



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 1EQ2 / pdb_00001eq2
Title : THE CRYSTAL STRUCTURE OF ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE
Authors : Deacon, A.M.; Ni, Y.S.; Coleman Jr., W.G.; Ealick, S.E.
Deposited on : 2000-03-31
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

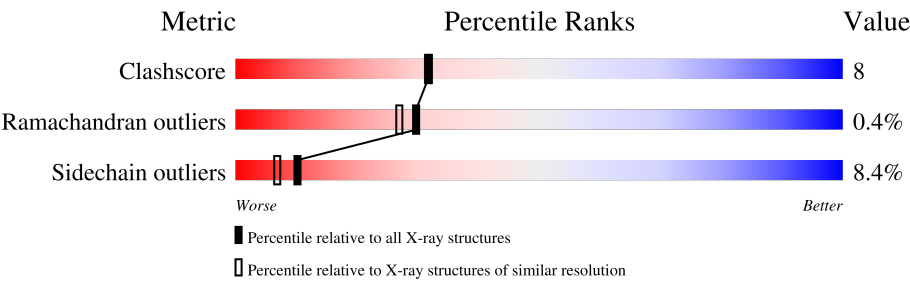
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	310	65%19%12%
1	B	310	75%17%
1	C	310	66%18%12%
1	D	310	75%21%
1	E	310	74%18%5%
1	F	310	74%21%
1	G	310	81%16%
1	H	310	74%19%

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Mol	Chain	Length	Quality of chain
1	I	310	
1	J	310	

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
2	NAP	G	2406	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25435 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 ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2150	1375	349	417	9			
1	B	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	C	272	Total	C	N	O	S	0	0	0
			2160	1385	348	418	9			
1	D	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	E	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			
1	F	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	G	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	H	297	Total	C	N	O	S	0	0	0
			2360	1511	381	459	9			
1	I	307	Total	C	N	O	S	0	0	0
			2442	1566	396	471	9			
1	J	300	Total	C	N	O	S	0	0	0
			2386	1531	384	462	9			

There are 10 discrepancies between the modelled and reference sequences:

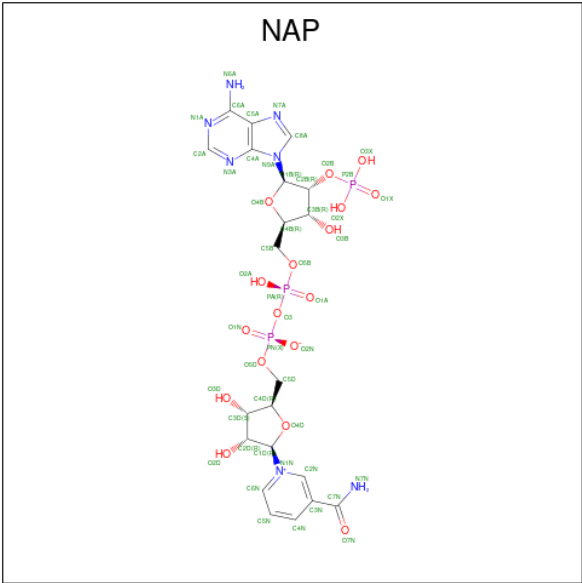
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	CSO	CYS	modified residue	UNP P67910
B	78	CSO	CYS	modified residue	UNP P67910
C	78	CSO	CYS	modified residue	UNP P67910
D	78	CSO	CYS	modified residue	UNP P67910
E	78	CSO	CYS	modified residue	UNP P67910
F	78	CSO	CYS	modified residue	UNP P67910
G	78	CSO	CYS	modified residue	UNP P67910
H	78	CSO	CYS	modified residue	UNP P67910
I	78	CSO	CYS	modified residue	UNP P67910

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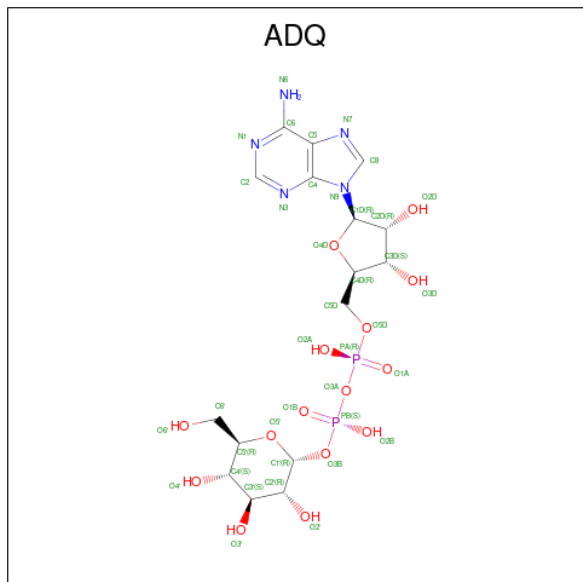
Chain	Residue	Modelled	Actual	Comment	Reference
J	78	CSO	CYS	modified residue	UNP P67910

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE-GLUCOSE (CCD ID: ADQ) (formula: $C_{16}H_{25}N_5O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	119	Total 119	O 119	0	0
4	C	82	Total 82	O 82	0	0
4	D	118	Total 118	O 118	0	0
4	E	105	Total 105	O 105	0	0
4	F	106	Total 106	O 106	0	0
4	G	118	Total 118	O 118	0	0
4	H	114	Total 114	O 114	0	0
4	I	123	Total 123	O 123	0	0
4	J	101	Total 101	O 101	0	0

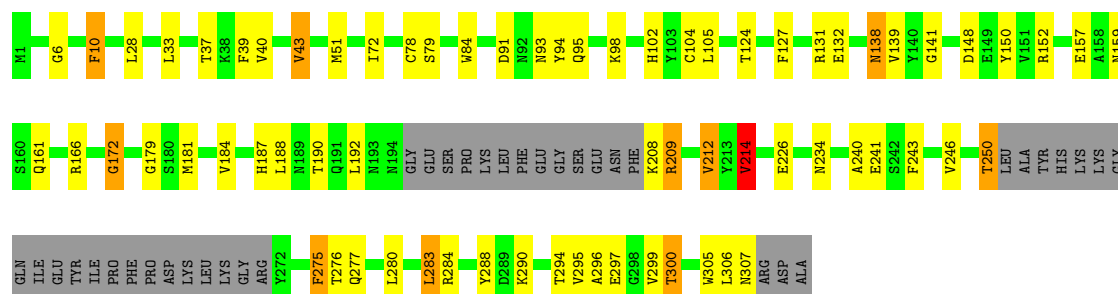
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

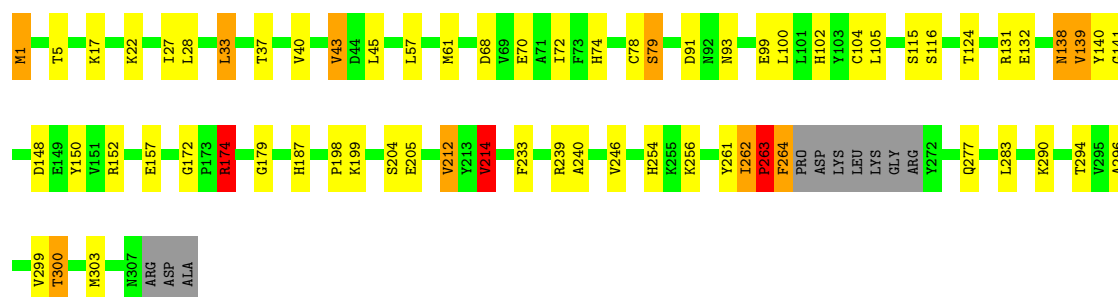
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain A: 



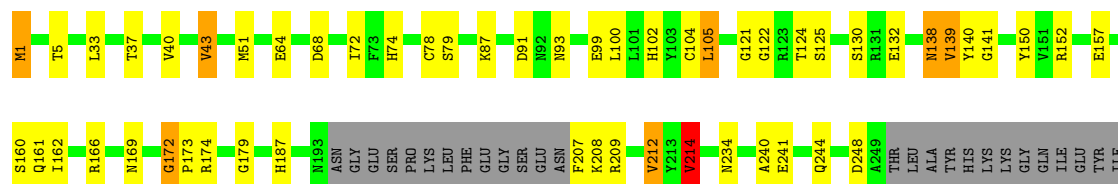
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain B: 



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

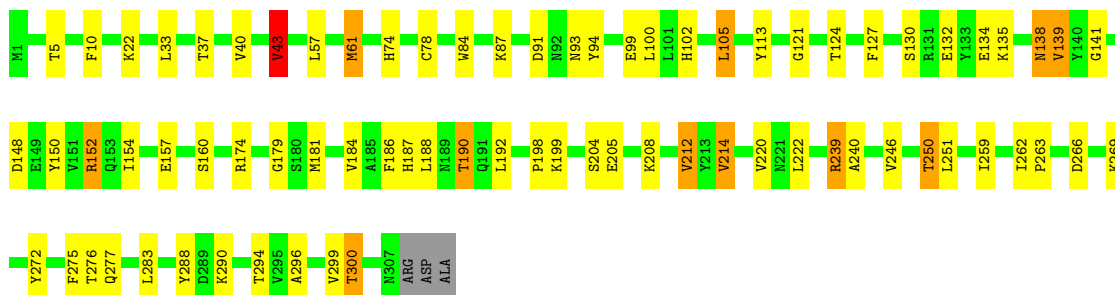
Chain C: 





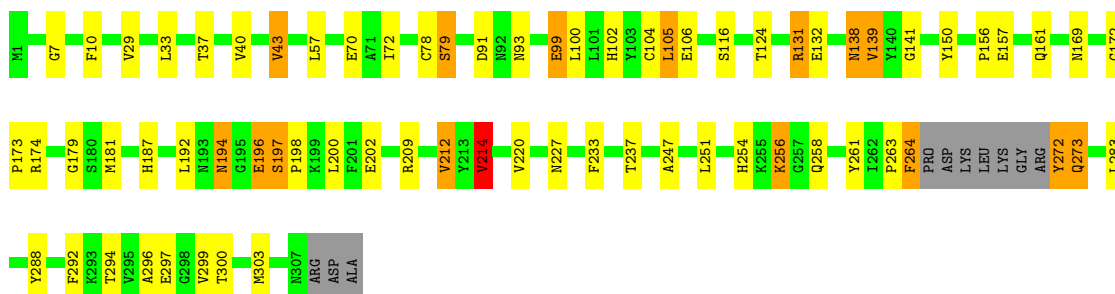
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain D: 75% 21%



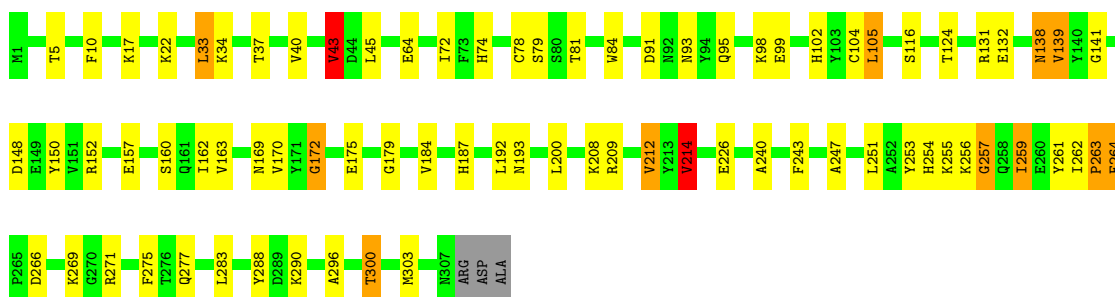
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain E: 74% 18% 5%



