:O	1:H:353:TRP:NE1	2.23	0.72
1:C:301:ARG:HG2	5:C:1396:GOL:H11	1.71	0.72
2:A:1395:CNA:O2N	2:A:1395:CNA:C4D	2.34	0.71
1:C:301:ARG:O	1:C:304:LEU:HD12	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:C	1:D:306:VAL:N	2.49	0.71
1:H:318:LEU:HD13	1:H:343:ILE:HB	1.72	0.71
1:A:304:LEU:HD23	1:C:303:LEU:HD12	1.73	0.71
1:A:279:ARG:HG3	1:A:284:THR:O	1.91	0.70
1:G:149:SER:OG	1:G:231:ASP:OD2	2.05	0.70
1:H:292:VAL:O	3:H:1396:SR7:HBHA	1.92	0.70
1:J:157:PHE:CZ	1:J:179:ILE:HD11	2.26	0.70
1:D:304:LEU:O	1:D:305:HIS:C	2.35	0.69
1:K:156:ASP:HA	3:K:1397:SR7:HAP	1.73	0.69
1:A:256:CYS:SG	1:A:259:CYS:N	2.65	0.69
1:B:280:CYS:SG	1:B:283:CYS:N	2.65	0.69
1:K:137:CYS:HA	1:K:313:ASP:OD2	1.92	0.69
2:H:1395:CNA:H21	3:H:1396:SR7:CAZ	2.06	0.69
1:H:366:VAL:HG23	2:H:1395:CNA:N1A	2.07	0.69
1:F:280:CYS:SG	1:F:283:CYS:N	2.64	0.68
2:I:1395:CNA:H21	3:I:1396:SR7:CAX	2.06	0.68
1:I:199:LEU:HD11	3:I:1396:SR7:HAN	1.76	0.68
1:A:305:HIS:HE1	1:B:305:HIS:NE2	1.81	0.68
1:A:304:LEU:O	1:A:305:HIS:C	2.37	0.67
1:I:280:CYS:SG	1:I:283:CYS:N	2.65	0.67
1:D:304:LEU:O	1:D:306:VAL:N	2.27	0.67
1:F:142:VAL:HG12	1:F:225:LEU:HD13	1.76	0.67
1:C:305:HIS:NE2	1:D:305:HIS:CD2	2.62	0.67
1:K:325:GLU:OE1	1:K:326:PRO:HA	1.95	0.67
1:L:325:GLU:OE1	1:L:328:ALA:HB3	1.95	0.67
1:D:150:THR:O	1:D:153:GLY:N	2.26	0.67
2:G:1395:CNA:H24	3:G:1396:SR7:HAJ	1.76	0.67
1:E:133:ARG:C	1:E:135:ARG:H	2.02	0.67
1:E:128:VAL:HG11	1:E:341:LEU:HD22	1.76	0.66
1:G:346:ASP:HA	1:G:363:LEU:HD22	1.75	0.66
1:K:342:LEU:HD23	1:K:347:LEU:HD12	1.78	0.66
1:J:156:ASP:HA	3:J:1396:SR7:HAP	1.78	0.66
1:B:301:ARG:HG2	5:D:1395:GOL:H2	1.78	0.66
1:I:318:LEU:HD13	1:I:343:ILE:HB	1.77	0.66
1:L:175:TYR:CE2	1:L:178:ALA:HB2	2.31	0.65
2:G:1395:CNA:H24	3:G:1396:SR7:CAJ	2.26	0.65
1:C:317:ILE:HD12	1:C:351:LEU:HD11	1.78	0.65
1:A:303:LEU:CD1	1:B:306:VAL:HG11	2.28	0.65
1:A:305:HIS:NE2	1:B:305:HIS:HE1	1.87	0.65
1:D:150:THR:HG22	1:D:151:PRO:N	2.09	0.65
1:A:233:LEU:HA	1:A:236:VAL:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:VAL:HG23	1:J:225:LEU:HD13	1.79	0.64
1:B:205:LYS:HE2	1:B:394:LEU:HD22	1.79	0.64
1:G:248:HIS:CE1	3:G:1396:SR7:HARA	2.31	0.64
1:I:158:ARG:HE	3:I:1396:SR7:HAA	1.61	0.64
2:L:1395:CNA:H19	3:L:1397:SR7:NBE	2.12	0.64
1:B:304:LEU:O	1:B:305:HIS:C	2.41	0.64
1:G:280:CYS:SG	1:G:283:CYS:N	2.63	0.64
1:H:386:LEU:HA	1:H:389:ARG:HD2	1.78	0.64
1:B:303:LEU:HD23	1:D:304:LEU:HD12	1.80	0.63
1:A:156:ASP:HA	3:A:1396:SR7:HAP	1.80	0.63
1:B:134:ALA:O	1:B:135:ARG:HB2	1.97	0.63
1:C:280:CYS:SG	1:C:283:CYS:N	2.60	0.63
1:E:346:ASP:HA	1:E:363:LEU:HD22	1.80	0.63
1:E:133:ARG:O	1:E:135:ARG:N	2.31	0.63
1:D:304:LEU:C	1:D:306:VAL:H	2.05	0.62
1:H:199:LEU:HD11	3:H:1396:SR7:HAN	1.80	0.62
1:C:345:ARG:HA	1:C:364:GLY:O	1.99	0.62
1:K:303:LEU:CD1	1:L:306:VAL:HG11	2.29	0.62
1:C:342:LEU:HD22	1:C:351:LEU:HD12	1.80	0.62
1:G:122:LYS:C	1:G:122:LYS:HE3	2.23	0.62
3:F:1396:SR7:NAY	3:F:1396:SR7:HAJ	2.14	0.62
1:A:279:ARG:CG	1:A:284:THR:O	2.48	0.62
1:A:305:HIS:CE1	1:B:305:HIS:CD2	2.83	0.62
1:G:171:TYR:O	1:G:173:LEU:N	2.32	0.62
1:A:162:SER:O	1:A:163:GLY:C	2.43	0.62
1:E:353:TRP:H	1:E:353:TRP:CD1	2.16	0.62
1:L:366:VAL:HG23	2:L:1395:CNA:C2A	2.30	0.61
2:G:1395:CNA:C6N	3:G:1396:SR7:CAJ	2.78	0.61
1:D:353:TRP:O	1:D:354:HIS:CB	2.48	0.61
1:C:156:ASP:HA	3:C:1397:SR7:HAP	1.82	0.61
1:E:317:ILE:C	1:E:318:LEU:HD23	2.25	0.61
1:L:135:ARG:NH1	1:L:138:GLN:HG2	2.16	0.61
1:B:342:LEU:HB2	1:B:351:LEU:HD12	1.83	0.61
1:C:346:ASP:HA	1:C:363:LEU:HD22	1.83	0.61
1:L:224:ARG:HG2	1:L:226:TYR:CE1	2.35	0.61
1:G:256:CYS:SG	1:G:259:CYS:N	2.74	0.60
1:B:345:ARG:HH11	1:B:345:ARG:HB3	1.66	0.60
1:H:188:ASN:OD1	1:H:190:LYS:N	2.33	0.60
1:B:322:LEU:HD12	1:B:348:VAL:HG23	1.82	0.60
1:H:143:MET:HE1	1:H:331:THR:HG23	1.82	0.60
1:E:175:TYR:CE1	1:E:178:ALA:HB2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:HIS:CE1	3:H:1396:SR7:HARA	2.37	0.60
1:J:232:GLY:O	1:J:236:VAL:HG23	2.01	0.60
1:K:155:PRO:O	3:K:1397:SR7:HAM	2.02	0.60
1:C:317:ILE:C	1:C:318:LEU:HD23	2.26	0.60
1:G:218:ASP:O	1:H:261:ARG:HG3	2.01	0.60
1:K:342:LEU:HD12	1:K:343:ILE:H	1.67	0.60
1:E:292:VAL:O	3:E:1396:SR7:HBHA	2.02	0.59
1:A:304:LEU:HD23	1:C:303:LEU:CD1	2.32	0.59
2:D:1394:CNA:H19	3:D:1396:SR7:NBE	2.18	0.59
2:G:1395:CNA:H17	2:G:1395:CNA:O2N	2.02	0.59
1:K:302:PHE:O	1:K:305:HIS:HB2	2.01	0.59
1:L:279:ARG:HG2	1:L:286:VAL:HA	1.84	0.59
2:L:1395:CNA:H19	3:L:1397:SR7:HNBE	1.66	0.59
1:F:248:HIS:CE1	3:F:1396:SR7:HAR	2.37	0.59
1:H:278:PRO:C	1:H:279:ARG:HG3	2.28	0.59
1:F:148:ILE:HG22	1:F:209:THR:HG21	1.83	0.59
1:G:157:PHE:CE2	1:G:179:ILE:HD11	2.37	0.59
1:B:325:GLU:OE1	1:B:328:ALA:HB3	2.03	0.58
1:J:257:THR:HB	1:J:286:VAL:O	2.02	0.58
1:K:306:VAL:HG21	1:L:306:VAL:HG21	1.85	0.58
1:A:304:LEU:C	1:A:306:VAL:N	2.61	0.58
1:I:230:ILE:HD12	1:I:291:ILE:HD12	1.85	0.58
1:F:157:PHE:CZ	1:F:179:ILE:HD11	2.39	0.58
2:D:1394:CNA:H17	2:D:1394:CNA:O2N	2.03	0.58
1:B:303:LEU:HD12	1:B:303:LEU:O	2.04	0.58
1:C:301:ARG:O	1:C:304:LEU:CD1	2.51	0.58
1:F:339:PRO:HA	1:F:358:ARG:HB3	1.86	0.58
1:A:280:CYS:SG	1:A:282:VAL:HB	2.44	0.58
2:H:1395:CNA:O3D	3:H:1396:SR7:NAY	2.31	0.57
1:L:175:TYR:CD2	1:L:178:ALA:HB2	2.40	0.57
1:C:306:VAL:HG11	1:D:303:LEU:HD21	1.85	0.57
1:K:347:LEU:HB2	1:K:363:LEU:HD11	1.86	0.57
1:J:182:LEU:O	1:J:183:PRO:C	2.46	0.57
1:D:125:LEU:HD22	1:D:362:GLN:OE1	2.04	0.57
1:D:191:PRO:O	1:D:194:THR:HB	2.04	0.57
1:A:325:GLU:OE1	1:A:328:ALA:HB3	2.05	0.56
1:E:234:GLU:CB	1:E:244:LEU:HD21	2.36	0.56
1:K:366:VAL:HG23	2:K:1395:CNA:C2A	2.35	0.56
1:H:173:LEU:HD13	1:H:174:PRO:HD2	1.87	0.56
1:C:304:LEU:HD12	1:C:304:LEU:H	1.70	0.56
1:H:233:LEU:N	1:H:233:LEU:HD23	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1395:CNA:O2N	2:J:1395:CNA:C4D	2.52	0.56
1:F:236:VAL:C	1:F:238:GLY:H	2.13	0.56
1:H:150:THR:HG21	2:H:1395:CNA:H11	1.71	0.56
2:H:1395:CNA:O3D	3:H:1396:SR7:CAZ	2.54	0.56
1:L:254:ALA:HA	1:L:289:PRO:HA	1.87	0.56
1:B:235:ARG:HD2	1:B:246:GLU:OE2	2.06	0.55
1:E:173:LEU:HD23	1:E:174:PRO:HD2	1.88	0.55
1:B:384:ARG:NH1	1:B:384:ARG:HB3	2.21	0.55
1:D:150:THR:O	1:D:152:SER:N	2.39	0.55
3:J:1396:SR7:HAJ	3:J:1396:SR7:NAY	2.21	0.55
1:A:303:LEU:HD13	1:B:306:VAL:HG11	1.87	0.55
1:K:303:LEU:HD12	1:L:306:VAL:HG11	1.86	0.55
1:C:356:ARG:N	1:C:359:ASP:OD2	2.40	0.55
1:D:256:CYS:SG	1:D:259:CYS:N	2.75	0.55
1:F:160:PRO:HA	1:F:165:TYR:CD2	2.41	0.55
2:K:1395:CNA:H19	3:K:1397:SR7:HNBE	1.72	0.55
1:C:303:LEU:O	1:C:306:VAL:HG23	2.06	0.55
2:K:1395:CNA:H19	3:K:1397:SR7:NBE	2.21	0.55
1:L:342:LEU:HD22	1:L:351:LEU:HD12	1.89	0.55
1:B:248:HIS:CD2	3:B:1396:SR7:HAR	2.41	0.55
1:D:283:CYS:HB2	1:D:285:GLY:H	1.71	0.55
1:A:138:GLN:HA	1:A:221:LEU:CD2	2.37	0.55
1:C:283:CYS:O	1:C:284:THR:OG1	2.19	0.54
1:D:322:LEU:HD13	1:D:331:THR:HG21	1.89	0.54
1:K:149:SER:O	1:K:150:THR:C	2.50	0.54
1:K:377:LEU:HD23	1:K:379:TRP:CZ3	2.42	0.54
1:B:176:PRO:O	1:B:179:ILE:HG22	2.08	0.54
1:B:195:LEU:O	1:B:196:ALA:C	2.50	0.54
1:F:248:HIS:CE1	3:F:1396:SR7:CAR	2.90	0.54
1:K:344:ASN:HB3	1:K:346:ASP:O	2.08	0.54
1:D:179:ILE:HG22	1:D:192:PHE:HA	1.90	0.54
1:I:374:VAL:HG13	1:I:379:TRP:HB2	1.90	0.54
1:A:306:VAL:HG21	1:B:306:VAL:CG2	2.35	0.54
1:C:327:PHE:O	1:C:328:ALA:C	2.49	0.54
1:C:340:ARG:HB2	1:C:359:ASP:OD1	2.08	0.54
1:J:207:ASN:O	1:J:210:HIS:N	2.40	0.54
1:D:182:LEU:O	1:D:183:PRO:C	2.51	0.54
1:A:301:ARG:HA	5:C:1396:GOL:H2	1.90	0.54
1:C:133:ARG:C	1:C:135:ARG:H	2.16	0.53
1:F:278:PRO:C	1:F:279:ARG:HG2	2.32	0.53
1:C:130:GLU:HA	1:C:130:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:HIS:NE2	1:D:305:HIS:ND1	2.45	0.53
1:G:158:ARG:HG3	1:G:158:ARG:HH11	1.73	0.53
2:G:1395:CNA:O2N	2:G:1395:CNA:C4D	2.56	0.53
1:B:320:THR:HG23	1:B:322:LEU:HG	1.90	0.53
1:C:304:LEU:O	1:C:305:HIS:C	2.50	0.53
1:K:125:LEU:HD23	1:K:376:LEU:HD12	1.91	0.53
1:J:148:ILE:HG22	1:J:209:THR:HG21	1.90	0.53
1:J:366:VAL:HG22	2:J:1395:CNA:N1A	2.23	0.53
3:A:1396:SR7:HAJ	3:A:1396:SR7:NAY	2.23	0.53
1:D:148:ILE:O	1:D:207:ASN:ND2	2.37	0.53
1:E:214:ARG:HD3	1:E:237:SER:O	2.09	0.53
1:J:313:ASP:C	1:J:338:VAL:HG13	2.33	0.53
1:E:214:ARG:O	1:E:217:HIS:HB3	2.09	0.53
1:I:347:LEU:HD23	1:I:352:ALA:HB2	1.91	0.53
1:K:342:LEU:HD12	1:K:343:ILE:N	2.23	0.53
1:A:302:PHE:O	1:A:305:HIS:HB2	2.08	0.52
1:A:225:LEU:C	1:A:225:LEU:HD12	2.34	0.52
1:C:316:LEU:CD1	1:C:341:LEU:HD23	2.39	0.52
1:E:259:CYS:O	1:E:260:GLN:HB2	2.10	0.52
1:G:173:LEU:HD13	1:G:174:PRO:HD2	1.91	0.52
1:C:241:ALA:HA	1:C:244:LEU:HD12	1.92	0.52
1:F:310:PRO:O	1:F:335:ARG:NH2	2.43	0.52
1:D:157:PHE:CZ	1:D:179:ILE:HD11	2.44	0.52
1:E:234:GLU:HB3	1:E:244:LEU:HD21	1.90	0.52
1:J:225:LEU:C	1:J:225:LEU:HD12	2.34	0.52
1:B:133:ARG:NH1	1:B:377:LEU:O	2.43	0.52
1:B:304:LEU:C	1:B:306:VAL:N	2.67	0.52
1:C:317:ILE:O	1:C:342:LEU:HD12	2.09	0.52
1:D:351:LEU:O	1:D:355:PRO:HB3	2.08	0.52
1:G:344:ASN:O	1:G:345:ARG:C	2.52	0.52
1:H:188:ASN:OD1	1:H:191:PRO:HD3	2.10	0.52
1:A:176:PRO:O	1:A:179:ILE:HG22	2.10	0.52
1:I:325:GLU:OE1	1:I:326:PRO:HA	2.10	0.52
1:C:307:VAL:CG2	1:C:311:MET:HE2	2.40	0.52
1:G:321:SER:O	1:G:322:LEU:HB2	2.09	0.52
1:L:135:ARG:NE	1:L:221:LEU:HD21	2.24	0.52
1:E:353:TRP:CD1	1:E:353:TRP:N	2.77	0.52
1:I:225:LEU:HD12	1:I:225:LEU:C	2.34	0.52
1:D:195:LEU:C	1:D:195:LEU:HD23	2.35	0.52
1:B:138:GLN:HA	1:B:221:LEU:HD23	1.90	0.51
1:A:214:ARG:O	1:A:217:HIS:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:PHE:CD1	3:G:1396:SR7:NAL	2.77	0.51
1:I:386:LEU:HD12	1:I:386:LEU:O	2.10	0.51
1:J:337:SER:O	1:J:358:ARG:HD2	2.10	0.51
1:K:350:PRO:HA	1:K:353:TRP:HB2	1.92	0.51
1:A:305:HIS:CD2	1:B:305:HIS:CE1	2.92	0.51
1:B:248:HIS:NE2	3:B:1396:SR7:HAR	2.25	0.51
1:F:182:LEU:O	1:F:183:PRO:C	2.51	0.51
2:J:1395:CNA:H24	3:J:1396:SR7:CAJ	2.41	0.51
1:L:134:ALA:O	1:L:136:ALA:N	2.44	0.51
2:I:1395:CNA:H21	3:I:1396:SR7:CAZ	2.15	0.51
1:A:303:LEU:HG	1:C:303:LEU:HD13	1.92	0.51
1:A:316:LEU:HG	1:A:318:LEU:HD21	1.92	0.51
1:D:256:CYS:HA	1:D:287:VAL:HA	1.93	0.51
1:E:313:ASP:OD1	1:E:313:ASP:C	2.53	0.51
1:G:288:LYS:NZ	1:G:291:ILE:O	2.44	0.51
2:B:1395:CNA:H17	2:B:1395:CNA:O2N	2.11	0.51
1:D:339:PRO:HA	1:D:358:ARG:O	2.10	0.51
1:J:235:ARG:HD2	1:J:246:GLU:OE2	2.11	0.51
1:G:126:GLN:O	1:G:129:ALA:HB3	2.11	0.51
1:A:307:VAL:HB	1:D:307:VAL:HG12	1.92	0.50
1:C:305:HIS:HE1	1:D:305:HIS:ND1	1.99	0.50
1:J:139:ARG:HG3	1:J:223:LEU:HD22	1.93	0.50
1:A:129:ALA:HA	1:A:377:LEU:HD21	1.93	0.50
1:A:154:ILE:HG21	2:A:1395:CNA:N7N	2.26	0.50
1:B:304:LEU:O	1:B:306:VAL:N	2.44	0.50
1:K:271:ASP:OD1	1:K:276:ARG:NH2	2.44	0.50
1:C:306:VAL:HG11	1:D:303:LEU:CD2	2.42	0.50
1:F:307:VAL:HG12	1:L:307:VAL:HA	1.93	0.50
1:K:224:ARG:HG2	1:K:226:TYR:CE1	2.47	0.50
1:A:298:LEU:O	1:A:299:PRO:C	2.52	0.50
1:A:304:LEU:CD2	1:C:303:LEU:HD12	2.41	0.50
1:A:383:MET:O	1:A:387:VAL:HG23	2.11	0.50
1:F:156:ASP:HA	3:F:1396:SR7:HAP	1.94	0.50
1:F:162:SER:O	1:F:165:TYR:N	2.44	0.50
1:I:160:PRO:HA	1:I:165:TYR:CG	2.46	0.50
1:I:206:PRO:HG3	1:I:236:VAL:HG12	1.94	0.50
1:I:327:PHE:HA	1:I:330:LEU:HD12	1.93	0.50
1:I:379:TRP:O	1:I:380:THR:C	2.54	0.50
1:A:307:VAL:HA	1:D:307:VAL:HG12	1.93	0.50
1:D:146:ALA:HB2	2:D:1394:CNA:H16	1.94	0.50
1:A:266:GLU:OE1	1:A:266:GLU:N	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:157:PHE:CD1	3:G:1396:SR7:HAP	2.47	0.50
2:H:1395:CNA:C4N	3:H:1396:SR7:HAP	2.41	0.50
1:A:188:ASN:OD1	1:A:188:ASN:C	2.55	0.49
1:C:168:LEU:HD23	1:C:194:THR:HG21	1.94	0.49
1:I:215:LEU:HD22	1:I:383:MET:HG2	1.93	0.49
2:I:1395:CNA:O3D	3:I:1396:SR7:CAX	2.58	0.49
1:K:227:THR:HG23	1:K:246:GLU:HA	1.95	0.49
2:C:1395:CNA:H17	2:C:1395:CNA:O2N	2.13	0.49
1:F:319:GLY:HA2	1:F:344:ASN:OD1	2.12	0.49
1:J:157:PHE:CE1	3:J:1396:SR7:NAL	2.80	0.49
1:C:123:LEU:HD22	1:C:127:ASP:CB	2.42	0.49
1:F:283:CYS:O	1:F:284:THR:HB	2.11	0.49
1:H:345:ARG:HG2	2:H:1395:CNA:N3A	2.27	0.49
1:L:341:LEU:HD12	1:L:360:VAL:O	2.12	0.49
1:H:302:PHE:CZ	1:H:326:PRO:HG2	2.48	0.49
1:L:156:ASP:HA	3:L:1397:SR7:HAP	1.93	0.49
1:G:125:LEU:HD11	1:G:373:LEU:HD13	1.94	0.49
1:H:348:VAL:O	1:H:351:LEU:HB2	2.13	0.49
1:A:304:LEU:O	1:A:306:VAL:N	2.45	0.49
1:B:234:GLU:HB3	1:B:244:LEU:HD21	1.95	0.49
1:D:195:LEU:HD23	1:D:195:LEU:O	2.12	0.49
1:A:156:ASP:OD1	1:A:158:ARG:HB2	2.12	0.49
1:E:173:LEU:O	1:E:174:PRO:C	2.56	0.49
1:B:368:HIS:ND1	1:B:368:HIS:O	2.47	0.48
1:C:224:ARG:HG2	1:C:226:TYR:CE1	2.48	0.48
1:D:227:THR:OG1	1:D:229:ASN:HB2	2.13	0.48
1:L:122:LYS:HA	1:L:122:LYS:HE3	1.95	0.48
1:A:342:LEU:HB2	1:A:351:LEU:HD12	1.96	0.48
1:J:225:LEU:HD12	1:J:226:TYR:N	2.29	0.48
1:A:182:LEU:HB2	1:A:183:PRO:HD3	1.95	0.48
1:C:256:CYS:SG	1:C:259:CYS:N	2.86	0.48
1:B:160:PRO:HA	1:B:165:TYR:CD2	2.49	0.48
1:H:366:VAL:O	1:H:370:VAL:HG23	2.13	0.48
1:A:266:GLU:CD	1:A:266:GLU:H	2.21	0.48
1:B:169:GLN:O	1:B:170:GLN:C	2.57	0.48
1:H:209:THR:HG23	1:H:370:VAL:HG21	1.95	0.48
1:C:304:LEU:C	1:C:306:VAL:N	2.72	0.48
1:K:166:SER:HA	1:K:169:GLN:HG2	1.94	0.48
1:A:199:LEU:HD11	3:A:1396:SR7:HAN	1.96	0.48
1:E:327:PHE:O	1:E:328:ALA:C	2.57	0.48
1:F:236:VAL:C	1:F:238:GLY:N	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:332:GLU:OE2	1:K:350:PRO:HB3	2.14	0.48
1:A:208:VAL:HG11	1:A:367:VAL:HG13	1.96	0.48
1:F:148:ILE:HD12	1:F:210:HIS:CE1	2.49	0.48
1:H:377:LEU:HD13	1:H:379:TRP:CH2	2.49	0.48
1:H:254:ALA:HA	1:H:289:PRO:HA	1.95	0.48
1:B:269:ARG:O	1:B:270:ALA:C	2.57	0.47
1:K:150:THR:HB	1:K:151:PRO:CD	2.43	0.47
1:E:299:PRO:O	1:E:300:GLN:C	2.57	0.47
1:E:344:ASN:O	1:E:345:ARG:C	2.57	0.47
1:G:381:GLU:HA	1:G:384:ARG:NH1	2.29	0.47
1:I:205:LYS:HE3	1:I:205:LYS:HA	1.97	0.47
2:K:1395:CNA:H24	3:K:1397:SR7:CAJ	2.45	0.47
1:L:366:VAL:HG23	2:L:1395:CNA:N1A	2.29	0.47
1:C:150:THR:HG22	1:C:151:PRO:N	2.29	0.47
1:D:341:LEU:HD12	1:D:360:VAL:O	2.14	0.47
1:I:379:TRP:O	1:I:382:GLU:N	2.48	0.47
1:A:366:VAL:O	1:A:370:VAL:HG23	2.15	0.47
1:I:292:VAL:O	3:I:1396:SR7:HBHA	2.14	0.47
1:C:182:LEU:O	1:C:183:PRO:C	2.58	0.47
1:E:259:CYS:O	1:E:260:GLN:CB	2.63	0.47
1:F:199:LEU:HD11	3:F:1396:SR7:HAN	1.96	0.47
1:G:326:PRO:O	1:G:329:SER:HB3	2.13	0.47
2:G:1395:CNA:C4N	3:G:1396:SR7:CAO	2.90	0.47
1:H:386:LEU:O	1:H:387:VAL:C	2.58	0.47
1:D:235:ARG:HD2	1:D:246:GLU:OE2	2.15	0.47
1:G:190:LYS:N	1:G:191:PRO:CD	2.78	0.47
1:H:192:PHE:O	1:H:195:LEU:HB3	2.15	0.47
1:I:349:GLY:O	1:I:353:TRP:HB3	2.14	0.47
1:K:250:THR:HG23	1:K:252:ALA:H	1.80	0.47
1:K:304:LEU:O	1:K:305:HIS:C	2.56	0.47
1:L:345:ARG:CB	2:L:1395:CNA:O2B	2.62	0.47
3:L:1397:SR7:NBE	3:L:1397:SR7:NAY	2.62	0.47
1:D:213:LEU:HD21	1:D:318:LEU:HD11	1.97	0.47
3:E:1396:SR7:HAJ	3:E:1396:SR7:NAY	2.30	0.47
1:L:260:GLN:O	1:L:261:ARG:C	2.57	0.47
1:L:377:LEU:HD13	1:L:379:TRP:CZ3	2.50	0.47
1:F:157:PHE:CE2	3:F:1396:SR7:NAL	2.83	0.47
1:F:303:LEU:O	1:F:306:VAL:HG23	2.14	0.47
1:G:192:PHE:O	1:G:195:LEU:HB3	2.15	0.47
1:J:300:GLN:O	1:J:302:PHE:N	2.48	0.47
1:K:322:LEU:HD23	1:K:348:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:283:CYS:HB2	1:F:285:GLY:H	1.79	0.46
1:G:306:VAL:HG12	1:G:307:VAL:HG13	1.96	0.46
1:B:302:PHE:O	1:B:305:HIS:HB2	2.14	0.46
1:B:344:ASN:O	1:B:345:ARG:C	2.58	0.46
1:A:184:PHE:O	1:A:185:PHE:C	2.58	0.46
1:A:351:LEU:N	1:A:351:LEU:HD23	2.31	0.46
1:B:333:ALA:O	1:B:334:VAL:C	2.58	0.46
1:E:141:VAL:HG23	1:E:312:ALA:HB2	1.96	0.46
1:K:182:LEU:O	1:K:185:PHE:N	2.49	0.46
1:A:175:TYR:O	1:A:176:PRO:C	2.56	0.46
1:H:126:GLN:HA	1:H:376:LEU:HD22	1.97	0.46
1:H:366:VAL:HG23	2:H:1395:CNA:C6A	2.45	0.46
1:J:123:LEU:HB2	1:J:360:VAL:CG2	2.45	0.46
1:A:302:PHE:CZ	1:A:326:PRO:HG2	2.49	0.46
1:D:195:LEU:C	1:D:195:LEU:CD2	2.88	0.46
1:F:309:PHE:CE2	1:F:330:LEU:HD22	2.50	0.46
1:H:225:LEU:C	1:H:225:LEU:HD12	2.40	0.46
1:D:342:LEU:HB2	1:D:351:LEU:CD1	2.46	0.46
1:H:233:LEU:N	1:H:233:LEU:CD2	2.78	0.46
1:K:339:PRO:HA	1:K:358:ARG:O	2.16	0.46
1:A:268:ILE:HG21	1:A:287:VAL:HG11	1.98	0.46
1:B:205:LYS:CE	1:B:394:LEU:HD22	2.45	0.46
2:F:1395:CNA:O3D	3:F:1396:SR7:NAY	2.47	0.46
1:I:215:LEU:HD23	1:I:379:TRP:CE3	2.51	0.46
1:K:254:ALA:HA	1:K:289:PRO:HA	1.97	0.46
1:H:285:GLY:O	1:H:286:VAL:C	2.58	0.46
1:K:134:ALA:O	1:K:136:ALA:N	2.49	0.46
1:K:147:GLY:HA3	1:K:319:GLY:HA3	1.97	0.46
1:B:258:VAL:O	1:B:260:GLN:HG2	2.16	0.46
1:F:142:VAL:CG1	1:F:225:LEU:HD13	2.46	0.46
1:F:328:ALA:O	1:F:331:THR:OG1	2.34	0.46
1:J:300:GLN:C	1:J:302:PHE:N	2.73	0.46
1:L:133:ARG:O	1:L:135:ARG:N	2.48	0.46
1:B:195:LEU:C	1:B:195:LEU:CD2	2.89	0.45
1:D:327:PHE:O	1:D:328:ALA:C	2.58	0.45
1:H:157:PHE:HB2	3:H:1396:SR7:NAI	2.32	0.45
1:K:228:GLN:O	2:K:1395:CNA:H22	2.16	0.45
1:A:193:PHE:CE2	1:A:277:VAL:HG13	2.51	0.45
1:D:125:LEU:O	1:D:126:GLN:C	2.58	0.45
1:E:176:PRO:C	1:E:178:ALA:H	2.24	0.45
1:H:302:PHE:C	1:H:304:LEU:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:125:LEU:CD1	1:L:373:LEU:HD13	2.46	0.45
1:L:304:LEU:O	1:L:305:HIS:C	2.60	0.45
1:D:150:THR:CG2	1:D:151:PRO:N	2.79	0.45
1:F:283:CYS:O	1:F:284:THR:CB	2.64	0.45
1:I:253:SER:OG	1:I:290:ASP:OD2	2.33	0.45
1:K:128:VAL:O	1:K:132:ILE:HG12	2.16	0.45
1:L:307:VAL:O	1:L:311:MET:HB2	2.17	0.45
1:A:307:VAL:HG23	1:A:311:MET:HE2	1.98	0.45
1:A:379:TRP:CD1	1:A:379:TRP:N	2.80	0.45
1:B:256:CYS:SG	1:B:259:CYS:N	2.89	0.45
1:D:123:LEU:HD22	1:D:127:ASP:CB	2.46	0.45
1:G:157:PHE:HD1	3:G:1396:SR7:HAP	1.82	0.45
1:C:207:ASN:O	1:C:210:HIS:N	2.50	0.45
1:E:171:TYR:O	1:E:172:ASP:C	2.59	0.45
1:G:383:MET:O	1:G:384:ARG:C	2.59	0.45
1:J:162:SER:O	1:J:165:TYR:HB3	2.16	0.45
1:K:145:GLY:O	1:K:146:ALA:C	2.60	0.45
1:L:135:ARG:HB3	1:L:135:ARG:HH11	1.81	0.45
1:A:212:PHE:O	1:A:213:LEU:C	2.59	0.45
1:B:266:GLU:CD	1:B:266:GLU:H	2.24	0.45
1:E:182:LEU:HD23	1:E:293:PHE:CD2	2.52	0.45
1:E:301:ARG:O	1:E:302:PHE:C	2.59	0.45
1:F:342:LEU:HD23	1:F:347:LEU:HD12	1.97	0.45
1:G:195:LEU:O	1:G:196:ALA:C	2.60	0.45
1:G:264:PRO:HD2	1:G:267:ASP:CG	2.42	0.45
2:I:1395:CNA:C5N	3:I:1396:SR7:CAP	2.95	0.45
1:K:176:PRO:O	1:K:179:ILE:HG22	2.16	0.45
1:L:167:ASN:HB3	1:L:194:THR:HG21	1.98	0.45
1:A:259:CYS:HB3	1:A:283:CYS:HB3	1.69	0.45
1:B:195:LEU:C	1:B:195:LEU:HD23	2.42	0.45
1:C:365:ASP:O	1:C:366:VAL:C	2.58	0.45
1:E:141:VAL:CG2	1:E:312:ALA:HB2	2.47	0.45
1:I:169:GLN:O	1:I:171:TYR:N	2.50	0.45
1:A:261:ARG:NH2	1:A:282:VAL:HG11	2.32	0.45
1:C:206:PRO:HB2	1:C:211:TYR:CE2	2.52	0.45
1:H:191:PRO:O	1:H:192:PHE:C	2.59	0.45
1:A:302:PHE:O	1:A:305:HIS:CB	2.65	0.45
1:D:224:ARG:NE	1:D:308:ASP:OD2	2.43	0.45
1:F:196:ALA:O	1:F:197:LYS:C	2.58	0.45
1:L:314:LEU:HD13	1:L:339:PRO:HG2	1.99	0.45
1:A:255:THR:O	1:A:256:CYS:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:O	1:B:195:LEU:HD23	2.17	0.44
1:B:343:ILE:HG12	1:B:362:GLN:HB3	1.99	0.44
1:C:267:ASP:C	1:C:269:ARG:H	2.25	0.44
1:L:148:ILE:O	1:L:151:PRO:HD2	2.17	0.44
1:L:155:PRO:O	3:L:1397:SR7:HAM	2.16	0.44
1:D:224:ARG:HG2	1:D:226:TYR:CE1	2.51	0.44
1:D:235:ARG:HH11	1:D:235:ARG:HG2	1.82	0.44
1:C:316:LEU:HD13	1:C:341:LEU:HD23	1.99	0.44
1:F:301:ARG:HA	5:K:1396:GOL:H2	1.99	0.44
1:A:160:PRO:HA	1:A:165:TYR:CD2	2.53	0.44
1:B:342:LEU:HD11	1:B:344:ASN:HB2	1.99	0.44
1:H:331:THR:O	1:H:340:ARG:NH1	2.45	0.44
1:A:196:ALA:O	1:A:197:LYS:C	2.60	0.44
1:D:133:ARG:C	1:D:135:ARG:N	2.75	0.44
1:E:383:MET:O	1:E:387:VAL:HG13	2.17	0.44
1:F:387:VAL:O	1:F:391:THR:OG1	2.16	0.44
1:L:316:LEU:CD1	1:L:341:LEU:HD23	2.47	0.44
1:E:248:HIS:C	1:E:292:VAL:HG23	2.42	0.44
1:G:302:PHE:C	1:G:304:LEU:H	2.25	0.44
1:I:129:ALA:HB2	1:I:373:LEU:HD12	2.00	0.44
1:I:129:ALA:HB2	1:I:373:LEU:CD1	2.47	0.44
1:K:122:LYS:HA	1:K:122:LYS:CE	2.46	0.44
1:K:379:TRP:O	1:K:383:MET:N	2.44	0.44
1:L:190:LYS:N	1:L:191:PRO:HD2	2.32	0.44
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.87	0.44
1:C:173:LEU:C	1:C:175:TYR:HA	2.43	0.44
1:C:231:ASP:O	1:C:233:LEU:HG	2.18	0.44
1:C:298:LEU:HB3	1:C:299:PRO:HD2	2.00	0.44
1:K:182:LEU:CB	1:K:183:PRO:CD	2.96	0.44
1:L:261:ARG:CZ	1:L:282:VAL:HG21	2.48	0.44
1:B:200:TYR:O	1:B:201:PRO:C	2.60	0.44
1:C:123:LEU:HB3	1:C:360:VAL:CG2	2.48	0.44
1:D:232:GLY:O	1:D:236:VAL:HG23	2.17	0.44
1:E:234:GLU:HB2	1:E:244:LEU:HD21	1.99	0.44
1:E:269:ARG:O	1:E:273:MET:HG2	2.18	0.44
1:J:205:LYS:HE2	1:J:394:LEU:HD22	2.00	0.44
1:B:301:ARG:HA	5:D:1395:GOL:H2	1.99	0.43
1:E:367:VAL:O	1:E:368:HIS:C	2.59	0.43
1:A:344:ASN:O	1:A:363:LEU:HA	2.18	0.43
1:B:302:PHE:O	1:B:305:HIS:CB	2.66	0.43
1:G:248:HIS:CE1	3:G:1396:SR7:CAR	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:374:VAL:HG13	1:H:379:TRP:HB2	2.00	0.43
1:J:156:ASP:HA	3:J:1396:SR7:CAP	2.46	0.43
1:J:304:LEU:O	1:J:305:HIS:C	2.61	0.43
1:L:274:ALA:HB3	1:L:276:ARG:NH1	2.33	0.43
1:D:304:LEU:CD1	1:D:304:LEU:N	2.81	0.43
1:B:298:LEU:O	1:B:299:PRO:C	2.58	0.43
1:D:196:ALA:O	1:D:197:LYS:C	2.59	0.43
1:D:374:VAL:HG11	1:D:383:MET:HG3	2.01	0.43
1:C:135:ARG:HD2	1:C:135:ARG:HA	1.75	0.43
1:D:383:MET:O	1:D:384:ARG:C	2.61	0.43
1:H:149:SER:HB3	1:H:154:ILE:HD12	2.01	0.43
1:J:300:GLN:C	1:J:302:PHE:H	2.27	0.43
1:J:327:PHE:O	1:J:328:ALA:C	2.61	0.43
1:K:189:PRO:C	1:K:191:PRO:HD2	2.43	0.43
1:F:155:PRO:O	3:F:1396:SR7:HAM	2.18	0.43
1:F:235:ARG:NH2	1:F:246:GLU:OE1	2.52	0.43
1:G:144:VAL:HG12	1:G:318:LEU:HB2	1.99	0.43
2:G:1395:CNA:C5N	3:G:1396:SR7:NAI	2.76	0.43
1:K:149:SER:O	1:K:152:SER:N	2.42	0.43
1:K:292:VAL:O	3:K:1397:SR7:HBC	2.19	0.43
1:C:347:LEU:HD23	1:C:352:ALA:HA	2.01	0.43
1:D:144:VAL:HG21	1:D:148:ILE:CD1	2.49	0.43
1:D:228:GLN:HG3	1:D:327:PHE:CZ	2.53	0.43
1:F:226:TYR:CE2	1:F:245:VAL:HG21	2.53	0.43
1:H:173:LEU:HA	1:H:174:PRO:HD2	1.92	0.43
1:H:256:CYS:SG	1:H:259:CYS:N	2.91	0.43
1:H:328:ALA:O	1:H:331:THR:OG1	2.37	0.43
1:I:155:PRO:O	3:I:1396:SR7:HAM	2.19	0.43
1:K:307:VAL:O	1:K:311:MET:HB2	2.18	0.43
1:K:321:SER:C	1:K:323:GLU:N	2.76	0.43
1:E:339:PRO:HA	1:E:358:ARG:O	2.19	0.43
1:F:157:PHE:CE2	1:F:179:ILE:HD11	2.53	0.43
2:K:1395:CNA:H18	2:K:1395:CNA:H30	1.79	0.43
1:L:125:LEU:HD11	1:L:373:LEU:HD13	2.00	0.43
1:B:256:CYS:HA	1:B:287:VAL:HA	2.00	0.42
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.92	0.42
1:D:185:PHE:O	1:D:189:PRO:HD3	2.19	0.42
1:G:345:ARG:HD3	1:G:345:ARG:HA	1.88	0.42
1:I:248:HIS:O	1:I:292:VAL:HG23	2.18	0.42
3:K:1397:SR7:NAY	3:K:1397:SR7:HAJ	2.34	0.42
1:A:150:THR:HB	1:A:151:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HE3	1:A:273:MET:HA	2.00	0.42
1:A:342:LEU:HD22	1:A:351:LEU:HD12	2.00	0.42
1:B:269:ARG:HG2	1:B:270:ALA:N	2.33	0.42
1:C:344:ASN:HD22	1:C:346:ASP:H	1.66	0.42
1:C:368:HIS:O	1:C:368:HIS:CD2	2.72	0.42
1:D:298:LEU:O	1:D:299:PRO:C	2.63	0.42
1:J:214:ARG:HG3	1:J:386:LEU:HD21	2.01	0.42
1:A:204:TYR:O	1:A:233:LEU:HD21	2.18	0.42
1:A:368:HIS:O	1:A:368:HIS:CG	2.72	0.42
1:C:318:LEU:HD23	1:C:318:LEU:N	2.34	0.42
1:D:379:TRP:O	1:D:381:GLU:N	2.52	0.42
1:A:258:VAL:O	1:A:260:GLN:HG2	2.19	0.42
1:B:235:ARG:HG2	1:B:235:ARG:HH11	1.85	0.42
1:B:235:ARG:HG2	1:B:235:ARG:NH1	2.34	0.42
1:F:303:LEU:O	1:F:303:LEU:HD12	2.19	0.42
1:G:123:LEU:N	1:G:123:LEU:HD23	2.34	0.42
1:H:321:SER:O	1:H:322:LEU:HB2	2.20	0.42
1:B:301:ARG:CG	5:D:1395:GOL:H2	2.47	0.42
1:G:158:ARG:NH1	3:G:1396:SR7:CBF	2.82	0.42
1:K:190:LYS:N	1:K:191:PRO:HD2	2.33	0.42
1:L:361:ALA:HB1	1:L:363:LEU:HG	2.01	0.42
1:A:227:THR:OG1	1:A:229:ASN:HB2	2.19	0.42
1:A:303:LEU:HD13	1:B:306:VAL:CG1	2.49	0.42
1:E:133:ARG:C	1:E:135:ARG:N	2.71	0.42
1:E:199:LEU:HD11	3:E:1396:SR7:HAN	2.02	0.42
2:E:1395:CNA:H17	2:E:1395:CNA:O2N	2.20	0.42
1:G:258:VAL:O	1:G:259:CYS:C	2.62	0.42
1:H:354:HIS:N	1:H:355:PRO:CD	2.82	0.42
1:B:303:LEU:HD23	1:D:304:LEU:CD1	2.47	0.42
1:B:374:VAL:HG11	1:B:383:MET:HG3	2.02	0.42
1:C:131:LEU:O	1:C:132:ILE:C	2.62	0.42
1:E:190:LYS:N	1:E:191:PRO:CD	2.83	0.42
1:G:150:THR:HB	1:G:151:PRO:HD3	2.01	0.42
1:K:162:SER:O	1:K:163:GLY:C	2.63	0.42
1:A:182:LEU:O	1:A:183:PRO:C	2.61	0.42
1:B:140:VAL:HG13	1:B:221:LEU:O	2.20	0.42
1:E:190:LYS:N	1:E:191:PRO:HD2	2.35	0.42
1:I:222:LEU:O	1:I:243:LYS:NZ	2.50	0.42
1:A:146:ALA:HB2	2:A:1395:CNA:H16	2.01	0.42
1:B:248:HIS:O	1:B:292:VAL:HG23	2.19	0.42
3:C:1397:SR7:NAY	3:C:1397:SR7:HAJ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ALA:HB1	1:D:363:LEU:HD21	2.02	0.42
1:F:141:VAL:CG2	1:F:312:ALA:HB2	2.49	0.42
1:F:157:PHE:CE2	3:F:1396:SR7:CAG	3.03	0.42
1:F:160:PRO:HA	1:F:165:TYR:CG	2.55	0.42
1:H:383:MET:O	1:H:387:VAL:HG13	2.20	0.42
1:I:386:LEU:HD12	1:I:386:LEU:C	2.44	0.42
1:J:294:PHE:CD1	3:J:1396:SR7:HAU	2.54	0.42
1:J:271:ASP:OD1	1:J:271:ASP:N	2.53	0.42
2:A:1395:CNA:H24	3:A:1396:SR7:CAJ	2.50	0.41
1:D:364:GLY:O	2:D:1394:CNA:H13	2.20	0.41
1:H:228:GLN:HG3	1:H:327:PHE:CE1	2.54	0.41
1:I:205:LYS:HD2	1:I:205:LYS:N	2.34	0.41
1:K:361:ALA:HB1	1:K:363:LEU:HG	2.02	0.41
1:A:279:ARG:CG	1:A:284:THR:C	2.87	0.41
1:F:157:PHE:H	3:F:1396:SR7:HAP	1.85	0.41
2:F:1395:CNA:H24	3:F:1396:SR7:CAJ	2.50	0.41
1:H:184:PHE:CD1	1:H:184:PHE:C	2.97	0.41
1:H:346:ASP:HA	1:H:363:LEU:HD22	2.02	0.41
1:I:328:ALA:O	1:I:331:THR:OG1	2.27	0.41
1:I:352:ALA:O	1:I:353:TRP:C	2.63	0.41
1:A:233:LEU:HA	1:A:236:VAL:CG1	2.47	0.41
1:A:234:GLU:HB3	1:A:244:LEU:HD21	2.01	0.41
1:B:127:ASP:O	1:B:130:GLU:HB2	2.20	0.41
1:B:302:PHE:O	1:B:302:PHE:CD2	2.74	0.41
1:C:157:PHE:CE2	3:C:1397:SR7:CAG	3.03	0.41
1:F:149:SER:HB3	1:F:154:ILE:HD13	2.02	0.41
1:F:342:LEU:HD11	1:F:344:ASN:HB2	2.01	0.41
1:G:261:ARG:HG2	1:G:263:PHE:CE1	2.56	0.41
1:G:328:ALA:O	1:G:329:SER:C	2.63	0.41
1:H:125:LEU:O	1:H:126:GLN:C	2.62	0.41
1:I:375:GLU:HA	1:I:380:THR:HG23	2.02	0.41
1:K:199:LEU:HD11	3:K:1397:SR7:HAN	2.02	0.41
1:A:387:VAL:O	1:A:391:THR:OG1	2.39	0.41
1:C:259:CYS:O	1:C:260:GLN:HB2	2.20	0.41
1:D:190:LYS:N	1:D:191:PRO:CD	2.84	0.41
1:K:256:CYS:SG	1:K:258:VAL:HG13	2.61	0.41
1:L:195:LEU:HD21	1:L:199:LEU:HD12	2.02	0.41
1:B:345:ARG:HG2	2:B:1395:CNA:N3A	2.35	0.41
1:C:192:PHE:CD1	1:C:192:PHE:C	2.98	0.41
1:C:195:LEU:C	1:C:195:LEU:HD23	2.46	0.41
1:E:302:PHE:C	1:E:304:LEU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:GLU:O	1:H:237:SER:OG	2.30	0.41
1:B:192:PHE:CD1	1:B:192:PHE:C	2.98	0.41
2:B:1395:CNA:H19	3:B:1396:SR7:NBE	2.36	0.41
1:C:292:VAL:HG21	1:C:299:PRO:HD3	2.03	0.41
1:E:305:HIS:O	1:E:307:VAL:N	2.54	0.41
1:F:370:VAL:O	1:F:373:LEU:N	2.53	0.41
1:H:209:THR:HG21	1:H:366:VAL:HG11	2.02	0.41
1:I:242:SER:O	1:I:301:ARG:NH2	2.54	0.41
1:B:345:ARG:HH11	1:B:345:ARG:CB	2.32	0.41
1:C:341:LEU:HD12	1:C:360:VAL:O	2.20	0.41
1:E:223:LEU:O	1:E:223:LEU:HD12	2.21	0.41
1:F:176:PRO:HG2	1:F:177:GLU:OE2	2.21	0.41
1:G:337:SER:O	1:G:358:ARG:NH1	2.53	0.41
1:L:316:LEU:HD11	1:L:341:LEU:HD23	2.03	0.41
1:A:311:MET:HG2	1:D:311:MET:HG3	2.03	0.41
1:D:149:SER:O	1:D:154:ILE:HB	2.21	0.41
1:E:388:GLN:O	1:E:389:ARG:C	2.63	0.41
1:F:321:SER:N	2:F:1395:CNA:O2N	2.40	0.41
1:K:193:PHE:CZ	1:K:278:PRO:HD2	2.55	0.41
1:K:377:LEU:HD23	1:K:379:TRP:CH2	2.56	0.41
1:L:352:ALA:O	1:L:353:TRP:C	2.63	0.41
1:A:165:TYR:O	1:A:169:GLN:HG2	2.21	0.41
1:A:195:LEU:HD12	1:A:199:LEU:HG	2.03	0.41
1:B:175:TYR:CD1	1:B:175:TYR:N	2.89	0.41
1:B:198:GLU:O	1:B:203:ASN:ND2	2.54	0.41
1:B:351:LEU:HD23	1:B:351:LEU:N	2.35	0.41
1:D:234:GLU:O	1:D:235:ARG:C	2.64	0.41
1:D:283:CYS:O	1:D:284:THR:OG1	2.28	0.41
1:E:248:HIS:CE1	3:E:1396:SR7:HAR	2.56	0.41
1:G:125:LEU:O	1:G:126:GLN:C	2.64	0.41
1:H:261:ARG:HE	1:H:261:ARG:HB2	1.50	0.41
1:H:388:GLN:O	1:H:389:ARG:C	2.63	0.41
1:B:150:THR:HB	1:B:151:PRO:HD3	2.03	0.41
1:B:302:PHE:O	1:B:302:PHE:CG	2.74	0.41
1:C:137:CYS:HA	1:C:313:ASP:OD2	2.21	0.41
3:D:1396:SR7:NBE	3:D:1396:SR7:NAY	2.67	0.41
1:F:150:THR:HB	1:F:151:PRO:CD	2.51	0.41
1:K:182:LEU:HB2	1:K:183:PRO:CD	2.51	0.41
1:B:178:ALA:O	1:B:179:ILE:C	2.64	0.40
1:B:384:ARG:HB3	1:B:384:ARG:HH11	1.86	0.40
1:H:318:LEU:CD1	1:H:343:ILE:HB	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:227:THR:OG1	1:L:229:ASN:HB2	2.22	0.40
1:C:228:GLN:HG3	1:C:327:PHE:CZ	2.56	0.40
1:D:150:THR:C	1:D:152:SER:N	2.79	0.40
1:I:150:THR:HB	1:I:151:PRO:CD	2.51	0.40
1:J:154:ILE:HA	1:J:155:PRO:HD3	1.93	0.40
1:J:248:HIS:NE2	3:J:1396:SR7:HAR	2.36	0.40
1:J:277:VAL:O	1:J:277:VAL:HG12	2.21	0.40
1:A:148:ILE:HD12	1:A:210:HIS:CD2	2.57	0.40
1:A:269:ARG:O	1:A:270:ALA:C	2.64	0.40
1:B:298:LEU:HB3	1:B:299:PRO:HD2	2.02	0.40
2:B:1395:CNA:H19	3:B:1396:SR7:HNBE	1.86	0.40
1:C:321:SER:O	1:C:322:LEU:C	2.65	0.40
1:D:134:ALA:O	1:D:135:ARG:HB2	2.22	0.40
1:F:162:SER:O	1:F:165:TYR:HB3	2.21	0.40
1:F:385:ASP:O	1:F:386:LEU:C	2.64	0.40
1:G:182:LEU:HD23	1:G:293:PHE:CD2	2.55	0.40
1:G:189:PRO:C	1:G:191:PRO:HD2	2.45	0.40
1:H:195:LEU:HD11	3:H:1396:SR7:HAO	2.01	0.40
1:I:173:LEU:HD23	1:I:173:LEU:HA	1.96	0.40
1:J:160:PRO:HA	1:J:165:TYR:CD1	2.56	0.40
1:J:188:ASN:O	1:J:191:PRO:HD2	2.21	0.40
1:K:304:LEU:O	1:K:307:VAL:N	2.53	0.40
1:L:164:LEU:HD11	1:L:195:LEU:HA	2.03	0.40
1:B:128:VAL:O	1:B:129:ALA:C	2.61	0.40
1:D:146:ALA:HB2	2:D:1394:CNA:C5D	2.51	0.40
1:E:132:ILE:HG23	1:E:221:LEU:HD13	2.03	0.40
1:G:225:LEU:HD22	1:G:244:LEU:CD2	2.52	0.40
2:G:1395:CNA:H30	3:G:1396:SR7:CAJ	2.52	0.40
1:I:179:ILE:HG23	1:I:180:PHE:CD2	2.56	0.40
1:J:207:ASN:O	1:J:208:VAL:C	2.65	0.40
1:J:374:VAL:HG11	1:J:383:MET:HG3	2.03	0.40
1:K:304:LEU:O	1:K:306:VAL:N	2.54	0.40
1:L:320:THR:O	1:L:320:THR:HG23	2.20	0.40
3:L:1397:SR7:NAY	3:L:1397:SR7:HAJ	2.37	0.40
1:A:160:PRO:HA	1:A:165:TYR:CG	2.57	0.40
1:A:163:GLY:O	1:A:167:ASN:ND2	2.54	0.40
1:A:268:ILE:O	1:A:269:ARG:C	2.64	0.40
1:E:171:TYR:CD2	1:E:191:PRO:HB3	2.56	0.40
1:E:215:LEU:HD11	1:E:219:LYS:HE2	2.03	0.40
1:F:199:LEU:O	1:F:200:TYR:C	2.63	0.40
1:G:209:THR:HG23	1:G:370:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:ASP:C	1:H:233:LEU:HD23	2.46	0.40
1:K:139:ARG:O	1:K:313:ASP:OD1	2.39	0.40
1:K:150:THR:HB	1:K:151:PRO:HD3	2.03	0.40
1:K:312:ALA:O	1:K:338:VAL:HG21	2.21	0.40