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain F: 74% 21%



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

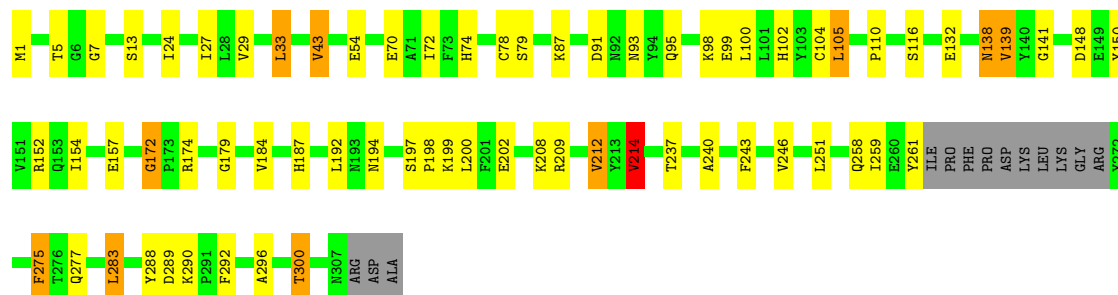
Chain G: 81% 16%





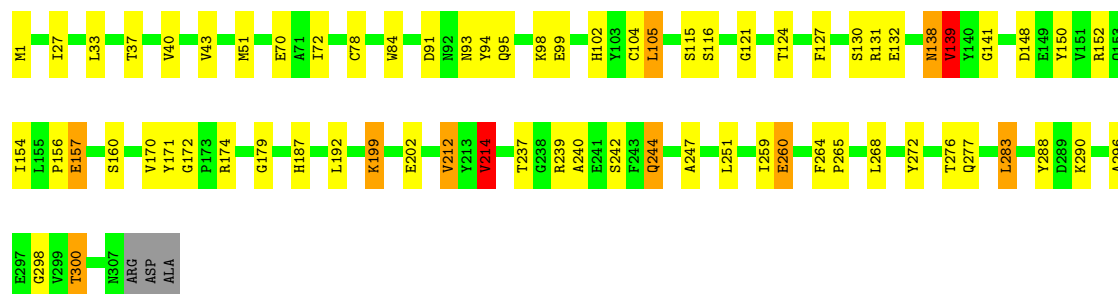
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain H: 74% 19%



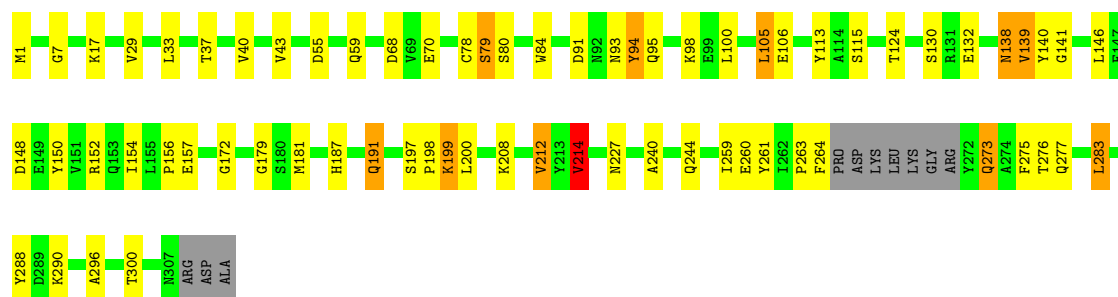
• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain I: 76% 19%



• Molecule 1: ADP-L-GLYCERO-D-MANNOHEPTOSE 6-EPIMERASE

Chain J: 75% 19%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.46 Å 109.76 Å 181.54 Å 90.00° 91.04° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.3 (20.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.212 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25435	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CSO, NAP, ADQ

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	0.68	1/2188 (0.0%)	1.01	12/2958 (0.4%)
1	B	0.68	0/2434	1.06	18/3290 (0.5%)
1	C	0.72	0/2200	1.01	9/2973 (0.3%)
1	D	0.69	1/2492 (0.0%)	1.02	9/3368 (0.3%)
1	E	0.69	0/2434	1.04	12/3290 (0.4%)
1	F	0.69	0/2492	1.04	11/3368 (0.3%)
1	G	0.69	0/2492	1.03	11/3368 (0.3%)
1	H	0.69	1/2406 (0.0%)	1.03	13/3251 (0.4%)
1	I	0.69	0/2492	1.02	9/3368 (0.3%)
1	J	0.68	0/2434	1.02	8/3290 (0.2%)
All	All	0.69	3/24064 (0.0%)	1.03	112/32524 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	MET	SD-CE	5.39	1.93	1.79
1	D	61	MET	SD-CE	5.32	1.92	1.79
1	H	24	ILE	CA-CB	5.00	1.60	1.54