All (1) 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)
1:E:305:HIS:NE2	1:E:305:HIS:NE2[2_756]	1.96	0.24

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/281 (96%)	230 (85%)	37 (14%)	4 (2%)	8	32
1	B	271/281 (96%)	231 (85%)	35 (13%)	5 (2%)	6	29
1	C	271/281 (96%)	223 (82%)	36 (13%)	12 (4%)	2	12
1	D	270/281 (96%)	227 (84%)	33 (12%)	10 (4%)	2	15
1	E	271/281 (96%)	241 (89%)	23 (8%)	7 (3%)	4	21
1	F	271/281 (96%)	239 (88%)	29 (11%)	3 (1%)	11	38
1	G	271/281 (96%)	249 (92%)	18 (7%)	4 (2%)	8	32
1	H	271/281 (96%)	244 (90%)	24 (9%)	3 (1%)	11	38
1	I	271/281 (96%)	237 (88%)	29 (11%)	5 (2%)	6	29
1	J	271/281 (96%)	246 (91%)	21 (8%)	4 (2%)	8	32
1	K	271/281 (96%)	237 (88%)	26 (10%)	8 (3%)	3	19
1	L	271/281 (96%)	237 (88%)	29 (11%)	5 (2%)	6	29
All	All	3251/3372 (96%)	2841 (87%)	340 (10%)	70 (2%)	5	25

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	305	HIS
1	B	305	HIS
1	C	176	PRO
1	C	242	SER
1	C	305	HIS
1	C	381	GLU
1	D	305	HIS
1	E	172	ASP
1	E	260	GLN
1	E	306	VAL
1	J	328	ALA
1	K	135	ARG
1	K	305	HIS
1	L	135	ARG
1	L	305	HIS
1	A	282	VAL
1	B	257	THR
1	C	132	ILE
1	C	258	VAL
1	D	354	HIS
1	D	380	THR
1	E	134	ALA
1	E	258	VAL
1	F	172	ASP
1	G	306	VAL
1	H	258	VAL
1	I	170	GLN
1	I	380	THR
1	J	208	VAL
1	J	301	ARG
1	K	150	THR
1	K	258	VAL
1	K	322	LEU
1	L	345	ARG
1	B	259	CYS
1	B	336	SER
1	F	284	THR
1	K	300	GLN
1	C	131	LEU
1	C	134	ALA
1	C	349	GLY
1	C	355	PRO

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Mol	Chain	Res	Type
1	D	270	ALA
1	E	177	GLU
1	E	350	PRO
1	I	126	GLN
1	I	176	PRO
1	L	300	GLN
1	A	354	HIS
1	B	201	PRO
1	C	174	PRO
1	D	151	PRO
1	D	206	PRO
1	D	232	GLY
1	G	126	GLN
1	G	241	ALA
1	H	164	LEU
1	H	303	LEU
1	K	134	ALA
1	L	353	TRP
1	D	134	ALA
1	D	150	THR
1	G	258	VAL
1	F	208	VAL
1	C	268	ILE
1	D	370	VAL
1	I	258	VAL
1	J	201	PRO
1	K	147	GLY
1	A	258	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	237/243 (98%)	201 (85%)	36 (15%)	3	12
1	B	237/243 (98%)	198 (84%)	39 (16%)	2	10
1	C	234/243 (96%)	198 (85%)	36 (15%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	219/243 (90%)	191 (87%)	28 (13%)	4	18
1	E	227/243 (93%)	204 (90%)	23 (10%)	7	26
1	F	237/243 (98%)	207 (87%)	30 (13%)	4	18
1	G	237/243 (98%)	210 (89%)	27 (11%)	5	22
1	H	237/243 (98%)	208 (88%)	29 (12%)	5	20
1	I	232/243 (96%)	201 (87%)	31 (13%)	4	16
1	J	237/243 (98%)	212 (90%)	25 (10%)	6	24
1	K	237/243 (98%)	211 (89%)	26 (11%)	6	23
1	L	235/243 (97%)	210 (89%)	25 (11%)	6	24
All	All	2806/2916 (96%)	2451 (87%)	355 (13%)	4	18

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	LYS
1	A	123	LEU
1	A	135	ARG
1	A	139	ARG
1	A	154	ILE
1	A	170	GLN
1	A	173	LEU
1	A	195	LEU
1	A	203	ASN
1	A	225	LEU
1	A	243	LYS
1	A	256	CYS
1	A	261	ARG
1	A	266	GLU
1	A	272	VAL
1	A	279	ARG
1	A	286	VAL
1	A	289	PRO
1	A	300	GLN
1	A	305	HIS
1	A	307	VAL
1	A	311	MET
1	A	318	LEU
1	A	323	GLU
1	A	329	SER

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Mol	Chain	Res	Type
1	A	332	GLU
1	A	336	SER
1	A	341	LEU
1	A	345	ARG
1	A	347	LEU
1	A	351	LEU
1	A	353	TRP
1	A	360	VAL
1	A	383	MET
1	A	385	ASP
1	A	386	LEU
1	B	122	LYS
1	B	123	LEU
1	B	135	ARG
1	B	138	GLN
1	B	139	ARG
1	B	140	VAL
1	B	150	THR
1	B	170	GLN
1	B	173	LEU
1	B	175	TYR
1	B	190	LYS
1	B	195	LEU
1	B	203	ASN
1	B	205	LYS
1	B	208	VAL
1	B	230	ILE
1	B	231	ASP
1	B	235	ARG
1	B	243	LYS
1	B	253	SER
1	B	256	CYS
1	B	258	VAL
1	B	269	ARG
1	B	282	VAL
1	B	283	CYS
1	B	286	VAL
1	B	303	LEU
1	B	305	HIS
1	B	306	VAL
1	B	311	MET
1	B	318	LEU

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Mol	Chain	Res	Type
1	B	345	ARG
1	B	351	LEU
1	B	360	VAL
1	B	366	VAL
1	B	372	SER
1	B	375	GLU
1	B	380	THR
1	B	383	MET
1	C	135	ARG
1	C	138	GLN
1	C	139	ARG
1	C	150	THR
1	C	152	SER
1	C	179	ILE
1	C	190	LYS
1	C	200	TYR
1	C	208	VAL
1	C	209	THR
1	C	227	THR
1	C	230	ILE
1	C	231	ASP
1	C	242	SER
1	C	250	THR
1	C	256	CYS
1	C	257	THR
1	C	272	VAL
1	C	277	VAL
1	C	283	CYS
1	C	300	GLN
1	C	303	LEU
1	C	305	HIS
1	C	306	VAL
1	C	307	VAL
1	C	318	LEU
1	C	323	GLU
1	C	324	VAL
1	C	329	SER
1	C	336	SER
1	C	347	LEU
1	C	354	HIS
1	C	356	ARG
1	C	376	LEU

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Mol	Chain	Res	Type
1	C	380	THR
1	C	384	ARG
1	D	123	LEU
1	D	135	ARG
1	D	139	ARG
1	D	150	THR
1	D	175	TYR
1	D	177	GLU
1	D	179	ILE
1	D	190	LYS
1	D	200	TYR
1	D	208	VAL
1	D	225	LEU
1	D	230	ILE
1	D	256	CYS
1	D	259	CYS
1	D	272	VAL
1	D	282	VAL
1	D	283	CYS
1	D	300	GLN
1	D	304	LEU
1	D	306	VAL
1	D	316	LEU
1	D	318	LEU
1	D	324	VAL
1	D	329	SER
1	D	336	SER
1	D	347	LEU
1	D	375	GLU
1	D	376	LEU
1	E	122	LYS
1	E	123	LEU
1	E	125	LEU
1	E	127	ASP
1	E	150	THR
1	E	173	LEU
1	E	190	LYS
1	E	200	TYR
1	E	203	ASN
1	E	208	VAL
1	E	209	THR
1	E	216	LEU

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Mol	Chain	Res	Type
1	E	250	THR
1	E	284	THR
1	E	304	LEU
1	E	311	MET
1	E	318	LEU
1	E	327	PHE
1	E	351	LEU
1	E	353	TRP
1	E	366	VAL
1	E	370	VAL
1	E	376	LEU
1	F	122	LYS
1	F	135	ARG
1	F	154	ILE
1	F	162	SER
1	F	166	SER
1	F	172	ASP
1	F	179	ILE
1	F	182	LEU
1	F	194	THR
1	F	199	LEU
1	F	200	TYR
1	F	203	ASN
1	F	205	LYS
1	F	216	LEU
1	F	250	THR
1	F	256	CYS
1	F	258	VAL
1	F	280	CYS
1	F	283	CYS
1	F	284	THR
1	F	303	LEU
1	F	306	VAL
1	F	316	LEU
1	F	318	LEU
1	F	331	THR
1	F	345	ARG
1	F	347	LEU
1	F	366	VAL
1	F	375	GLU
1	F	390	GLU
1	G	122	LYS

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Mol	Chain	Res	Type
1	G	123	LEU
1	G	173	LEU
1	G	177	GLU
1	G	190	LYS
1	G	200	TYR
1	G	205	LYS
1	G	208	VAL
1	G	253	SER
1	G	256	CYS
1	G	258	VAL
1	G	259	CYS
1	G	266	GLU
1	G	269	ARG
1	G	283	CYS
1	G	304	LEU
1	G	306	VAL
1	G	311	MET
1	G	318	LEU
1	G	320	THR
1	G	327	PHE
1	G	341	LEU
1	G	345	ARG
1	G	353	TRP
1	G	366	VAL
1	G	376	LEU
1	G	381	GLU
1	H	122	LYS
1	H	139	ARG
1	H	150	THR
1	H	152	SER
1	H	156	ASP
1	H	173	LEU
1	H	194	THR
1	H	200	TYR
1	H	216	LEU
1	H	225	LEU
1	H	233	LEU
1	H	235	ARG
1	H	244	LEU
1	H	256	CYS
1	H	258	VAL
1	H	261	ARG

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Mol	Chain	Res	Type
1	H	282	VAL
1	H	283	CYS
1	H	311	MET
1	H	318	LEU
1	H	320	THR
1	H	324	VAL
1	H	329	SER
1	H	336	SER
1	H	345	ARG
1	H	351	LEU
1	H	353	TRP
1	H	376	LEU
1	H	381	GLU
1	I	122	LYS
1	I	123	LEU
1	I	125	LEU
1	I	126	GLN
1	I	139	ARG
1	I	166	SER
1	I	171	TYR
1	I	173	LEU
1	I	194	THR
1	I	195	LEU
1	I	200	TYR
1	I	216	LEU
1	I	225	LEU
1	I	253	SER
1	I	256	CYS
1	I	258	VAL
1	I	266	GLU
1	I	279	ARG
1	I	280	CYS
1	I	283	CYS
1	I	306	VAL
1	I	311	MET
1	I	320	THR
1	I	327	PHE
1	I	336	SER
1	I	346	ASP
1	I	351	LEU
1	I	353	TRP
1	I	366	VAL

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Mol	Chain	Res	Type
1	I	380	THR
1	I	386	LEU
1	J	122	LYS
1	J	124	SER
1	J	139	ARG
1	J	159	SER
1	J	170	GLN
1	J	179	ILE
1	J	182	LEU
1	J	195	LEU
1	J	200	TYR
1	J	215	LEU
1	J	216	LEU
1	J	223	LEU
1	J	225	LEU
1	J	250	THR
1	J	255	THR
1	J	266	GLU
1	J	271	ASP
1	J	279	ARG
1	J	303	LEU
1	J	318	LEU
1	J	320	THR
1	J	345	ARG
1	J	358	ARG
1	J	366	VAL
1	J	380	THR
1	K	122	LYS
1	K	154	ILE
1	K	162	SER
1	K	173	LEU
1	K	175	TYR
1	K	177	GLU
1	K	187	HIS
1	K	194	THR
1	K	200	TYR
1	K	222	LEU
1	K	225	LEU
1	K	227	THR
1	K	230	ILE
1	K	250	THR
1	K	258	VAL

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Mol	Chain	Res	Type
1	K	266	GLU
1	K	306	VAL
1	K	322	LEU
1	K	329	SER
1	K	336	SER
1	K	344	ASN
1	K	348	VAL
1	K	351	LEU
1	K	366	VAL
1	K	377	LEU
1	K	387	VAL
1	L	122	LYS
1	L	131	LEU
1	L	135	ARG
1	L	138	GLN
1	L	154	ILE
1	L	158	ARG
1	L	175	TYR
1	L	190	LYS
1	L	194	THR
1	L	200	TYR
1	L	216	LEU
1	L	225	LEU
1	L	235	ARG
1	L	258	VAL
1	L	266	GLU
1	L	269	ARG
1	L	303	LEU
1	L	306	VAL
1	L	307	VAL
1	L	347	LEU
1	L	348	VAL
1	L	380	THR
1	L	387	VAL
1	L	388	GLN
1	L	389	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	217	HIS

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Mol	Chain	Res	Type
1	A	344	ASN
1	A	368	HIS
1	C	203	ASN
1	C	300	GLN
1	C	368	HIS
1	D	203	ASN
1	D	228	GLN
1	D	300	GLN
1	D	305	HIS
1	E	169	GLN
1	E	203	ASN
1	E	228	GLN
1	E	354	HIS
1	F	167	ASN
1	F	210	HIS
1	F	248	HIS
1	F	354	HIS
1	G	138	GLN
1	G	228	GLN
1	G	305	HIS
1	G	354	HIS
1	G	368	HIS
1	I	217	HIS
1	I	228	GLN
1	I	354	HIS
1	J	228	GLN
1	K	203	ASN
1	K	228	GLN
1	K	344	ASN
1	L	167	ASN
1	L	169	GLN
1	L	203	ASN
1	L	354	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 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$
3	SR7	J	1396	-	39,39,39	2.19	12 (30%)	51,55,55	2.79	22 (43%)
3	SR7	F	1396	-	39,39,39	2.26	13 (33%)	51,55,55	2.94	22 (43%)
5	GOL	C	1396	-	5,5,5	0.40	0	5,5,5	0.99	0
3	SR7	L	1397	-	39,39,39	1.96	13 (33%)	51,55,55	2.31	17 (33%)
5	GOL	L	1396	-	5,5,5	0.30	0	5,5,5	0.68	0
2	CNA	A	1395	-	47,48,48	2.26	13 (27%)	65,73,73	2.24	20 (30%)
5	GOL	D	1395	-	5,5,5	0.37	0	5,5,5	1.25	0
3	SR7	I	1396	-	39,39,39	2.52	13 (33%)	51,55,55	2.75	24 (47%)
2	CNA	E	1395	-	47,48,48	2.15	12 (25%)	65,73,73	2.11	21 (32%)
2	CNA	H	1395	-	47,48,48	2.22	13 (27%)	65,73,73	2.10	17 (26%)
3	SR7	B	1396	-	39,39,39	2.95	15 (38%)	51,55,55	3.25	23 (45%)
2	CNA	G	1395	-	47,48,48	2.27	13 (27%)	65,73,73	2.09	17 (26%)
2	CNA	D	1394	-	47,48,48	2.47	15 (31%)	65,73,73	1.98	17 (26%)
2	CNA	K	1395	-	47,48,48	3.09	22 (46%)	65,73,73	2.48	21 (32%)
2	CNA	B	1395	-	47,48,48	2.40	13 (27%)	65,73,73	2.26	18 (27%)
2	CNA	J	1395	-	47,48,48	2.11	14 (29%)	65,73,73	1.85	18 (27%)
2	CNA	C	1395	-	47,48,48	2.13	13 (27%)	65,73,73	1.89	18 (27%)
3	SR7	A	1396	-	39,39,39	2.81	15 (38%)	51,55,55	3.35	25 (49%)
3	SR7	C	1397	-	39,39,39	2.71	15 (38%)	51,55,55	2.44	21 (41%)
3	SR7	K	1397	-	39,39,39	2.42	13 (33%)	51,55,55	1.95	15 (29%)
2	CNA	F	1395	-	47,48,48	2.01	10 (21%)	65,73,73	1.90	16 (24%)
5	GOL	K	1396	-	5,5,5	0.26	0	5,5,5	0.60	0
3	SR7	E	1396	-	39,39,39	2.48	12 (30%)	51,55,55	3.22	25 (49%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CNA	I	1395	-	47,48,48	2.15	12 (25%)	65,73,73	2.06	19 (29%)
3	SR7	G	1396	-	39,39,39	2.54	13 (33%)	51,55,55	2.83	26 (50%)
3	SR7	H	1396	-	39,39,39	2.33	11 (28%)	51,55,55	2.37	17 (33%)
3	SR7	D	1396	-	39,39,39	2.82	11 (28%)	51,55,55	1.97	12 (23%)
2	CNA	L	1395	-	47,48,48	3.86	17 (36%)	65,73,73	2.22	19 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SR7	J	1396	-	-	5/16/24/24	1/6/6/6
3	SR7	F	1396	-	-	5/16/24/24	1/6/6/6
5	GOL	C	1396	-	-	2/4/4/4	-
3	SR7	L	1397	-	-	4/16/24/24	0/6/6/6
5	GOL	L	1396	-	-	1/4/4/4	-
2	CNA	A	1395	-	-	5/28/62/62	0/5/5/5
5	GOL	D	1395	-	-	2/4/4/4	-
3	SR7	I	1396	-	-	5/16/24/24	0/6/6/6
2	CNA	E	1395	-	-	14/28/62/62	0/5/5/5
2	CNA	H	1395	-	-	16/28/62/62	0/5/5/5
3	SR7	B	1396	-	-	5/16/24/24	1/6/6/6
2	CNA	G	1395	-	-	15/28/62/62	0/5/5/5
2	CNA	D	1394	-	-	5/28/62/62	0/5/5/5
2	CNA	K	1395	-	-	12/28/62/62	0/5/5/5
2	CNA	B	1395	-	-	7/28/62/62	0/5/5/5
2	CNA	J	1395	-	-	10/28/62/62	0/5/5/5
2	CNA	C	1395	-	-	3/28/62/62	0/5/5/5
3	SR7	A	1396	-	-	5/16/24/24	1/6/6/6
3	SR7	C	1397	-	-	6/16/24/24	0/6/6/6
3	SR7	K	1397	-	-	4/16/24/24	0/6/6/6
2	CNA	F	1395	-	-	13/28/62/62	0/5/5/5
5	GOL	K	1396	-	-	1/4/4/4	-
3	SR7	E	1396	-	-	6/16/24/24	0/6/6/6
2	CNA	I	1395	-	-	13/28/62/62	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SR7	G	1396	-	-	5/16/24/24	0/6/6/6
3	SR7	H	1396	-	-	5/16/24/24	0/6/6/6
3	SR7	D	1396	-	-	1/16/24/24	0/6/6/6
2	CNA	L	1395	-	-	14/28/62/62	0/5/5/5

All (323) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1395	CNA	PA-O3	15.85	1.76	1.59
2	L	1395	CNA	PN-O3	14.23	1.74	1.59
2	K	1395	CNA	PA-O3	10.64	1.71	1.59
3	D	1396	SR7	CAX-SBB	-9.19	1.55	1.74
3	C	1397	SR7	CAX-SBB	-9.09	1.55	1.74
3	B	1396	SR7	CAX-SBB	-8.74	1.56	1.74
2	K	1395	CNA	C2N-N1N	8.39	1.44	1.35
2	L	1395	CNA	C3N-C7N	-8.29	1.38	1.50
2	D	1394	CNA	C3N-C7N	-8.15	1.38	1.50
2	B	1395	CNA	C3N-C7N	-7.99	1.38	1.50
2	C	1395	CNA	C3N-C7N	-7.98	1.38	1.50
3	A	1396	SR7	CAX-SBB	-7.82	1.58	1.74
2	H	1395	CNA	C2N-N1N	7.81	1.43	1.35
2	D	1394	CNA	PA-O3	7.69	1.67	1.59
2	A	1395	CNA	C3N-C7N	-7.60	1.39	1.50
3	B	1396	SR7	CBD-NAW	-7.40	1.32	1.39
2	K	1395	CNA	PN-O3	7.33	1.67	1.59
2	I	1395	CNA	C3N-C7N	-7.31	1.39	1.50
3	D	1396	SR7	CAC-CAZ	-7.23	1.34	1.47
3	D	1396	SR7	CBD-NAW	-7.10	1.32	1.39
3	A	1396	SR7	CBD-NAW	-6.99	1.32	1.39
3	K	1397	SR7	CBD-NAW	-6.88	1.32	1.39
3	C	1397	SR7	CAC-CAZ	-6.79	1.35	1.47
3	G	1396	SR7	CAX-SBB	-6.76	1.60	1.74
2	J	1395	CNA	C3N-C7N	-6.72	1.40	1.50
2	E	1395	CNA	C2N-N1N	6.72	1.42	1.35
2	F	1395	CNA	C2N-N1N	6.54	1.42	1.35
2	H	1395	CNA	C3N-C7N	-6.48	1.40	1.50
2	G	1395	CNA	PN-O3	-6.43	1.52	1.59
2	F	1395	CNA	C3N-C7N	-6.40	1.41	1.50
3	A	1396	SR7	CAH-NAI	-6.40	1.26	1.37
2	G	1395	CNA	C3N-C7N	-6.26	1.41	1.50
2	G	1395	CNA	C2N-N1N	6.25	1.41	1.35
3	I	1396	SR7	CAC-CAZ	-6.06	1.36	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1395	CNA	C2N-N1N	6.04	1.41	1.35
2	E	1395	CNA	PN-O3	-6.00	1.53	1.59
3	I	1396	SR7	CAX-SBB	-5.96	1.62	1.74
3	B	1396	SR7	CAC-CAZ	-5.95	1.36	1.47
3	F	1396	SR7	CAC-CAZ	-5.94	1.36	1.47
3	B	1396	SR7	CAH-NAI	-5.89	1.27	1.37
3	E	1396	SR7	CAX-SBB	-5.84	1.62	1.74
3	K	1397	SR7	CAC-CAZ	-5.79	1.36	1.47
3	J	1396	SR7	CAC-CAZ	-5.72	1.37	1.47
2	B	1395	CNA	C5A-N7A	-5.65	1.28	1.39
3	G	1396	SR7	CAC-CAZ	-5.61	1.37	1.47
3	E	1396	SR7	CAH-NAI	-5.54	1.28	1.37
2	L	1395	CNA	C2N-N1N	5.51	1.41	1.35
3	C	1397	SR7	CBD-NAW	-5.48	1.34	1.39
2	J	1395	CNA	C2N-N1N	5.38	1.40	1.35
2	K	1395	CNA	C3N-C7N	-5.36	1.42	1.50
3	F	1396	SR7	CAH-NAI	-5.33	1.28	1.37
3	H	1396	SR7	CAJ-NAI	5.30	1.40	1.31
2	I	1395	CNA	C2N-N1N	5.28	1.40	1.35
2	E	1395	CNA	C3N-C7N	-5.18	1.42	1.50
3	E	1396	SR7	CAC-CAZ	-5.10	1.38	1.47
3	H	1396	SR7	CAC-CAZ	-5.03	1.38	1.47
3	E	1396	SR7	CBC-SBB	-5.03	1.59	1.71
3	I	1396	SR7	CBD-NAW	-5.02	1.34	1.39
2	K	1395	CNA	C2A-N3A	5.01	1.42	1.33
3	G	1396	SR7	CBC-SBB	-4.99	1.59	1.71
3	H	1396	SR7	CBD-NAW	-4.96	1.34	1.39
3	F	1396	SR7	CBH-CBD	4.94	1.56	1.50
2	K	1395	CNA	C2A-N1A	4.93	1.42	1.33
2	L	1395	CNA	C2A-N3A	4.87	1.42	1.33
3	A	1396	SR7	CBC-SBB	-4.84	1.60	1.71
3	J	1396	SR7	CAH-NAI	-4.80	1.29	1.37
3	A	1396	SR7	CAB-NBE	-4.77	1.32	1.41
3	A	1396	SR7	CAC-CAZ	-4.77	1.38	1.47
3	K	1397	SR7	CAJ-NAI	4.77	1.39	1.31
3	K	1397	SR7	CAB-NBE	-4.73	1.32	1.41
3	I	1396	SR7	CAJ-NAI	4.70	1.39	1.31
3	H	1396	SR7	CBC-SBB	-4.69	1.60	1.71
3	L	1397	SR7	CAC-CAZ	-4.66	1.38	1.47
2	A	1395	CNA	C5A-N7A	-4.65	1.30	1.39
3	H	1396	SR7	CAK-CBF	-4.63	1.37	1.50
3	D	1396	SR7	CAJ-NAI	4.63	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1397	SR7	CAH-NAI	-4.62	1.29	1.37
2	C	1395	CNA	C2N-N1N	4.58	1.40	1.35
3	K	1397	SR7	CAK-CBF	-4.57	1.38	1.50
2	L	1395	CNA	C2A-N1A	4.55	1.42	1.33
3	G	1396	SR7	CAH-NAI	-4.50	1.29	1.37
2	A	1395	CNA	C2N-N1N	4.48	1.39	1.35
2	B	1395	CNA	C5A-C4A	-4.45	1.31	1.39
3	J	1396	SR7	CBH-CBD	4.44	1.55	1.50
3	E	1396	SR7	CAB-NBE	-4.40	1.33	1.41
2	B	1395	CNA	C8A-N9A	-4.34	1.30	1.37
3	E	1396	SR7	CBH-CBD	4.32	1.55	1.50
3	I	1396	SR7	CAK-CBF	-4.30	1.38	1.50
2	A	1395	CNA	C5A-C4A	-4.29	1.31	1.39
3	B	1396	SR7	CBC-SBB	-4.26	1.61	1.71
2	I	1395	CNA	C5A-N7A	-4.25	1.31	1.39
3	G	1396	SR7	CBH-CBD	4.23	1.55	1.50
3	F	1396	SR7	CAB-NBE	-4.18	1.33	1.41
2	G	1395	CNA	C2A-N3A	4.18	1.41	1.33
2	E	1395	CNA	C2A-N3A	4.14	1.41	1.33
3	B	1396	SR7	CAZ-NAY	-4.13	1.32	1.39
3	J	1396	SR7	CBD-NAW	-4.13	1.35	1.39
3	G	1396	SR7	CAB-NBE	-4.13	1.33	1.41
3	G	1396	SR7	CBD-NAW	-4.11	1.35	1.39
2	D	1394	CNA	C5A-N7A	-4.11	1.31	1.39
3	G	1396	SR7	CAJ-NAI	4.08	1.38	1.31
2	C	1395	CNA	C5A-N7A	-4.06	1.31	1.39
3	I	1396	SR7	CAB-NBE	-4.03	1.33	1.41
3	E	1396	SR7	CAZ-NAY	-4.02	1.32	1.39
2	A	1395	CNA	C8A-N9A	-4.02	1.30	1.37
2	D	1394	CNA	C2N-N1N	3.98	1.39	1.35
2	A	1395	CNA	C2D-C1D	-3.98	1.48	1.53
2	J	1395	CNA	C2A-N1A	3.97	1.41	1.33
3	C	1397	SR7	CAB-NBE	-3.95	1.34	1.41
2	D	1394	CNA	PN-O3	3.93	1.63	1.59
3	E	1396	SR7	CAJ-NAI	3.91	1.38	1.31
3	D	1396	SR7	CAZ-NAY	-3.90	1.32	1.39
3	J	1396	SR7	CAJ-NAI	3.86	1.38	1.31
3	I	1396	SR7	CAH-NAI	-3.85	1.31	1.37
3	H	1396	SR7	CAX-SBB	-3.85	1.66	1.74
2	E	1395	CNA	C5A-C4A	-3.85	1.32	1.39
3	L	1397	SR7	CAK-CBF	-3.80	1.40	1.50
2	J	1395	CNA	C2A-N3A	3.79	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	1397	SR7	CBD-NAW	-3.78	1.35	1.39
2	I	1395	CNA	C2A-N3A	3.76	1.40	1.33
3	B	1396	SR7	CAP-CAG	-3.75	1.35	1.41
2	K	1395	CNA	PN-O2N	3.73	1.72	1.55
2	J	1395	CNA	C5A-N7A	-3.73	1.32	1.39
3	B	1396	SR7	CAB-NBE	-3.71	1.34	1.41
3	I	1396	SR7	CBC-SBB	-3.67	1.62	1.71
3	F	1396	SR7	CBD-NAW	-3.66	1.36	1.39
2	B	1395	CNA	C5A-C6A	-3.64	1.30	1.41
2	E	1395	CNA	C5A-N7A	-3.64	1.32	1.39
3	F	1396	SR7	CAZ-NAY	-3.63	1.32	1.39
3	L	1397	SR7	CAJ-NAI	3.62	1.37	1.31
2	F	1395	CNA	C5A-N7A	-3.61	1.32	1.39
3	J	1396	SR7	CAB-NBE	-3.58	1.34	1.41
3	L	1397	SR7	CAH-NAI	-3.58	1.31	1.37
3	D	1396	SR7	CBC-SBB	-3.58	1.63	1.71
3	J	1396	SR7	CAZ-NAY	-3.58	1.33	1.39
2	H	1395	CNA	C2A-N3A	3.56	1.40	1.33
2	K	1395	CNA	C5A-N7A	-3.56	1.32	1.39
2	I	1395	CNA	C2A-N1A	3.56	1.40	1.33
3	I	1396	SR7	CBH-CBD	3.55	1.54	1.50
3	F	1396	SR7	CAP-CAG	-3.55	1.35	1.41
2	I	1395	CNA	C5A-C4A	-3.53	1.32	1.39
2	D	1394	CNA	C4A-N9A	-3.53	1.30	1.37
2	K	1395	CNA	O3B-C3B	3.51	1.51	1.43
3	K	1397	SR7	CAH-NAI	-3.47	1.31	1.37
2	I	1395	CNA	C5A-C6A	-3.46	1.31	1.41
2	G	1395	CNA	C5A-N7A	-3.46	1.32	1.39
3	C	1397	SR7	CAZ-NAY	-3.44	1.33	1.39
2	F	1395	CNA	C2A-N3A	3.44	1.40	1.33
3	C	1397	SR7	CAK-CBF	-3.44	1.41	1.50
2	B	1395	CNA	C2A-N3A	3.44	1.40	1.33
3	H	1396	SR7	CAB-NBE	-3.43	1.35	1.41
2	K	1395	CNA	PA-O1A	3.41	1.71	1.55
3	A	1396	SR7	CAP-CAG	-3.41	1.36	1.41
2	G	1395	CNA	C6N-N1N	3.39	1.43	1.35
3	G	1396	SR7	CAZ-NAY	-3.39	1.33	1.39
3	I	1396	SR7	CAZ-NAY	-3.38	1.33	1.39
3	B	1396	SR7	CAK-CBF	-3.38	1.41	1.50
3	A	1396	SR7	CAK-CBF	-3.37	1.41	1.50
2	A	1395	CNA	C5A-C6A	-3.34	1.31	1.41
2	H	1395	CNA	C5A-C4A	-3.33	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1395	CNA	C2A-N3A	3.32	1.39	1.33
3	L	1397	SR7	CAB-NBE	-3.32	1.35	1.41
2	D	1394	CNA	C2A-N1A	3.31	1.39	1.33
2	F	1395	CNA	C5A-C6A	-3.30	1.31	1.41
3	D	1396	SR7	CAK-CBF	-3.27	1.41	1.50
2	H	1395	CNA	C5A-N7A	-3.26	1.33	1.39
2	D	1394	CNA	C2A-N3A	3.26	1.39	1.33
2	C	1395	CNA	C2A-N1A	3.24	1.39	1.33
2	D	1394	CNA	C8A-N9A	-3.24	1.32	1.37
2	L	1395	CNA	PA-O1A	3.23	1.70	1.55
3	B	1396	SR7	CBA-NAW	-3.22	1.32	1.38
3	H	1396	SR7	CBH-CBD	3.22	1.54	1.50
3	J	1396	SR7	CAP-CAG	-3.22	1.36	1.41
2	J	1395	CNA	PN-O3	-3.22	1.56	1.59
2	H	1395	CNA	C2A-N1A	3.21	1.39	1.33
2	F	1395	CNA	C5A-C4A	-3.18	1.33	1.39
3	E	1396	SR7	CAP-CAG	-3.18	1.36	1.41
2	F	1395	CNA	C2A-N1A	3.18	1.39	1.33
2	H	1395	CNA	C6N-N1N	3.18	1.42	1.35
3	D	1396	SR7	CBA-NAW	-3.18	1.32	1.38
2	A	1395	CNA	C2A-N3A	3.16	1.39	1.33
2	C	1395	CNA	C8A-N9A	-3.14	1.32	1.37
2	C	1395	CNA	C4A-N9A	-3.14	1.31	1.37
3	E	1396	SR7	CAK-CBF	-3.14	1.41	1.50
2	C	1395	CNA	C5A-C4A	-3.12	1.33	1.39
2	L	1395	CNA	C5A-N7A	-3.12	1.33	1.39
3	A	1396	SR7	CAZ-NAY	-3.11	1.33	1.39
2	G	1395	CNA	C2A-N1A	3.08	1.39	1.33
3	H	1396	SR7	CAZ-NAY	-3.08	1.33	1.39
2	G	1395	CNA	C5A-C4A	-3.08	1.33	1.39
2	B	1395	CNA	C4A-N9A	-3.06	1.31	1.37
2	D	1394	CNA	C5A-C4A	-3.06	1.33	1.39
2	K	1395	CNA	C2D-C1D	3.06	1.57	1.53
2	E	1395	CNA	C5A-C6A	-3.06	1.32	1.41
3	C	1397	SR7	CAJ-NAI	3.03	1.36	1.31
2	H	1395	CNA	C5A-C6A	-3.01	1.32	1.41
2	L	1395	CNA	O3B-C3B	2.99	1.50	1.43
2	C	1395	CNA	PA-O3	2.99	1.62	1.59
2	B	1395	CNA	PN-O5D	-2.98	1.47	1.59
2	J	1395	CNA	C5A-C6A	-2.98	1.32	1.41
3	D	1396	SR7	CAB-NBE	-2.96	1.35	1.41
2	A	1395	CNA	PN-O3	-2.95	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1396	SR7	CAQ-CAR	-2.92	1.44	1.51
2	E	1395	CNA	C2A-N1A	2.90	1.39	1.33
3	E	1396	SR7	CBD-NAW	-2.90	1.36	1.39
2	C	1395	CNA	PN-O3	2.89	1.62	1.59
3	J	1396	SR7	CAK-CBF	-2.88	1.42	1.50
2	I	1395	CNA	C4A-N9A	-2.88	1.31	1.37
3	F	1396	SR7	CAJ-NAI	2.88	1.36	1.31
2	L	1395	CNA	C6N-N1N	2.87	1.41	1.35
3	B	1396	SR7	CAJ-NAI	2.87	1.36	1.31
3	L	1397	SR7	CBH-CBD	2.85	1.53	1.50
3	G	1396	SR7	CAP-CAG	-2.81	1.37	1.41
3	F	1396	SR7	CAK-CBF	-2.81	1.42	1.50
3	G	1396	SR7	CAH-CAG	-2.80	1.36	1.42
2	J	1395	CNA	C5A-C4A	-2.80	1.34	1.39
2	L	1395	CNA	PN-O5D	2.78	1.70	1.59
3	K	1397	SR7	CBH-CBD	2.78	1.53	1.50
3	A	1396	SR7	CBA-NAW	-2.77	1.33	1.38
3	H	1396	SR7	CAP-CAG	-2.77	1.37	1.41
2	K	1395	CNA	C4A-N9A	-2.76	1.31	1.37
3	L	1397	SR7	CAZ-NAY	-2.75	1.34	1.39
2	H	1395	CNA	O3B-C3B	2.75	1.49	1.43
2	L	1395	CNA	C8A-N9A	-2.74	1.32	1.37
2	G	1395	CNA	C1B-N9A	2.74	1.53	1.46
2	A	1395	CNA	C5D-C4D	2.73	1.57	1.51
3	I	1396	SR7	CBA-NAW	-2.72	1.33	1.38
2	D	1394	CNA	C5A-C6A	-2.72	1.33	1.41
3	K	1397	SR7	CAU-CAT	2.69	1.58	1.51
2	G	1395	CNA	O4B-C1B	2.69	1.48	1.42
3	B	1396	SR7	CBA-CAZ	-2.68	1.32	1.37
2	I	1395	CNA	C6N-N1N	2.66	1.41	1.35
2	A	1395	CNA	PN-O5D	-2.66	1.49	1.59
2	K	1395	CNA	C8A-N9A	-2.65	1.33	1.37
3	C	1397	SR7	CAQ-CAR	-2.61	1.45	1.51
3	D	1396	SR7	CAH-NAI	-2.60	1.33	1.37
2	K	1395	CNA	C6N-N1N	2.58	1.41	1.35
2	H	1395	CNA	C2N-C3N	2.58	1.43	1.39
2	J	1395	CNA	O2B-C2B	2.57	1.49	1.43
2	J	1395	CNA	C8A-N9A	-2.56	1.33	1.37
2	K	1395	CNA	C2N-C3N	2.55	1.43	1.39
3	G	1396	SR7	CAK-CBF	-2.54	1.43	1.50
2	G	1395	CNA	C5A-C6A	-2.54	1.33	1.41
2	F	1395	CNA	C8A-N9A	-2.53	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1395	CNA	C2D-C1D	2.51	1.56	1.53
2	L	1395	CNA	PN-O2N	2.51	1.67	1.55
3	K	1397	SR7	CAQ-CAR	2.51	1.57	1.51
3	C	1397	SR7	CAU-CAT	2.50	1.57	1.51
2	B	1395	CNA	C2A-N1A	2.49	1.38	1.33
3	D	1396	SR7	CBA-CAZ	-2.49	1.33	1.37
2	I	1395	CNA	C8A-N9A	-2.48	1.33	1.37
2	J	1395	CNA	C4A-N9A	-2.48	1.32	1.37
2	C	1395	CNA	C5A-C6A	-2.48	1.34	1.41
3	A	1396	SR7	CAO-CAH	-2.48	1.37	1.41
2	L	1395	CNA	C5B-C4B	2.48	1.59	1.51
3	C	1397	SR7	CBH-CBD	2.47	1.53	1.50
3	B	1396	SR7	CAX-NAW	-2.47	1.32	1.37
2	A	1395	CNA	C4D-C3D	-2.43	1.47	1.54
2	B	1395	CNA	C2D-C1D	-2.41	1.50	1.53
3	I	1396	SR7	CAP-CAG	-2.41	1.37	1.41
2	L	1395	CNA	C5A-C4A	-2.39	1.34	1.39
3	B	1396	SR7	CAM-CAP	2.38	1.41	1.36
2	E	1395	CNA	C8A-N9A	-2.37	1.33	1.37
2	J	1395	CNA	C6N-N1N	2.36	1.40	1.35
3	A	1396	SR7	CAJ-NAI	2.35	1.35	1.31
3	F	1396	SR7	CAO-CAH	-2.35	1.37	1.41
2	D	1394	CNA	PA-O1A	2.35	1.66	1.55
3	A	1396	SR7	CAX-NAW	-2.35	1.32	1.37
3	J	1396	SR7	CBA-NAW	-2.35	1.33	1.38
2	H	1395	CNA	C4A-N9A	-2.34	1.32	1.37
3	L	1397	SR7	CAM-CAP	2.33	1.41	1.36
3	F	1396	SR7	CBC-SBB	-2.33	1.66	1.71
2	A	1395	CNA	C4A-N9A	-2.33	1.32	1.37
3	C	1397	SR7	CAP-CAG	-2.33	1.38	1.41
3	H	1396	SR7	CBA-NAW	-2.33	1.33	1.38
2	B	1395	CNA	C4'-C4D	-2.30	1.47	1.53
2	G	1395	CNA	C2N-C3N	2.30	1.42	1.39
2	L	1395	CNA	C4A-N9A	-2.30	1.32	1.37
3	C	1397	SR7	CBC-SBB	-2.29	1.66	1.71
2	H	1395	CNA	O2B-C2B	2.29	1.48	1.43
2	K	1395	CNA	C5A-C4A	-2.28	1.35	1.39
3	G	1396	SR7	CAO-CAH	-2.27	1.38	1.41
3	E	1396	SR7	CAO-CAH	-2.27	1.38	1.41
3	K	1397	SR7	CBA-NAW	-2.26	1.34	1.38
2	K	1395	CNA	O3D-C3D	2.25	1.48	1.43
2	K	1395	CNA	PA-O5B	2.23	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1396	SR7	CBC-SBB	-2.23	1.66	1.71
2	H	1395	CNA	C4D-C3D	-2.22	1.48	1.54
2	E	1395	CNA	C4A-N9A	-2.20	1.33	1.37
3	K	1397	SR7	CAP-CAG	-2.19	1.38	1.41
3	L	1397	SR7	CAC-CAB	2.19	1.44	1.41
2	J	1395	CNA	O4B-C1B	2.18	1.47	1.42
3	K	1397	SR7	CAZ-NAY	-2.17	1.35	1.39
2	L	1395	CNA	PA-O5B	2.16	1.67	1.59
3	F	1396	SR7	CBA-NAW	-2.16	1.34	1.38
2	E	1395	CNA	O4B-C1B	2.16	1.47	1.42
3	L	1397	SR7	CAD-CAC	2.15	1.43	1.39
3	L	1397	SR7	CAP-CAG	-2.15	1.38	1.41
3	L	1397	SR7	CAU-CAT	2.15	1.56	1.51
2	K	1395	CNA	C5A-C6A	-2.14	1.35	1.41
2	J	1395	CNA	O3B-C3B	2.13	1.48	1.43
3	F	1396	SR7	CBA-CAZ	-2.13	1.33	1.37
2	D	1394	CNA	O2D-C2D	-2.13	1.37	1.43
2	D	1394	CNA	C5D-C4D	2.12	1.55	1.51
2	F	1395	CNA	C4'-C1D	-2.11	1.46	1.53
2	D	1394	CNA	C2B-C1B	-2.10	1.46	1.53
3	A	1396	SR7	CAQ-CAR	-2.09	1.46	1.51
2	I	1395	CNA	PN-O3	2.09	1.61	1.59
2	C	1395	CNA	O3D-C3D	2.08	1.48	1.43
2	F	1395	CNA	C4A-N9A	-2.08	1.33	1.37
3	J	1396	SR7	CAQ-CAR	-2.08	1.46	1.51
3	C	1397	SR7	CAM-CAP	2.07	1.41	1.36
2	G	1395	CNA	C8A-N9A	-2.06	1.34	1.37
3	C	1397	SR7	CBA-NAW	-2.06	1.34	1.38
2	K	1395	CNA	C5D-C4D	2.06	1.55	1.51
2	K	1395	CNA	PN-O5D	2.06	1.67	1.59
3	I	1396	SR7	CBA-CAZ	-2.06	1.33	1.37
3	K	1397	SR7	CAM-CAP	2.05	1.41	1.36
2	C	1395	CNA	O3B-C3B	2.04	1.48	1.43
3	A	1396	SR7	CAM-CAP	2.03	1.41	1.36
2	B	1395	CNA	PN-O3	-2.01	1.57	1.59
2	K	1395	CNA	C2D-C3D	2.01	1.58	1.53
2	E	1395	CNA	O2B-C2B	2.01	1.47	1.43