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	GLU	N-CA-C	-11.19	95.45	110.55
1	A	214	VAL	CB-CA-C	-8.48	100.93	112.04
1	F	43	VAL	N-CA-C	8.24	120.02	110.62
1	B	262	ILE	CA-C-N	7.84	129.64	119.84
1	B	262	ILE	C-N-CA	7.84	129.64	119.84
1	E	197	SER	N-CA-C	7.82	119.63	109.93
1	C	214	VAL	CB-CA-C	-7.79	100.68	112.05
1	F	257	GLY	N-CA-C	7.71	121.81	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	214	VAL	CB-CA-C	-7.65	102.01	112.04
1	B	43	VAL	N-CA-C	7.26	117.99	110.36
1	D	214	VAL	CB-CA-C	-7.17	102.65	112.04
1	G	214	VAL	CB-CA-C	-7.13	102.70	112.04
1	E	43	VAL	N-CA-C	7.05	118.66	110.62
1	F	84	TRP	N-CA-C	7.01	120.71	112.72
1	H	139	VAL	CB-CA-C	-7.01	102.67	112.14
1	B	214	VAL	CB-CA-C	-7.00	101.83	112.05
1	H	214	VAL	CB-CA-C	-6.95	101.39	112.16
1	I	214	VAL	CB-CA-C	-6.92	102.80	112.14
1	H	43	VAL	N-CA-C	6.91	117.62	110.36
1	J	43	VAL	N-CA-C	6.88	118.47	110.62
1	D	272	TYR	N-CA-C	6.88	121.04	109.76
1	J	84	TRP	N-CA-C	6.86	121.35	112.92
1	I	199	LYS	N-CA-C	6.83	121.43	109.96
1	A	84	TRP	N-CA-C	6.78	121.26	112.92
1	G	43	VAL	N-CA-C	6.73	118.29	110.62
1	J	212	VAL	CB-CA-C	-6.67	100.68	110.62
1	A	212	VAL	CB-CA-C	-6.65	100.70	110.81
1	C	139	VAL	CB-CA-C	-6.65	103.16	112.14
1	I	212	VAL	CB-CA-C	-6.64	100.73	110.62
1	B	174	ARG	N-CA-C	6.54	120.55	112.58
1	F	43	VAL	CB-CA-C	-6.54	103.48	112.04
1	E	194	ASN	N-CA-C	-6.50	105.31	112.72
1	H	87	LYS	N-CA-C	-6.45	104.18	111.14
1	F	259	ILE	N-CA-C	6.42	118.88	109.63
1	B	212	VAL	CB-CA-C	-6.42	101.06	110.81
1	E	139	VAL	CB-CA-C	-6.39	103.51	112.14
1	J	139	VAL	CB-CA-C	-6.35	102.32	112.16
1	E	214	VAL	CB-CA-C	-6.34	102.33	112.16
1	F	214	VAL	CB-CA-C	-6.32	102.36	112.16
1	E	273	GLN	N-CA-C	-6.31	97.35	110.80
1	B	263	PRO	N-CA-C	6.31	125.47	112.47
1	C	212	VAL	CB-CA-C	-6.30	101.23	110.62
1	D	139	VAL	CB-CA-C	-6.28	103.66	112.14
1	I	272	TYR	N-CA-C	6.25	119.66	109.59
1	E	131	ARG	N-CA-C	6.21	118.84	111.33
1	E	212	VAL	CB-CA-C	-6.05	101.61	110.62
1	A	6	GLY	N-CA-C	-6.02	106.93	115.30
1	B	27	ILE	N-CA-C	5.97	116.71	108.12
1	G	212	VAL	CB-CA-C	-5.88	101.86	110.62
1	F	172	GLY	CA-C-N	5.86	125.88	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	172	GLY	C-N-CA	5.86	125.88	119.90
1	A	94	TYR	N-CA-C	5.82	117.31	110.97
1	I	27	ILE	N-CA-C	5.77	116.44	108.12
1	H	275	PHE	N-CA-C	5.77	117.78	108.32
1	J	227	ASN	N-CA-C	5.75	120.46	113.38
1	B	261	TYR	N-CA-C	5.75	118.44	107.75
1	H	43	VAL	N-CA-CB	5.75	116.89	110.51
1	B	139	VAL	CB-CA-C	-5.71	103.31	112.16
1	H	43	VAL	CB-CA-C	-5.70	104.59	111.88
1	G	43	VAL	CB-CA-C	-5.69	104.58	112.04
1	A	172	GLY	CA-C-N	5.68	125.68	119.89
1	A	172	GLY	C-N-CA	5.68	125.68	119.89
1	G	139	VAL	CB-CA-C	-5.67	104.48	112.14
1	D	212	VAL	CB-CA-C	-5.62	102.24	110.62
1	H	27	ILE	N-CA-C	5.55	116.12	108.12
1	H	259	ILE	N-CA-C	5.54	116.23	109.30
1	G	199	LYS	N-CA-C	5.54	118.58	109.72
1	A	290	LYS	CA-C-N	5.53	125.51	120.03
1	A	290	LYS	C-N-CA	5.53	125.51	120.03
1	I	131	ARG	N-CA-C	5.50	117.99	111.33
1	E	196	GLU	N-CA-C	5.50	118.38	109.86
1	F	139	VAL	CB-CA-C	-5.48	103.67	112.16
1	I	115	SER	N-CA-C	-5.47	101.48	109.63
1	C	43	VAL	N-CA-C	5.46	120.70	109.34
1	E	233	PHE	N-CA-C	5.43	118.31	109.24
1	B	199	LYS	N-CA-C	5.42	118.31	109.59
1	D	204	SER	N-CA-C	5.35	118.91	112.38
1	G	272	TYR	N-CA-C	5.34	118.19	109.59
1	D	43	VAL	N-CA-C	5.31	120.38	109.34
1	G	131	ARG	N-CA-C	5.29	117.73	111.33
1	D	290	LYS	CA-C-N	5.28	125.75	120.52
1	D	290	LYS	C-N-CA	5.28	125.75	120.52
1	D	94	TYR	N-CA-C	5.28	116.73	110.97
1	F	254	HIS	N-CA-C	5.26	117.02	111.28
1	A	290	LYS	N-CA-C	5.25	116.30	109.64
1	G	172	GLY	CA-C-N	5.24	125.23	119.89
1	G	172	GLY	C-N-CA	5.24	125.23	119.89
1	C	87	LYS	N-CA-C	-5.24	105.49	111.14
1	I	139	VAL	CB-CA-C	-5.22	104.07	112.16
1	B	115	SER	N-CA-C	-5.21	101.86	109.63
1	G	94	TYR	N-CA-C	5.21	116.65	110.97
1	H	212	VAL	CB-CA-C	-5.21	102.86	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	172	GLY	CA-C-N	5.20	125.20	119.90
1	H	172	GLY	C-N-CA	5.20	125.20	119.90
1	F	212	VAL	CB-CA-C	-5.17	102.91	110.62
1	A	131	ARG	N-CA-C	5.17	118.36	111.75
1	E	227	ASN	N-CA-C	5.11	119.66	113.38
1	B	290	LYS	CA-C-N	-5.09	115.48	120.52
1	B	290	LYS	C-N-CA	-5.09	115.48	120.52
1	H	202	GLU	N-CA-C	-5.07	102.98	110.48
1	B	198	PRO	N-CA-C	-5.06	102.55	110.50
1	C	161	GLN	N-CA-C	5.06	117.64	110.10
1	J	94	TYR	N-CA-C	5.06	116.48	110.97
1	J	115	SER	N-CA-C	-5.05	102.10	109.63
1	A	161	GLN	N-CA-C	5.05	117.55	110.23
1	B	256	LYS	N-CA-C	5.04	115.81	108.14
1	C	172	GLY	CA-C-N	5.04	126.14	119.84
1	C	172	GLY	C-N-CA	5.04	126.14	119.84
1	E	161	GLN	N-CA-C	5.03	117.59	110.10
1	I	94	TYR	N-CA-C	5.02	116.44	110.97
1	B	233	PHE	N-CA-C	5.02	117.62	109.24
1	C	305	TRP	N-CA-C	-5.01	106.31	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2150	0	2045	39	0
1	B	2386	0	2272	30	0
1	C	2160	0	2056	32	0
1	D	2442	0	2337	41	0
1	E	2386	0	2272	37	0
1	F	2442	0	2337	44	0
1	G	2442	0	2337	38	0
1	H	2360	0	2245	36	0
1	I	2442	0	2337	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	2386	0	2272	36	0
2	A	48	0	25	1	0
2	B	48	0	25	1	0
2	C	48	0	25	0	0
2	D	48	0	25	0	0
2	E	48	0	25	1	0
2	F	48	0	25	1	0
2	G	48	0	25	1	0
2	H	48	0	25	1	0
2	I	48	0	25	1	0
2	J	48	0	25	0	0
3	A	27	0	12	3	0
3	B	38	0	23	2	0
3	C	27	0	12	2	0
3	D	38	0	23	1	0
3	E	27	0	12	3	0
3	F	38	0	23	3	0
3	G	27	0	12	0	0
3	H	27	0	12	1	0
3	I	27	0	12	3	0
3	J	27	0	12	0	0
4	A	70	0	0	4	0
4	B	119	0	0	5	0
4	C	82	0	0	5	0
4	D	118	0	0	4	0
4	E	105	0	0	2	0
4	F	106	0	0	6	0
4	G	118	0	0	3	0
4	H	114	0	0	4	0
4	I	123	0	0	6	0
4	J	101	0	0	7	0
All	All	25435	0	22913	382	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (382) 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)
3:A:2500:ADQ:H5'1	3:A:2500:ADQ:H8	1.30	1.13
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:H8	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:H8	1.41	1.01
3:C:2502:ADQ:H5'1	3:C:2502:ADQ:H8	1.40	1.00
1:F:296:ALA:O	1:F:300:THR:HG23	1.64	0.95
1:A:296:ALA:O	1:A:300:THR:HG23	1.69	0.93
1:D:296:ALA:O	1:D:300:THR:HG23	1.69	0.93
1:H:296:ALA:O	1:H:300:THR:HG23	1.70	0.92
1:J:296:ALA:O	1:J:300:THR:HG23	1.70	0.91
1:B:296:ALA:O	1:B:300:THR:HG23	1.71	0.90
1:G:296:ALA:O	1:G:300:THR:HG23	1.72	0.88
1:E:296:ALA:O	1:E:300:THR:HG23	1.76	0.84
1:D:239:ARG:HH22	1:D:294:THR:HA	1.41	0.84
1:D:246:VAL:O	1:D:250:THR:HG23	1.80	0.81
1:F:169:ASN:HD21	1:F:209:ARG:HH11	1.28	0.81
1:C:169:ASN:HD21	1:C:209:ARG:HH11	1.28	0.81
1:H:78:CSO:H	1:H:93:ASN:HD21	1.31	0.79
1:J:240:ALA:H	1:J:277:GLN:HE21	1.31	0.78
1:B:240:ALA:H	1:B:277:GLN:HE21	1.30	0.77
1:C:296:ALA:O	1:C:300:THR:HG23	1.83	0.77
1:I:296:ALA:O	1:I:300:THR:HG23	1.84	0.77
1:I:78:CSO:H	1:I:93:ASN:HD21	1.34	0.76
1:D:78:CSO:H	1:D:93:ASN:HD21	1.33	0.75
1:C:78:CSO:H	1:C:93:ASN:HD21	1.34	0.75
1:D:57:LEU:HG	1:D:61:MET:HE2	1.69	0.75
1:B:78:CSO:H	1:B:93:ASN:HD21	1.36	0.74
1:E:263:PRO:O	1:E:264:PHE:HB2	1.86	0.74
3:B:2501:ADQ:H8	3:B:2501:ADQ:H5'1	1.69	0.74
3:I:2508:ADQ:H5'1	3:I:2508:ADQ:C8	2.16	0.74
1:H:240:ALA:H	1:H:277:GLN:HE21	1.35	0.73
1:H:300:THR:HG22	4:H:979:HOH:O	1.89	0.73
1:F:300:THR:HG22	4:F:798:HOH:O	1.90	0.72
1:G:138:ASN:HD22	1:G:141:GLY:H	1.36	0.71
1:B:138:ASN:ND2	1:B:141:GLY:H	1.88	0.71
1:E:78:CSO:H	1:E:93:ASN:HD21	1.38	0.71
3:E:2504:ADQ:H8	3:E:2504:ADQ:C5D	2.22	0.70
1:I:138:ASN:ND2	1:I:141:GLY:H	1.88	0.70
1:A:138:ASN:ND2	1:A:141:GLY:H	1.89	0.69
1:F:138:ASN:ND2	1:F:141:GLY:H	1.89	0.69
1:I:268:LEU:HD11	3:I:2508:ADQ:H5'2	1.73	0.69
1:G:138:ASN:ND2	1:G:141:GLY:H	1.88	0.69
1:G:240:ALA:H	1:G:277:GLN:HE21	1.37	0.69
1:E:138:ASN:ND2	1:E:141:GLY:H	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:ASN:ND2	1:H:141:GLY:H	1.91	0.68
1:I:290:LYS:HB3	4:I:1653:HOH:O	1.92	0.68
1:I:138:ASN:HD22	1:I:141:GLY:H	1.41	0.68
1:B:262:ILE:HG23	1:B:263:PRO:HD2	1.74	0.68
1:D:138:ASN:HD22	1:D:141:GLY:H	1.40	0.67
1:A:159:ASN:HB3	4:A:1472:HOH:O	1.95	0.67
1:A:72:ILE:HD12	1:A:104:CYS:SG	2.35	0.67
1:B:300:THR:HG22	4:B:898:HOH:O	1.94	0.67
1:F:262:ILE:HG23	1:F:263:PRO:HD2	1.77	0.67
1:D:300:THR:HG22	4:D:1467:HOH:O	1.94	0.65
1:D:190:THR:HG22	4:D:901:HOH:O	1.97	0.65
1:F:78:CSO:H	1:F:93:ASN:HD21	1.44	0.65
1:A:138:ASN:HD22	1:A:141:GLY:H	1.45	0.65
1:J:78:CSO:H	1:J:93:ASN:HD21	1.45	0.64
3:C:2502:ADQ:H5'1	3:C:2502:ADQ:C8	2.21	0.64
1:F:240:ALA:H	1:F:277:GLN:HE21	1.45	0.64
1:A:78:CSO:H	1:A:93:ASN:HD21	1.46	0.63
1:J:80:SER:HA	1:J:181:MET:HE1	1.79	0.63
3:E:2504:ADQ:H8	3:E:2504:ADQ:H5'1	1.80	0.63
1:G:78:CSO:H	1:G:93:ASN:HD21	1.44	0.63
1:H:72:ILE:HD12	1:H:104:CYS:SG	2.40	0.61
1:H:174:ARG:NH1	4:H:852:HOH:O	2.33	0.61
1:J:37:THR:O	1:J:40:VAL:HG22	1.99	0.61
1:C:138:ASN:HD22	1:C:141:GLY:H	1.49	0.61
1:G:9:GLY:HA3	2:G:2406:NAP:H52A	1.82	0.61
1:I:260:GLU:O	1:I:260:GLU:HG3	2.00	0.60
1:D:138:ASN:ND2	1:D:141:GLY:H	1.99	0.60
1:A:240:ALA:H	1:A:277:GLN:HE21	1.49	0.59
3:B:2501:ADQ:H5'1	3:B:2501:ADQ:C8	2.32	0.59
1:H:138:ASN:HD22	1:H:141:GLY:H	1.48	0.59
1:I:240:ALA:H	1:I:277:GLN:HE21	1.49	0.59
1:E:138:ASN:HD22	1:E:141:GLY:H	1.48	0.59
1:H:13:SER:OG	1:H:174:ARG:HD3	2.02	0.59
1:J:7:GLY:HA3	1:J:29:VAL:HG13	1.84	0.59
1:C:283:LEU:HD22	1:C:288:TYR:HB3	1.84	0.58
1:F:37:THR:O	1:F:40:VAL:HG22	2.02	0.58
1:D:148:ASP:O	1:D:152:ARG:HG3	2.02	0.58
1:J:138:ASN:ND2	1:J:141:GLY:H	2.00	0.58
1:B:72:ILE:HD12	1:B:104:CYS:SG	2.43	0.58
1:F:138:ASN:HD22	1:F:141:GLY:H	1.50	0.58
1:C:72:ILE:HD12	1:C:104:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:ARG:HD3	4:C:1634:HOH:O	2.04	0.58
1:C:240:ALA:H	1:C:277:GLN:HE21	1.50	0.58
1:E:272:TYR:O	1:E:273:GLN:HG3	2.04	0.58
1:H:197:SER:OG	1:H:199:LYS:HE3	2.04	0.58
1:B:138:ASN:HD22	1:B:141:GLY:H	1.51	0.57
1:B:254:HIS:HD2	4:B:1497:HOH:O	1.86	0.57
1:E:294:THR:OG1	1:E:297:GLU:HG3	2.04	0.57
1:H:192:LEU:HD11	1:H:251:LEU:CD2	2.33	0.57
1:A:190:THR:HG23	4:A:1230:HOH:O	2.03	0.57
1:D:239:ARG:NH2	1:D:294:THR:HA	2.18	0.57
1:H:289:ASP:HB3	4:H:1534:HOH:O	2.04	0.57
1:I:199:LYS:HG2	1:I:260:GLU:HG2	1.85	0.57
1:I:290:LYS:HG2	4:I:1455:HOH:O	2.05	0.57
1:C:138:ASN:ND2	1:C:141:GLY:H	2.01	0.57
3:F:2505:ADQ:H8	3:F:2505:ADQ:C5D	2.25	0.56
1:A:37:THR:O	1:A:40:VAL:HG22	2.05	0.56
1:G:148:ASP:O	1:G:152:ARG:HG3	2.06	0.56
1:F:169:ASN:ND2	1:F:209:ARG:HH11	1.99	0.56
1:E:256:LYS:HB2	1:E:256:LYS:NZ	2.21	0.56
1:D:174:ARG:HD2	4:D:747:HOH:O	2.05	0.56
1:E:200:LEU:O	1:E:261:TYR:HA	2.06	0.56
1:J:150:TYR:HB2	4:J:1538:HOH:O	2.06	0.56
1:C:207:PHE:HA	1:C:274:ALA:O	2.06	0.56
1:H:192:LEU:HD21	1:H:198:PRO:HG3	1.89	0.55
1:J:138:ASN:HD22	1:J:141:GLY:H	1.52	0.55
1:G:174:ARG:HD2	4:G:700:HOH:O	2.06	0.55
1:J:197:SER:O	1:J:199:LYS:HG3	2.07	0.55
1:A:10:PHE:HB3	2:A:2400:NAP:O2N	2.06	0.55
1:F:105:LEU:HD11	1:F:162:ILE:HD11	1.87	0.55
1:G:240:ALA:N	1:G:277:GLN:HE21	2.04	0.55
1:H:148:ASP:O	1:H:152:ARG:HG3	2.06	0.55
1:I:148:ASP:O	1:I:152:ARG:HG3	2.07	0.55
1:I:283:LEU:HD22	1:I:288:TYR:HB3	1.89	0.55
1:C:37:THR:O	1:C:40:VAL:HG22	2.07	0.55
1:G:169:ASN:HD21	1:G:209:ARG:HH11	1.55	0.55
1:A:166:ARG:HB2	1:A:234:ASN:HA	1.89	0.54
1:F:72:ILE:HD12	1:F:104:CYS:SG	2.48	0.54
1:F:259:ILE:HD12	4:F:1513:HOH:O	2.06	0.54
1:I:37:THR:O	1:I:40:VAL:HG22	2.07	0.54
1:I:51:MET:HG3	4:I:755:HOH:O	2.06	0.54
1:B:239:ARG:HH21	1:B:294:THR:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LYS:HD3	4:J:1594:HOH:O	2.07	0.54
1:G:208:LYS:O	1:G:275:PHE:HA	2.07	0.54
1:F:81:THR:HG23	4:F:1210:HOH:O	2.07	0.54
1:I:174:ARG:HD2	4:I:808:HOH:O	2.08	0.54
1:F:169:ASN:HD21	1:F:209:ARG:NH1	2.01	0.53
1:B:57:LEU:O	1:B:61:MET:HG3	2.08	0.53
1:G:300:THR:HG22	4:G:1022:HOH:O	2.08	0.53
1:J:273:GLN:NE2	1:J:276:THR:HG22	2.23	0.53