All (470) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1395	CNA	O4B-C1B-N9A	-11.65	85.71	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1396	SR7	CBH-CBD-CBC	-11.23	116.99	130.68
3	B	1396	SR7	CAO-CAH-CAG	9.54	130.53	119.25
3	G	1396	SR7	CBH-CBD-CBC	-9.49	119.10	130.68
2	L	1395	CNA	O4B-C1B-N9A	-9.19	90.45	108.09
3	A	1396	SR7	CAO-CAH-CAG	8.72	129.56	119.25
3	L	1397	SR7	CBH-CBD-CBC	-8.43	120.40	130.68
3	J	1396	SR7	CBH-CBD-CBC	-8.13	120.77	130.68
3	H	1396	SR7	CBH-CBD-CBC	-7.81	121.15	130.68
3	B	1396	SR7	CAJ-CAK-CBF	-7.79	109.75	119.71
3	A	1396	SR7	CAJ-CAK-CBF	-7.65	109.94	119.71
2	H	1395	CNA	C6N-N1N-C2N	-7.61	115.41	121.88
3	E	1396	SR7	CAO-CAH-CAG	7.43	128.03	119.25
3	F	1396	SR7	CBH-CBD-CBC	-7.37	121.70	130.68
3	F	1396	SR7	CAO-CAH-CAG	7.24	127.81	119.25
3	B	1396	SR7	CAP-CAG-CAH	-6.77	111.24	119.25
3	J	1396	SR7	CAO-CAH-CAG	6.77	127.25	119.25
2	E	1395	CNA	N3A-C2A-N1A	-6.76	118.35	128.58
3	A	1396	SR7	CBF-CAK-NAL	6.75	134.50	116.86
2	H	1395	CNA	N3A-C2A-N1A	-6.73	118.40	128.58
3	B	1396	SR7	CBF-CAK-NAL	6.68	134.31	116.86
3	A	1396	SR7	CAP-CAG-CAH	-6.68	111.35	119.25
2	B	1395	CNA	O4B-C1B-N9A	-6.66	95.29	108.09
2	F	1395	CNA	N3A-C2A-N1A	-6.57	118.64	128.58
3	I	1396	SR7	CAJ-CAK-CBF	-6.54	111.36	119.71
2	L	1395	CNA	N3A-C2A-N1A	-6.32	119.01	128.58
2	A	1395	CNA	C5A-C4A-N3A	-6.31	118.03	126.72
3	D	1396	SR7	CBH-CBD-CBC	-6.24	123.07	130.68
3	A	1396	SR7	CBA-CAZ-NAY	-6.23	104.78	110.75
3	I	1396	SR7	CBH-CBD-CBC	-6.22	123.09	130.68
2	A	1395	CNA	O4B-C1B-N9A	-6.19	96.21	108.09
2	B	1395	CNA	C5A-C4A-N3A	-6.13	118.27	126.72
2	A	1395	CNA	N3A-C2A-N1A	-6.12	119.32	128.58
2	G	1395	CNA	N3A-C2A-N1A	-6.10	119.34	128.58
3	E	1396	SR7	CBA-CAZ-NAY	-6.10	104.91	110.75
2	J	1395	CNA	N3A-C2A-N1A	-6.08	119.37	128.58
2	I	1395	CNA	N3A-C2A-N1A	-6.01	119.49	128.58
3	E	1396	SR7	CAJ-CAK-CBF	-5.97	112.08	119.71
2	I	1395	CNA	C6N-N1N-C2N	-5.92	116.84	121.88
3	E	1396	SR7	CBF-CAK-NAL	5.87	132.19	116.86
2	G	1395	CNA	C6N-N1N-C2N	-5.80	116.94	121.88
2	B	1395	CNA	N3A-C2A-N1A	-5.79	119.82	128.58
3	C	1397	SR7	CAO-CAH-CAG	5.75	126.05	119.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1395	CNA	N3A-C2A-N1A	-5.73	119.91	128.58
3	F	1396	SR7	CBA-CAZ-NAY	-5.71	105.28	110.75
3	B	1396	SR7	CBH-CBD-CBC	-5.69	123.74	130.68
3	F	1396	SR7	CBF-CAK-NAL	5.62	131.55	116.86
3	L	1397	SR7	CAJ-CAK-CBF	-5.54	112.63	119.71
3	G	1396	SR7	CBF-CAK-NAL	5.53	131.32	116.86
3	I	1396	SR7	CAO-CAH-CAG	5.50	125.75	119.25
2	G	1395	CNA	C5A-C4A-N3A	-5.49	119.16	126.72
3	A	1396	SR7	CBH-CBD-CBC	-5.44	124.04	130.68
3	F	1396	SR7	SBB-CAX-NAY	5.30	145.31	135.84
2	C	1395	CNA	N3A-C2A-N1A	-5.27	120.60	128.58
3	J	1396	SR7	CBF-CAK-NAL	5.24	130.56	116.86
3	F	1396	SR7	CAJ-CAK-CBF	-5.22	113.04	119.71
3	A	1396	SR7	CBC-SBB-CAX	5.19	98.23	89.41
3	A	1396	SR7	CAC-CAZ-NAY	5.11	129.25	118.86
3	C	1397	SR7	CBD-CBC-SBB	-5.06	106.01	113.11
2	K	1395	CNA	C6N-N1N-C2N	-5.04	117.59	121.88
3	A	1396	SR7	SBB-CAX-NAY	5.02	144.81	135.84
2	E	1395	CNA	C5A-C4A-N3A	-4.99	119.84	126.72
3	I	1396	SR7	CBC-SBB-CAX	4.99	97.89	89.41
2	G	1395	CNA	C4'-C1D-N1N	-4.98	107.25	113.50
3	G	1396	SR7	CBA-CAZ-NAY	-4.94	106.02	110.75
3	D	1396	SR7	CBD-CBC-SBB	-4.94	106.19	113.11
3	B	1396	SR7	CBD-CBC-SBB	-4.93	106.20	113.11
3	B	1396	SR7	CAG-CAH-NAI	-4.93	116.56	121.00
3	I	1396	SR7	CBF-CAK-NAL	4.90	129.66	116.86
3	K	1397	SR7	SBB-CAX-NAY	4.88	144.55	135.84
3	I	1396	SR7	SBB-CAX-NAW	-4.88	106.64	110.55
2	C	1395	CNA	C5A-C4A-N3A	-4.86	120.02	126.72
3	C	1397	SR7	CBF-CAK-NAL	4.82	129.47	116.86
3	C	1397	SR7	CAJ-CAK-CBF	-4.82	113.55	119.71
3	A	1396	SR7	CBD-CBC-SBB	-4.82	106.36	113.11
3	J	1396	SR7	CAJ-CAK-CBF	-4.82	113.56	119.71
3	C	1397	SR7	CBH-CBD-CBC	-4.76	124.87	130.68
2	E	1395	CNA	N9A-C8A-N7A	-4.75	107.20	113.94
2	B	1395	CNA	C6N-N1N-C2N	-4.73	117.85	121.88
3	D	1396	SR7	CBC-SBB-CAX	4.73	97.46	89.41
3	I	1396	SR7	CAC-CAZ-NAY	4.73	128.48	118.86
2	I	1395	CNA	O4B-C1B-N9A	-4.72	99.02	108.09
3	C	1397	SR7	CBC-SBB-CAX	4.72	97.43	89.41
3	I	1396	SR7	CBD-CBC-SBB	-4.71	106.50	113.11
3	I	1396	SR7	SBB-CAX-NAY	4.71	144.26	135.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1395	CNA	C6A-C5A-C4A	4.71	123.61	117.18
3	G	1396	SR7	CBC-SBB-CAX	4.71	97.41	89.41
3	L	1397	SR7	CBF-CAK-NAL	4.64	128.99	116.86
3	J	1396	SR7	CBA-CAZ-NAY	-4.64	106.31	110.75
3	J	1396	SR7	SBB-CAX-NAY	4.60	144.05	135.84
2	L	1395	CNA	C5A-C4A-N3A	-4.59	120.40	126.72
3	F	1396	SR7	CAP-CAG-CAH	-4.58	113.83	119.25
2	D	1394	CNA	C5A-C4A-N3A	-4.56	120.44	126.72
3	B	1396	SR7	CBC-SBB-CAX	4.55	97.14	89.41
3	H	1396	SR7	SBB-CAX-NAY	4.53	143.93	135.84
3	E	1396	SR7	CBC-SBB-CAX	4.50	97.06	89.41
2	D	1394	CNA	N3A-C2A-N1A	-4.47	121.82	128.58
2	E	1395	CNA	C6N-N1N-C2N	-4.46	118.08	121.88
3	K	1397	SR7	CAC-CAZ-NAY	4.40	127.80	118.86
2	F	1395	CNA	N9A-C8A-N7A	-4.38	107.72	113.94
2	C	1395	CNA	C5A-C4A-N9A	4.38	110.59	105.81
3	F	1396	SR7	CAC-CAZ-NAY	4.38	127.77	118.86
2	A	1395	CNA	C4'-C1D-N1N	-4.38	108.01	113.50
2	D	1394	CNA	C4D-C3D-C2D	-4.37	98.72	103.87
2	K	1395	CNA	C5A-C4A-N3A	-4.35	120.73	126.72
3	H	1396	SR7	CBA-CAZ-NAY	-4.34	106.60	110.75
3	D	1396	SR7	CBH-NAV-CAU	-4.30	104.45	111.14
3	B	1396	SR7	CBA-CAZ-NAY	-4.28	106.66	110.75
2	F	1395	CNA	C4'-C1D-C2D	-4.27	96.99	104.22
3	K	1397	SR7	NAW-CAX-NAY	-4.27	106.83	113.23
3	H	1396	SR7	CBC-SBB-CAX	4.27	96.66	89.41
2	I	1395	CNA	C5A-C4A-N3A	-4.25	120.87	126.72
2	H	1395	CNA	N9A-C8A-N7A	-4.24	107.93	113.94
3	A	1396	SR7	SBB-CAX-NAW	-4.22	107.16	110.55
2	J	1395	CNA	C5A-C4A-N3A	-4.21	120.92	126.72
2	L	1395	CNA	C6N-N1N-C2N	-4.21	118.30	121.88
2	F	1395	CNA	C5A-C4A-N3A	-4.19	120.94	126.72
2	D	1394	CNA	O4B-C1B-N9A	-4.17	100.08	108.09
2	J	1395	CNA	C6N-N1N-C2N	-4.16	118.34	121.88
2	L	1395	CNA	N9A-C8A-N7A	-4.15	108.04	113.94
3	L	1397	SR7	CAO-CAH-CAG	4.15	124.16	119.25
2	G	1395	CNA	C3D-C2D-C1D	-4.14	96.14	102.46
2	H	1395	CNA	C4'-C1D-N1N	-4.13	108.32	113.50
3	E	1396	SR7	CAP-CAG-CAH	-4.13	114.36	119.25
2	D	1394	CNA	O3-PN-O1N	4.12	123.10	110.70
3	F	1396	SR7	SBB-CAX-NAW	-4.12	107.24	110.55
2	D	1394	CNA	C5A-C4A-N9A	4.10	110.28	105.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1396	SR7	SBB-CAX-NAY	4.10	143.17	135.84
3	A	1396	SR7	CAG-CAH-NAI	-4.10	117.30	121.00
3	H	1396	SR7	CBD-CBC-SBB	-4.09	107.37	113.11
2	J	1395	CNA	N9A-C8A-N7A	-4.06	108.17	113.94
3	G	1396	SR7	CAG-CAH-NAI	-4.03	117.36	121.00
3	L	1397	SR7	CAP-CAG-CAH	-4.02	114.49	119.25
3	E	1396	SR7	CAB-CAC-CAZ	4.01	128.58	124.14
3	H	1396	SR7	CAC-CAZ-NAY	4.00	127.00	118.86
3	K	1397	SR7	CBD-CBC-SBB	-3.99	107.52	113.11
3	C	1397	SR7	CAP-CAG-CAH	-3.98	114.54	119.25
3	G	1396	SR7	CAJ-CAK-CBF	-3.95	114.66	119.71
3	G	1396	SR7	CAO-CAH-CAG	3.94	123.91	119.25
3	J	1396	SR7	CBH-NAV-CAU	-3.94	105.02	111.14
2	L	1395	CNA	C2N-C3N-C4N	3.93	122.83	118.26
3	B	1396	SR7	CAN-CAM-CAP	3.89	125.61	120.40
3	B	1396	SR7	CAH-CAG-NAL	3.87	125.92	121.18
3	J	1396	SR7	CAC-CAZ-NAY	3.86	126.70	118.86
3	F	1396	SR7	NAW-CAX-NAY	-3.86	107.45	113.23
3	B	1396	SR7	NAW-CAX-NAY	-3.85	107.46	113.23
2	A	1395	CNA	N9A-C8A-N7A	-3.84	108.49	113.94
3	C	1397	SR7	SBB-CAX-NAY	3.83	142.68	135.84
2	A	1395	CNA	C6N-N1N-C2N	-3.82	118.63	121.88
2	D	1394	CNA	C6A-C5A-C4A	3.82	122.39	117.18
3	J	1396	SR7	CAP-CAG-CAH	-3.81	114.73	119.25
2	K	1395	CNA	O1A-PA-O3	-3.80	96.99	107.27
3	G	1396	SR7	SBB-CAX-NAY	3.80	142.63	135.84
2	H	1395	CNA	C5A-C4A-N3A	-3.80	121.49	126.72
2	I	1395	CNA	N9A-C8A-N7A	-3.79	108.56	113.94
3	A	1396	SR7	CAH-CAG-NAL	3.79	125.82	121.18
3	E	1396	SR7	CAD-CAC-CAB	-3.78	114.55	118.81
3	G	1396	SR7	CBD-CBC-SBB	-3.78	107.82	113.11
2	A	1395	CNA	C6A-C5A-C4A	3.77	122.32	117.18
2	C	1395	CNA	O4B-C1B-N9A	-3.76	100.87	108.09
3	F	1396	SR7	CBH-NAV-CAU	-3.73	105.34	111.14
3	J	1396	SR7	NAW-CAX-NAY	-3.73	107.64	113.23
3	H	1396	SR7	SBB-CAX-NAW	-3.72	107.56	110.55
2	A	1395	CNA	O3-PN-O1N	3.71	121.88	110.70
3	K	1397	SR7	CAO-CAH-CAG	3.68	123.60	119.25
2	I	1395	CNA	C6A-C5A-C4A	3.67	122.19	117.18
3	E	1396	SR7	CAZ-CBA-NAW	3.66	111.10	105.81
2	E	1395	CNA	C5A-C6A-N6A	-3.66	114.23	123.29
3	B	1396	SR7	CAM-CAN-CAO	-3.64	115.53	120.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1396	SR7	CAG-CAH-NAI	-3.63	117.73	121.00
2	A	1395	CNA	C2A-N3A-C4A	3.63	120.70	111.83
3	E	1396	SR7	CAH-CAG-NAL	3.62	125.62	121.18
3	G	1396	SR7	CAJ-CAK-NAL	-3.62	113.81	121.62
2	D	1394	CNA	C4'-C4D-C5D	-3.59	105.67	112.78
2	G	1395	CNA	N9A-C8A-N7A	-3.56	108.88	113.94
3	E	1396	SR7	SBB-CAX-NAY	3.56	142.20	135.84
2	B	1395	CNA	C4'-C4D-C5D	-3.56	105.74	112.78
2	B	1395	CNA	N9A-C8A-N7A	-3.55	108.89	113.94
2	E	1395	CNA	C2A-N3A-C4A	3.55	120.51	111.83
3	F	1396	SR7	CAZ-CBA-NAW	3.55	110.94	105.81
2	A	1395	CNA	N3A-C4A-N9A	3.53	133.16	127.17
3	F	1396	SR7	CAG-CAH-NAI	-3.52	117.82	121.00
2	I	1395	CNA	C5A-C6A-N6A	-3.52	114.57	123.29
3	B	1396	SR7	CAO-CAH-NAI	-3.51	112.91	118.55
2	H	1395	CNA	C5A-C6A-N6A	-3.50	114.63	123.29
2	H	1395	CNA	C4A-N9A-C1B	-3.48	118.49	126.63
3	I	1396	SR7	CAP-CAG-CAH	-3.48	115.13	119.25
2	D	1394	CNA	C4A-C5A-N7A	-3.48	106.61	110.58
3	A	1396	SR7	NAW-CAX-NAY	-3.47	108.03	113.23
2	F	1395	CNA	C5A-C6A-N6A	-3.47	114.70	123.29
2	G	1395	CNA	C2A-N3A-C4A	3.46	120.28	111.83
2	B	1395	CNA	O3-PN-O1N	3.45	121.08	110.70
2	B	1395	CNA	C5A-C4A-N9A	3.44	109.56	105.81
3	H	1396	SR7	CAR-CAQ-NAV	-3.44	104.31	111.14
3	B	1396	SR7	CAC-CAZ-NAY	3.44	125.85	118.86
3	D	1396	SR7	SBB-CAX-NAY	3.43	141.97	135.84
3	G	1396	SR7	CAP-CAG-CAH	-3.42	115.20	119.25
2	C	1395	CNA	C4A-C5A-N7A	-3.42	106.67	110.58
3	I	1396	SR7	CBA-CAZ-NAY	-3.41	107.49	110.75
2	K	1395	CNA	C6A-C5A-C4A	3.40	121.83	117.18
3	E	1396	SR7	CBD-CBC-SBB	-3.40	108.35	113.11
3	J	1396	SR7	CAH-CAG-NAL	3.40	125.34	121.18
3	B	1396	SR7	CBH-NAV-CAU	-3.38	105.89	111.14
3	L	1397	SR7	CBA-CAZ-NAY	-3.37	107.52	110.75
2	C	1395	CNA	C6A-C5A-C4A	3.37	121.78	117.18
3	A	1396	SR7	CAO-CAH-NAI	-3.37	113.14	118.55
3	A	1396	SR7	CAZ-CBA-NAW	3.36	110.67	105.81
2	D	1394	CNA	C6N-N1N-C2N	-3.35	119.03	121.88
2	D	1394	CNA	N9A-C8A-N7A	-3.33	109.21	113.94
2	K	1395	CNA	N9A-C8A-N7A	-3.32	109.22	113.94
2	K	1395	CNA	C2B-C1B-N9A	3.32	121.55	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1396	SR7	CAM-CAN-CAO	-3.30	115.98	120.40
3	G	1396	SR7	CAD-CAC-CAB	-3.30	115.09	118.81
2	A	1395	CNA	C5A-C6A-N6A	-3.27	115.18	123.29
2	J	1395	CNA	O1A-PA-O3	-3.25	98.50	107.27
2	G	1395	CNA	C5A-C6A-N6A	-3.24	115.27	123.29
2	C	1395	CNA	C6N-N1N-C2N	-3.22	119.14	121.88
2	E	1395	CNA	N3A-C4A-N9A	3.21	132.63	127.17
2	I	1395	CNA	C2B-C1B-N9A	3.20	121.26	113.30
3	A	1396	SR7	CAB-CAC-CAZ	3.19	127.68	124.14
3	C	1397	SR7	NAW-CAX-NAY	-3.19	108.45	113.23
2	K	1395	CNA	C4N-C3N-C7N	-3.19	112.37	121.06
3	H	1396	SR7	CAJ-CAK-CBF	-3.17	115.66	119.71
3	C	1397	SR7	CAC-CAZ-NAY	3.17	125.30	118.86
2	L	1395	CNA	C2A-N3A-C4A	3.16	119.55	111.83
3	H	1396	SR7	NAW-CAX-NAY	-3.15	108.50	113.23
2	B	1395	CNA	C2A-N3A-C4A	3.15	119.53	111.83
2	J	1395	CNA	O4B-C1B-N9A	-3.15	102.04	108.09
3	I	1396	SR7	CBH-NAV-CAQ	3.14	116.03	111.14
3	K	1397	SR7	CBA-CAZ-NAY	-3.14	107.74	110.75
2	E	1395	CNA	C5A-N7A-C8A	3.13	108.37	103.45
2	L	1395	CNA	C5A-N7A-C8A	3.13	108.36	103.45
3	C	1397	SR7	CBD-CBH-NAV	-3.12	104.97	112.71
2	A	1395	CNA	C5A-N7A-C8A	3.11	108.33	103.45
3	F	1396	SR7	CBD-CBC-SBB	-3.10	108.76	113.11
2	J	1395	CNA	C6A-C5A-C4A	3.10	121.41	117.18
3	L	1397	SR7	NAW-CAX-NAY	-3.10	108.58	113.23
3	A	1396	SR7	CAM-CAN-CAO	-3.09	116.26	120.40
2	B	1395	CNA	C5A-N7A-C8A	3.09	108.31	103.45
2	H	1395	CNA	C2A-N3A-C4A	3.09	119.37	111.83
3	G	1396	SR7	CAK-NAL-CAG	3.08	122.22	117.56
2	D	1394	CNA	O4B-C4B-C5B	-3.07	99.50	109.33
3	L	1397	SR7	CAG-CAH-NAI	-3.06	118.24	121.00
3	K	1397	SR7	CBH-NAV-CAQ	-3.05	106.40	111.14
3	I	1396	SR7	CAH-CAG-NAL	3.05	124.91	121.18
3	H	1396	SR7	CBH-NAV-CAQ	3.03	115.86	111.14
3	E	1396	SR7	CAO-CAH-NAI	-3.03	113.68	118.55
3	E	1396	SR7	CAC-CAZ-NAY	3.03	125.02	118.86
3	E	1396	SR7	CAG-CAH-NAI	-3.01	118.29	121.00
3	G	1396	SR7	CAZ-CBA-NAW	3.00	110.15	105.81
2	E	1395	CNA	O2N-PN-O5D	-3.00	93.97	107.57
2	B	1395	CNA	C4A-C5A-N7A	-3.00	107.16	110.58
2	C	1395	CNA	N9A-C8A-N7A	-2.98	109.70	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1396	SR7	CBD-CBC-SBB	-2.98	108.93	113.11
2	B	1395	CNA	C5A-C6A-N6A	-2.98	115.91	123.29
2	C	1395	CNA	C2A-N3A-C4A	2.97	119.09	111.83
2	L	1395	CNA	C4A-C5A-N7A	-2.96	107.20	110.58
2	I	1395	CNA	C4'-C1D-N1N	-2.95	109.79	113.50
2	C	1395	CNA	O5B-PA-O2A	2.95	120.63	108.94
2	I	1395	CNA	O4B-C1B-C2B	-2.93	100.33	106.62
2	B	1395	CNA	N3A-C4A-N9A	2.93	132.16	127.17
3	G	1396	SR7	NAW-CAX-NAY	-2.93	108.84	113.23
2	J	1395	CNA	C5A-N7A-C8A	2.92	108.04	103.45
3	H	1396	SR7	CAK-CAJ-NAI	-2.91	118.34	122.77
3	E	1396	SR7	CAQ-CAR-NAS	-2.91	103.47	110.90
3	L	1397	SR7	CAM-CAN-CAO	-2.91	116.51	120.40
3	I	1396	SR7	CAC-CAZ-CBA	-2.91	124.03	130.77
2	F	1395	CNA	O3-PN-O1N	2.91	119.45	110.70
2	F	1395	CNA	C6N-N1N-C2N	-2.91	119.40	121.88
2	G	1395	CNA	N3A-C4A-N9A	2.88	132.07	127.17
3	F	1396	SR7	CAJ-CAK-NAL	-2.88	115.40	121.62
2	E	1395	CNA	C5A-C6A-N1A	2.88	124.82	117.51
2	L	1395	CNA	C4'-C4D-C5D	-2.87	107.09	112.78
2	H	1395	CNA	C1B-N9A-C8A	2.86	133.45	127.09
3	G	1396	SR7	CAC-CAZ-NAY	2.86	124.68	118.86
2	F	1395	CNA	C5A-N7A-C8A	2.85	107.93	103.45
3	B	1396	SR7	CAP-CAG-NAL	2.85	122.85	118.69
2	E	1395	CNA	O2N-PN-O3	-2.85	99.58	107.27
2	F	1395	CNA	C2A-N3A-C4A	2.84	118.77	111.83
3	A	1396	SR7	CAP-CAG-NAL	2.84	122.84	118.69
2	L	1395	CNA	C6A-C5A-C4A	2.83	121.04	117.18
3	A	1396	SR7	CAJ-CAK-NAL	-2.83	115.51	121.62
3	E	1396	SR7	CAK-CBF-NBE	-2.82	106.92	113.99
3	B	1396	SR7	CAB-CAC-CAZ	2.82	127.27	124.14
2	G	1395	CNA	C6A-C5A-C4A	2.81	121.02	117.18
2	K	1395	CNA	O3-PA-O2A	2.80	119.12	110.70
3	J	1396	SR7	CAZ-CBA-NAW	2.80	109.85	105.81
3	J	1396	SR7	SBB-CAX-NAW	-2.79	108.31	110.55
2	G	1395	CNA	C5A-N7A-C8A	2.79	107.84	103.45
3	F	1396	SR7	CAH-CAG-NAL	2.79	124.60	121.18
3	C	1397	SR7	CAG-CAH-NAI	-2.78	118.50	121.00
2	K	1395	CNA	C2N-C3N-C7N	2.77	127.46	119.46
3	A	1396	SR7	CAN-CAM-CAP	2.77	124.11	120.40
3	B	1396	SR7	CAD-CAC-CAZ	-2.76	114.54	119.25
3	E	1396	SR7	CAJ-CAK-NAL	-2.76	115.66	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1395	CNA	O1A-PA-O3	-2.75	99.83	107.27
3	J	1396	SR7	CAN-CAO-CAH	-2.75	116.33	120.09
3	I	1396	SR7	NAW-CAX-NAY	-2.75	109.11	113.23
2	A	1395	CNA	C5A-C4A-N9A	2.75	108.81	105.81
3	I	1396	SR7	CAZ-CBA-NAW	2.75	109.78	105.81
3	I	1396	SR7	CBD-CBH-NAV	-2.75	105.90	112.71
3	K	1397	SR7	CAC-CAZ-CBA	-2.74	124.41	130.77
2	K	1395	CNA	C4D-C3D-C2D	-2.74	100.64	103.87
3	K	1397	SR7	CAQ-CAR-NAS	-2.73	103.92	110.90
3	H	1396	SR7	CAK-CBF-NBE	-2.73	107.15	113.99
3	L	1397	SR7	CBH-NAV-CAU	-2.73	106.90	111.14
2	G	1395	CNA	O3D-C3D-C4D	-2.72	105.45	112.56
2	A	1395	CNA	C4A-C5A-N7A	-2.72	107.47	110.58
2	K	1395	CNA	C2A-N3A-C4A	2.72	118.47	111.83
3	C	1397	SR7	CAM-CAN-CAO	-2.72	116.76	120.40
2	G	1395	CNA	C5A-C4A-N9A	2.72	108.77	105.81
2	L	1395	CNA	C5A-C6A-N6A	-2.71	116.57	123.29
3	L	1397	SR7	SBB-CAX-NAY	2.69	140.66	135.84
3	H	1396	SR7	OBG-CBF-NBE	2.69	130.57	123.75
3	E	1396	SR7	NAW-CAX-NAY	-2.68	109.20	113.23
3	K	1397	SR7	CAH-CAG-NAL	2.68	124.46	121.18
3	G	1396	SR7	CAK-CBF-NBE	-2.68	107.28	113.99
2	I	1395	CNA	C2A-N3A-C4A	2.67	118.36	111.83
3	E	1396	SR7	CAK-CAJ-NAI	2.67	126.83	122.77
3	G	1396	SR7	CBH-NAV-CAU	-2.67	106.99	111.14
3	E	1396	SR7	CAN-CAO-CAH	-2.67	116.44	120.09
3	J	1396	SR7	CAJ-CAK-NAL	-2.67	115.86	121.62
2	F	1395	CNA	N3A-C4A-N9A	2.67	131.70	127.17
2	F	1395	CNA	C6A-C5A-C4A	2.66	120.81	117.18
3	G	1396	SR7	CAJ-NAI-CAH	2.66	120.04	116.96
3	D	1396	SR7	NAW-CAX-NAY	-2.66	109.25	113.23
3	I	1396	SR7	CAT-CAU-NAV	2.65	116.42	111.14
2	C	1395	CNA	O3-PN-O1N	2.65	118.68	110.70
2	C	1395	CNA	O2N-PN-O3	2.65	114.44	107.27
2	J	1395	CNA	C5A-C6A-N6A	-2.65	116.73	123.29
2	J	1395	CNA	C2A-N3A-C4A	2.65	118.29	111.83
2	B	1395	CNA	O2N-PN-O3	2.64	114.41	107.27
2	J	1395	CNA	C3N-C7N-N7N	-2.64	114.49	117.74
3	C	1397	SR7	CAH-CAG-NAL	2.64	124.41	121.18
3	B	1396	SR7	CAJ-CAK-NAL	-2.63	115.94	121.62
2	K	1395	CNA	C4A-C5A-N7A	-2.62	107.59	110.58
2	D	1394	CNA	C5A-N7A-C8A	2.61	107.55	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1396	SR7	CAO-CAH-NAI	-2.60	114.36	118.55
3	A	1396	SR7	CAK-CAJ-NAI	2.60	126.72	122.77
2	K	1395	CNA	C5A-C4A-N9A	2.60	108.64	105.81
3	C	1397	SR7	CBA-CAZ-NAY	-2.59	108.27	110.75
3	I	1396	SR7	CAR-CAQ-NAV	-2.57	106.03	111.14
3	F	1396	SR7	CBC-SBB-CAX	2.56	93.77	89.41
2	K	1395	CNA	C5A-C6A-N6A	-2.55	116.97	123.29
3	H	1396	SR7	CAZ-CBA-NAW	2.53	109.47	105.81
2	E	1395	CNA	C4A-N9A-C8A	2.53	108.39	105.74
2	I	1395	CNA	N3A-C4A-N9A	2.53	131.47	127.17
2	L	1395	CNA	N3A-C4A-N9A	2.53	131.46	127.17
2	F	1395	CNA	C4A-N9A-C8A	2.51	108.38	105.74
2	G	1395	CNA	C5A-C6A-N1A	2.51	123.89	117.51
3	G	1396	SR7	SBB-CAX-NAW	-2.51	108.53	110.55
3	K	1397	SR7	CBF-CAK-NAL	2.51	123.41	116.86
2	A	1395	CNA	O2B-C2B-C3B	-2.50	103.81	111.82
2	H	1395	CNA	C5A-N7A-C8A	2.49	107.37	103.45
2	C	1395	CNA	C5A-N7A-C8A	2.49	107.36	103.45
2	E	1395	CNA	C4'-C4D-C5D	-2.48	107.87	112.78
3	C	1397	SR7	CAD-CAC-CAZ	-2.48	115.03	119.25
2	E	1395	CNA	O3-PN-O1N	2.48	118.15	110.70
3	D	1396	SR7	CBF-CAK-NAL	2.47	123.32	116.86
2	K	1395	CNA	C5A-N7A-C8A	2.47	107.33	103.45
2	H	1395	CNA	O3D-C3D-C4D	-2.47	106.12	112.56
2	A	1395	CNA	C4D-C3D-C2D	-2.46	100.96	103.87
3	E	1396	SR7	CAN-CAM-CAP	2.46	123.69	120.40
2	J	1395	CNA	C4A-C5A-N7A	-2.45	107.78	110.58
3	J	1396	SR7	CAK-CBF-NBE	-2.44	107.88	113.99
3	E	1396	SR7	SBB-CAX-NAW	-2.44	108.59	110.55
3	J	1396	SR7	CBC-SBB-CAX	2.44	93.56	89.41
3	F	1396	SR7	CAN-CAO-CAH	-2.44	116.76	120.09
3	G	1396	SR7	CAB-CAC-CAZ	2.42	126.82	124.14
2	D	1394	CNA	C2A-N3A-C4A	2.41	117.73	111.83
3	L	1397	SR7	CAU-NAV-CAQ	2.41	114.03	108.84
3	A	1396	SR7	CBH-NAV-CAU	-2.41	107.40	111.14
3	K	1397	SR7	SBB-CAX-NAW	-2.40	108.62	110.55
2	C	1395	CNA	C4D-C3D-C2D	-2.40	101.04	103.87
2	B	1395	CNA	C3N-C7N-N7N	-2.40	114.79	117.74
3	J	1396	SR7	CAB-NBE-CBF	2.39	133.55	126.90
2	A	1395	CNA	C4'-C4D-C5D	-2.38	108.06	112.78
3	G	1396	SR7	CAP-CAG-NAL	2.38	122.17	118.69
2	L	1395	CNA	C4A-N9A-C8A	2.38	108.24	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1396	SR7	OBG-CBF-CAK	2.38	126.33	121.08
3	F	1396	SR7	CBH-NAV-CAQ	2.37	114.83	111.14
2	H	1395	CNA	C4'-C4D-C5D	2.37	117.47	112.78
3	L	1397	SR7	CBD-CBC-SBB	-2.37	109.79	113.11
2	E	1395	CNA	O5B-PA-O2A	2.36	118.31	108.94
3	I	1396	SR7	CAK-CBF-NBE	-2.36	108.07	113.99
3	B	1396	SR7	CAN-CAO-CAH	-2.36	116.86	120.09
2	G	1395	CNA	C4A-C5A-N7A	-2.36	107.89	110.58
3	D	1396	SR7	CAK-NAL-CAG	2.35	121.12	117.56
2	C	1395	CNA	C4'-C4D-C5D	-2.34	108.14	112.78
2	I	1395	CNA	N6A-C6A-N1A	2.34	123.59	118.38
2	E	1395	CNA	O5B-C5B-C4B	-2.33	101.07	108.99
3	G	1396	SR7	CAR-CAQ-NAV	-2.32	106.54	111.14
2	C	1395	CNA	C3B-C2B-C1B	2.31	105.84	101.46
3	C	1397	SR7	CAU-NAV-CAQ	2.30	113.81	108.84
3	F	1396	SR7	CAN-CAM-CAP	2.30	123.48	120.40
3	G	1396	SR7	CBH-NAV-CAQ	2.30	114.72	111.14
2	J	1395	CNA	O3-PN-O1N	2.29	117.61	110.70
2	I	1395	CNA	C2N-C3N-C4N	2.29	120.92	118.26
2	D	1394	CNA	C3D-C2D-C1D	2.29	105.96	102.46
3	L	1397	SR7	CAC-CAZ-NAY	2.29	123.52	118.86
2	G	1395	CNA	O2D-C2D-C3D	-2.28	104.50	111.82
2	A	1395	CNA	C5A-C6A-N1A	2.28	123.30	117.51
3	H	1396	SR7	CAM-CAP-CAG	2.26	123.18	120.09
2	B	1395	CNA	C1B-N9A-C8A	-2.26	122.08	127.09
2	E	1395	CNA	O4B-C4B-C5B	2.26	116.57	109.33
2	A	1395	CNA	C2B-C1B-N9A	2.26	118.91	113.30
2	J	1395	CNA	C5A-C4A-N9A	2.25	108.26	105.81
2	K	1395	CNA	O7N-C7N-C3N	2.24	122.34	119.60
3	C	1397	SR7	CAN-CAM-CAP	2.24	123.40	120.40
2	H	1395	CNA	C2N-C3N-C4N	2.23	120.86	118.26
2	J	1395	CNA	O2N-PN-O5D	-2.22	97.50	107.57
2	I	1395	CNA	PA-O5B-C5B	-2.22	108.62	121.35
3	B	1396	SR7	CAK-CAJ-NAI	2.22	126.14	122.77
2	C	1395	CNA	C2N-C3N-C4N	2.22	120.83	118.26
2	F	1395	CNA	O4B-C1B-N9A	-2.21	103.84	108.09
2	J	1395	CNA	O5B-PA-O2A	2.21	117.69	108.94
3	D	1396	SR7	CAC-CAZ-NAY	2.20	123.34	118.86
2	E	1395	CNA	C6A-C5A-C4A	2.20	120.18	117.18
3	D	1396	SR7	SBB-CAX-NAW	-2.20	108.78	110.55
2	H	1395	CNA	C4A-N9A-C8A	2.20	108.05	105.74
2	L	1395	CNA	C4'-C1D-C2D	2.20	107.94	104.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1396	SR7	CAO-CAH-NAI	-2.20	115.02	118.55
3	J	1396	SR7	CAK-CAJ-NAI	2.19	126.10	122.77
2	B	1395	CNA	C4A-N9A-C1B	2.18	131.73	126.63
2	D	1394	CNA	O5B-PA-O2A	2.18	117.58	108.94
2	I	1395	CNA	C5A-N7A-C8A	2.18	106.87	103.45
2	L	1395	CNA	O7N-C7N-C3N	-2.17	116.94	119.60
2	F	1395	CNA	C3D-C2D-C1D	-2.17	99.15	102.46
3	A	1396	SR7	CAC-CAZ-CBA	-2.17	125.74	130.77
2	H	1395	CNA	N3A-C4A-N9A	2.16	130.85	127.17
2	A	1395	CNA	O2N-PN-O3	2.16	113.12	107.27
3	A	1396	SR7	CAD-CAC-CAZ	-2.16	115.56	119.25
3	I	1396	SR7	CAG-CAH-NAI	-2.16	119.06	121.00
3	C	1397	SR7	CAJ-CAK-NAL	-2.15	116.97	121.62
2	L	1395	CNA	C4'-C4D-C3D	2.15	108.34	102.89
2	J	1395	CNA	N3A-C4A-N9A	2.15	130.82	127.17
2	K	1395	CNA	O4B-C1B-C2B	-2.14	102.03	106.62
3	D	1396	SR7	CAT-CAU-NAV	2.14	115.39	111.14
2	J	1395	CNA	O3-PA-O2A	2.14	117.14	110.70
2	I	1395	CNA	C4'-C4D-C3D	2.13	108.30	102.89
3	K	1397	SR7	CAP-CAG-CAH	-2.13	116.73	119.25
2	L	1395	CNA	C5A-C4A-N9A	2.13	108.13	105.81
2	C	1395	CNA	O4B-C4B-C5B	-2.12	102.55	109.33
3	L	1397	SR7	CAZ-CBA-NAW	2.12	108.87	105.81
2	K	1395	CNA	C3B-C2B-C1B	2.11	105.46	101.46
3	L	1397	SR7	CAH-CAG-NAL	2.11	123.76	121.18
3	K	1397	SR7	CAJ-CAK-CBF	-2.11	117.02	119.71
2	E	1395	CNA	C3N-C7N-N7N	-2.11	115.14	117.74
2	I	1395	CNA	C5N-C4N-C3N	-2.11	118.29	120.36
2	H	1395	CNA	C6A-C5A-C4A	2.10	120.04	117.18
3	D	1396	SR7	CAJ-NAI-CAH	2.10	119.39	116.96
3	L	1397	SR7	CAP-CAG-NAL	2.09	121.75	118.69
2	H	1395	CNA	C5A-C6A-N1A	2.09	122.82	117.51
3	I	1396	SR7	CAN-CAO-CAH	-2.09	117.23	120.09
3	I	1396	SR7	CAO-CAH-NAI	-2.09	115.19	118.55
3	C	1397	SR7	SBB-CAX-NAW	-2.09	108.87	110.55
2	F	1395	CNA	O1A-PA-O3	-2.08	101.64	107.27
2	E	1395	CNA	O3-PA-O2A	2.08	116.95	110.70
2	E	1395	CNA	O7N-C7N-C3N	2.05	122.11	119.60
2	L	1395	CNA	C5A-C6A-N1A	2.05	122.73	117.51
3	F	1396	SR7	CAD-CAC-CAB	-2.05	116.49	118.81
3	K	1397	SR7	CAG-CAH-NAI	-2.05	119.15	121.00
3	H	1396	SR7	CAB-CAC-CAZ	2.04	126.41	124.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1394	CNA	O4B-C1B-C2B	-2.04	102.24	106.62
3	C	1397	SR7	CAR-CAQ-NAV	-2.03	107.10	111.14
2	F	1395	CNA	C4D-C4'-C1D	-2.03	96.15	102.60
3	I	1396	SR7	OBG-CBF-NBE	2.03	128.89	123.75
3	E	1396	SR7	CAE-CAD-CAC	2.02	123.45	119.80
2	K	1395	CNA	N3A-C4A-N9A	2.01	130.58	127.17
2	G	1395	CNA	O2N-PN-O3	-2.00	101.87	107.27

There are no chirality outliers.

All (189) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1395	CNA	C4D-C5D-O5D-PN
2	A	1395	CNA	C4'-C4D-C5D-O5D
2	A	1395	CNA	C3D-C4D-C5D-O5D
2	A	1395	CNA	C2D-C1D-N1N-C2N
2	A	1395	CNA	C2D-C1D-N1N-C6N
2	B	1395	CNA	C4D-C5D-O5D-PN
2	B	1395	CNA	C2D-C1D-N1N-C2N
2	B	1395	CNA	C2D-C1D-N1N-C6N
2	C	1395	CNA	C2D-C1D-N1N-C2N
2	C	1395	CNA	C2D-C1D-N1N-C6N
2	D	1394	CNA	C2D-C1D-N1N-C2N
2	D	1394	CNA	C2D-C1D-N1N-C6N
2	E	1395	CNA	C5B-O5B-PA-O1A
2	E	1395	CNA	C4D-C5D-O5D-PN
2	E	1395	CNA	C4'-C4D-C5D-O5D
2	E	1395	CNA	C3D-C4D-C5D-O5D
2	E	1395	CNA	C2D-C1D-N1N-C2N
2	E	1395	CNA	C2D-C1D-N1N-C6N
2	F	1395	CNA	C5D-O5D-PN-O3
2	F	1395	CNA	C5D-O5D-PN-O1N
2	F	1395	CNA	C5D-O5D-PN-O2N
2	F	1395	CNA	C2D-C1D-N1N-C2N
2	F	1395	CNA	C2D-C1D-N1N-C6N
2	F	1395	CNA	C2N-C3N-C7N-O7N
2	F	1395	CNA	C2N-C3N-C7N-N7N
2	G	1395	CNA	C5B-O5B-PA-O1A
2	G	1395	CNA	C5B-O5B-PA-O2A
2	G	1395	CNA	C5B-O5B-PA-O3
2	G	1395	CNA	C5D-O5D-PN-O3
2	G	1395	CNA	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	G	1395	CNA	C4'-C4D-C5D-O5D
2	G	1395	CNA	C2D-C1D-N1N-C2N
2	G	1395	CNA	C2D-C1D-N1N-C6N
2	H	1395	CNA	C5D-O5D-PN-O3
2	H	1395	CNA	C5D-O5D-PN-O1N
2	H	1395	CNA	C4D-C5D-O5D-PN
2	H	1395	CNA	C4'-C4D-C5D-O5D
2	H	1395	CNA	C2D-C1D-N1N-C2N
2	H	1395	CNA	C2D-C1D-N1N-C6N
2	I	1395	CNA	C5D-O5D-PN-O3
2	I	1395	CNA	C5D-O5D-PN-O2N
2	I	1395	CNA	C4'-C4D-C5D-O5D
2	I	1395	CNA	C3D-C4D-C5D-O5D
2	I	1395	CNA	C2D-C1D-N1N-C2N
2	I	1395	CNA	C2D-C1D-N1N-C6N
2	J	1395	CNA	C4'-C4D-C5D-O5D
2	J	1395	CNA	C3D-C4D-C5D-O5D
2	J	1395	CNA	C2D-C1D-N1N-C2N
2	J	1395	CNA	C2D-C1D-N1N-C6N
2	K	1395	CNA	C4D-C5D-O5D-PN
2	K	1395	CNA	C2D-C1D-N1N-C2N
2	K	1395	CNA	C2D-C1D-N1N-C6N
2	K	1395	CNA	C2N-C3N-C7N-O7N
2	K	1395	CNA	C2N-C3N-C7N-N7N
2	L	1395	CNA	C4'-C4D-C5D-O5D
2	L	1395	CNA	C3D-C4D-C5D-O5D
2	L	1395	CNA	C2D-C1D-N1N-C2N
2	L	1395	CNA	C2D-C1D-N1N-C6N
2	L	1395	CNA	C2N-C3N-C7N-O7N
3	A	1396	SR7	CAJ-CAK-CBF-OBG
3	B	1396	SR7	CAD-CAC-CAZ-NAY
3	B	1396	SR7	CAJ-CAK-CBF-OBG
3	C	1397	SR7	CAJ-CAK-CBF-OBG
3	D	1396	SR7	CAD-CAC-CAZ-NAY
3	E	1396	SR7	CAD-CAC-CAZ-NAY
3	E	1396	SR7	CAJ-CAK-CBF-OBG
3	G	1396	SR7	CAD-CAC-CAZ-NAY
3	G	1396	SR7	CAJ-CAK-CBF-NBE
3	H	1396	SR7	CAD-CAC-CAZ-NAY
3	H	1396	SR7	CAJ-CAK-CBF-NBE
3	H	1396	SR7	CAJ-CAK-CBF-OBG
3	H	1396	SR7	NAL-CAK-CBF-NBE

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Mol	Chain	Res	Type	Atoms
3	I	1396	SR7	CAD-CAC-CAZ-NAY
3	I	1396	SR7	CAJ-CAK-CBF-NBE
3	I	1396	SR7	CAJ-CAK-CBF-OBG
3	J	1396	SR7	CAD-CAC-CAZ-NAY
3	K	1397	SR7	CAJ-CAK-CBF-NBE
3	K	1397	SR7	CAJ-CAK-CBF-OBG
3	L	1397	SR7	CAJ-CAK-CBF-NBE
3	L	1397	SR7	CAJ-CAK-CBF-OBG
3	H	1396	SR7	NAL-CAK-CBF-OBG
2	K	1395	CNA	C4N-C3N-C7N-O7N
2	K	1395	CNA	C4N-C3N-C7N-N7N
3	I	1396	SR7	NAL-CAK-CBF-OBG
2	E	1395	CNA	C2N-C3N-C7N-N7N
3	E	1396	SR7	NAL-CAK-CBF-OBG
3	F	1396	SR7	NAL-CAK-CBF-OBG
3	G	1396	SR7	NAL-CAK-CBF-OBG
3	K	1397	SR7	NAL-CAK-CBF-OBG
2	F	1395	CNA	C4N-C3N-C7N-N7N
3	B	1396	SR7	NAL-CAK-CBF-OBG
3	C	1397	SR7	NAL-CAK-CBF-OBG
3	J	1396	SR7	NAL-CAK-CBF-OBG
3	L	1397	SR7	NAL-CAK-CBF-OBG
3	C	1397	SR7	NAL-CAK-CBF-NBE
3	I	1396	SR7	NAL-CAK-CBF-NBE
3	A	1396	SR7	NAL-CAK-CBF-OBG
3	A	1396	SR7	NAL-CAK-CBF-NBE
3	B	1396	SR7	NAL-CAK-CBF-NBE
3	E	1396	SR7	NAL-CAK-CBF-NBE
3	G	1396	SR7	NAL-CAK-CBF-NBE
3	J	1396	SR7	NAL-CAK-CBF-NBE
3	K	1397	SR7	NAL-CAK-CBF-NBE
3	F	1396	SR7	NAL-CAK-CBF-NBE
3	L	1397	SR7	NAL-CAK-CBF-NBE
2	E	1395	CNA	C2N-C3N-C7N-O7N
2	F	1395	CNA	C4N-C3N-C7N-O7N
2	E	1395	CNA	C4N-C3N-C7N-N7N
3	F	1396	SR7	CAJ-CAK-CBF-OBG
3	G	1396	SR7	CAJ-CAK-CBF-OBG
3	J	1396	SR7	CAJ-CAK-CBF-OBG
2	L	1395	CNA	C4N-C3N-C7N-O7N
2	L	1395	CNA	C2N-C3N-C7N-N7N
3	A	1396	SR7	CAJ-CAK-CBF-NBE

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Mol	Chain	Res	Type	Atoms
3	B	1396	SR7	CAJ-CAK-CBF-NBE
3	C	1397	SR7	CAJ-CAK-CBF-NBE
3	E	1396	SR7	CAJ-CAK-CBF-NBE
3	F	1396	SR7	CAJ-CAK-CBF-NBE
3	J	1396	SR7	CAJ-CAK-CBF-NBE
2	E	1395	CNA	C4N-C3N-C7N-O7N
2	L	1395	CNA	C4N-C3N-C7N-N7N
2	J	1395	CNA	C2N-C3N-C7N-N7N
2	H	1395	CNA	O4B-C4B-C5B-O5B
2	E	1395	CNA	C3B-C4B-C5B-O5B
2	E	1395	CNA	O4B-C4B-C5B-O5B
2	J	1395	CNA	C2N-C3N-C7N-O7N
2	J	1395	CNA	C4N-C3N-C7N-N7N
3	A	1396	SR7	CAD-CAC-CAZ-NAY
3	C	1397	SR7	CAD-CAC-CAZ-NAY
3	F	1396	SR7	CAD-CAC-CAZ-NAY
5	C	1396	GOL	O2-C2-C3-O3
5	D	1395	GOL	O1-C1-C2-O2
5	K	1396	GOL	O1-C1-C2-O2
5	L	1396	GOL	O2-C2-C3-O3
5	C	1396	GOL	C1-C2-C3-O3
2	L	1395	CNA	PA-O3-PN-O1N
2	D	1394	CNA	C4D-C5D-O5D-PN
2	F	1395	CNA	C4D-C5D-O5D-PN
5	D	1395	GOL	O2-C2-C3-O3
2	F	1395	CNA	C3D-C4D-C5D-O5D
2	H	1395	CNA	C3D-C4D-C5D-O5D
2	J	1395	CNA	C4N-C3N-C7N-O7N
2	E	1395	CNA	C5B-O5B-PA-O2A
2	E	1395	CNA	C5D-O5D-PN-O3
2	H	1395	CNA	C5B-O5B-PA-O1A
2	H	1395	CNA	C5B-O5B-PA-O2A
2	H	1395	CNA	C5B-O5B-PA-O3
2	I	1395	CNA	C5D-O5D-PN-O1N
2	L	1395	CNA	C5D-O5D-PN-O3
2	L	1395	CNA	C5D-O5D-PN-O1N
2	L	1395	CNA	C5D-O5D-PN-O2N
2	H	1395	CNA	C4B-C5B-O5B-PA
2	G	1395	CNA	C2N-C3N-C7N-O7N
2	H	1395	CNA	C3B-C4B-C5B-O5B
2	B	1395	CNA	C4N-C3N-C7N-N7N
2	G	1395	CNA	C2N-C3N-C7N-N7N

Continued on next page...

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Mol	Chain	Res	Type	Atoms
2	D	1394	CNA	O4B-C4B-C5B-O5B
2	G	1395	CNA	C4N-C3N-C7N-O7N
2	I	1395	CNA	C2N-C3N-C7N-N7N
2	K	1395	CNA	PA-O3-PN-O2N
2	G	1395	CNA	C4N-C3N-C7N-N7N
2	I	1395	CNA	C2N-C3N-C7N-O7N
2	F	1395	CNA	O4B-C4B-C5B-O5B
2	H	1395	CNA	C2N-C3N-C7N-N7N
2	G	1395	CNA	O4B-C4B-C5B-O5B
2	I	1395	CNA	PA-O3-PN-O1N
2	I	1395	CNA	PA-O3-PN-O2N
2	K	1395	CNA	PA-O3-PN-O1N
2	L	1395	CNA	PA-O3-PN-O2N
2	I	1395	CNA	C4N-C3N-C7N-N7N
3	C	1397	SR7	CBD-CBH-NAV-CAU
2	C	1395	CNA	C4D-C5D-O5D-PN
2	G	1395	CNA	C4D-C5D-O5D-PN
2	J	1395	CNA	C4D-C5D-O5D-PN
3	E	1396	SR7	NAW-CBD-CBH-NAV
2	B	1395	CNA	C2N-C3N-C7N-N7N
2	G	1395	CNA	C3D-C4D-C5D-O5D
2	K	1395	CNA	C3D-C4D-C5D-O5D
2	K	1395	CNA	O4B-C4B-C5B-O5B
2	H	1395	CNA	C2B-C1B-N9A-C8A
2	H	1395	CNA	C2N-C3N-C7N-O7N
2	F	1395	CNA	C3B-C4B-C5B-O5B
2	B	1395	CNA	PN-O3-PA-O1A
2	D	1394	CNA	PN-O3-PA-O1A
2	I	1395	CNA	PN-O3-PA-O1A
2	J	1395	CNA	PN-O3-PA-O1A
2	K	1395	CNA	PN-O3-PA-O1A
2	L	1395	CNA	PN-O3-PA-O1A
2	B	1395	CNA	O4B-C4B-C5B-O5B

All (4) ring outliers are listed below:

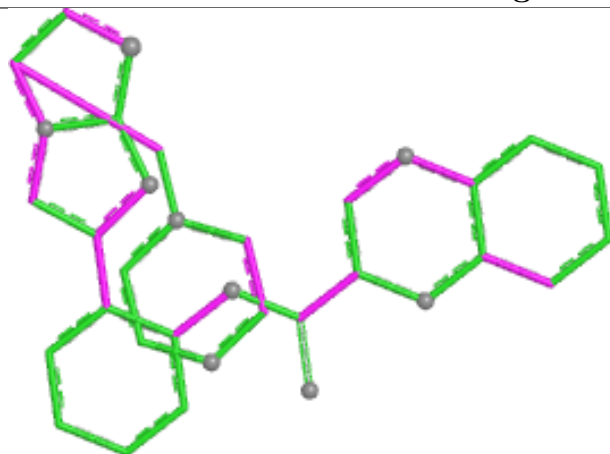
Mol	Chain	Res	Type	Atoms
3	B	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	A	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	F	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV
3	J	1396	SR7	CAQ-CAR-CAT-CAU-NAS-NAV

27 monomers are involved in 125 short contacts:

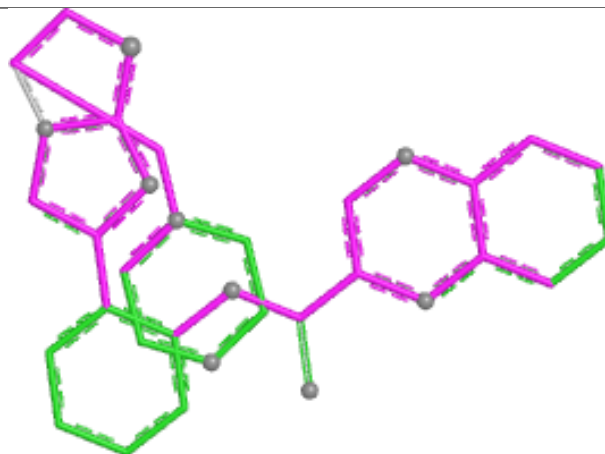
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	1396	SR7	7	0
3	F	1396	SR7	11	0
5	C	1396	GOL	2	0
3	L	1397	SR7	6	0
2	A	1395	CNA	5	0
5	D	1395	GOL	3	0
3	I	1396	SR7	10	0
2	E	1395	CNA	1	0
2	H	1395	CNA	10	0
3	B	1396	SR7	5	0
2	G	1395	CNA	12	0
2	D	1394	CNA	5	0
2	K	1395	CNA	6	0
2	B	1395	CNA	4	0
2	J	1395	CNA	4	0
2	C	1395	CNA	1	0
3	A	1396	SR7	4	0
3	C	1397	SR7	4	0
3	K	1397	SR7	8	0
2	F	1395	CNA	3	0
5	K	1396	GOL	1	0
3	E	1396	SR7	5	0
2	I	1395	CNA	5	0
3	G	1396	SR7	18	0
3	H	1396	SR7	11	0
3	D	1396	SR7	2	0
2	L	1395	CNA	5	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.