1:J:55:ASP:O	1:J:59:GLN:HG3	2.09	0.53
1:F:192:LEU:HD11	1:F:251:LEU:HD22	1.90	0.53
1:H:200:LEU:O	1:H:261:TYR:HA	2.08	0.53
1:I:105:LEU:HD21	1:I:154:ILE:HG21	1.91	0.53
1:B:17:LYS:HE3	4:B:1402:HOH:O	2.09	0.52
1:G:102:HIS:HE1	1:G:150:TYR:OH	1.92	0.52
1:C:179:GLY:O	1:C:187:HIS:HE1	1.93	0.52
1:I:102:HIS:HE1	1:I:150:TYR:OH	1.93	0.52
1:B:148:ASP:O	1:B:152:ARG:HG3	2.10	0.52
1:D:113:TYR:HB2	4:D:1434:HOH:O	2.10	0.52
1:F:263:PRO:O	1:F:264:PHE:HB2	2.09	0.52
1:A:102:HIS:HE1	1:A:150:TYR:OH	1.93	0.52
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.24	0.52
1:B:240:ALA:N	1:B:277:GLN:HE21	2.02	0.52
1:E:7:GLY:HA3	1:E:29:VAL:HG13	1.91	0.52
1:B:1:MET:HE1	1:B:28:LEU:HB2	1.92	0.51
1:F:40:VAL:HA	1:F:43:VAL:HG22	1.92	0.51
1:G:179:GLY:O	1:G:187:HIS:HE1	1.94	0.51
1:F:256:LYS:HG2	1:F:257:GLY:N	2.25	0.51
3:A:2500:ADQ:H5'1	3:A:2500:ADQ:C8	2.22	0.51
1:C:208:LYS:O	1:C:275:PHE:HA	2.11	0.51
1:E:192:LEU:HD13	1:E:254:HIS:CG	2.46	0.51
1:A:172:GLY:HA3	1:A:214:VAL:HG22	1.93	0.51
1:F:179:GLY:O	1:F:187:HIS:HE1	1.93	0.51
1:F:187:HIS:HD2	4:F:1262:HOH:O	1.94	0.51
1:E:102:HIS:O	1:E:106:GLU:HG3	2.11	0.50
1:G:240:ALA:H	1:G:277:GLN:NE2	2.06	0.50
1:J:300:THR:HG22	4:J:1040:HOH:O	2.11	0.50
1:B:174:ARG:HD2	4:B:969:HOH:O	2.10	0.50
1:C:121:GLY:HA2	4:C:1017:HOH:O	2.12	0.50
1:I:172:GLY:HA3	1:I:214:VAL:HG22	1.93	0.50
1:J:208:LYS:O	1:J:275:PHE:HA	2.12	0.50
1:D:102:HIS:HE1	1:D:150:TYR:OH	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:THR:OG1	1:F:74:HIS:HA	2.12	0.50
1:D:240:ALA:H	1:D:277:GLN:HE21	1.60	0.49
1:A:246:VAL:O	1:A:250:THR:HG23	2.13	0.49
1:F:152:ARG:HD3	4:F:1237:HOH:O	2.11	0.49
1:H:283:LEU:HD22	1:H:288:TYR:HB3	1.94	0.49
1:J:240:ALA:N	1:J:277:GLN:HE21	2.06	0.49
1:C:102:HIS:HE1	1:C:150:TYR:OH	1.95	0.49
1:D:208:LYS:O	1:D:275:PHE:HA	2.12	0.49
3:A:2500:ADQ:H8	3:A:2500:ADQ:C5D	2.22	0.49
1:F:148:ASP:O	1:F:152:ARG:HG3	2.13	0.49
1:F:10:PHE:CD1	1:F:175:GLU:HB3	2.48	0.49
1:B:179:GLY:O	1:B:187:HIS:HE1	1.95	0.49
1:E:179:GLY:O	1:E:187:HIS:HE1	1.95	0.49
3:F:2505:ADQ:H5'1	3:F:2505:ADQ:C8	2.26	0.49
1:H:172:GLY:HA3	1:H:214:VAL:HG22	1.93	0.49
1:I:157:GLU:HB3	4:I:1496:HOH:O	2.12	0.49
1:A:283:LEU:HD22	1:A:288:TYR:HB3	1.95	0.48
1:J:172:GLY:HA3	1:J:214:VAL:HG22	1.95	0.48
1:J:288:TYR:CZ	1:J:290:LYS:HB2	2.48	0.48
1:C:172:GLY:HA3	1:C:214:VAL:HG22	1.96	0.48
1:D:102:HIS:CE1	1:D:150:TYR:OH	2.66	0.48
1:F:288:TYR:CZ	1:F:290:LYS:HB2	2.48	0.48
1:I:121:GLY:HA2	4:I:1159:HOH:O	2.12	0.48
1:A:296:ALA:HB3	4:A:994:HOH:O	2.14	0.48
1:D:87:LYS:HE2	4:E:1358:HOH:O	2.13	0.48
1:J:261:TYR:N	1:J:261:TYR:CD1	2.81	0.48
1:F:200:LEU:O	1:F:261:TYR:HA	2.13	0.48
1:H:198:PRO:HD2	1:H:258:GLN:O	2.14	0.48
1:A:184:VAL:O	1:A:188:LEU:HG	2.13	0.48
1:H:209:ARG:NH1	3:H:2507:ADQ:O2B	2.45	0.48
1:J:105:LEU:HD21	1:J:154:ILE:HG21	1.95	0.48
1:B:264:PHE:CD1	1:B:264:PHE:C	2.92	0.48
1:G:82:THR:HG22	4:G:985:HOH:O	2.12	0.47
1:G:136:PRO:HD2	4:J:1524:HOH:O	2.13	0.47
1:A:208:LYS:O	1:A:275:PHE:HA	2.13	0.47
1:H:70:GLU:O	1:H:110:PRO:HD2	2.14	0.47
1:F:200:LEU:HD11	1:F:247:ALA:HB2	1.96	0.47
1:H:179:GLY:O	1:H:187:HIS:HE1	1.96	0.47
1:E:37:THR:O	1:E:40:VAL:HG22	2.14	0.47
1:J:283:LEU:HD22	1:J:288:TYR:HB3	1.97	0.47
1:C:125:SER:HA	4:C:1556:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:THR:HG22	1:D:299:VAL:HG11	1.97	0.47
1:E:102:HIS:HE1	1:E:150:TYR:OH	1.98	0.47
1:G:239:ARG:HA	1:G:277:GLN:HE21	1.79	0.47
1:I:199:LYS:HG2	1:I:260:GLU:CG	2.45	0.47
1:J:95:GLN:NE2	1:J:98:LYS:HE2	2.30	0.47
1:A:102:HIS:CE1	1:A:150:TYR:OH	2.68	0.47
1:D:37:THR:O	1:D:40:VAL:HG22	2.15	0.47
1:F:253:TYR:CD2	1:F:303:MET:HB3	2.50	0.47
1:A:28:LEU:HD11	1:A:51:MET:HE3	1.97	0.47
1:C:292:PHE:HD1	4:C:1544:HOH:O	1.96	0.47
1:D:186:PHE:O	1:D:190:THR:HG23	2.14	0.46
1:D:192:LEU:HD11	1:D:251:LEU:HD22	1.97	0.46
1:D:179:GLY:O	1:D:187:HIS:HE1	1.97	0.46
1:E:194:ASN:C	1:E:196:GLU:H	2.23	0.46
1:J:191:GLN:HG2	1:J:197:SER:O	2.15	0.46
1:D:5:THR:OG1	1:D:74:HIS:HA	2.14	0.46
1:D:22:LYS:HD2	1:D:222:LEU:CD1	2.46	0.46
1:G:102:HIS:CE1	1:G:150:TYR:OH	2.68	0.46
1:F:263:PRO:O	1:F:264:PHE:CB	2.63	0.46
1:B:246:VAL:HG11	4:B:1658:HOH:O	2.15	0.46
1:A:300:THR:HG22	4:A:1525:HOH:O	2.15	0.46
1:D:266:ASP:HA	1:D:269:LYS:HG3	1.97	0.46
1:H:102:HIS:CE1	1:H:150:TYR:OH	2.68	0.46
1:D:105:LEU:HD21	1:D:154:ILE:HG21	1.98	0.46
1:D:134:GLU:CD	1:D:152:ARG:HH22	2.22	0.46
1:D:134:GLU:OE1	1:D:152:ARG:NH2	2.49	0.46
1:D:199:LYS:HB3	1:D:262:ILE:HG12	1.96	0.46
1:E:173:PRO:O	1:E:174:ARG:HB2	2.15	0.46
1:E:202:GLU:OE1	1:E:263:PRO:HA	2.16	0.46
1:G:239:ARG:NH2	1:G:294:THR:HG22	2.31	0.46
1:C:244:GLN:NE2	1:C:248:ASP:OD1	2.48	0.46
1:J:264:PHE:HD2	4:J:1365:HOH:O	1.99	0.45
1:A:250:THR:HG22	1:A:299:VAL:HG11	1.97	0.45
1:C:288:TYR:CE1	1:C:290:LYS:HE2	2.51	0.45
1:D:181:MET:O	3:D:2503:ADQ:O3'	2.34	0.45
1:E:116:SER:HB2	2:E:2404:NAP:H6N	1.99	0.45
1:H:105:LEU:HD21	1:H:154:ILE:HG21	1.98	0.45
1:H:192:LEU:CD2	1:H:198:PRO:HG3	2.46	0.45
1:I:127:PHE:CZ	1:I:276:THR:HA	2.51	0.45
1:F:95:GLN:NE2	1:F:98:LYS:HE2	2.31	0.45
1:H:5:THR:OG1	1:H:74:HIS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:GLN:NE2	1:I:98:LYS:HE2	2.31	0.45
1:C:5:THR:OG1	1:C:74:HIS:HA	2.17	0.45
1:E:247:ALA:O	1:E:251:LEU:HD13	2.16	0.45
1:E:102:HIS:CE1	1:E:150:TYR:OH	2.69	0.45
1:E:131:ARG:O	1:E:131:ARG:HD3	2.17	0.45
1:G:132:GLU:CD	1:G:132:GLU:H	2.24	0.45
1:C:1:MET:N	1:C:68:ASP:O	2.49	0.45
1:H:197:SER:HA	1:H:198:PRO:HD3	1.86	0.45
1:J:179:GLY:O	1:J:187:HIS:HE1	2.00	0.45
1:A:95:GLN:NE2	1:A:98:LYS:HE2	2.32	0.45
1:A:148:ASP:O	1:A:152:ARG:HG3	2.17	0.45
1:B:172:GLY:HA3	1:B:214:VAL:HG22	1.99	0.45
1:H:237:THR:HG22	1:H:292:PHE:HB3	1.98	0.45
1:H:102:HIS:HE1	1:H:150:TYR:OH	2.00	0.44
1:B:172:GLY:HA3	1:B:214:VAL:CG2	2.47	0.44
1:E:220:VAL:HG22	1:E:288:TYR:CZ	2.52	0.44
1:H:7:GLY:HA3	1:H:29:VAL:HG13	1.99	0.44
1:H:246:VAL:HG11	4:H:1553:HOH:O	2.17	0.44
1:F:255:LYS:HD3	1:F:255:LYS:HA	1.79	0.44
1:J:148:ASP:O	1:J:152:ARG:HG3	2.16	0.44
1:I:72:ILE:HD12	1:I:104:CYS:SG	2.57	0.44
1:E:169:ASN:HD21	1:E:209:ARG:HH11	1.64	0.44
1:F:172:GLY:HA3	1:F:214:VAL:HG22	1.99	0.44
1:B:131:ARG:O	1:B:131:ARG:HD3	2.18	0.44
1:D:198:PRO:HB2	1:D:259:ILE:HD13	2.00	0.44
1:J:93:ASN:N	1:J:93:ASN:HD22	2.15	0.44
1:C:173:PRO:C	1:C:174:ARG:HG3	2.42	0.44
1:I:192:LEU:HD11	1:I:251:LEU:HD12	2.00	0.44
1:A:188:LEU:O	1:A:192:LEU:HD13	2.18	0.43
1:D:220:VAL:HG22	1:D:288:TYR:CZ	2.53	0.43
1:E:72:ILE:HD12	1:E:104:CYS:SG	2.58	0.43
1:C:102:HIS:CE1	1:C:150:TYR:OH	2.71	0.43
1:E:172:GLY:HA3	1:E:214:VAL:HG22	2.00	0.43
1:E:272:TYR:C	1:E:273:GLN:HG3	2.44	0.43
1:J:172:GLY:HA3	1:J:214:VAL:CG2	2.48	0.43
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.92	0.43
1:F:208:LYS:O	1:F:275:PHE:HA	2.18	0.43
1:H:208:LYS:O	1:H:275:PHE:HA	2.19	0.43
1:A:280:LEU:O	1:A:284:ARG:HG2	2.19	0.43
1:B:33:LEU:HD12	1:B:33:LEU:HA	1.85	0.43
1:B:45:LEU:HD21	1:B:174:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:VAL:HG21	1:F:243:PHE:CE2	2.54	0.43
1:G:105:LEU:HD12	1:G:105:LEU:HA	1.90	0.43
1:I:116:SER:HB2	2:I:2408:NAP:H6N	2.00	0.43
1:A:208:LYS:HA	1:A:241:GLU:O	2.19	0.43
1:C:284:ARG:HD2	1:C:288:TYR:O	2.19	0.43
1:F:193:ASN:HB2	4:F:1309:HOH:O	2.18	0.43
1:B:116:SER:HB2	2:B:2401:NAP:H6N	2.01	0.42
1:C:51:MET:HE2	4:C:1516:HOH:O	2.18	0.42
1:F:22:LYS:HE2	1:F:226:GLU:OE2	2.19	0.42
1:I:247:ALA:HB1	1:I:259:ILE:HD11	2.00	0.42
1:J:260:GLU:O	1:J:260:GLU:HG3	2.19	0.42
1:I:179:GLY:O	1:I:187:HIS:HE1	2.02	0.42
1:B:5:THR:OG1	1:B:74:HIS:HA	2.19	0.42
1:C:105:LEU:HD11	1:C:162:ILE:HD11	2.01	0.42
1:D:192:LEU:HD11	1:D:251:LEU:CD2	2.50	0.42
1:G:127:PHE:CZ	1:G:276:THR:HA	2.54	0.42
1:I:84:TRP:CE3	1:I:139:VAL:HG22	2.55	0.42
1:A:294:THR:OG1	1:A:297:GLU:HG3	2.19	0.42
1:G:170:VAL:CG1	1:G:214:VAL:HG13	2.49	0.42
1:G:170:VAL:HG12	1:G:214:VAL:HG13	2.01	0.42
1:G:239:ARG:NH2	1:G:294:THR:HA	2.34	0.42
1:I:237:THR:HB	1:I:239:ARG:NH2	2.34	0.42
1:A:179:GLY:O	1:A:187:HIS:HE1	2.03	0.42
1:F:170:VAL:CG1	1:F:214:VAL:HG13	2.49	0.42
1:J:79:SER:HA	1:J:140:TYR:CE1	2.55	0.42
1:A:51:MET:HE3	1:A:51:MET:HB2	1.78	0.42
1:J:200:LEU:O	1:J:261:TYR:HA	2.20	0.42
1:A:240:ALA:N	1:A:277:GLN:HE21	2.18	0.42
1:D:40:VAL:HA	1:D:43:VAL:HG22	2.02	0.42
1:G:105:LEU:HD21	1:G:154:ILE:HG21	2.02	0.42
1:H:184:VAL:HG21	1:H:243:PHE:CE2	2.55	0.42
1:I:242:SER:OG	1:I:244:GLN:HB2	2.19	0.42
1:A:305:TRP:C	1:A:307:ASN:H	2.27	0.42
1:B:79:SER:HA	1:B:140:TYR:CE1	2.55	0.42
1:D:184:VAL:O	1:D:188:LEU:HG	2.20	0.42
1:E:79:SER:HB2	4:E:1489:HOH:O	2.19	0.42
1:I:171:TYR:OH	1:I:298:GLY:HA3	2.19	0.42
1:A:172:GLY:HA3	1:A:214:VAL:CG2	2.49	0.41
1:D:262:ILE:HG23	1:D:263:PRO:HD2	2.02	0.41
1:E:237:THR:HG22	1:E:292:PHE:HB3	2.02	0.41
1:G:239:ARG:HH21	1:G:294:THR:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:GLY:HA3	1:D:135:LYS:O	2.20	0.41
1:G:134:GLU:OE1	1:G:152:ARG:NH2	2.53	0.41
1:H:116:SER:HB2	2:H:2407:NAP:H6N	2.02	0.41
1:A:241:GLU:OE1	1:A:295:VAL:HB	2.20	0.41
1:E:57:LEU:HD11	1:E:99:GLU:HG2	2.02	0.41
1:F:240:ALA:N	1:F:277:GLN:HE21	2.14	0.41
1:H:95:GLN:NE2	1:H:98:LYS:HE2	2.35	0.41
1:J:199:LYS:HA	1:J:260:GLU:O	2.20	0.41
1:A:209:ARG:HG3	1:A:276:THR:OG1	2.21	0.41
1:D:84:TRP:CH2	1:D:138:ASN:HA	2.55	0.41
1:D:127:PHE:CZ	1:D:276:THR:HA	2.55	0.41
3:E:2504:ADQ:H8	3:E:2504:ADQ:H5'2	2.00	0.41
1:F:33:LEU:O	1:F:34:LYS:C	2.63	0.41
1:F:116:SER:HB2	2:F:2405:NAP:H6N	2.02	0.41
1:G:93:ASN:N	1:G:93:ASN:HD22	2.17	0.41
1:C:166:ARG:HB2	1:C:234:ASN:HA	2.02	0.41
1:E:131:ARG:HD3	1:E:131:ARG:C	2.45	0.41
1:I:102:HIS:CE1	1:I:150:TYR:OH	2.73	0.41
1:J:17:LYS:HE2	4:J:906:HOH:O	2.20	0.41
1:B:299:VAL:O	1:B:303:MET:HG2	2.21	0.41
1:H:240:ALA:N	1:H:277:GLN:HE21	2.11	0.41
1:J:146:LEU:HD12	1:J:146:LEU:HA	1.93	0.41
1:E:198:PRO:HD2	1:E:258:GLN:O	2.21	0.41
1:E:299:VAL:O	1:E:303:MET:HG2	2.20	0.41
1:G:205:GLU:OE1	1:G:205:GLU:HA	2.19	0.41
1:B:102:HIS:HE1	1:B:150:TYR:OH	2.03	0.41
1:C:79:SER:HA	1:C:140:TYR:CE1	2.56	0.41
1:A:127:PHE:CZ	1:A:276:THR:HA	2.56	0.41
1:A:209:ARG:NH1	1:A:243:PHE:HZ	2.19	0.41
1:D:239:ARG:HE	1:D:239:ARG:HB2	1.78	0.41
1:E:105:LEU:HD12	1:E:105:LEU:HA	1.93	0.41
1:E:197:SER:HA	1:E:198:PRO:HD3	1.73	0.41
1:F:17:LYS:HD3	1:F:45:LEU:HD21	2.01	0.41
1:G:146:LEU:HA	1:G:146:LEU:HD12	1.89	0.41
1:C:241:GLU:OE1	1:C:295:VAL:HB	2.21	0.41
1:E:263:PRO:O	1:E:264:PHE:CB	2.64	0.41
1:E:264:PHE:HD2	1:E:264:PHE:HA	1.68	0.41
1:G:55:ASP:O	1:G:59:GLN:HG3	2.21	0.41
1:B:37:THR:O	1:B:40:VAL:HG22	2.21	0.40
1:G:10:PHE:CE1	1:G:214:VAL:HG11	2.56	0.40
1:H:33:LEU:HD12	1:H:33:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ASN:HD21	1:C:209:ARG:NH1	2.08	0.40
1:J:1:MET:O	1:J:70:GLU:HG2	2.21	0.40
1:J:113:TYR:HB2	4:J:1127:HOH:O	2.21	0.40
1:F:102:HIS:HE1	1:F:150:TYR:OH	2.04	0.40
1:F:131:ARG:HD3	1:F:131:ARG:C	2.47	0.40
1:G:239:ARG:HA	1:G:277:GLN:NE2	2.37	0.40
1:I:264:PHE:HA	1:I:265:PRO:HD3	1.89	0.40
1:J:94:TYR:CZ	1:J:98:LYS:HD3	2.56	0.40
1:A:39:PHE:CE1	1:A:43:VAL:CG1	3.05	0.40
1:G:10:PHE:CZ	1:G:214:VAL:HG13	2.57	0.40
1:G:170:VAL:HA	1:G:212:VAL:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	266/310 (86%)	254 (96%)	9 (3%)	3 (1%)	11	7
1	B	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	36	35
1	C	265/310 (86%)	251 (95%)	13 (5%)	1 (0%)	30	27
1	D	304/310 (98%)	292 (96%)	11 (4%)	1 (0%)	36	35
1	E	295/310 (95%)	284 (96%)	10 (3%)	1 (0%)	36	35
1	F	304/310 (98%)	290 (95%)	13 (4%)	1 (0%)	36	35
1	G	304/310 (98%)	291 (96%)	11 (4%)	2 (1%)	18	14
1	H	292/310 (94%)	282 (97%)	10 (3%)	0	100	100
1	I	304/310 (98%)	290 (95%)	14 (5%)	0	100	100
1	J	295/310 (95%)	280 (95%)	12 (4%)	3 (1%)	12	8
All	All	2924/3100 (94%)	2798 (96%)	113 (4%)	13 (0%)	30	27

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	B	263	PRO
1	F	264	PHE
1	J	263	PRO
1	J	259	ILE
1	A	306	LEU
1	G	10	PHE
1	G	204	SER
1	D	10	PHE
1	A	10	PHE
1	E	10	PHE
1	J	199	LYS
1	C	122	GLY

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	222/256 (87%)	205 (92%)	17 (8%)	12	8
1	B	248/256 (97%)	224 (90%)	24 (10%)	8	5
1	C	224/256 (88%)	205 (92%)	19 (8%)	10	7
1	D	254/256 (99%)	232 (91%)	22 (9%)	9	6
1	E	248/256 (97%)	227 (92%)	21 (8%)	10	7
1	F	254/256 (99%)	232 (91%)	22 (9%)	9	6
1	G	254/256 (99%)	237 (93%)	17 (7%)	15	11
1	H	245/256 (96%)	226 (92%)	19 (8%)	11	8
1	I	254/256 (99%)	231 (91%)	23 (9%)	9	6
1	J	248/256 (97%)	227 (92%)	21 (8%)	10	7
All	All	2451/2560 (96%)	2246 (92%)	205 (8%)	10	7

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	43	VAL
1	A	79	SER
1	A	91	ASP
1	A	105	LEU
1	A	124	THR
1	A	132	GLU
1	A	138	ASN
1	A	139	VAL
1	A	157	GLU
1	A	209	ARG
1	A	212	VAL
1	A	214	VAL
1	A	226	GLU
1	A	250	THR
1	A	283	LEU
1	A	300	THR
1	B	1	MET
1	B	22	LYS
1	B	33	LEU
1	B	43	VAL
1	B	68	ASP
1	B	70	GLU
1	B	79	SER
1	B	91	ASP
1	B	99	GLU
1	B	100	LEU
1	B	105	LEU
1	B	124	THR
1	B	132	GLU
1	B	138	ASN
1	B	139	VAL
1	B	157	GLU
1	B	174	ARG
1	B	204	SER
1	B	212	VAL
1	B	214	VAL
1	B	263	PRO
1	B	264	PHE
1	B	283	LEU
1	B	300	THR
1	C	1	MET
1	C	33	LEU

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Mol	Chain	Res	Type
1	C	43	VAL
1	C	64	GLU
1	C	91	ASP
1	C	99	GLU
1	C	100	LEU
1	C	105	LEU
1	C	124	THR
1	C	130	SER
1	C	132	GLU
1	C	138	ASN
1	C	139	VAL
1	C	157	GLU
1	C	160	SER
1	C	212	VAL
1	C	214	VAL
1	C	283	LEU
1	C	300	THR
1	D	33	LEU
1	D	43	VAL
1	D	91	ASP
1	D	99	GLU
1	D	100	LEU
1	D	105	LEU
1	D	124	THR
1	D	130	SER
1	D	132	GLU
1	D	138	ASN
1	D	139	VAL
1	D	152	ARG
1	D	157	GLU
1	D	160	SER
1	D	190	THR
1	D	205	GLU
1	D	212	VAL
1	D	214	VAL
1	D	239	ARG
1	D	250	THR
1	D	283	LEU
1	D	300	THR
1	E	33	LEU
1	E	43	VAL
1	E	70	GLU

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Mol	Chain	Res	Type
1	E	79	SER
1	E	91	ASP
1	E	99	GLU
1	E	100	LEU
1	E	105	LEU
1	E	124	THR
1	E	132	GLU
1	E	138	ASN
1	E	139	VAL
1	E	156	PRO
1	E	157	GLU
1	E	181	MET
1	E	212	VAL
1	E	214	VAL
1	E	256	LYS
1	E	264	PHE
1	E	272	TYR
1	E	283	LEU
1	F	33	LEU
1	F	43	VAL
1	F	64	GLU
1	F	79	SER
1	F	91	ASP
1	F	99	GLU
1	F	105	LEU
1	F	124	THR
1	F	132	GLU
1	F	138	ASN
1	F	139	VAL
1	F	157	GLU
1	F	160	SER
1	F	163	VAL
1	F	212	VAL
1	F	214	VAL
1	F	263	PRO
1	F	266	ASP
1	F	269	LYS
1	F	271	ARG
1	F	283	LEU
1	F	300	THR
1	G	33	LEU
1	G	70	GLU