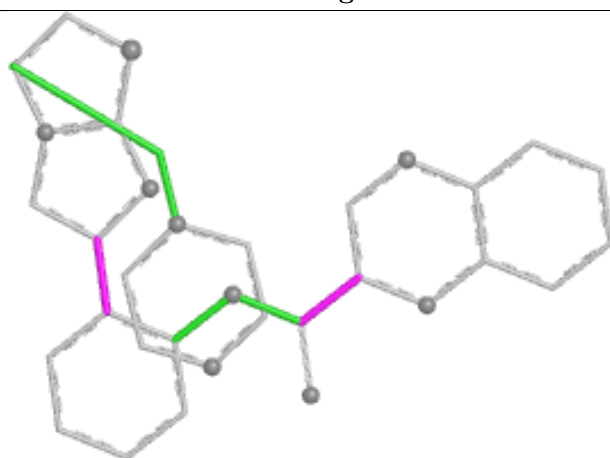
Ligand SR7 J 1396



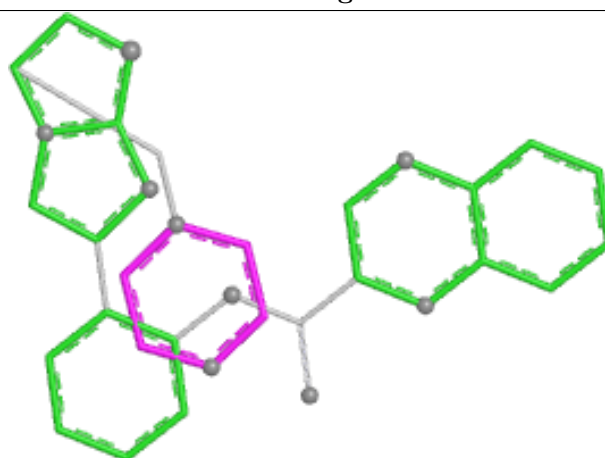
Bond lengths



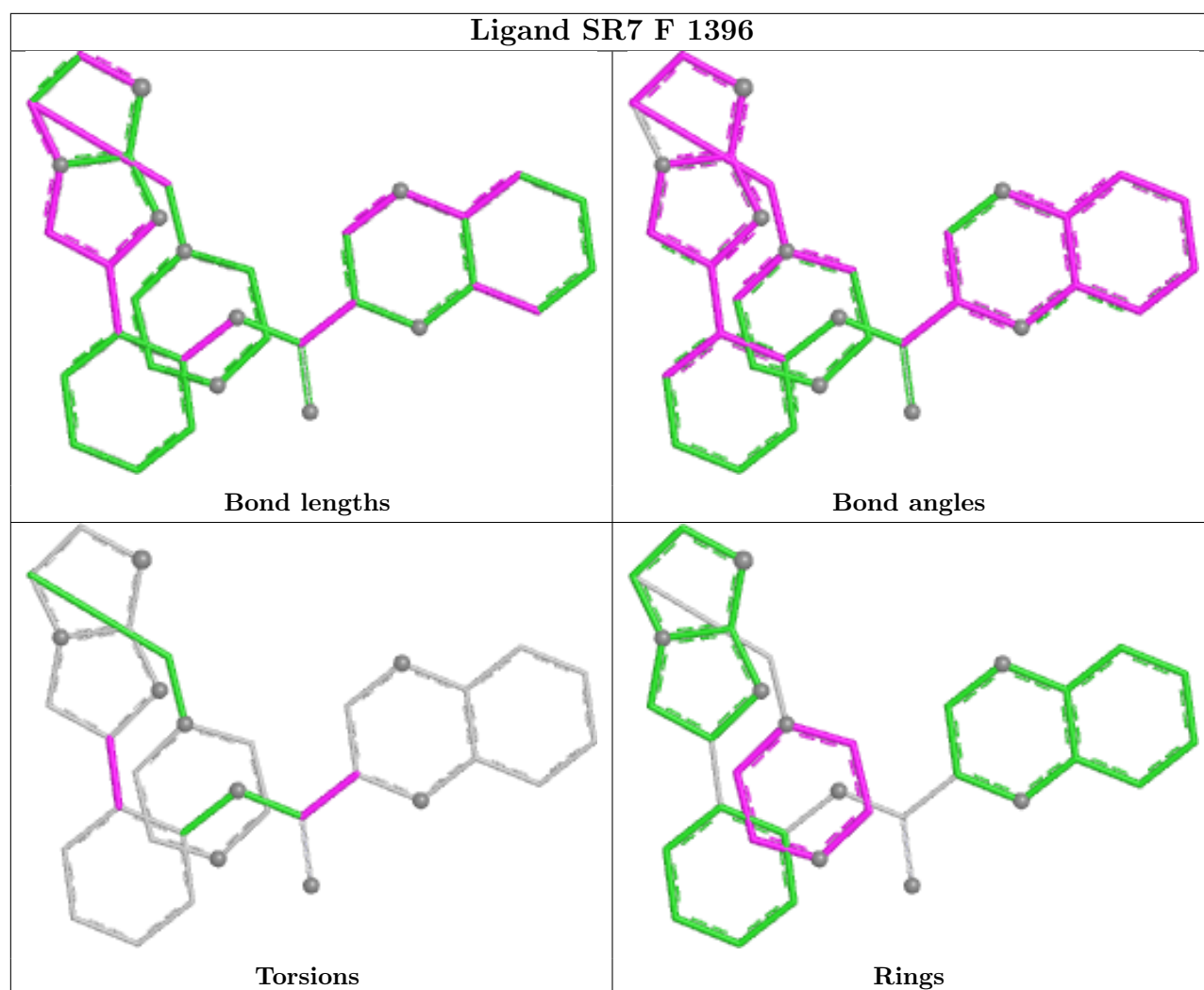
Bond angles

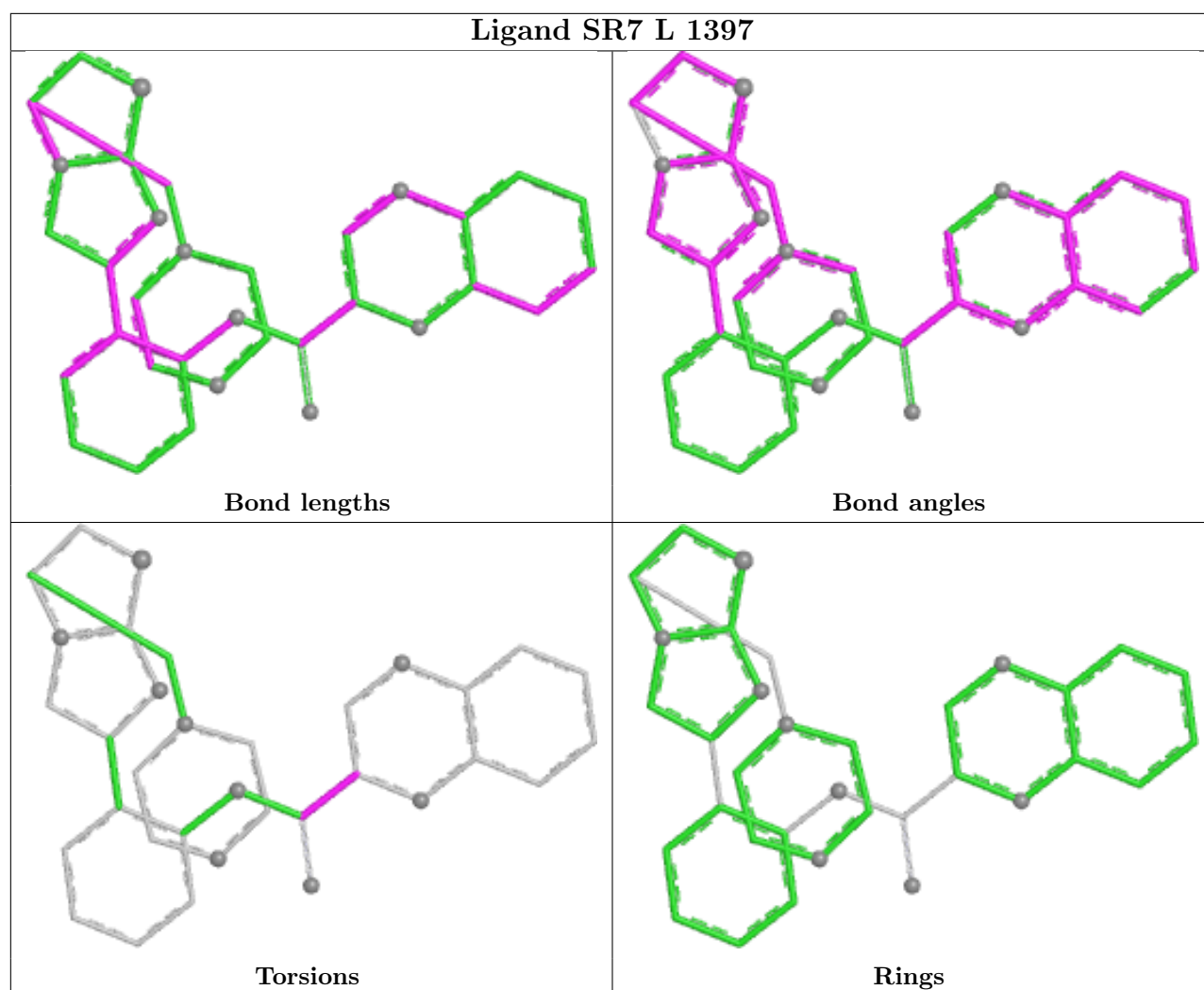


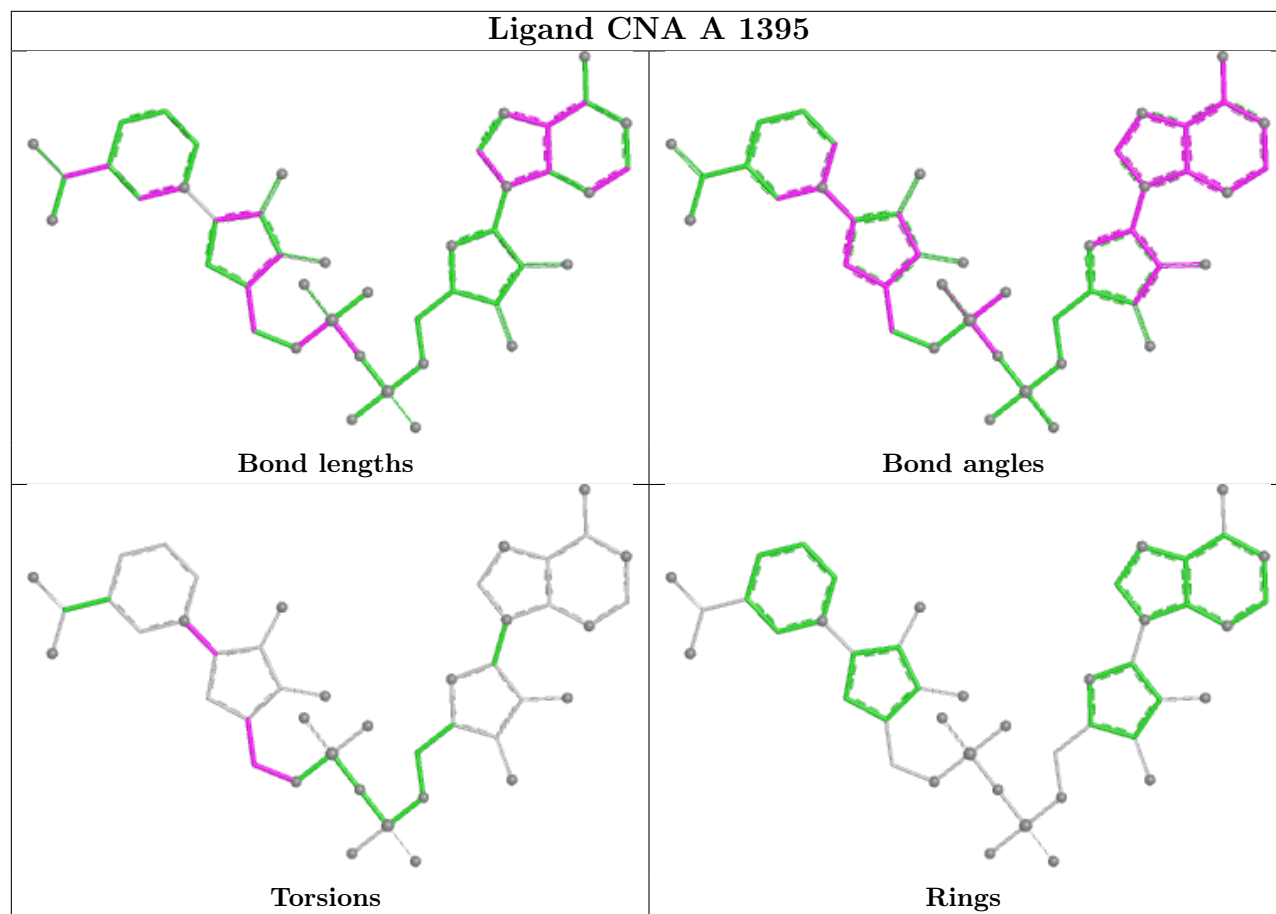
Torsions



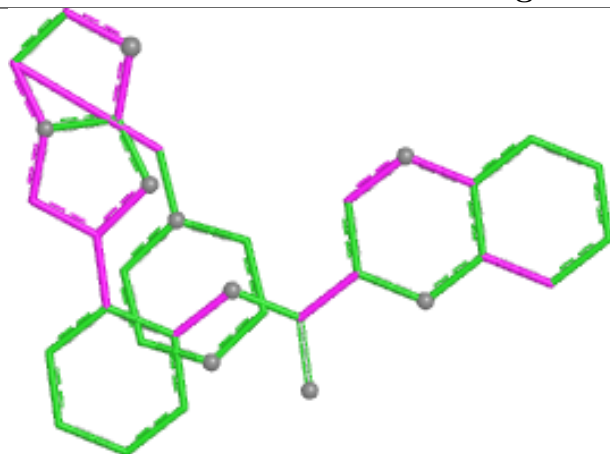
Rings



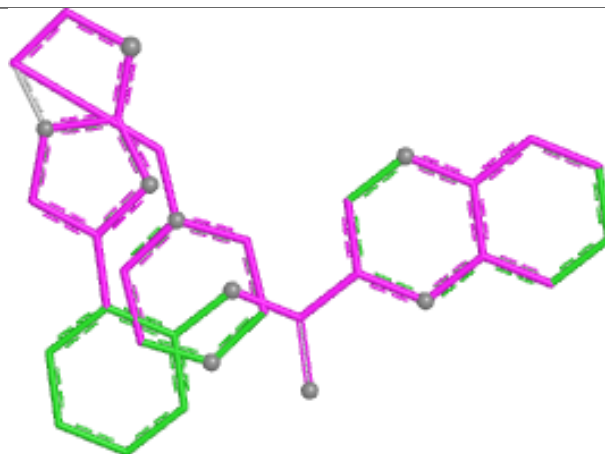




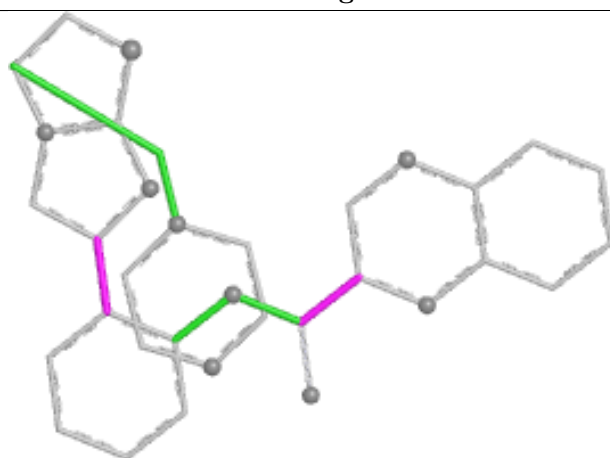
Ligand SR7 I 1396



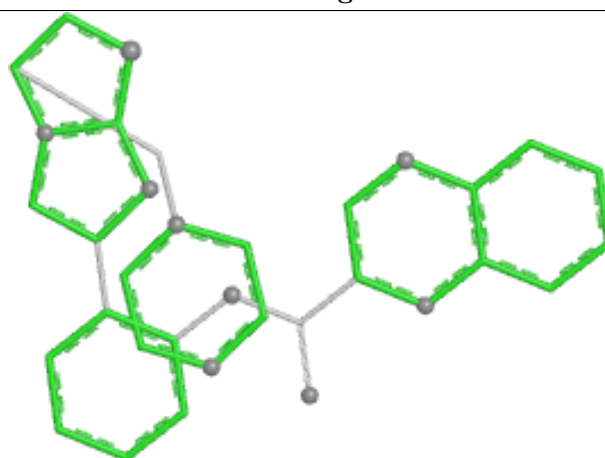
Bond lengths



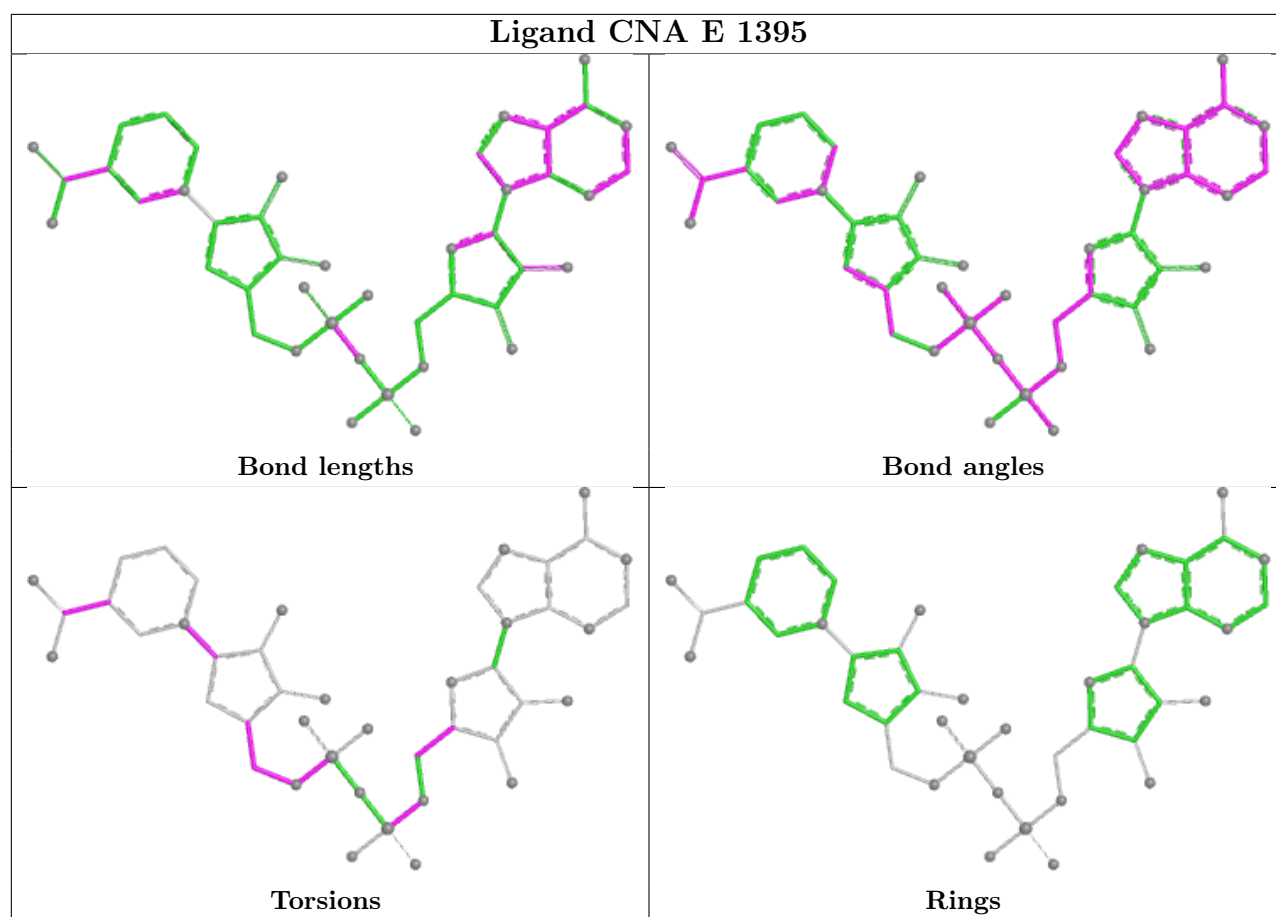
Bond angles

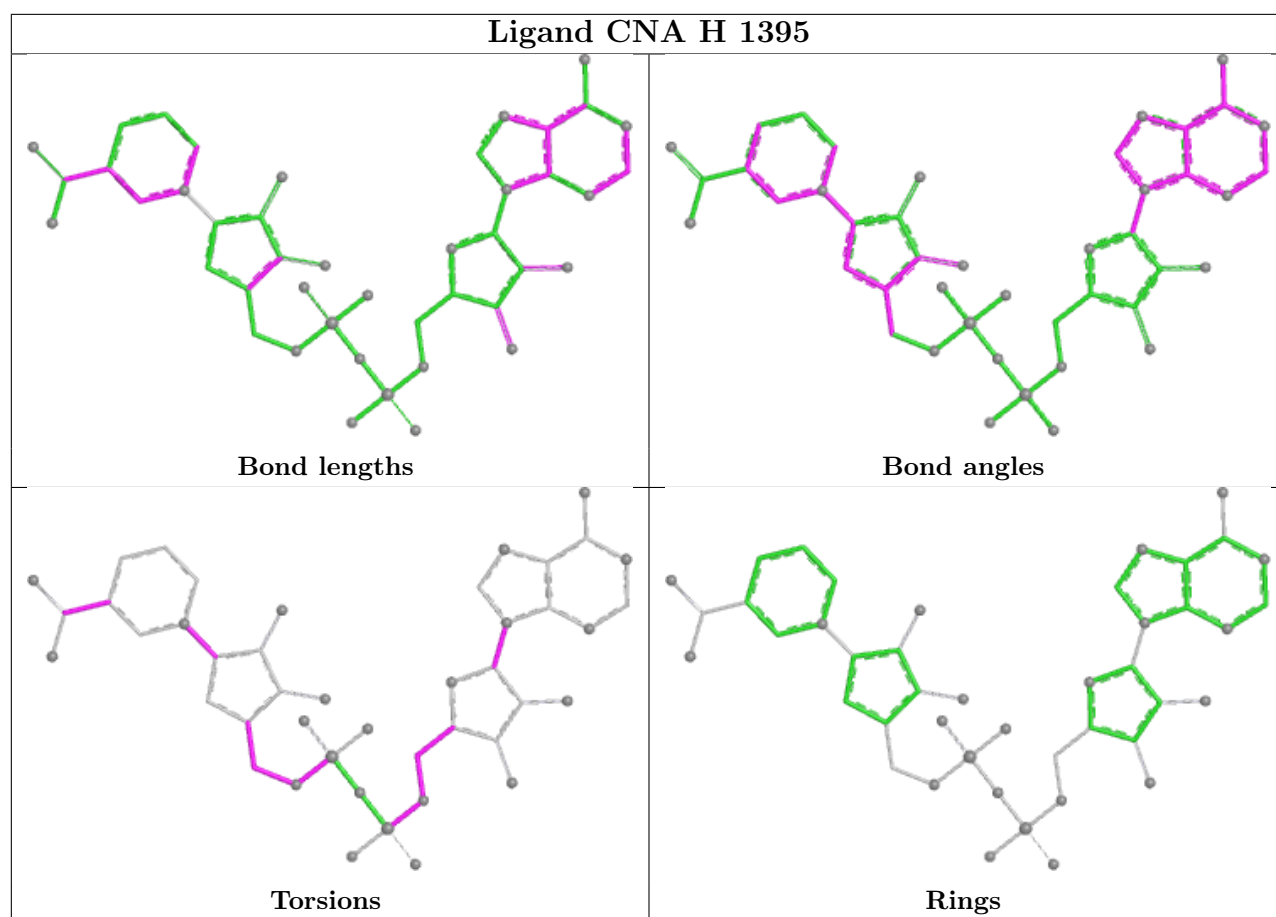


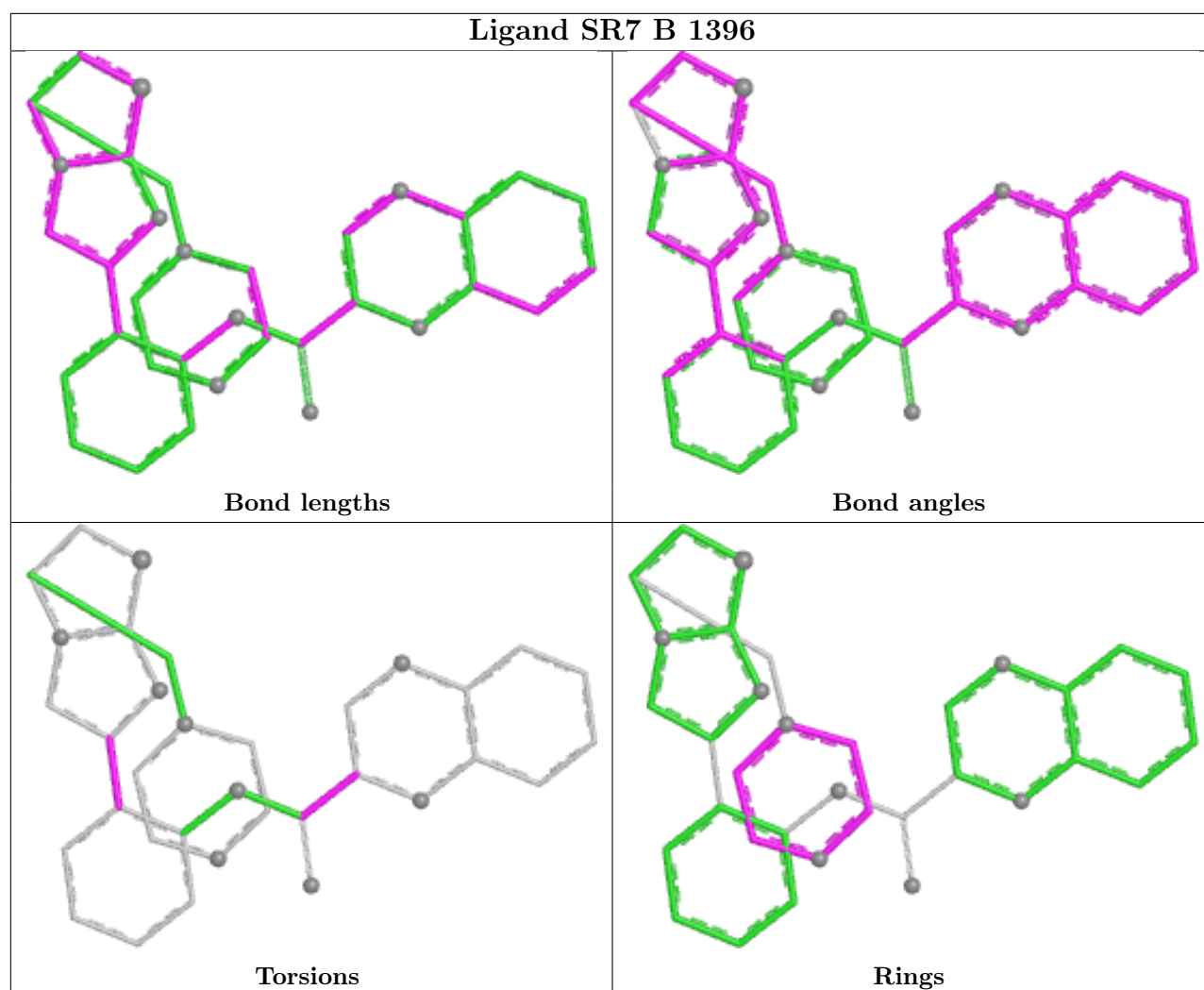
Torsions

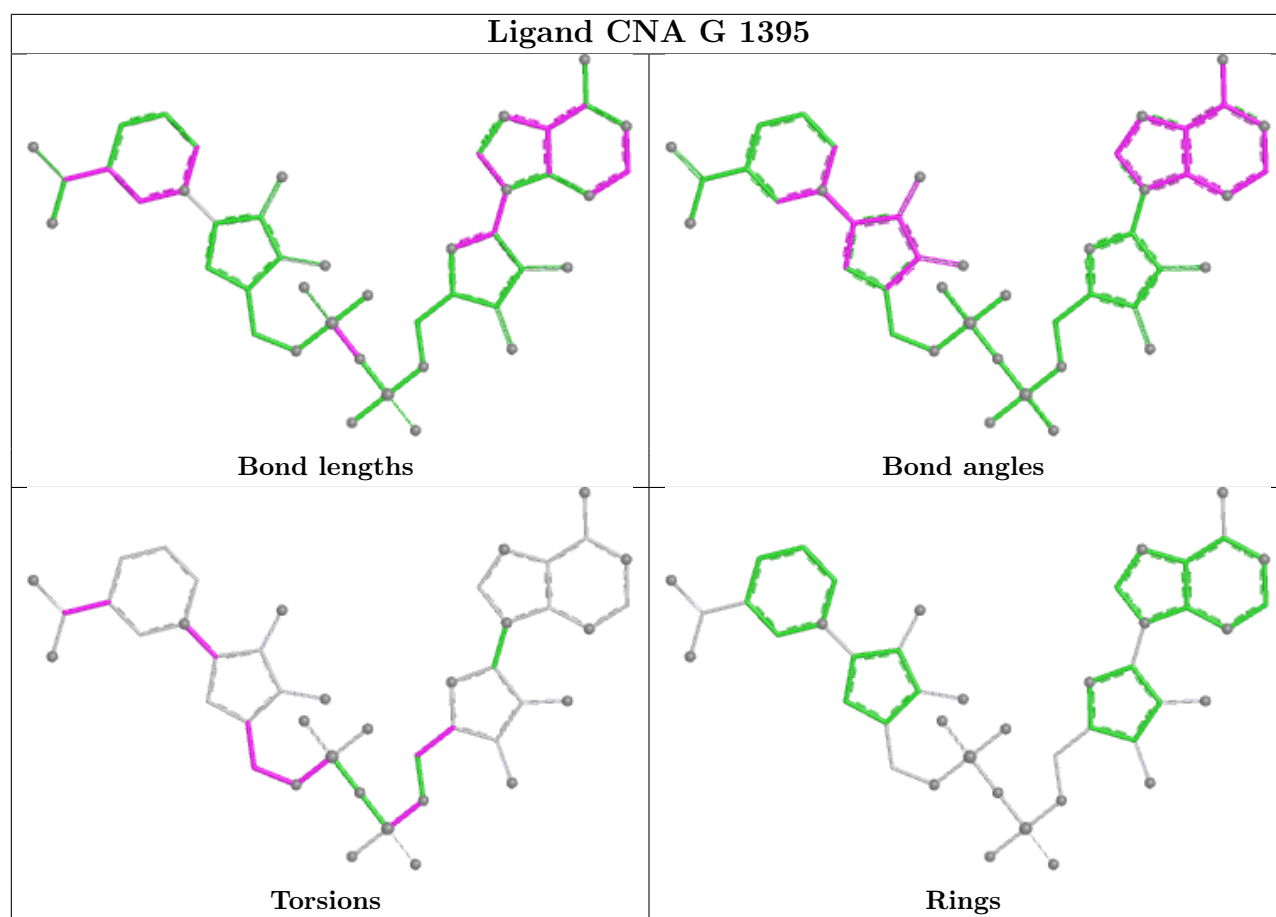


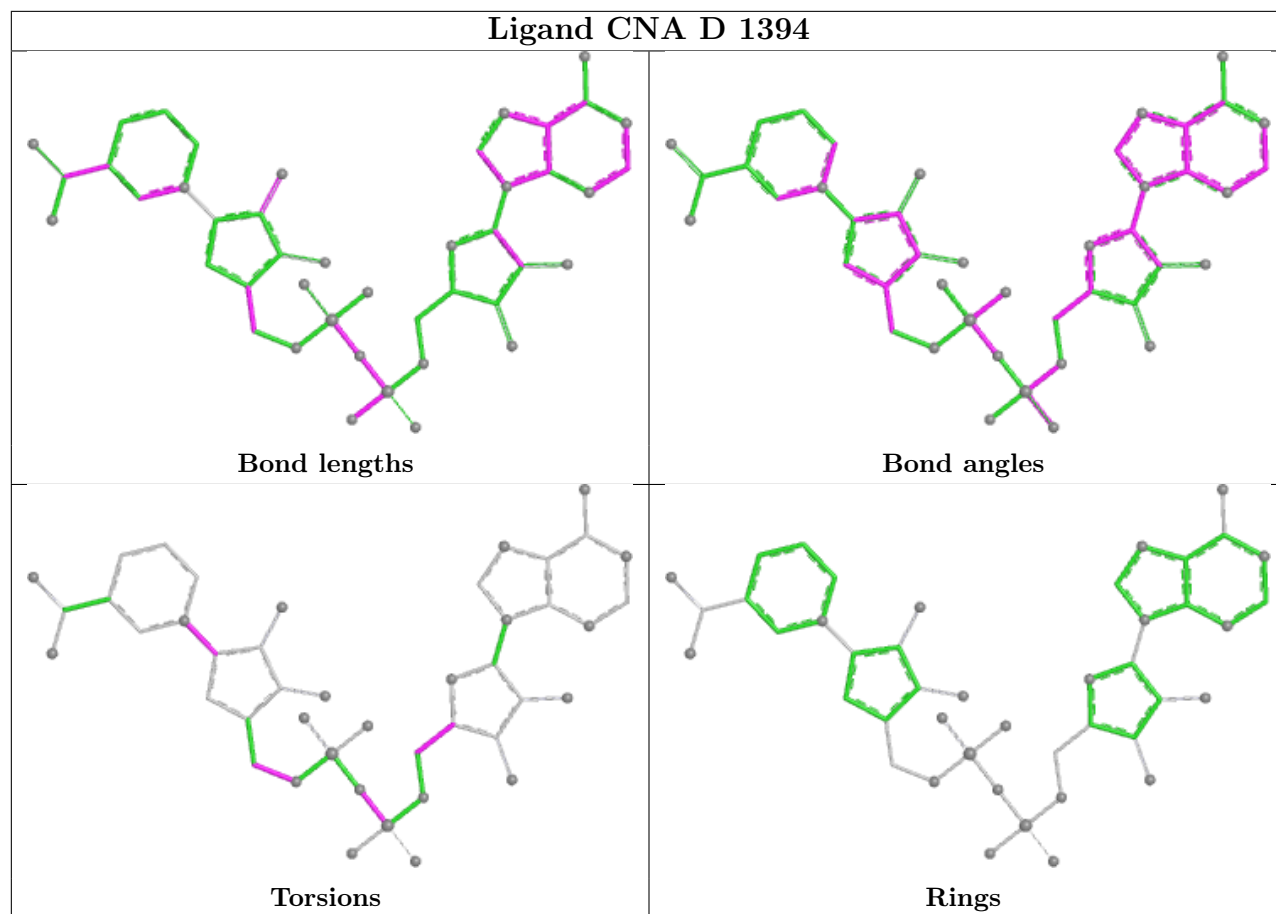
Rings

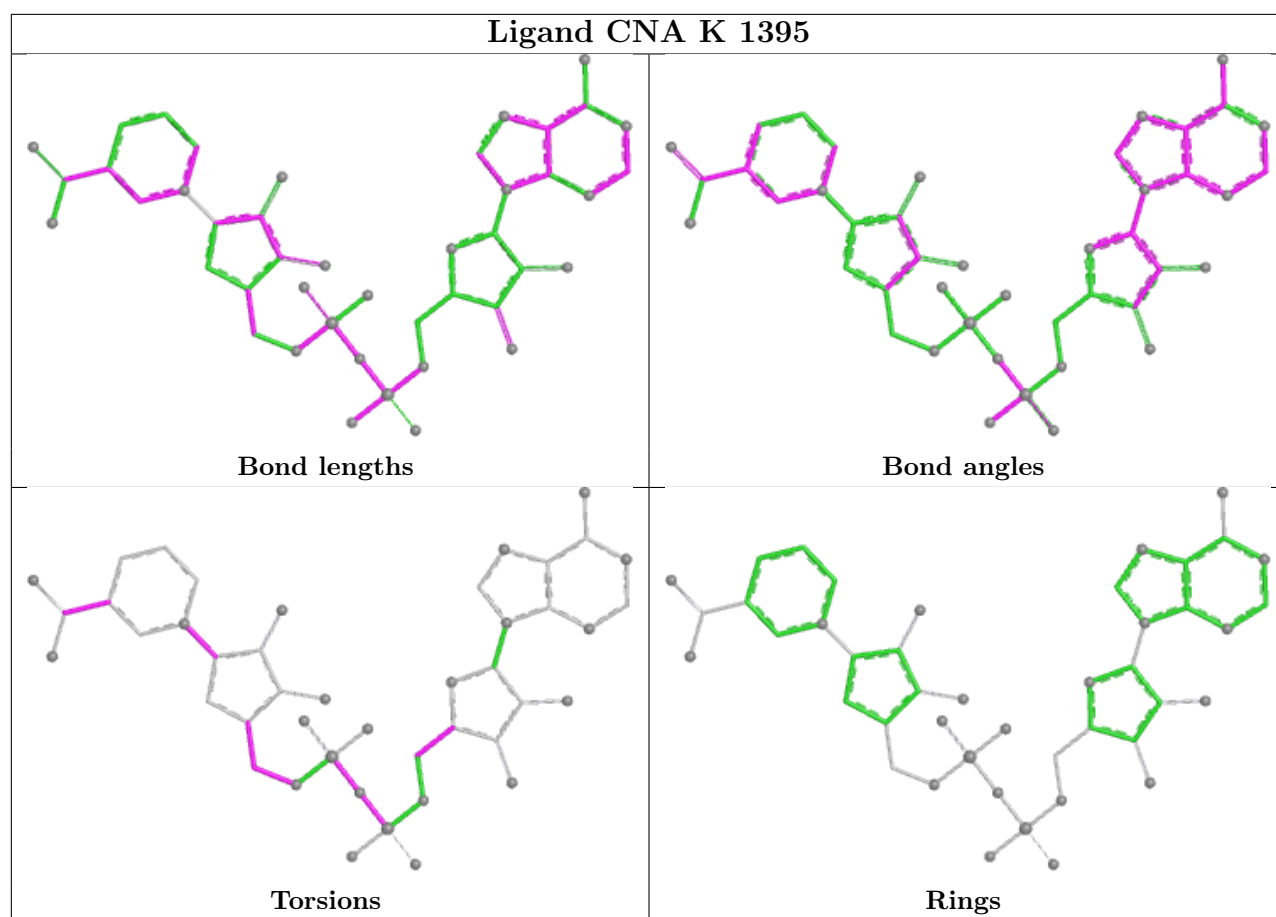


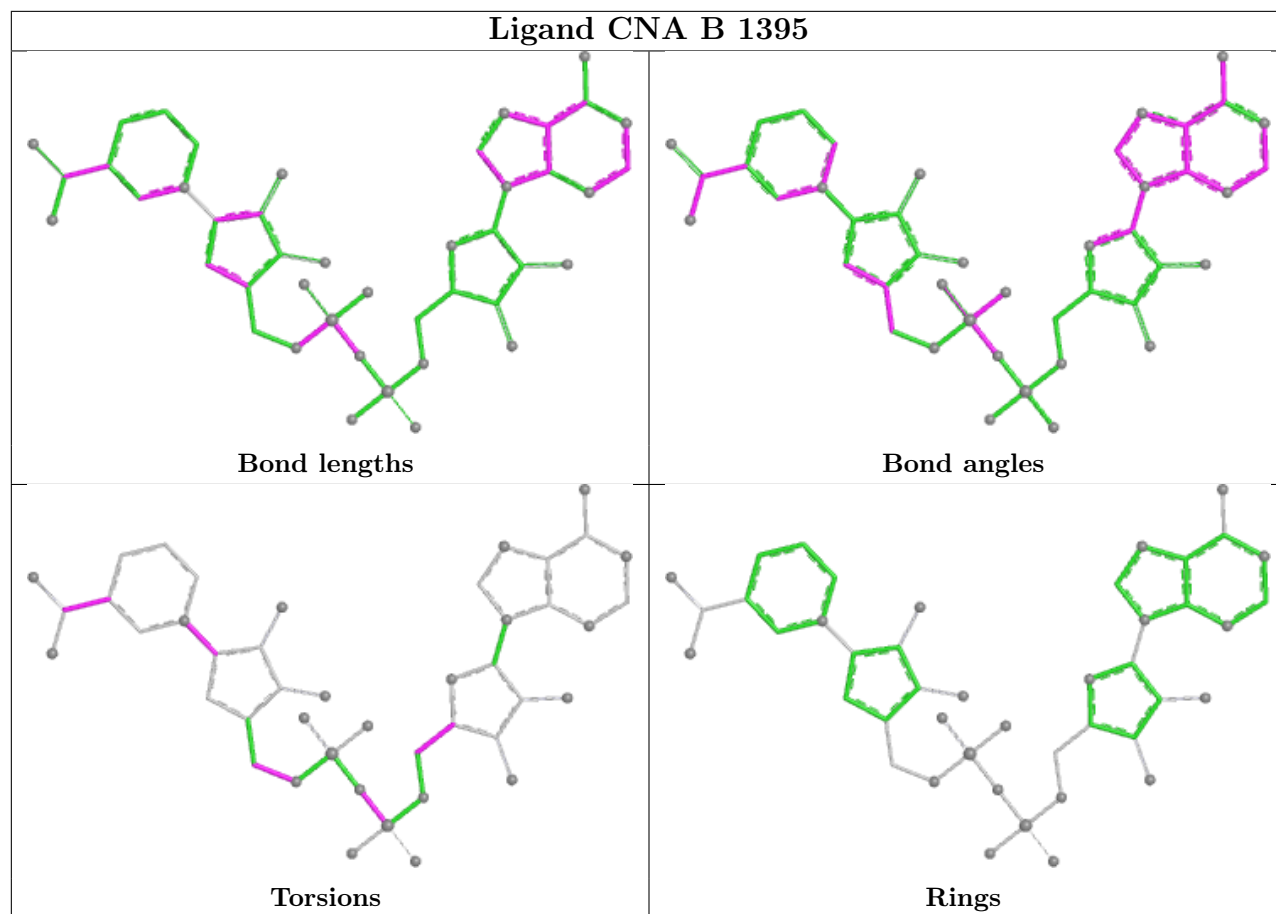


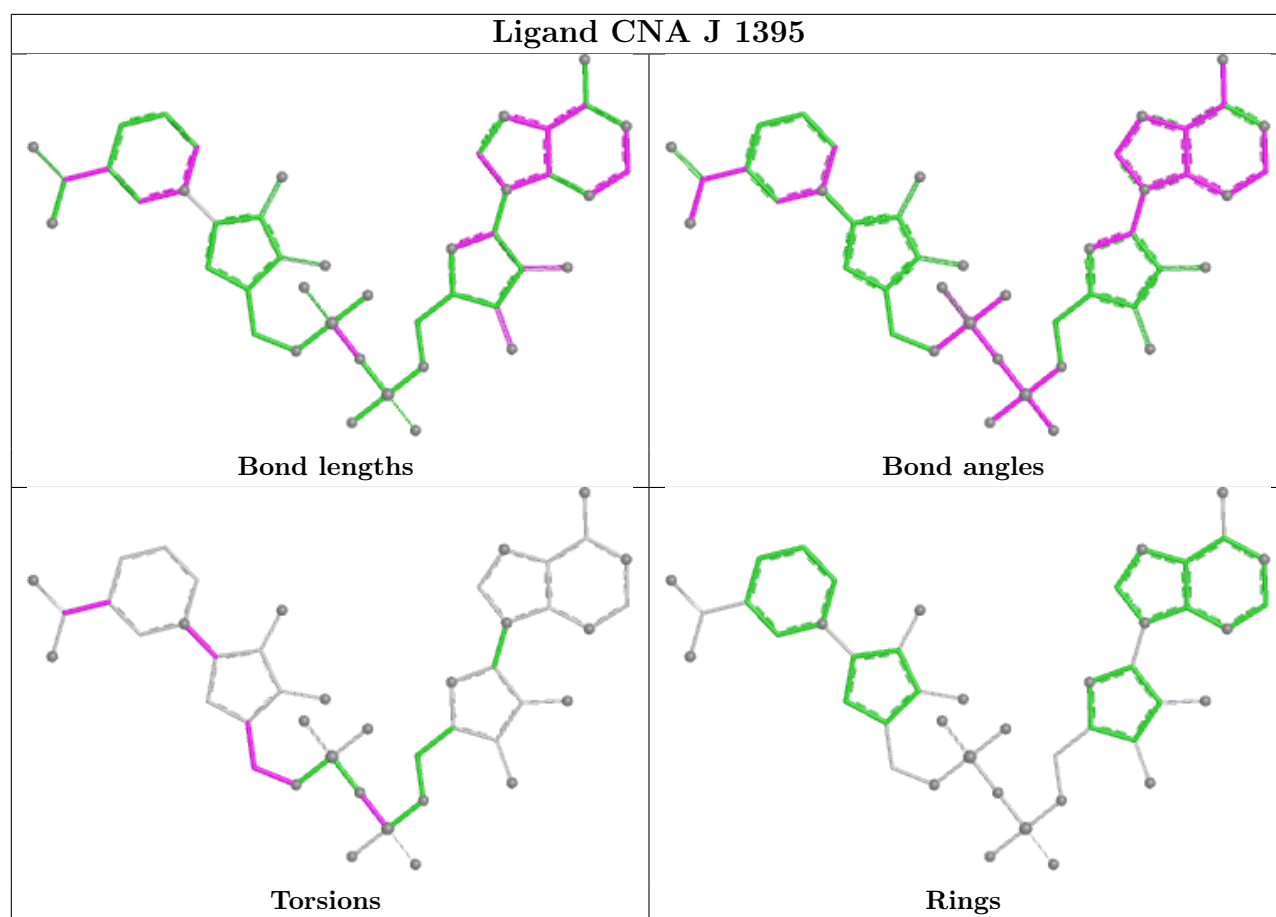


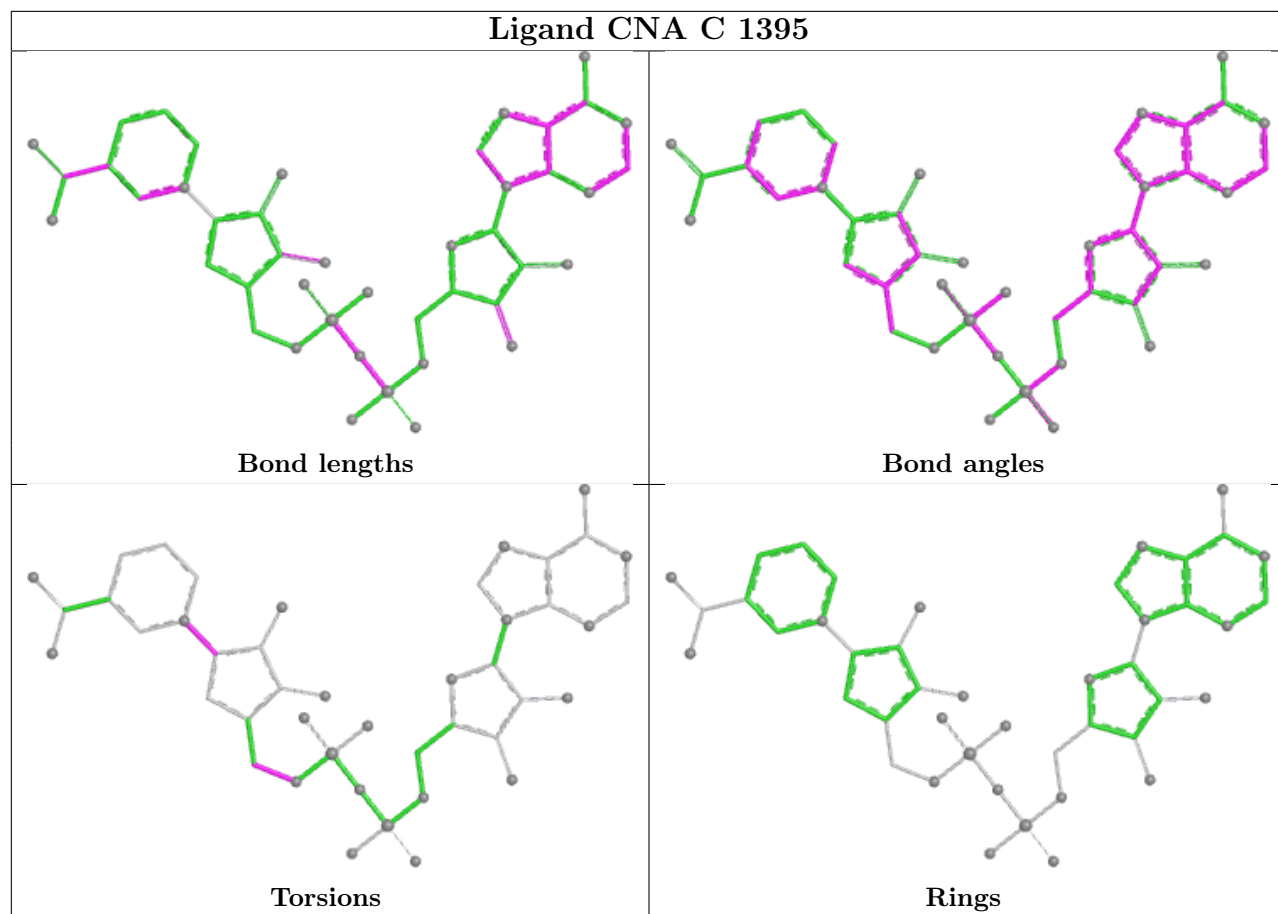


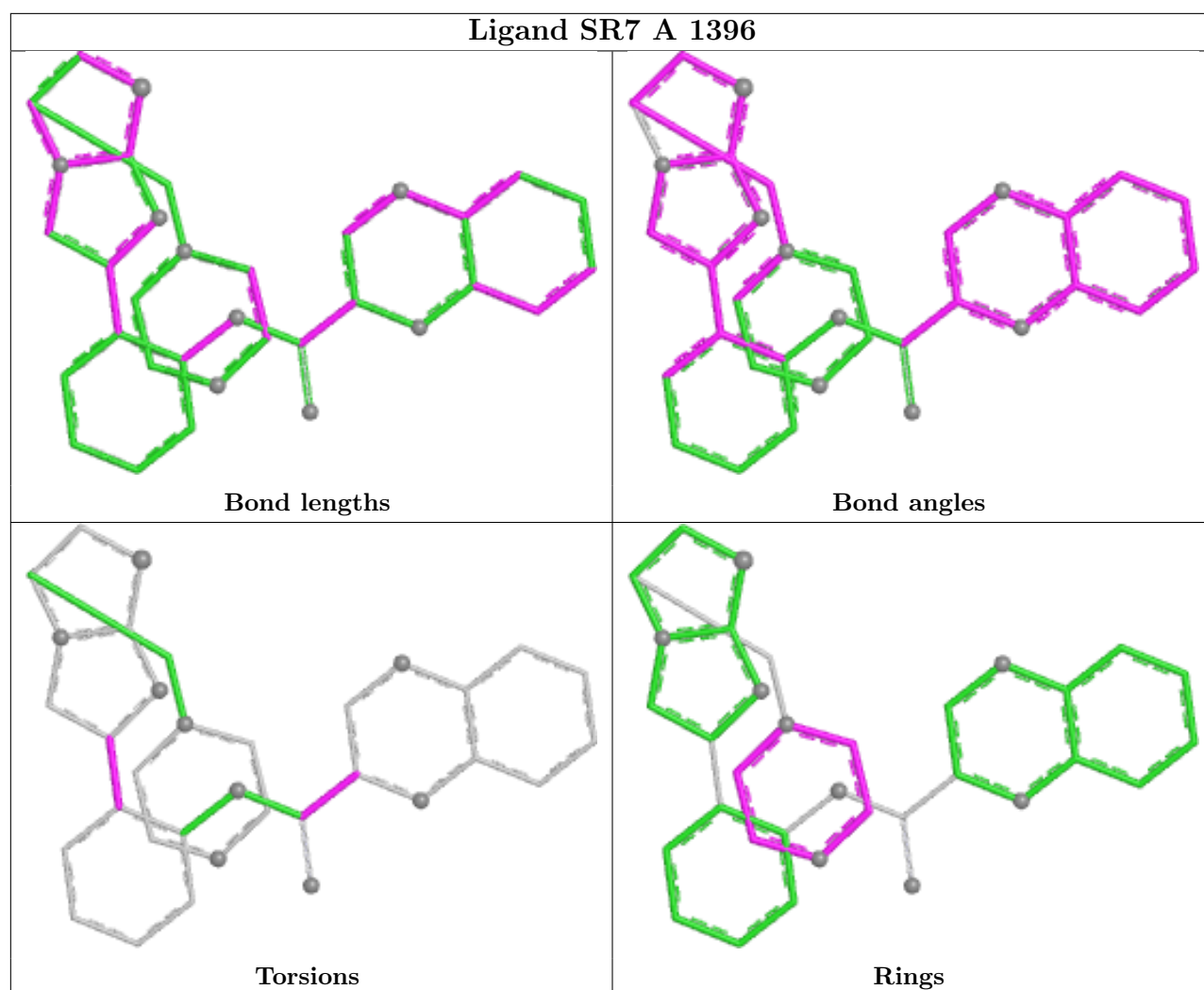


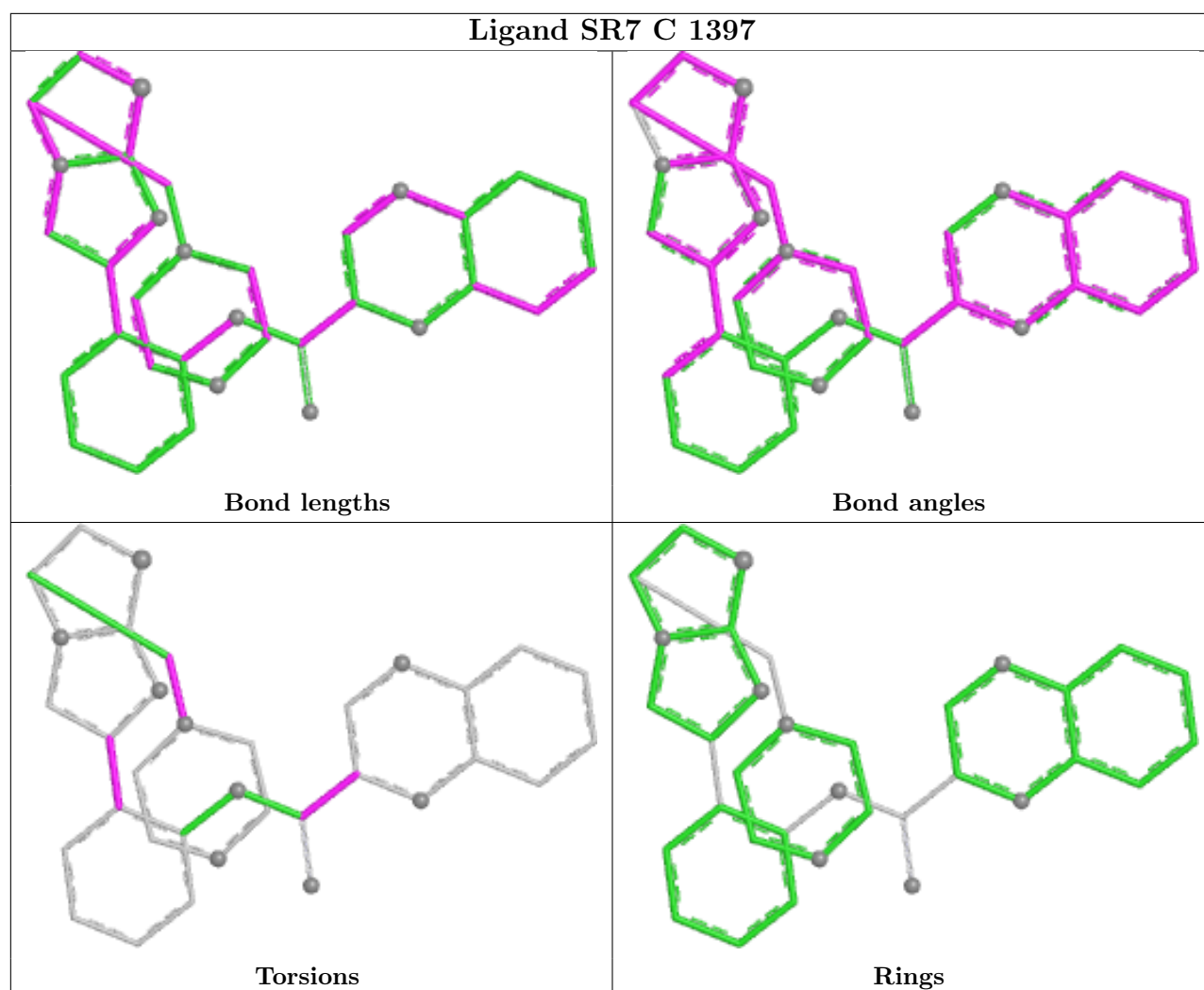


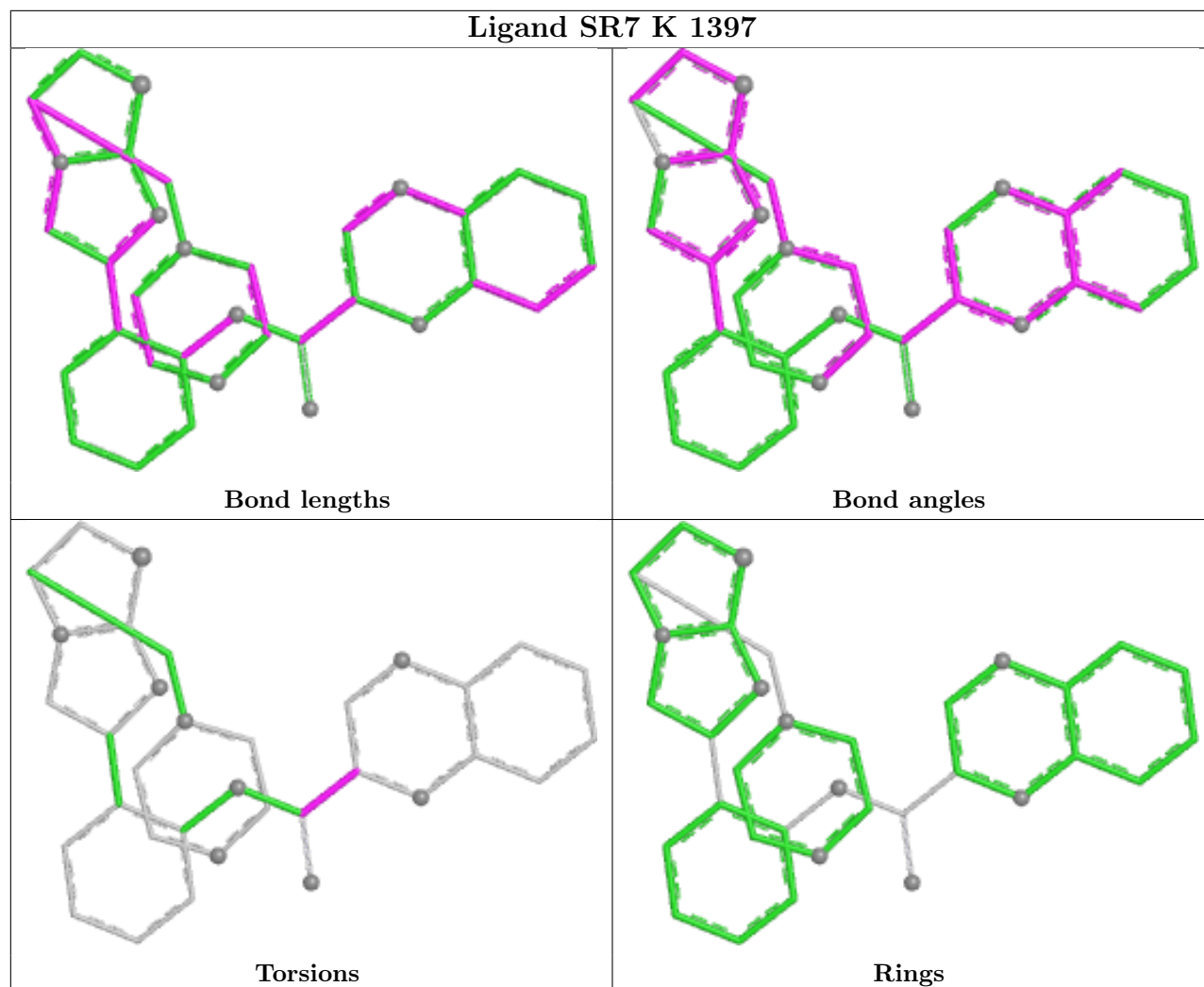


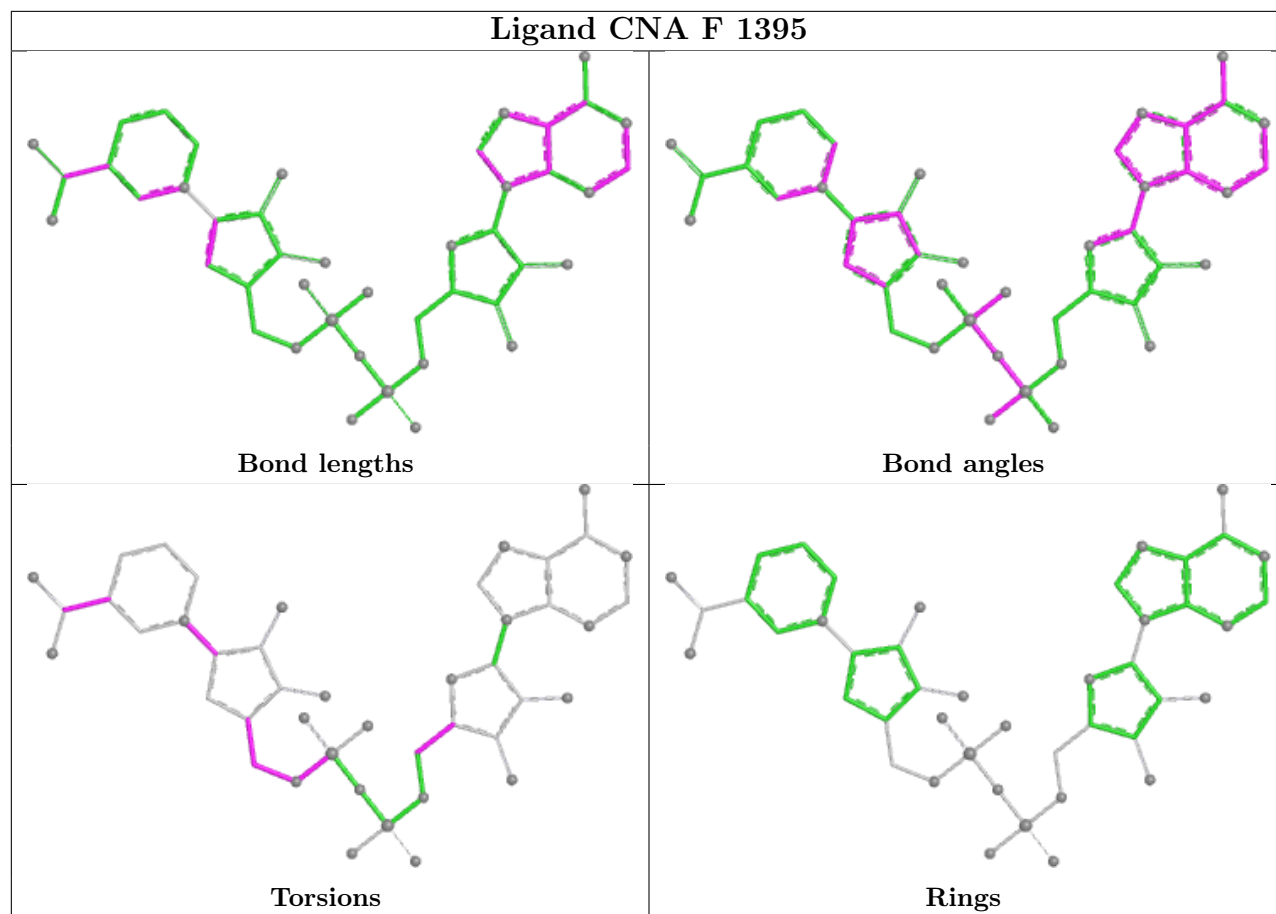


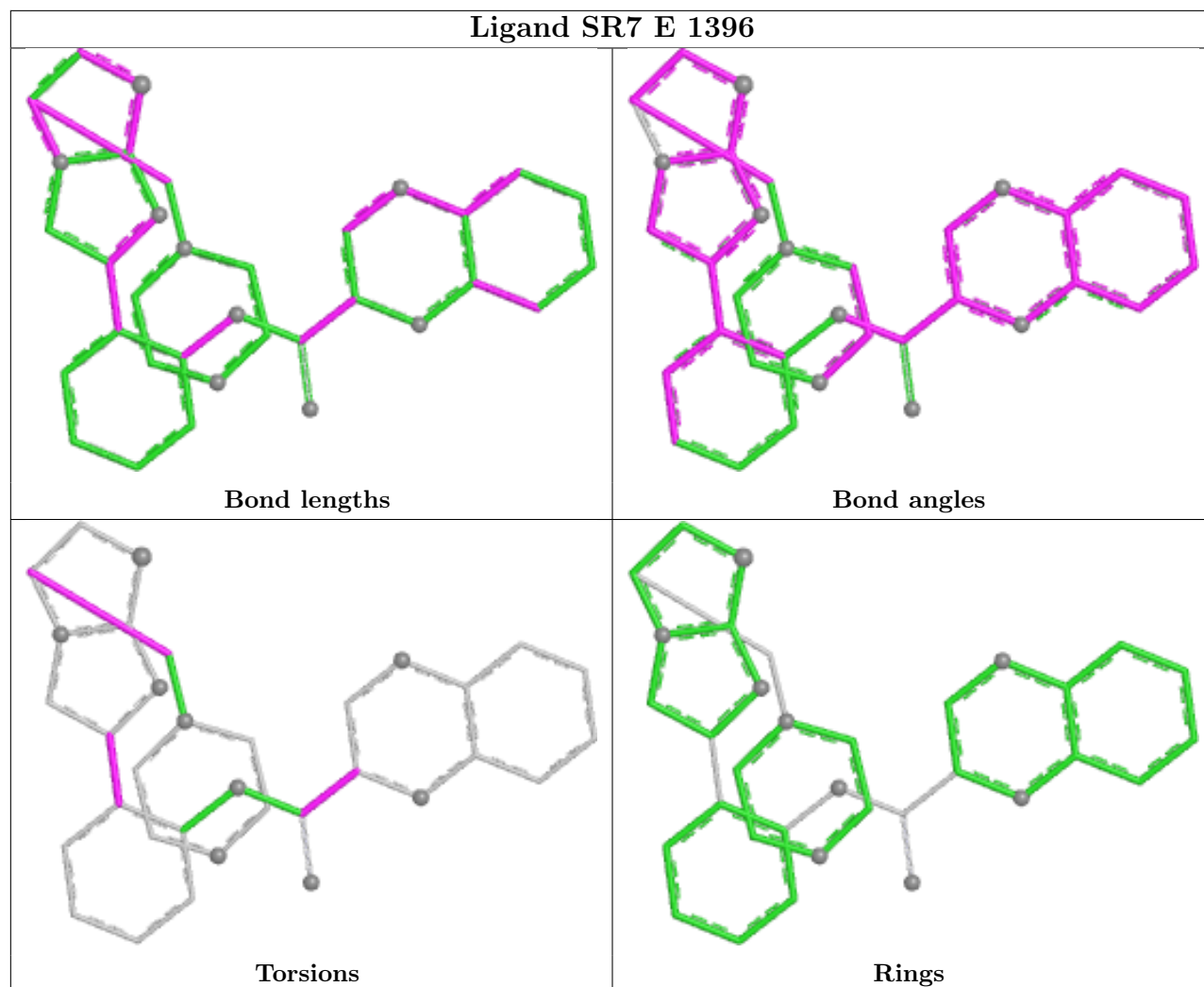


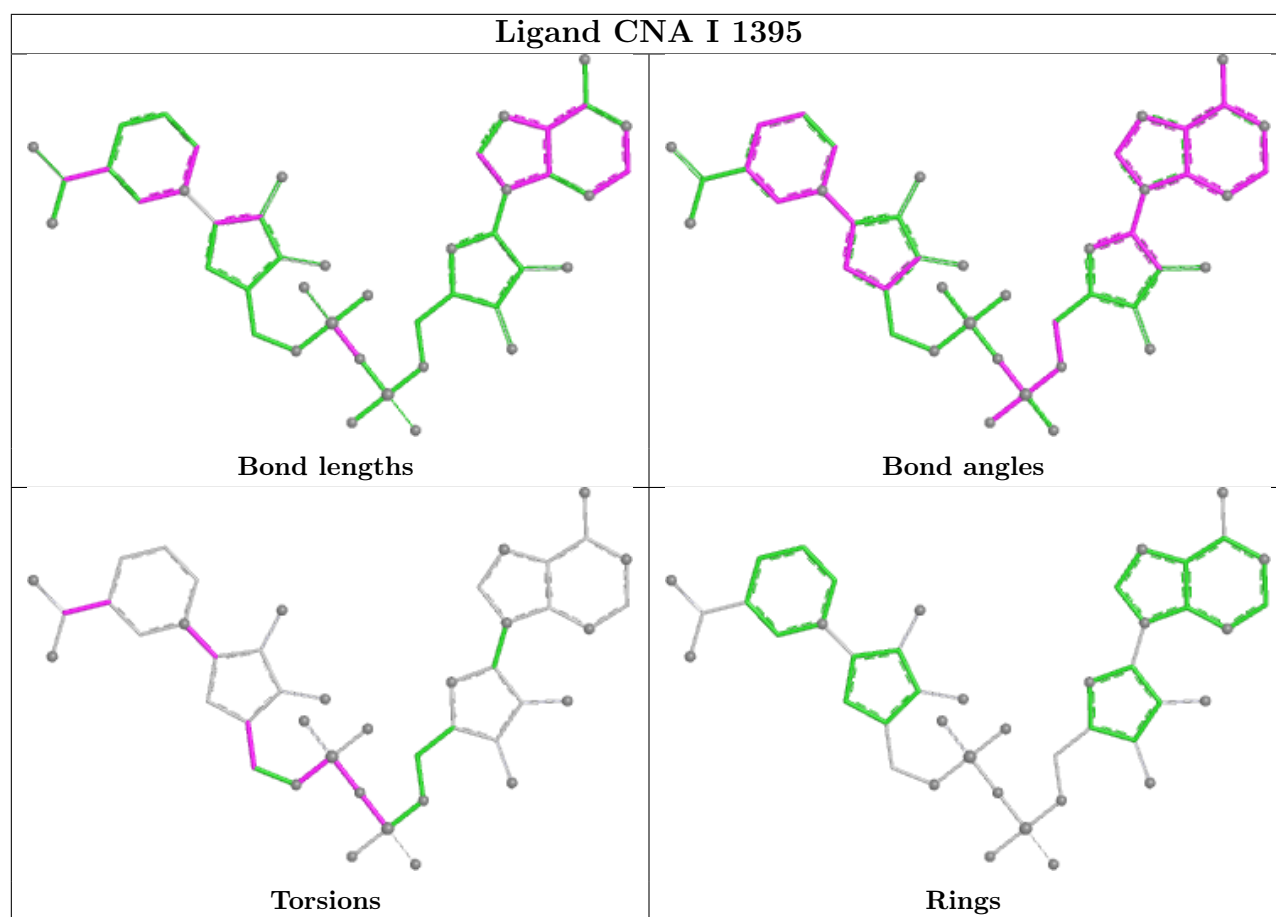


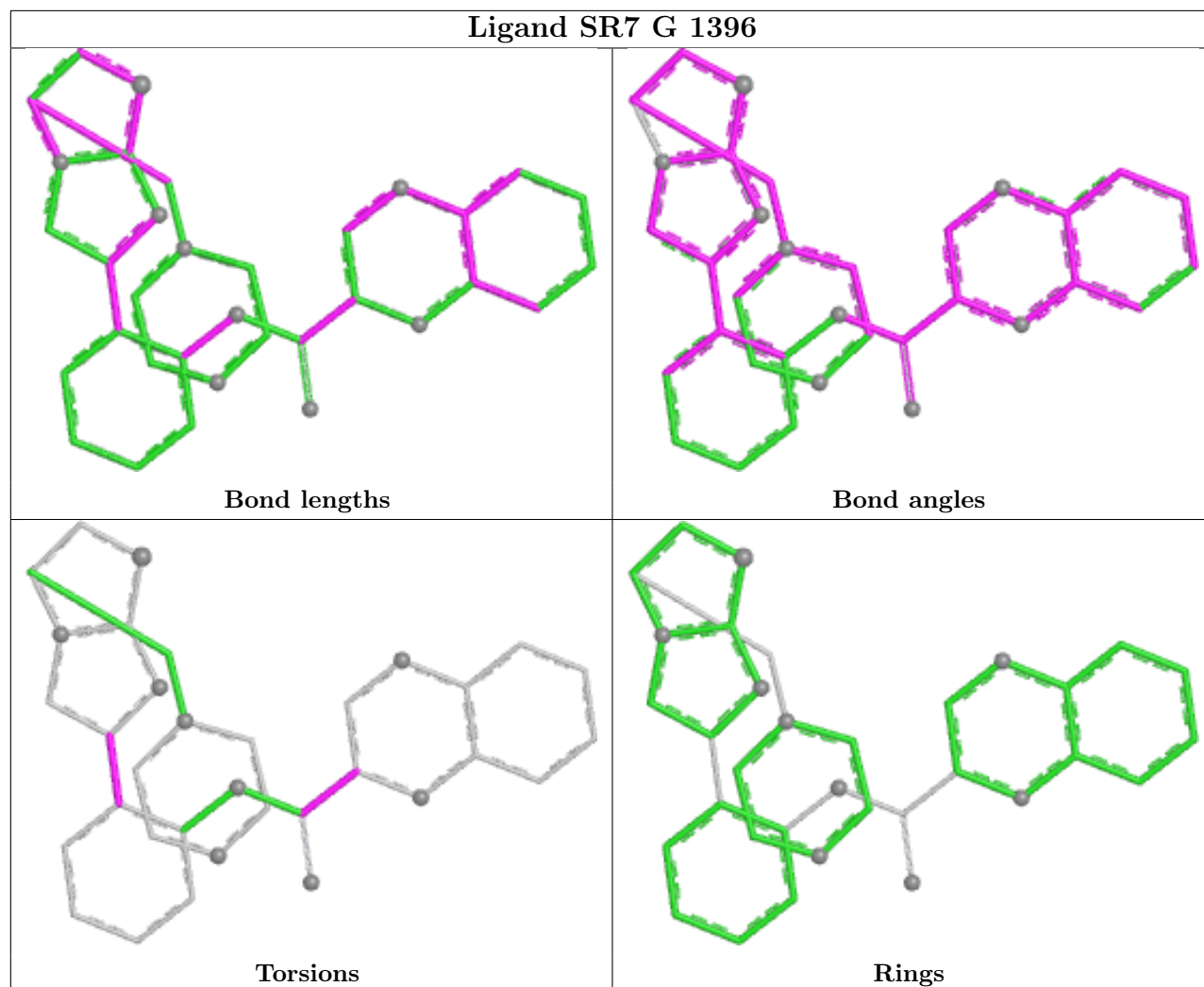


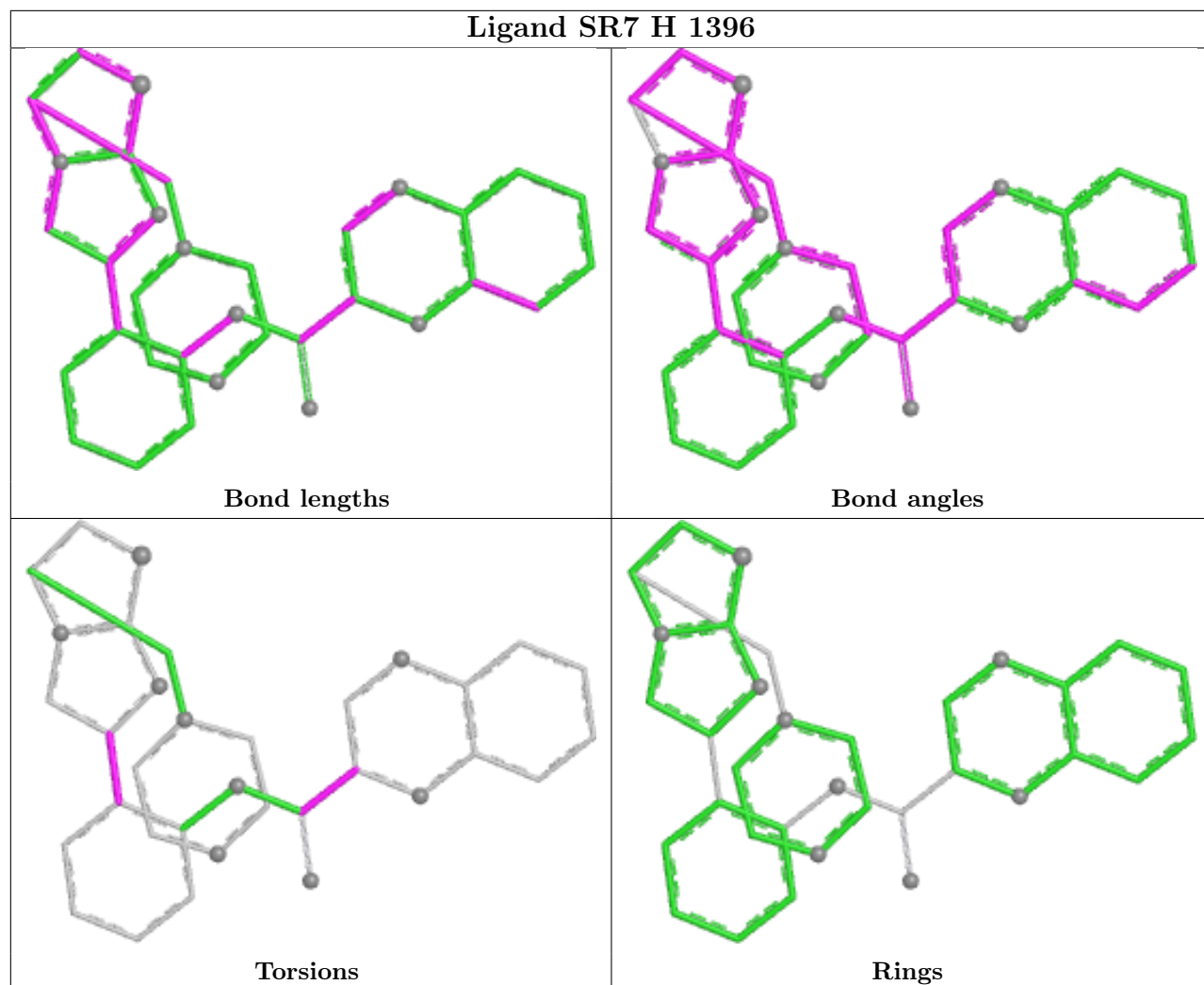




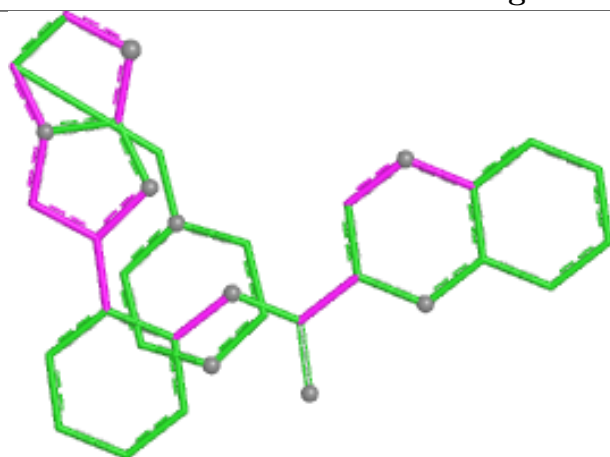




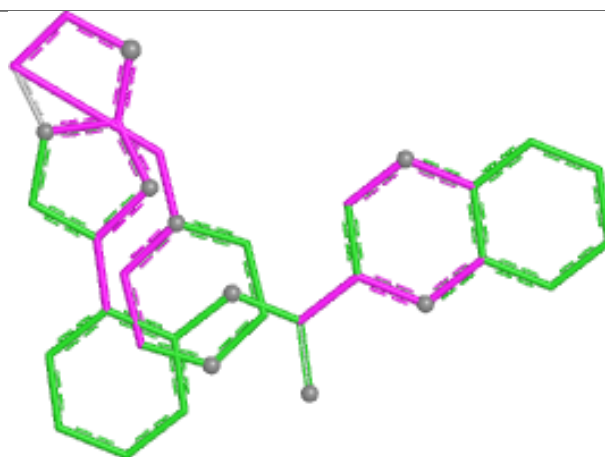




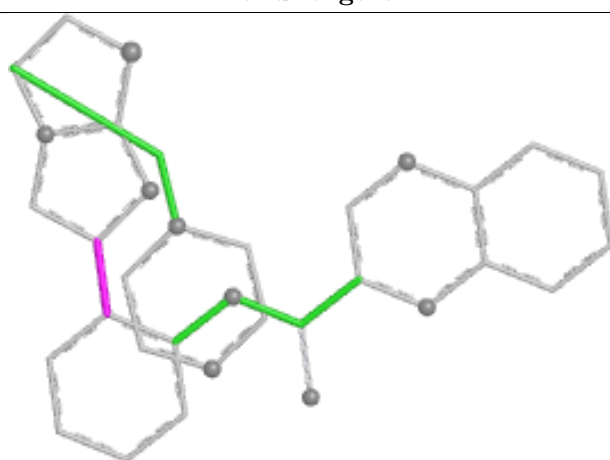
Ligand SR7 D 1396



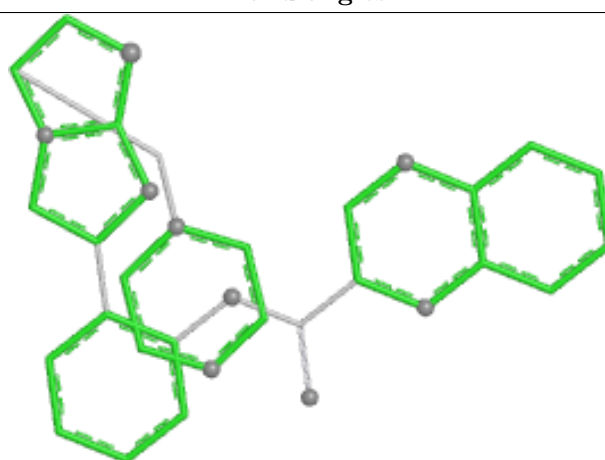
Bond lengths



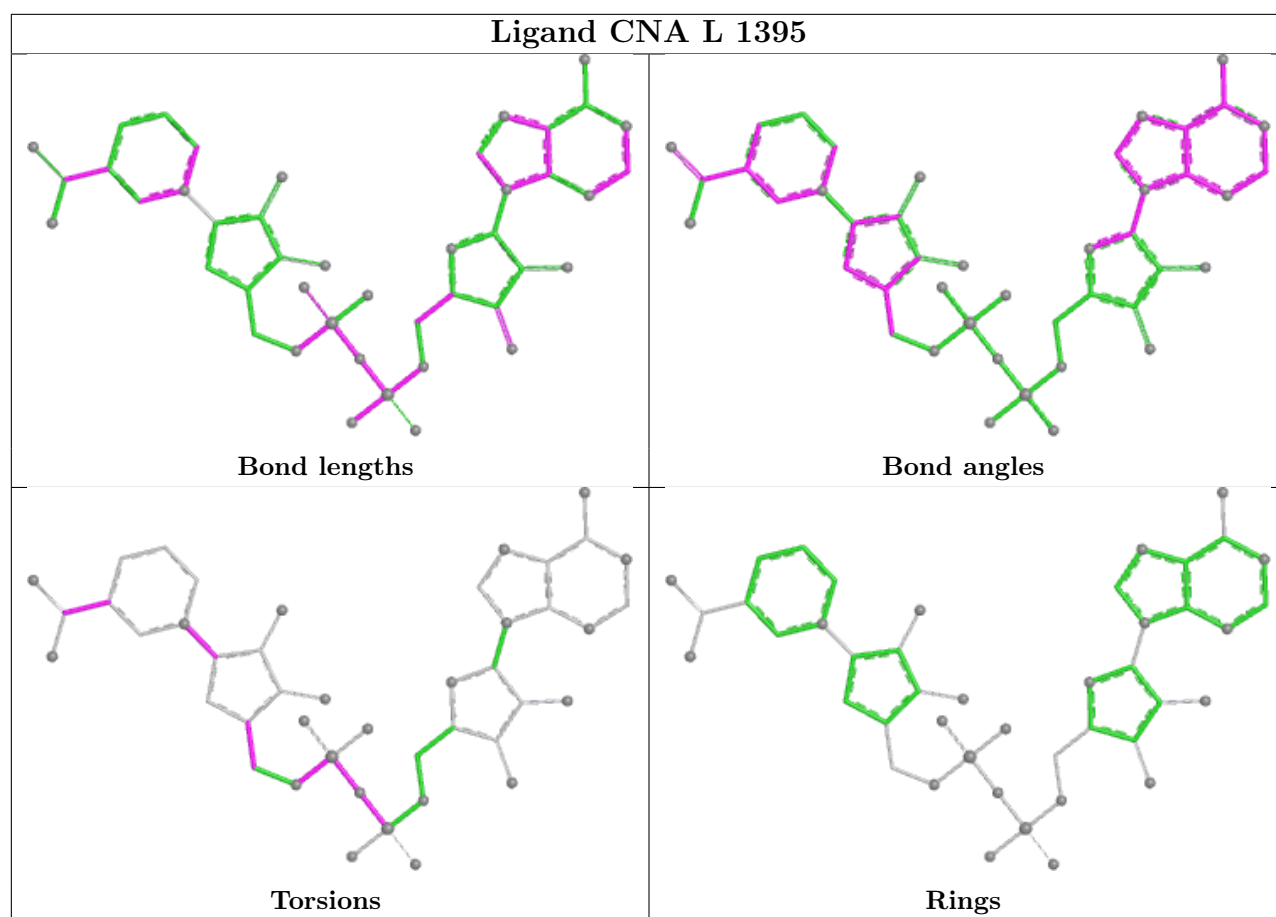
Bond angles



Torsions



Rings



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(Å²)	Q<0.9
1	A	273/281 (97%)	-1.31	0	100	100	56, 84, 116, 135	0
1	B	273/281 (97%)	-1.35	0	100	100	56, 81, 114, 133	0
1	C	273/281 (97%)	-1.18	0	100	100	62, 96, 131, 153	0
1	D	272/281 (96%)	-1.04	0	100	100	64, 98, 132, 144	0
1	E	273/281 (97%)	-1.46	0	100	100	64, 87, 112, 123	0
1	F	273/281 (97%)	-1.38	0	100	100	69, 92, 125, 139	0
1	G	273/281 (97%)	-1.49	0	100	100	66, 87, 110, 124	0
1	H	273/281 (97%)	-1.26	0	100	100	75, 101, 127, 141	0
1	I	273/281 (97%)	-1.27	0	100	100	73, 99, 127, 138	0
1	J	273/281 (97%)	-1.39	0	100	100	68, 91, 123, 136	0
1	K	273/281 (97%)	-0.55	2 (0%)	84	70	101, 132, 166, 177	0