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Mol	Chain	Res	Type
1	G	91	ASP
1	G	99	GLU
1	G	100	LEU
1	G	105	LEU
1	G	124	THR
1	G	132	GLU
1	G	138	ASN
1	G	139	VAL
1	G	157	GLU
1	G	160	SER
1	G	206	ASN
1	G	212	VAL
1	G	214	VAL
1	G	283	LEU
1	G	300	THR
1	H	1	MET
1	H	33	LEU
1	H	43	VAL
1	H	54	GLU
1	H	79	SER
1	H	91	ASP
1	H	99	GLU
1	H	100	LEU
1	H	105	LEU
1	H	132	GLU
1	H	138	ASN
1	H	139	VAL
1	H	157	GLU
1	H	194	ASN
1	H	212	VAL
1	H	214	VAL
1	H	283	LEU
1	H	290	LYS
1	H	300	THR
1	I	1	MET
1	I	33	LEU
1	I	43	VAL
1	I	70	GLU
1	I	91	ASP
1	I	99	GLU
1	I	105	LEU
1	I	124	THR

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Mol	Chain	Res	Type
1	I	130	SER
1	I	132	GLU
1	I	138	ASN
1	I	139	VAL
1	I	156	PRO
1	I	157	GLU
1	I	160	SER
1	I	170	VAL
1	I	202	GLU
1	I	212	VAL
1	I	214	VAL
1	I	244	GLN
1	I	260	GLU
1	I	283	LEU
1	I	300	THR
1	J	33	LEU
1	J	68	ASP
1	J	79	SER
1	J	91	ASP
1	J	100	LEU
1	J	105	LEU
1	J	106	GLU
1	J	124	THR
1	J	130	SER
1	J	132	GLU
1	J	138	ASN
1	J	139	VAL
1	J	156	PRO
1	J	157	GLU
1	J	191	GLN
1	J	198	PRO
1	J	212	VAL
1	J	214	VAL
1	J	244	GLN
1	J	273	GLN
1	J	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	102	HIS
1	A	138	ASN
1	A	221	ASN
1	A	227	ASN
1	A	277	GLN
1	A	282	ASN
1	B	93	ASN
1	B	95	GLN
1	B	102	HIS
1	B	138	ASN
1	B	187	HIS
1	B	206	ASN
1	B	227	ASN
1	B	254	HIS
1	B	277	GLN
1	B	282	ASN
1	C	93	ASN
1	C	95	GLN
1	C	102	HIS
1	C	138	ASN
1	C	169	ASN
1	C	187	HIS
1	C	221	ASN
1	C	227	ASN
1	C	273	GLN
1	C	277	GLN
1	C	282	ASN
1	D	93	ASN
1	D	95	GLN
1	D	102	HIS
1	D	138	ASN
1	D	187	HIS
1	D	206	ASN
1	D	221	ASN
1	D	227	ASN
1	D	244	GLN
1	D	254	HIS
1	D	258	GLN
1	D	273	GLN
1	D	277	GLN
1	D	282	ASN
1	E	93	ASN

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Mol	Chain	Res	Type
1	E	95	GLN
1	E	102	HIS
1	E	138	ASN
1	E	169	ASN
1	E	187	HIS
1	E	221	ASN
1	E	227	ASN
1	E	244	GLN
1	E	282	ASN
1	F	59	GLN
1	F	93	ASN
1	F	95	GLN
1	F	102	HIS
1	F	138	ASN
1	F	169	ASN
1	F	187	HIS
1	F	193	ASN
1	F	227	ASN
1	F	254	HIS
1	F	277	GLN
1	F	282	ASN
1	G	93	ASN
1	G	95	GLN
1	G	102	HIS
1	G	138	ASN
1	G	159	ASN
1	G	169	ASN
1	G	187	HIS
1	G	221	ASN
1	G	227	ASN
1	G	254	HIS
1	G	273	GLN
1	G	277	GLN
1	G	282	ASN
1	H	93	ASN
1	H	95	GLN
1	H	102	HIS
1	H	138	ASN
1	H	169	ASN
1	H	187	HIS
1	H	194	ASN
1	H	227	ASN

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Mol	Chain	Res	Type
1	H	254	HIS
1	H	277	GLN
1	H	282	ASN
1	I	93	ASN
1	I	95	GLN
1	I	102	HIS
1	I	138	ASN
1	I	169	ASN
1	I	187	HIS
1	I	221	ASN
1	I	227	ASN
1	I	254	HIS
1	I	258	GLN
1	I	273	GLN
1	I	277	GLN
1	I	282	ASN
1	J	41	ASN
1	J	93	ASN
1	J	95	GLN
1	J	102	HIS
1	J	138	ASN
1	J	169	ASN
1	J	187	HIS
1	J	221	ASN
1	J	227	ASN
1	J	254	HIS
1	J	273	GLN
1	J	277	GLN
1	J	282	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	B	78	1	3,6,7	0.57	0	1,6,8	0.21	0
1	CSO	G	78	1	3,6,7	0.80	0	1,6,8	0.07	0
1	CSO	H	78	1	3,6,7	0.70	0	1,6,8	0.41	0
1	CSO	D	78	1	3,6,7	0.79	0	1,6,8	0.60	0
1	CSO	I	78	1	3,6,7	0.73	0	1,6,8	0.45	0
1	CSO	F	78	1	3,6,7	0.62	0	1,6,8	0.71	0
1	CSO	J	78	1	3,6,7	0.71	0	1,6,8	0.43	0
1	CSO	A	78	1	3,6,7	0.62	0	1,6,8	0.11	0
1	CSO	E	78	1	3,6,7	0.86	0	1,6,8	0.03	0
1	CSO	C	78	1	3,6,7	0.80	0	1,6,8	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	78	1	-	0/1/5/7	-
1	CSO	G	78	1	-	1/1/5/7	-
1	CSO	H	78	1	-	1/1/5/7	-
1	CSO	D	78	1	-	1/1/5/7	-
1	CSO	I	78	1	-	1/1/5/7	-
1	CSO	F	78	1	-	1/1/5/7	-
1	CSO	J	78	1	-	1/1/5/7	-
1	CSO	A	78	1	-	0/1/5/7	-
1	CSO	E	78	1	-	0/1/5/7	-
1	CSO	C	78	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	78	CSO	N-CA-CB-SG
1	F	78	CSO	N-CA-CB-SG
1	G	78	CSO	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	H	78	CSO	N-CA-CB-SG
1	I	78	CSO	N-CA-CB-SG
1	J	78	CSO	N-CA-CB-SG

There are no ring outliers.

10 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	78	CSO	1	0
1	G	78	CSO	1	0
1	H	78	CSO	1	0
1	D	78	CSO	1	0
1	I	78	CSO	1	0
1	F	78	CSO	1	0
1	J	78	CSO	1	0
1	A	78	CSO	1	0
1	E	78	CSO	1	0
1	C	78	CSO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	E	2404	-	50,52,52	2.61	12 (24%)	71,80,80	1.80	11 (15%)
2	NAP	I	2408	-	50,52,52	2.75	12 (24%)	71,80,80	1.79	9 (12%)
2	NAP	D	2403	-	50,52,52	2.58	13 (26%)	71,80,80	1.74	8 (11%)
2	NAP	B	2401	-	50,52,52	2.62	12 (24%)	71,80,80	1.78	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADQ	G	2506	-	28,29,41	1.37	5 (17%)	43,45,63	1.89	8 (18%)
3	ADQ	D	2503	-	40,41,41	1.76	8 (20%)	60,63,63	2.09	16 (26%)
3	ADQ	A	2500	-	28,29,41	1.44	3 (10%)	43,45,63	2.00	9 (20%)
2	NAP	G	2406	-	50,52,52	2.44	14 (28%)	71,80,80	1.78	11 (15%)
3	ADQ	J	2509	-	28,29,41	1.37	3 (10%)	43,45,63	2.02	8 (18%)
2	NAP	C	2402	-	50,52,52	2.37	11 (22%)	71,80,80	1.82	8 (11%)
3	ADQ	C	2502	-	28,29,41	1.26	4 (14%)	43,45,63	1.92	7 (16%)
3	ADQ	H	2507	-	28,29,41	1.37	4 (14%)	43,45,63	1.99	9 (20%)
3	ADQ	I	2508	-	28,29,41	1.23	5 (17%)	43,45,63	1.96	11 (25%)
3	ADQ	B	2501	-	40,41,41	1.42	3 (7%)	60,63,63	1.90	13 (21%)
2	NAP	H	2407	-	50,52,52	2.50	12 (24%)	71,80,80	1.76	7 (9%)
2	NAP	A	2400	-	50,52,52	2.59	13 (26%)	71,80,80	1.77	10 (14%)
2	NAP	J	2409	-	50,52,52	2.61	11 (22%)	71,80,80	1.81	6 (8%)
2	NAP	F	2405	-	50,52,52	2.42	11 (22%)	71,80,80	1.86	9 (12%)
3	ADQ	F	2505	-	40,41,41	1.51	7 (17%)	60,63,63	1.86	13 (21%)
3	ADQ	E	2504	-	28,29,41	1.42	5 (17%)	43,45,63	1.98	9 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	E	2404	-	-	8/35/67/67	0/5/5/5
2	NAP	I	2408	-	-	8/35/67/67	0/5/5/5
2	NAP	D	2403	-	-	3/35/67/67	0/5/5/5
2	NAP	B	2401	-	-	2/35/67/67	0/5/5/5
3	ADQ	G	2506	-	-	1/16/32/59	0/3/3/4
3	ADQ	D	2503	-	-	8/23/59/59	0/4/4/4
3	ADQ	A	2500	-	-	2/16/32/59	0/3/3/4
2	NAP	G	2406	-	1/1/12/12	12/35/67/67	0/5/5/5
3	ADQ	J	2509	-	-	4/16/32/59	0/3/3/4
2	NAP	C	2402	-	-	3/35/67/67	0/5/5/5
3	ADQ	C	2502	-	-	5/16/32/59	0/3/3/4
3	ADQ	H	2507	-	-	5/16/32/59	0/3/3/4
3	ADQ	I	2508	-	-	4/16/32/59	0/3/3/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADQ	B	2501	-	-	5/23/59/59	0/4/4/4
2	NAP	H	2407	-	-	7/35/67/67	0/5/5/5
2	NAP	A	2400	-	-	3/35/67/67	0/5/5/5
2	NAP	J	2409	-	-	5/35/67/67	0/5/5/5
2	NAP	F	2405	-	-	3/35/67/67	0/5/5/5
3	ADQ	F	2505	-	-	5/23/59/59	0/4/4/4
3	ADQ	E	2504	-	-	2/16/32/59	0/3/3/4

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2408	NAP	PA-O3	-10.01	1.48	1.59
2	B	2401	NAP	P2B-O2B	9.33	1.75	1.59
2	J	2409	NAP	P2B-O2B	9.26	1.75	1.59
2	H	2407	NAP	P2B-O2B	9.06	1.75	1.59
2	E	2404	NAP	P2B-O2B	8.71	1.74	1.59
2	I	2408	NAP	P2B-O2B	8.52	1.74	1.59
2	A	2400	NAP	P2B-O2B	8.46	1.74	1.59
2	C	2402	NAP	P2B-O2B	8.41	1.74	1.59
2	F	2405	NAP	P2B-O2B	8.33	1.74	1.59
2	E	2404	NAP	PA-O3	-8.31	1.50	1.59
2	B	2401	NAP	PA-O3	-8.28	1.50	1.59
2	B	2401	NAP	C2N-N1N	8.11	1.43	1.35
2	D	2403	NAP	P2B-O2B	8.10	1.73	1.59
2	A	2400	NAP	C2N-N1N	8.07	1.43	1.35
2	F	2405	NAP	C2N-N1N	7.98	1.43	1.35
2	D	2403	NAP	C2N-N1N	7.83	1.43	1.35
2	D	2403	NAP	PA-O3	-7.73	1.51	1.59
2	G	2406	NAP	C2N-N1N	7.57	1.43	1.35
2	C	2402	NAP	C2N-N1N	7.47	1.43	1.35
2	H	2407	NAP	C2N-N1N	7.41	1.43	1.35
2	I	2408	NAP	C2N-N1N	7.40	1.43	1.35
2	J	2409	NAP	PA-O3	-7.37	1.51	1.59
2	H	2407	NAP	PA-O3	-7.05	1.51	1.59
2	G	2406	NAP	C3N-C7N	7.03	1.61	1.50
2	J	2409	NAP	C2N-N1N	7.02	1.42	1.35
2	A	2400	NAP	PA-O3	-6.96	1.52	1.59
2	G	2406	NAP	PA-O3	-6.59	1.52	1.59
2	J	2409	NAP	C3N-C7N	6.24	1.59	1.50
2	G	2406	NAP	P2B-O2B	6.18	1.70	1.59
2	E	2404	NAP	C2N-N1N	6.00	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2402	NAP	PA-O3	-5.97	1.53	1.59
2	E	2404	NAP	C3N-C7N	5.88	1.59	1.50
2	A	2400	NAP	C3N-C7N	5.87	1.59	1.50
2	D	2403	NAP	C3N-C7N	5.54	1.58	1.50
2	I	2408	NAP	C3N-C7N	5.52	1.58	1.50
2	F	2405	NAP	C3N-C7N	5.36	1.58	1.50
2	F	2405	NAP	PA-O3	-5.26	1.53	1.59
2	C	2402	NAP	C3N-C7N	4.92	1.57	1.50
2	H	2407	NAP	C3N-C7N	4.88	1.57	1.50
2	B	2401	NAP	C3N-C7N	4.87	1.57	1.50
2	E	2404	NAP	C4N-C3N	4.80	1.46	1.39
2	I	2408	NAP	PN-O3	-4.68	1.54	1.59
3	D	2503	ADQ	PB-O3A	-4.65	1.54	1.59
2	J	2409	NAP	C4N-C3N	4.64	1.46	1.39
3	E	2504	ADQ	C5-N7	-4.56	1.30	1.39
2	I	2408	NAP	C4N-C3N	4.14	1.45	1.39
3	A	2500	ADQ	C5-N7	-4.12	1.31	1.39
2	G	2406	NAP	C4N-C3N	4.11	1.45	1.39
3	D	2503	ADQ	PB-O3B	-4.01	1.47	1.59
2	A	2400	NAP	C4N-C3N	4.01	1.45	1.39
3	B	2501	ADQ	C5-N7	-3.96	1.31	1.39
3	D	2503	ADQ	PA-O3A	-3.89	1.55	1.59
2	H	2407	NAP	C4N-C3N	3.84	1.45	1.39
2	F	2405	NAP	C4N-C3N	3.84	1.45	1.39
2	A	2400	NAP	C3B-C2B	3.81	1.61	1.53
2	D	2403	NAP	C4N-C3N	3.81	1.45	1.39
3	J	2509	ADQ	C5-N7	-3.81	1.32	1.39
3	F	2505	ADQ	C5-N7	-3.77	1.32	1.39
3	H	2507	ADQ	C5-N7	-3.76	1.32	1.39
2	G	2406	NAP	C5N-C4N	3.68	1.45	1.38
2	F	2405	NAP	C5N-C4N	3.67	1.45	1.38
2	E	2404	NAP	C5N-C4N	3.63	1.45	1.38
2	J	2409	NAP	C3B-C2B	3.59	1.60	1.53
2	D	2403	NAP	C3B-C2B	3.49	1.60	1.53
2	C	2402	NAP	C4N-C3N	3.46	1.44	1.39
2	C	2402	NAP	C2A-N1A	3.45	1.40	1.33
2	H	2407	NAP	C3B-C2B	3.41	1.60	1.53
2	A	2400	NAP	C5N-C4N	3.40	1.44	1.38
2	B	2401	NAP	C7N-N7N	3.39	1.39	1.33
3	G	2506	ADQ	C5-N7	-3.39	1.32	1.39
2	I	2408	NAP	C3B-C2B	3.38	1.60	1.53
2	D	2403	NAP	C5N-C4N	3.37	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2404	NAP	C3B-C2B	3.36	1.60	1.53
2	D	2403	NAP	PN-O3	-3.36	1.55	1.59
2	G	2406	NAP	C2A-N1A	3.34	1.39	1.33
2	F	2405	NAP	C7N-N7N	3.31	1.39	1.33
2	I	2408	NAP	C5N-C4N	3.29	1.44	1.38
3	C	2502	ADQ	C5-N7	-3.29	1.33	1.39
2	J	2409	NAP	C5N-C4N	3.29	1.44	1.38
2	J	2409	NAP	C2A-N1A	3.28	1.39	1.33
3	F	2505	ADQ	C3'-C2'	3.20	1.60	1.52
3	F	2505	ADQ	PB-O3B	-3.20	1.49	1.59
2	E	2404	NAP	C7N-N7N	3.17	1.38	1.33
2	E	2404	NAP	PN-O3	-3.15	1.56	1.59
2	J	2409	NAP	C7N-N7N	3.13	1.38	1.33
3	D	2503	ADQ	C5-N7	-3.11	1.33	1.39
2	D	2403	NAP	C2A-N1A	3.11	1.39	1.33
2	B	2401	NAP	PN-O3	-3.10	1.56	1.59
2	A	2400	NAP	C7N-N7N	3.09	1.38	1.33
2	F	2405	NAP	C3B-C2B	3.07	1.59	1.53
3	A	2500	ADQ	C1D-N9	3.06	1.54	1.46
2	B	2401	NAP	C4N-C3N	3.05	1.44	1.39
2	D	2403	NAP	C7N-N7N	3.05	1.38	1.33
2	H	2407	NAP	C7N-N7N	3.01	1.38	1.33
2	H	2407	NAP	C2A-N1A	3.00	1.39	1.33
2	A	2400	NAP	C2A-N1A	2.97	1.39	1.33
2	C	2402	NAP	C3B-C2B	2.97	1.59	1.53
2	G	2406	NAP	C7N-N7N	2.94	1.38	1.33
2	I	2408	NAP	C7N-N7N	2.93	1.38	1.33
3	J	2509	ADQ	C1D-N9	2.93	1.54	1.46
3	I	2508	ADQ	C4-N9	-2.93	1.31	1.37
3	H	2507	ADQ	PB-O2B	2.91	1.65	1.54
3	C	2502	ADQ	PB-O2B	2.87	1.65	1.54
3	D	2503	ADQ	C4-N9	-2.84	1.31	1.37
2	I	2408	NAP	C6N-N1N	2.82	1.41	1.35
3	D	2503	ADQ	C1D-N9	2.82	1.54	1.46
3	F	2505	ADQ	C1D-N9	2.80	1.54	1.46
3	B	2501	ADQ	PB-O3B	-2.80	1.50	1.59
2	B	2401	NAP	C2A-N1A	2.77	1.38	1.33
2	B	2401	NAP	C3B-C2B	2.77	1.59	1.53
2	B	2401	NAP	C5N-C4N	2.76	1.43	1.38
3	A	2500	ADQ	PB-O2B	2.74	1.65	1.54
2	F	2405	NAP	C2A-N1A	2.70	1.38	1.33
3	I	2508	ADQ	C5-N7	-2.70	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2403	NAP	P2B-O3X	-2.70	1.44	1.54
2	G	2406	NAP	PN-O3	-2.67	1.56	1.59
2	C	2402	NAP	C5N-C4N	2.67	1.43	1.38
2	I	2408	NAP	C2A-N1A	2.67	1.38	1.33
2	C	2402	NAP	C7N-N7N	2.66	1.37	1.33
2	H	2407	NAP	C5N-C4N	2.66	1.43	1.38
2	I	2408	NAP	P2B-O3X	-2.56	1.45	1.54
3	D	2503	ADQ	C4'-C5'	2.54	1.58	1.53
2	G	2406	NAP	O4D-C1D	2.53	1.44	1.40
3	G	2506	ADQ	C4-N9	-2.50	1.32	1.37
2	E	2404	NAP	C2A-N1A	2.50	1.38	1.33
2	A	2400	NAP	O4D-C1D	2.48	1.44	1.40
2	G	2406	NAP	P2B-O3X	-2.48	1.45	1.54
2	J	2409	NAP	C6N-N1N	2.47	1.41	1.35
3	J	2509	ADQ	PB-O2B	2.46	1.63	1.54
2	A	2400	NAP	P2B-O3X	-2.45	1.45	1.54
3	E	2504	ADQ	C8-N9	-2.45	1.33	1.37
2	C	2402	NAP	P2B-O3X	-2.42	1.45	1.54
3	C	2502	ADQ	C4-N9	-2.41	1.32	1.37
2	E	2404	NAP	C6N-N1N	2.41	1.40	1.35
2	E	2404	NAP	P2B-O3X	-2.40	1.45	1.54
2	D	2403	NAP	C6N-N1N	2.39	1.40	1.35
2	A	2400	NAP	C5B-C4B	2.37	1.58	1.51
3	H	2507	ADQ	C1D-N9	2.36	1.52	1.46
3	I	2508	ADQ	PB-O2B	2.35	1.63	1.54
3	G	2506	ADQ	PB-O2B	2.30	1.63	1.54
2	F	2405	NAP	P2B-O3X	-2.30	1.46	1.54
2	D	2403	NAP	O4D-C1D	2.29	1.43	1.40
3	I	2508	ADQ	PA-O3A	-2.28	1.57	1.59
3	E	2504	ADQ	C1D-N9	2.28	1.52	1.46
3	G	2506	ADQ	O4D-C1D	2.27	1.47	1.42
2	J	2409	NAP	P2B-O3X	-2.26	1.46	1.54
3	F	2505	ADQ	C4-N9	-2.25	1.33	1.37
2	A	2400	NAP	C6N-N1N	2.21	1.40	1.35
3	C	2502	ADQ	C1D-N9	2.21	1.52	1.46
2	G	2406	NAP	C6N-N1N	2.21	1.40	1.35
2	B	2401	NAP	C5B-C4B	2.20	1.58	1.51
3	E	2504	ADQ	C4-N9	-2.20	1.33	1.37
2	H	2407	NAP	C6N-N1N	2.20	1.40	1.35
2	G	2406	NAP	C3B-C2B	2.20	1.57	1.53
3	G	2506	ADQ	C1D-N9	2.19	1.52	1.46
2	H	2407	NAP	P2B-O3X	-2.18	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2405	NAP	C6N-N1N	2.17	1.40	1.35
3	B	2501	ADQ	C3'-C2'	2.14	1.57	1.52
3	F	2505	ADQ	C4'-C3'	2.12	1.57	1.52
2	C	2402	NAP	C6N-N1N	2.11	1.40	1.35
3	D	2503	ADQ	O2'-C2'	2.08	1.48	1.43
3	F	2505	ADQ	O2'-C2'	2.08	1.48	1.43
2	G	2406	NAP	O4B-C1B	2.08	1.46	1.42
2	B	2401	NAP	P2B-O3X	-2.07	1.47	1.54
3	I	2508	ADQ	PA-O2A	-2.05	1.45	1.55
3	E	2504	ADQ	PB-O2B	2.04	1.62	1.54
3	H	2507	ADQ	O4D-C1D	2.03	1.46	1.42
2	H	2407	NAP	PN-O3	-2.02	1.57	1.59