1	L	273/281 (97%)	-0.54	1 (0%)	88	78	101, 132, 168, 182	0
All	All	3275/3372 (97%)	-1.19	3 (0%)	92	90	56, 96, 145, 182	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	174	PRO	3.3
1	L	160	PRO	2.8
1	K	160	PRO	2.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	CNA	K	1395	44/44	0.98	0.04	86,86,86,86	0
2	CNA	D	1394	44/44	0.99	0.04	86,86,86,86	0
2	CNA	F	1395	44/44	0.99	0.03	86,86,86,86	0
2	CNA	G	1395	44/44	0.99	0.03	86,86,86,86	0
2	CNA	H	1395	44/44	0.99	0.03	86,86,86,86	0
2	CNA	I	1395	44/44	0.99	0.03	86,86,86,86	0
2	CNA	J	1395	44/44	0.99	0.04	86,86,86,86	0
2	CNA	C	1395	44/44	0.99	0.04	86,86,86,86	0
2	CNA	L	1395	44/44	0.99	0.04	86,86,86,86	0
3	SR7	C	1397	34/34	0.99	0.05	86,86,86,86	0
3	SR7	D	1396	34/34	0.99	0.05	86,86,86,86	0
3	SR7	F	1396	34/34	0.99	0.04	86,86,86,86	0
3	SR7	G	1396	34/34	0.99	0.04	86,86,86,86	0
3	SR7	H	1396	34/34	0.99	0.05	86,86,86,86	0
3	SR7	I	1396	34/34	0.99	0.04	86,86,86,86	0
3	SR7	J	1396	34/34	0.99	0.04	86,86,86,86	0
3	SR7	K	1397	34/34	0.99	0.05	86,86,86,86	0
3	SR7	L	1397	34/34	0.99	0.05	86,86,86,86	0
5	GOL	C	1396	6/6	0.99	0.07	86,86,86,86	0
5	GOL	K	1396	6/6	0.99	0.09	86,86,86,86	0
5	GOL	L	1396	6/6	0.99	0.08	86,86,86,86	0
2	CNA	E	1395	44/44	1.00	0.03	86,86,86,86	0
3	SR7	E	1396	34/34	1.00	0.04	86,86,86,86	0
2	CNA	A	1395	44/44	1.00	0.03	86,86,86,86	0
4	ZN	A	1397	1/1	1.00	0.02	86,86,86,86	0
4	ZN	B	1397	1/1	1.00	0.02	86,86,86,86	0
4	ZN	C	1398	1/1	1.00	0.02	86,86,86,86	0
4	ZN	D	1397	1/1	1.00	0.02	86,86,86,86	0
4	ZN	E	1397	1/1	1.00	0.01	86,86,86,86	0
4	ZN	F	1397	1/1	1.00	0.01	86,86,86,86	0
4	ZN	G	1397	1/1	1.00	0.00	86,86,86,86	0
4	ZN	H	1397	1/1	1.00	0.01	86,86,86,86	0

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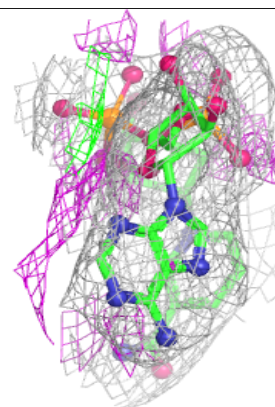
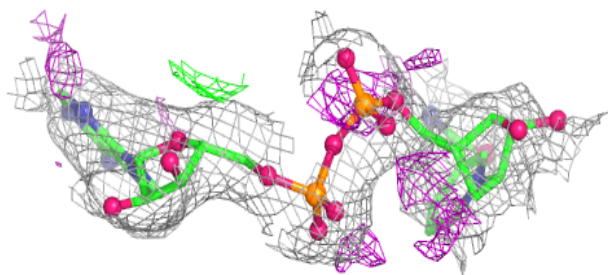
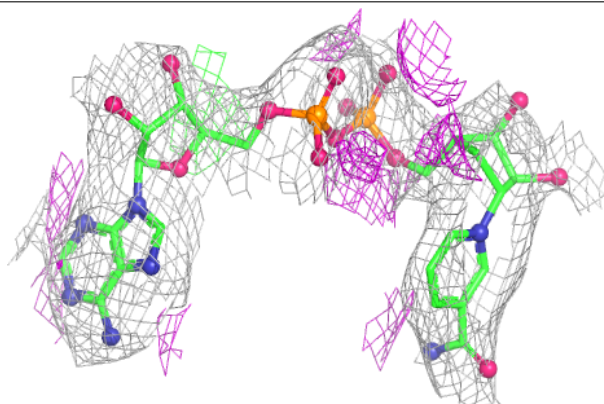
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	I	1397	1/1	1.00	0.02	86,86,86,86	0
4	ZN	J	1397	1/1	1.00	0.01	86,86,86,86	0
4	ZN	K	1398	1/1	1.00	0.02	86,86,86,86	0
4	ZN	L	1398	1/1	1.00	0.02	86,86,86,86	0
3	SR7	A	1396	34/34	1.00	0.04	86,86,86,86	0
5	GOL	D	1395	6/6	1.00	0.06	86,86,86,86	0
3	SR7	B	1396	34/34	1.00	0.04	86,86,86,86	0
2	CNA	B	1395	44/44	1.00	0.03	86,86,86,86	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.

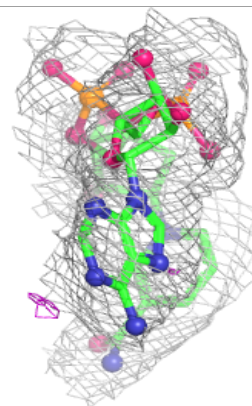
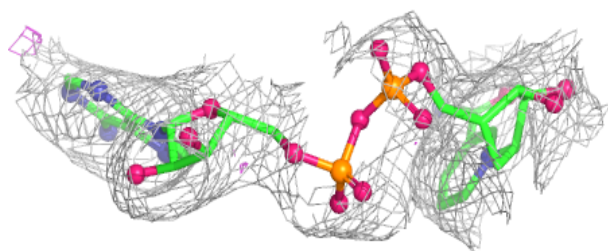
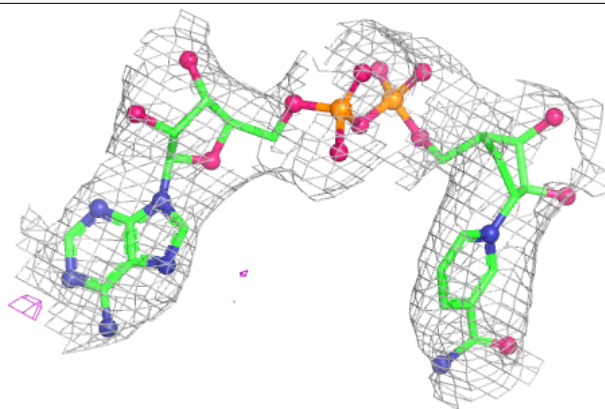
Electron density around CNA K 1395:

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

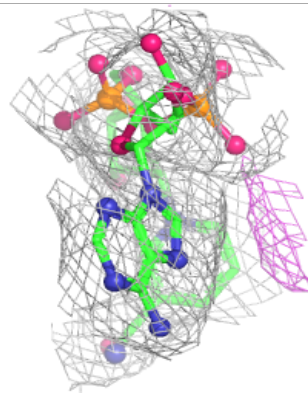
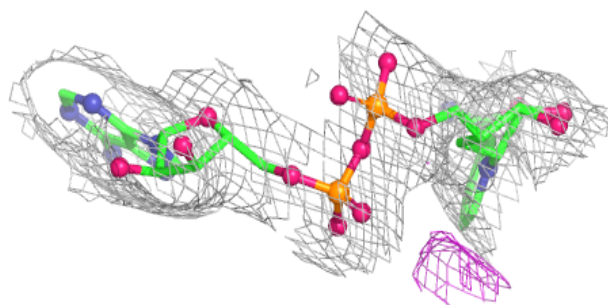
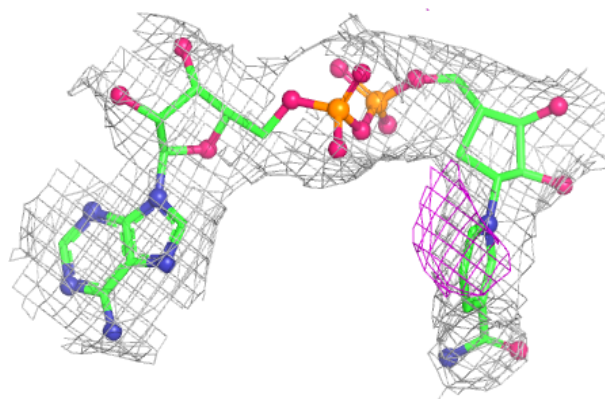


Electron density around CNA D 1394:

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

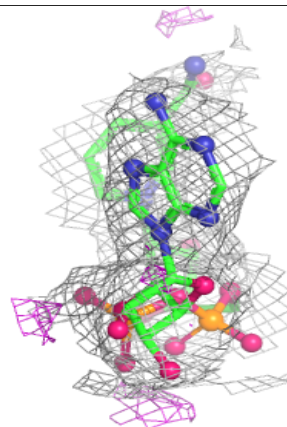
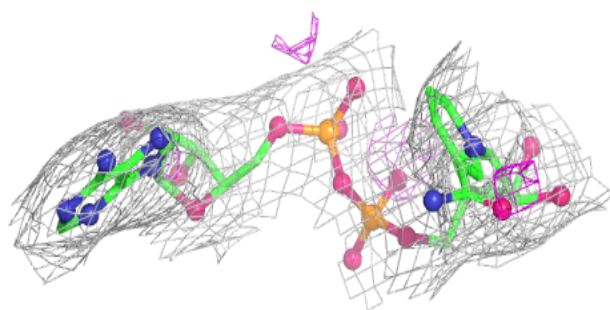
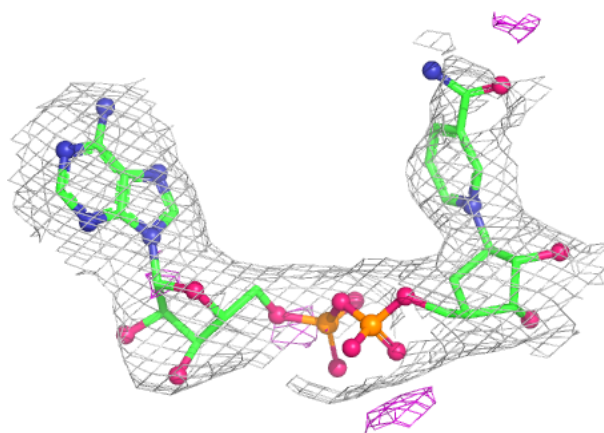
**Electron density around CNA F 1395:**

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

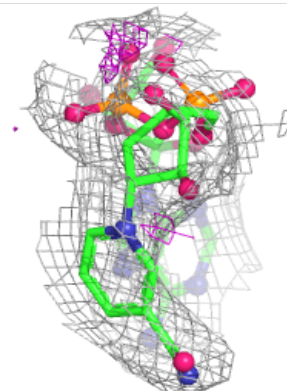
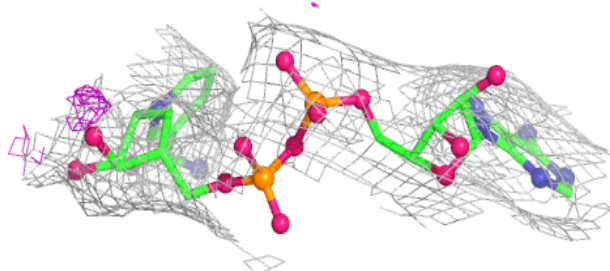
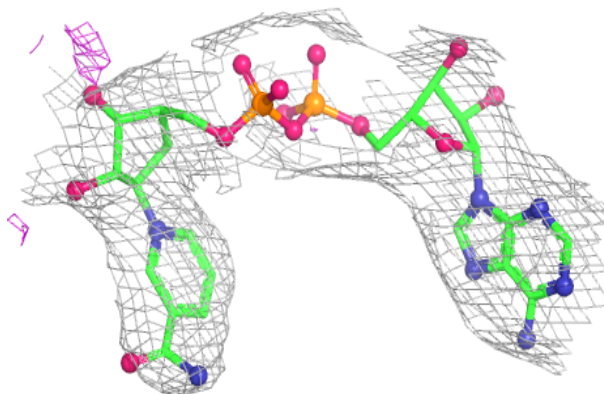


Electron density around CNA G 1395:

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

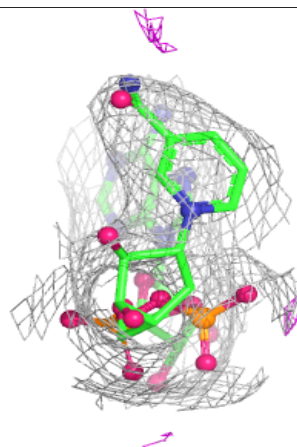
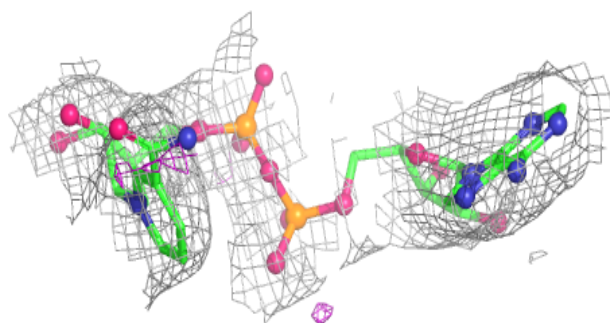
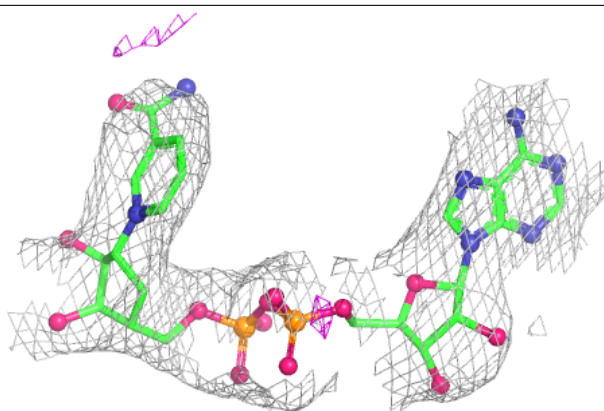
**Electron density around CNA H 1395:**

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

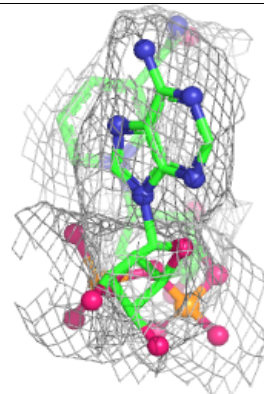
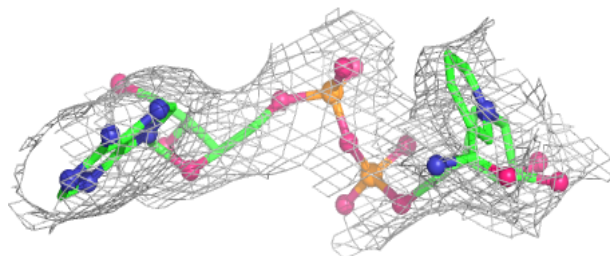
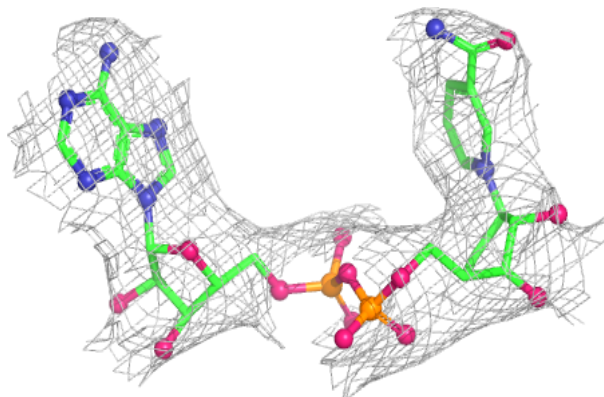


Electron density around CNA I 1395:

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

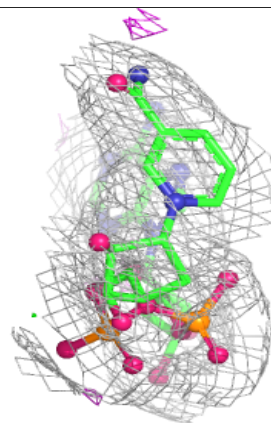
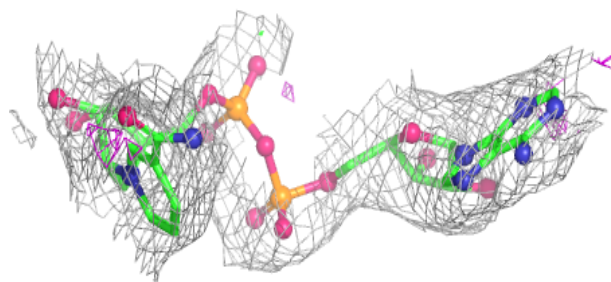
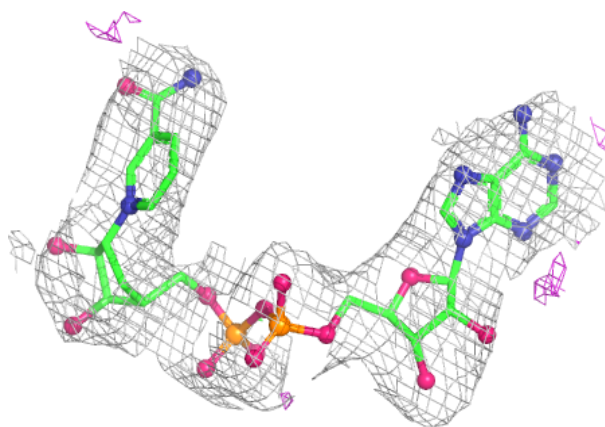
**Electron density around CNA J 1395:**

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



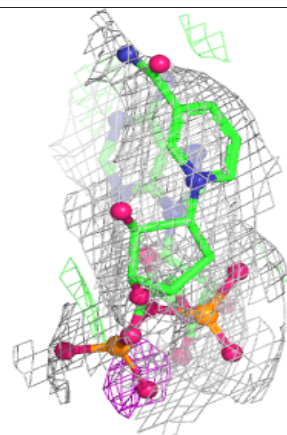
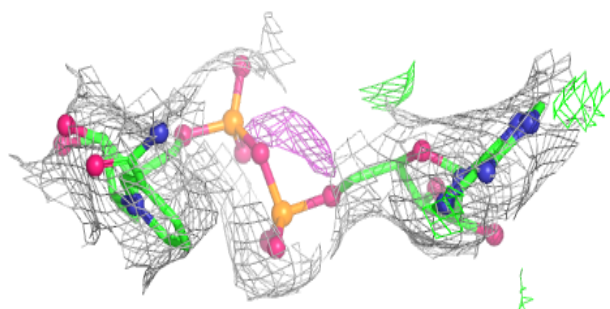
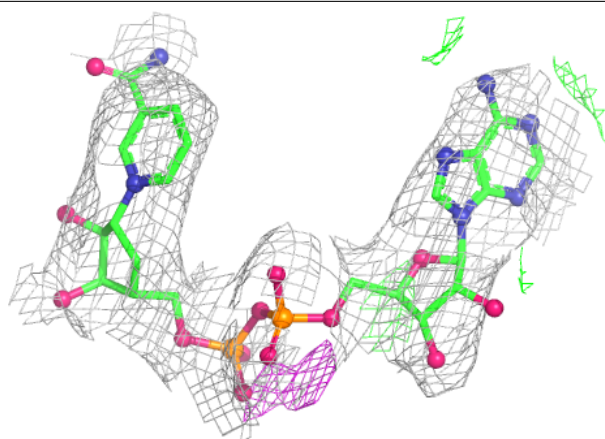
Electron density around CNA C 1395:

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

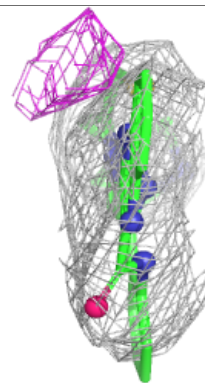
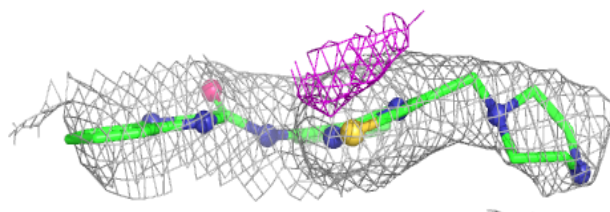
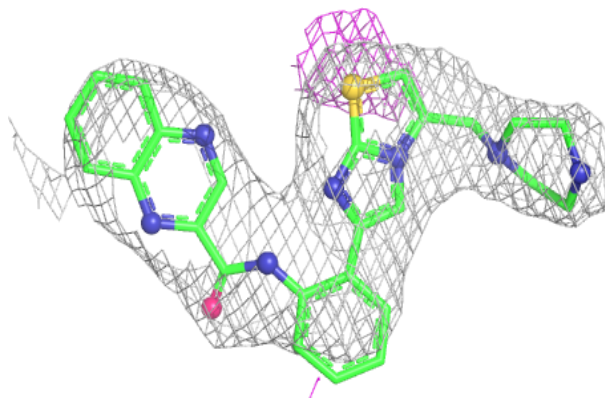


Electron density around CNA L 1395:

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

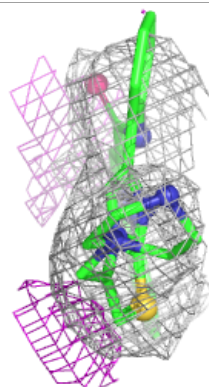
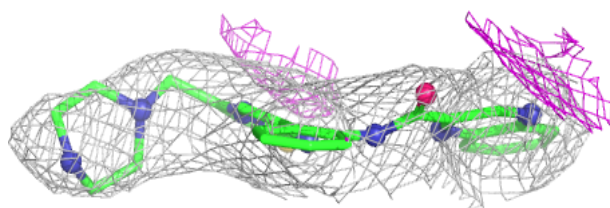
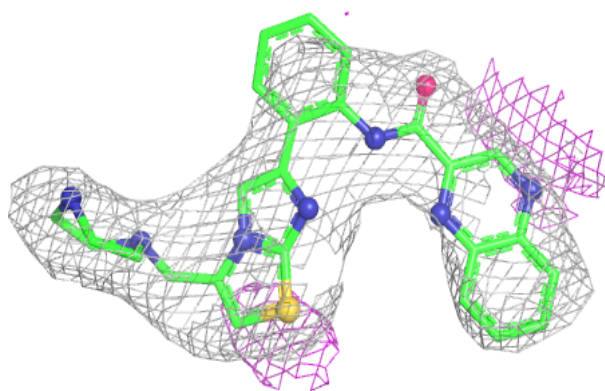
**Electron density around SR7 C 1397:**

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

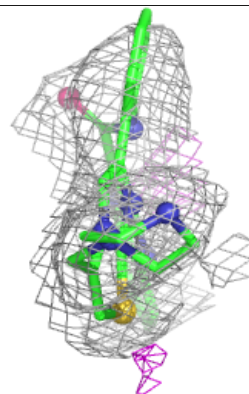
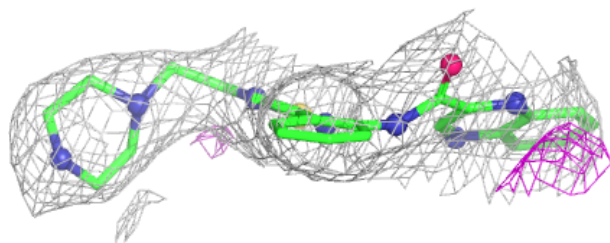
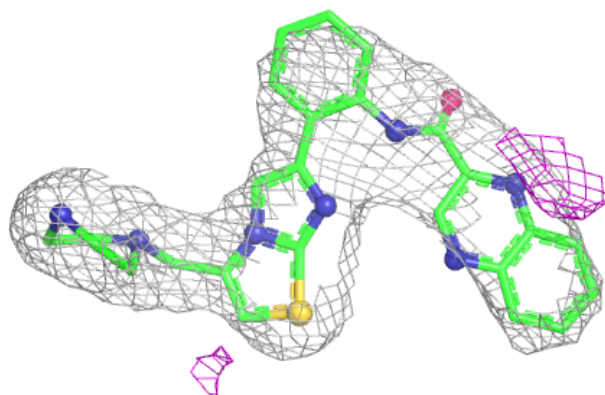


Electron density around SR7 D 1396:

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

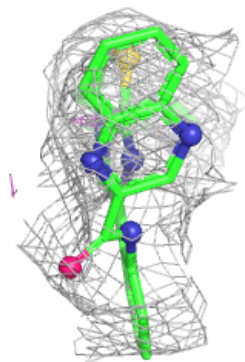
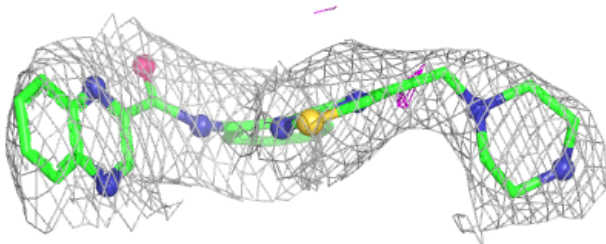
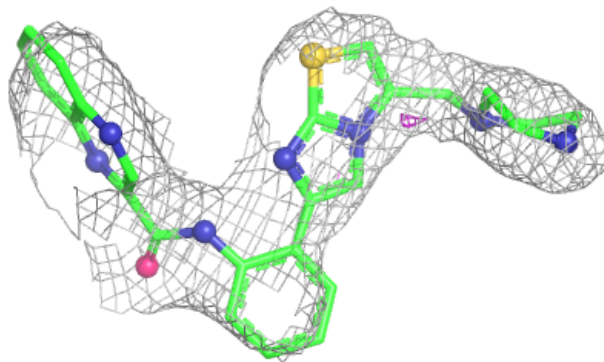
**Electron density around SR7 F 1396:**

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

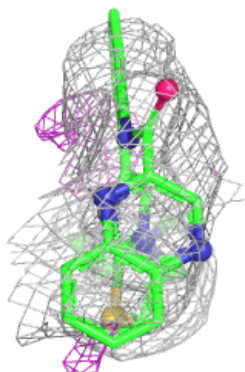
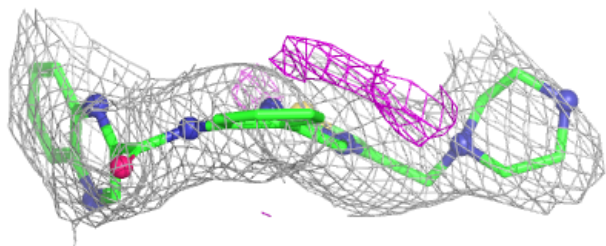
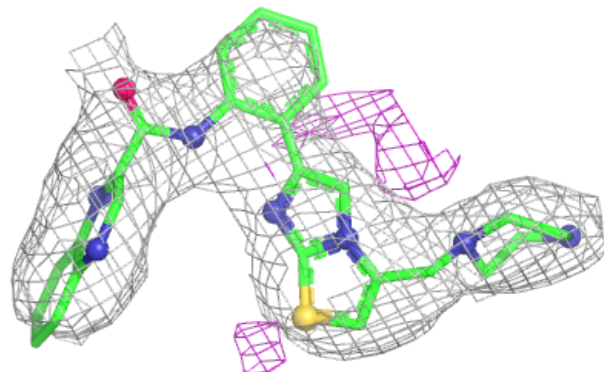


Electron density around SR7 G 1396:

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

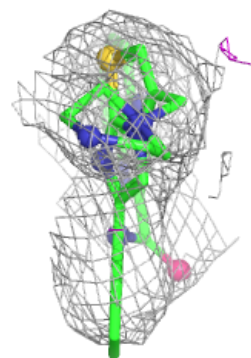
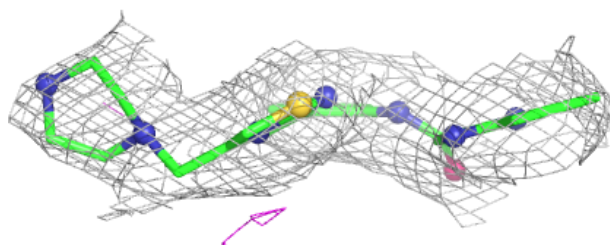
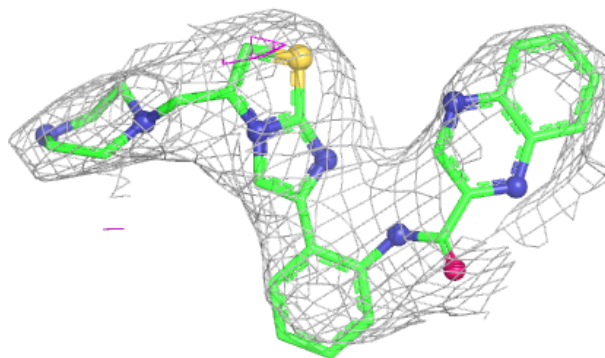
**Electron density around SR7 H 1396:**

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

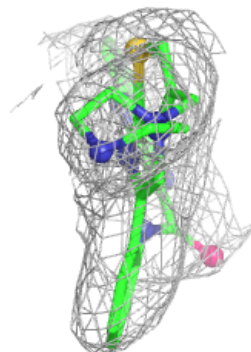
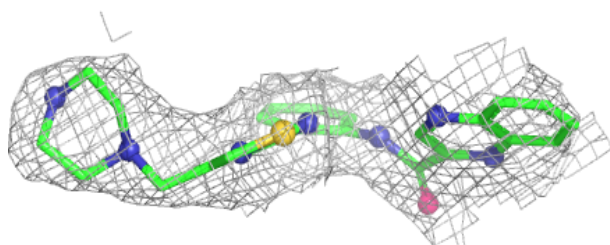
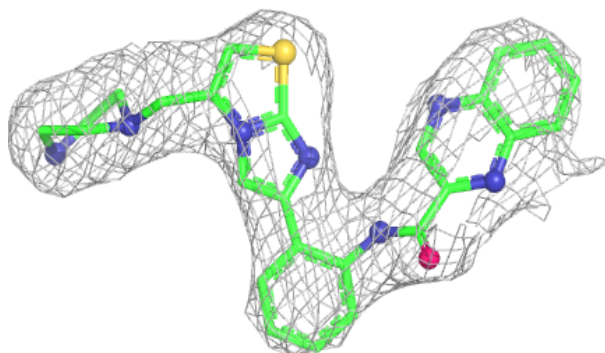


Electron density around SR7 I 1396:

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

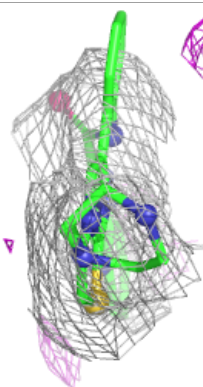
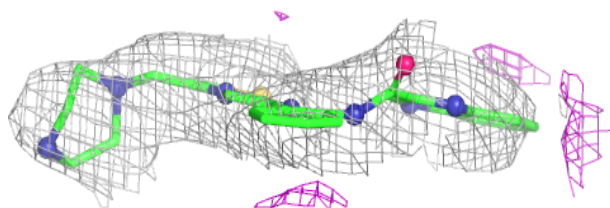
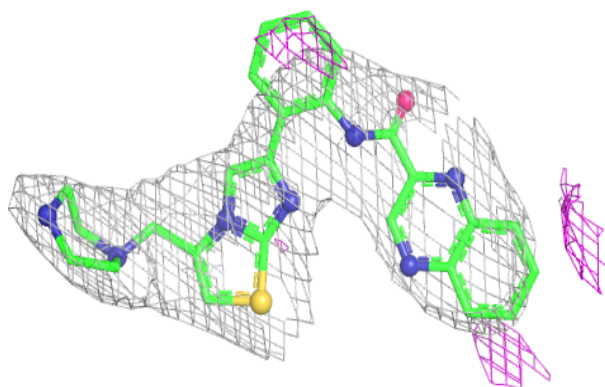
**Electron density around SR7 J 1396:**

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

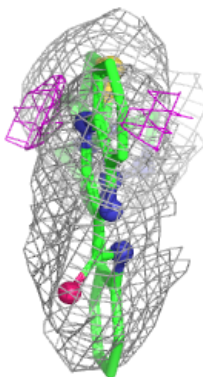
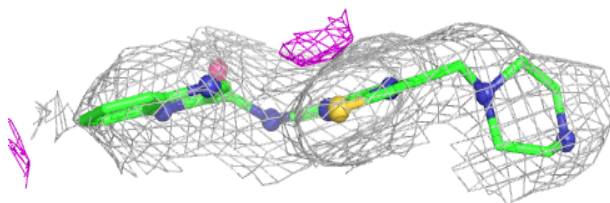
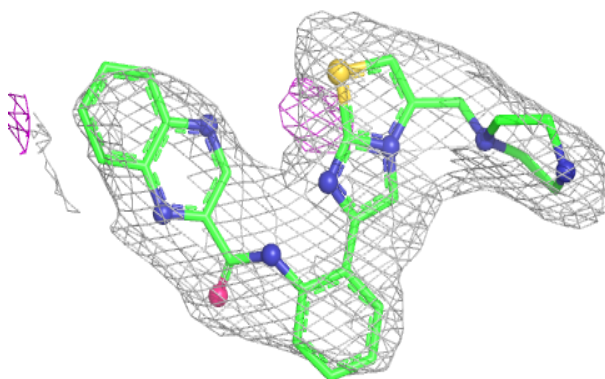


Electron density around SR7 K 1397:

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

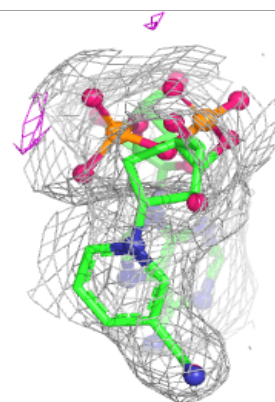
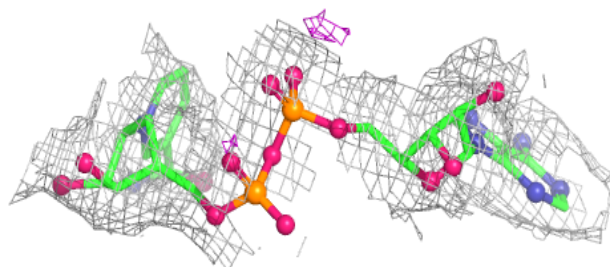
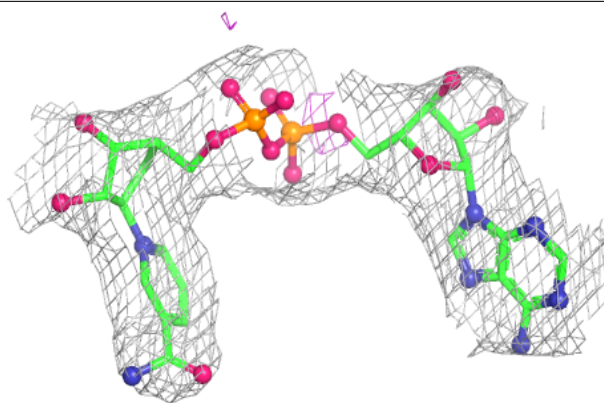
**Electron density around SR7 L 1397:**

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

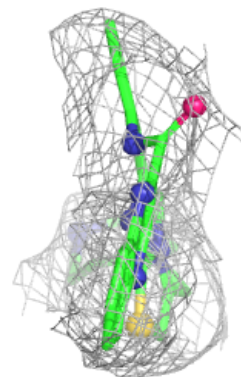
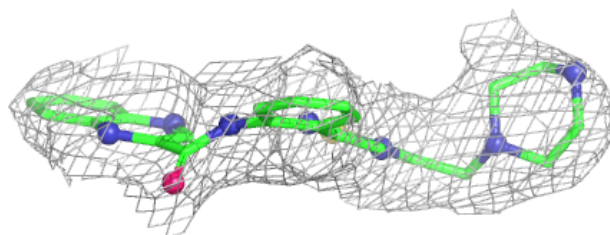
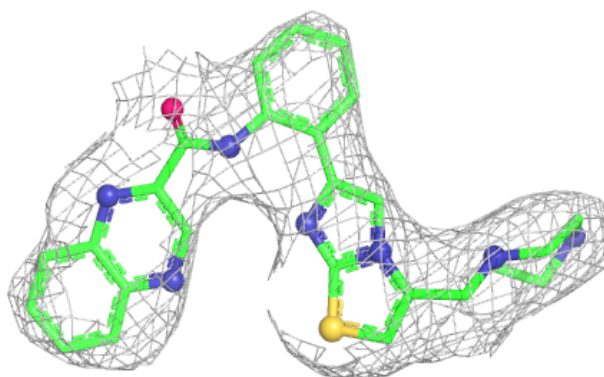


Electron density around CNA E 1395:

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

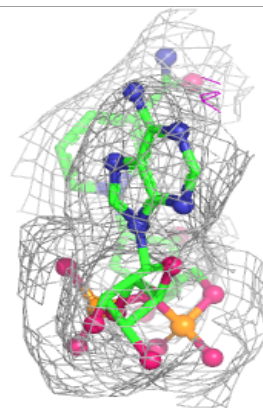
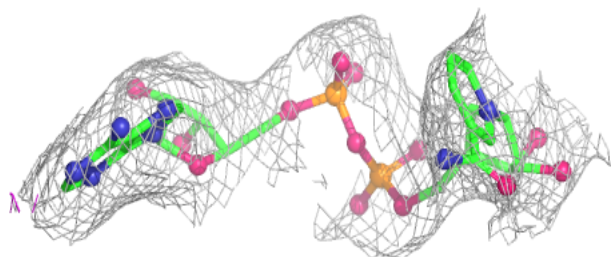
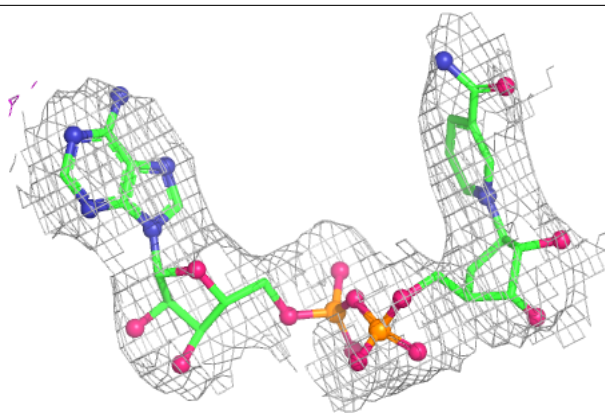
**Electron density around SR7 E 1396:**

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

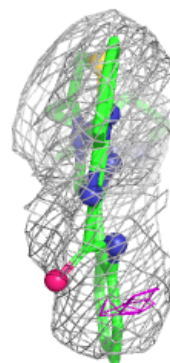
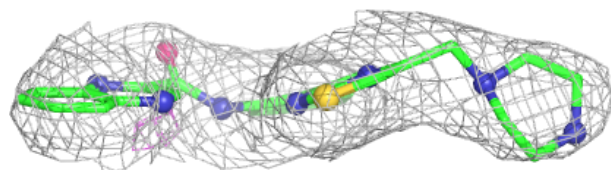
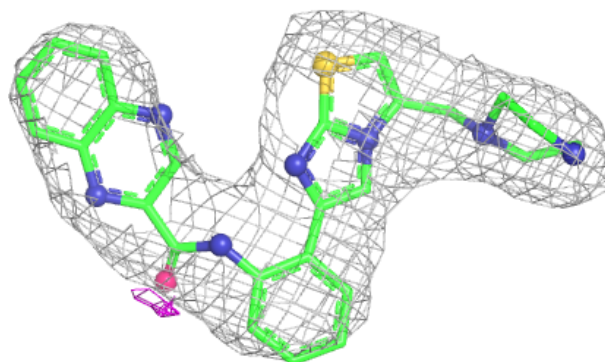


Electron density around CNA A 1395:

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

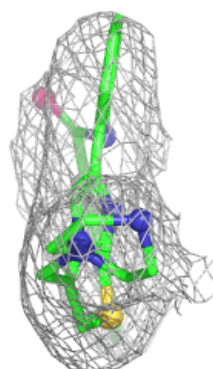
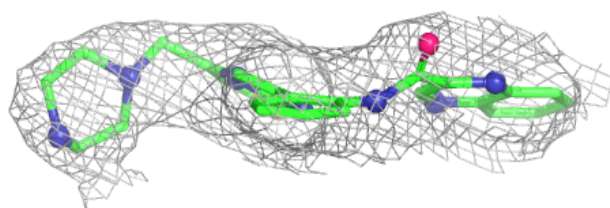
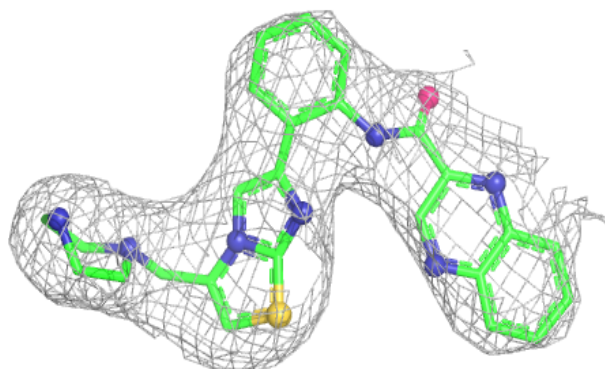
**Electron density around SR7 A 1396:**

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

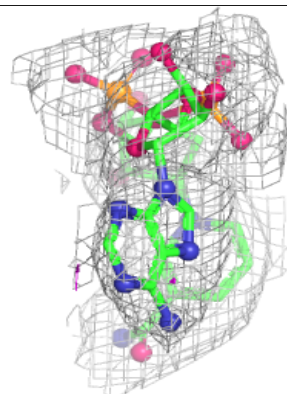
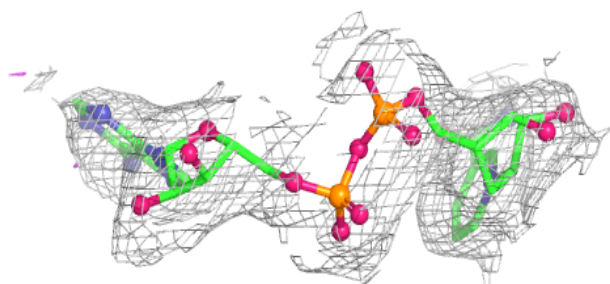
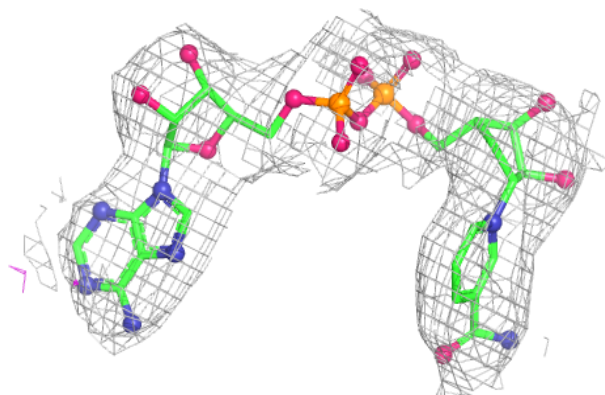


Electron density around SR7 B 1396:

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

**Electron density around CNA B 1395:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.