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	C5N-C4N-C3N	-9.13	111.39	120.36
2	J	2409	NAP	C5N-C4N-C3N	-9.02	111.50	120.36
2	E	2404	NAP	C5N-C4N-C3N	-8.97	111.55	120.36
2	B	2401	NAP	C5N-C4N-C3N	-8.96	111.56	120.36
2	H	2407	NAP	C5N-C4N-C3N	-8.88	111.63	120.36
2	C	2402	NAP	C5N-C4N-C3N	-8.83	111.68	120.36
2	A	2400	NAP	C5N-C4N-C3N	-8.83	111.68	120.36
2	I	2408	NAP	C5N-C4N-C3N	-8.63	111.88	120.36
2	G	2406	NAP	C5N-C4N-C3N	-8.48	112.03	120.36
2	D	2403	NAP	C5N-C4N-C3N	-8.32	112.19	120.36
3	D	2503	ADQ	O3B-C1'-C2'	7.42	121.97	108.38
2	C	2402	NAP	C2N-C3N-C4N	6.30	125.59	118.26
2	B	2401	NAP	C2N-C3N-C4N	6.28	125.57	118.26
2	I	2408	NAP	C2N-C3N-C4N	6.27	125.55	118.26
2	H	2407	NAP	C2N-C3N-C4N	6.24	125.52	118.26
3	J	2509	ADQ	N3-C2-N1	-6.20	119.20	128.58
3	F	2505	ADQ	N3-C2-N1	-6.15	119.27	128.58
2	J	2409	NAP	C2N-C3N-C4N	6.11	125.36	118.26
2	E	2404	NAP	C2N-C3N-C4N	6.10	125.35	118.26
3	E	2504	ADQ	N3-C2-N1	-6.08	119.38	128.58
3	A	2500	ADQ	C5-C4-N3	-6.05	118.38	126.72
3	B	2501	ADQ	N3-C2-N1	-6.02	119.47	128.58
3	D	2503	ADQ	N3-C2-N1	-6.01	119.48	128.58
3	A	2500	ADQ	N3-C2-N1	-6.01	119.48	128.58
3	H	2507	ADQ	N3-C2-N1	-6.00	119.50	128.58
3	C	2502	ADQ	N3-C2-N1	-5.98	119.53	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	C2N-C3N-C4N	5.97	125.21	118.26
3	G	2506	ADQ	N3-C2-N1	-5.92	119.62	128.58
2	D	2403	NAP	C2N-C3N-C4N	5.86	125.08	118.26
2	A	2400	NAP	C2N-C3N-C4N	5.83	125.04	118.26
3	B	2501	ADQ	C5-C4-N3	-5.78	118.76	126.72
3	H	2507	ADQ	C5-C4-N3	-5.76	118.78	126.72
3	I	2508	ADQ	N3-C2-N1	-5.75	119.88	128.58
3	J	2509	ADQ	C5-C4-N3	-5.74	118.81	126.72
3	E	2504	ADQ	C5-C4-N3	-5.70	118.87	126.72
3	F	2505	ADQ	C5-C4-N3	-5.63	118.96	126.72
3	G	2506	ADQ	C5-C4-N3	-5.60	119.00	126.72
2	G	2406	NAP	C2N-C3N-C4N	5.60	124.77	118.26
3	C	2502	ADQ	C5-C4-N3	-5.38	119.31	126.72
3	D	2503	ADQ	C5-C4-N3	-5.28	119.44	126.72
2	F	2405	NAP	C6N-C5N-C4N	5.24	127.01	119.45
3	I	2508	ADQ	C5-C4-N3	-5.24	119.51	126.72
2	B	2401	NAP	C6N-C5N-C4N	5.08	126.77	119.45
2	A	2400	NAP	C6N-C5N-C4N	5.04	126.71	119.45
2	H	2407	NAP	C6N-C5N-C4N	4.95	126.59	119.45
2	C	2402	NAP	C6N-C5N-C4N	4.95	126.58	119.45
2	G	2406	NAP	C6N-C5N-C4N	4.84	126.43	119.45
2	J	2409	NAP	C6N-C5N-C4N	4.78	126.34	119.45
2	D	2403	NAP	C6N-C5N-C4N	4.70	126.22	119.45
2	I	2408	NAP	C6N-C5N-C4N	4.64	126.13	119.45
3	G	2506	ADQ	C2-N3-C4	4.60	123.06	111.83
3	J	2509	ADQ	C2-N3-C4	4.55	122.94	111.83
3	B	2501	ADQ	C2-N3-C4	4.53	122.90	111.83
3	F	2505	ADQ	C2-N3-C4	4.52	122.87	111.83
3	A	2500	ADQ	C2-N3-C4	4.50	122.83	111.83
3	H	2507	ADQ	C2-N3-C4	4.45	122.69	111.83
3	C	2502	ADQ	C2-N3-C4	4.38	122.53	111.83
3	I	2508	ADQ	C2-N3-C4	4.37	122.51	111.83
2	E	2404	NAP	C6N-C5N-C4N	4.37	125.75	119.45
3	D	2503	ADQ	C2-N3-C4	4.37	122.50	111.83
3	E	2504	ADQ	C2-N3-C4	4.35	122.47	111.83
3	A	2500	ADQ	N3-C4-N9	4.12	134.17	127.17
2	F	2405	NAP	O4B-C1B-N9A	-4.05	100.31	108.09
3	E	2504	ADQ	N3-C4-N9	4.03	134.03	127.17
3	H	2507	ADQ	N3-C4-N9	4.02	134.01	127.17
2	C	2402	NAP	O4B-C1B-N9A	-3.99	100.42	108.09
3	J	2509	ADQ	N3-C4-N9	3.89	133.78	127.17
3	B	2501	ADQ	N3-C4-N9	3.86	133.74	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	2409	NAP	O4B-C1B-N9A	-3.73	100.93	108.09
3	F	2505	ADQ	N3-C4-N9	3.72	133.50	127.17
3	C	2502	ADQ	N3-C4-N9	3.61	133.31	127.17
2	D	2403	NAP	O4B-C1B-N9A	-3.60	101.18	108.09
3	I	2508	ADQ	N9-C8-N7	-3.58	108.85	113.94
3	D	2503	ADQ	C4-C5-N7	-3.56	106.51	110.58
3	G	2506	ADQ	N3-C4-N9	3.55	133.20	127.17
3	J	2509	ADQ	C5-N7-C8	3.48	108.92	103.45
3	B	2501	ADQ	O4'-C4'-C3'	3.46	118.53	110.38
3	B	2501	ADQ	C5-N7-C8	3.46	108.88	103.45
3	D	2503	ADQ	N9-C8-N7	-3.46	109.03	113.94
3	I	2508	ADQ	C4-C5-N7	-3.45	106.64	110.58
3	B	2501	ADQ	C4-C5-N7	-3.43	106.66	110.58
3	I	2508	ADQ	N3-C4-N9	3.40	132.95	127.17
3	A	2500	ADQ	C5-N7-C8	3.38	108.77	103.45
3	J	2509	ADQ	C4-C5-N7	-3.31	106.80	110.58
3	H	2507	ADQ	C5-N7-C8	3.29	108.62	103.45
3	E	2504	ADQ	C5-N7-C8	3.27	108.59	103.45
3	E	2504	ADQ	C4-C5-N7	-3.25	106.86	110.58
3	B	2501	ADQ	N9-C8-N7	-3.25	109.32	113.94
3	I	2508	ADQ	C5-N7-C8	3.25	108.56	103.45
3	A	2500	ADQ	C4-C5-N7	-3.19	106.94	110.58
3	F	2505	ADQ	C5-N7-C8	3.17	108.44	103.45
3	F	2505	ADQ	C4-C5-N7	-3.17	106.96	110.58
3	C	2502	ADQ	N9-C8-N7	-3.15	109.46	113.94
3	J	2509	ADQ	N9-C8-N7	-3.15	109.46	113.94
3	D	2503	ADQ	C5-N7-C8	3.15	108.41	103.45
3	D	2503	ADQ	N3-C4-N9	3.13	132.49	127.17
3	C	2502	ADQ	C4-C5-N7	-3.13	107.00	110.58
3	C	2502	ADQ	C5-N7-C8	3.12	108.36	103.45
3	H	2507	ADQ	C4-C5-N7	-3.10	107.04	110.58
3	D	2503	ADQ	C1'-O5'-C5'	3.09	119.75	113.72
3	F	2505	ADQ	O4'-C4'-C3'	3.06	117.59	110.38
3	H	2507	ADQ	N9-C8-N7	-3.06	109.60	113.94
3	G	2506	ADQ	N9-C8-N7	-3.05	109.60	113.94
3	G	2506	ADQ	C4-C5-N7	-2.98	107.17	110.58
3	D	2503	ADQ	PB-O3B-C1'	2.97	133.30	121.21
2	G	2406	NAP	C2B-C3B-C4B	-2.92	95.71	101.99
3	F	2505	ADQ	N9-C8-N7	-2.91	109.81	113.94
2	G	2406	NAP	O2B-P2B-O1X	-2.90	99.01	109.33
3	D	2503	ADQ	O4'-C4'-C3'	2.89	117.18	110.38
2	E	2404	NAP	O4B-C1B-N9A	-2.87	102.58	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2506	ADQ	C5-N7-C8	2.86	107.94	103.45
2	F	2405	NAP	O2B-P2B-O1X	-2.86	99.15	109.33
2	A	2400	NAP	O2B-P2B-O1X	-2.82	99.28	109.33
2	B	2401	NAP	O4B-C1B-N9A	-2.78	102.74	108.09
2	I	2408	NAP	O4B-C1B-N9A	-2.77	102.78	108.09
3	B	2501	ADQ	O5'-C5'-C4'	2.76	114.68	109.70
2	D	2403	NAP	O2B-P2B-O1X	-2.72	99.63	109.33
3	D	2503	ADQ	O5'-C5'-C4'	2.69	114.55	109.70
2	G	2406	NAP	O2N-PN-O3	2.68	114.51	107.27
3	A	2500	ADQ	N9-C8-N7	-2.67	110.15	113.94
3	E	2504	ADQ	N9-C8-N7	-2.65	110.17	113.94
3	E	2504	ADQ	O3B-PB-O3A	2.65	113.53	104.64
3	I	2508	ADQ	C4-N9-C8	2.54	108.40	105.74
2	A	2400	NAP	O4B-C1B-N9A	-2.53	103.23	108.09
3	F	2505	ADQ	O3B-C1'-C2'	2.52	112.99	108.38
3	F	2505	ADQ	C1'-C2'-C3'	2.49	115.25	110.01
3	B	2501	ADQ	O3B-C1'-C2'	2.46	112.89	108.38
2	H	2407	NAP	O2B-P2B-O1X	-2.45	100.59	109.33
3	H	2507	ADQ	O3B-PB-O3A	2.45	112.86	104.64
3	G	2506	ADQ	O3B-PB-O3A	2.43	112.77	104.64
2	I	2408	NAP	O5B-C5B-C4B	-2.42	100.75	108.99
3	B	2501	ADQ	C2D-C3D-C4D	2.41	107.27	102.61
3	F	2505	ADQ	C1'-O5'-C5'	2.35	118.31	113.72
2	H	2407	NAP	O4B-C1B-N9A	-2.35	103.58	108.09
2	I	2408	NAP	O2B-P2B-O1X	-2.34	101.00	109.33
2	E	2404	NAP	C3B-C2B-C1B	-2.34	98.33	102.81
3	J	2509	ADQ	C2D-C3D-C4D	2.33	107.11	102.61
2	F	2405	NAP	C3B-C2B-C1B	-2.32	98.37	102.81
3	E	2504	ADQ	C2D-C3D-C4D	2.31	107.08	102.61
2	G	2406	NAP	N6A-C6A-N1A	2.31	123.51	118.38
3	A	2500	ADQ	C2D-C3D-C4D	2.30	107.06	102.61
2	E	2404	NAP	O5B-C5B-C4B	-2.28	101.22	108.99
3	I	2508	ADQ	O3B-PB-O3A	2.27	112.24	104.64
3	A	2500	ADQ	O3B-PB-O3A	2.26	112.22	104.64
2	J	2409	NAP	O2B-P2B-O1X	-2.26	101.28	109.33
3	B	2501	ADQ	C1'-O5'-C5'	2.25	118.12	113.72
2	A	2400	NAP	O2N-PN-O3	2.25	113.36	107.27
2	H	2407	NAP	O3B-C3B-C2B	2.25	117.47	111.19
2	J	2409	NAP	N6A-C6A-N1A	2.24	123.37	118.38
2	B	2401	NAP	N6A-C6A-N1A	2.24	123.37	118.38
2	E	2404	NAP	N6A-C6A-N1A	2.24	123.37	118.38
2	I	2408	NAP	N6A-C6A-N1A	2.24	123.36	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2405	NAP	N6A-C6A-N1A	2.22	123.32	118.38
2	G	2406	NAP	P2B-O2B-C2B	-2.21	117.53	123.43
3	D	2503	ADQ	C6-C5-N7	2.20	136.34	132.09
2	E	2404	NAP	O2B-P2B-O1X	-2.19	101.53	109.33
2	G	2406	NAP	C5N-C6N-N1N	-2.19	117.39	120.38
2	C	2402	NAP	N6A-C6A-N1A	2.18	123.24	118.38
2	F	2405	NAP	O5B-C5B-C4B	-2.18	101.58	108.99
2	F	2405	NAP	O7N-C7N-N7N	2.17	125.75	122.62
2	C	2402	NAP	O3B-C3B-C2B	2.17	117.25	111.19
2	A	2400	NAP	N6A-C6A-N1A	2.15	123.18	118.38
2	H	2407	NAP	O7N-C7N-N7N	2.15	125.72	122.62
2	G	2406	NAP	O3X-P2B-O2X	2.14	115.84	107.80
3	F	2505	ADQ	O5'-C5'-C4'	2.14	113.56	109.70
3	D	2503	ADQ	C4-N9-C8	2.14	107.98	105.74
2	I	2408	NAP	O3X-P2B-O2X	2.14	115.81	107.80
3	H	2507	ADQ	O2D-C2D-C1D	2.12	117.42	110.10
2	E	2404	NAP	O3X-P2B-O2X	2.11	115.73	107.80
2	A	2400	NAP	O3X-P2B-O2X	2.11	115.73	107.80
2	D	2403	NAP	O2N-PN-O3	2.11	112.98	107.27
2	A	2400	NAP	O7N-C7N-N7N	2.09	125.63	122.62
2	C	2402	NAP	O2B-P2B-O1X	-2.08	101.92	109.33
2	B	2401	NAP	O2B-P2B-O1X	-2.08	101.93	109.33
2	D	2403	NAP	N6A-C6A-N1A	2.08	123.00	118.38
2	E	2404	NAP	C2N-N1N-C1D	-2.07	114.56	119.13
3	D	2503	ADQ	C5-C4-N9	2.06	108.06	105.81
3	D	2503	ADQ	O4'-C4'-C5'	-2.06	104.25	109.32
2	C	2402	NAP	O3X-P2B-O2X	2.06	115.52	107.80
2	B	2401	NAP	O7N-C7N-N7N	2.06	125.59	122.62
2	B	2401	NAP	O3X-P2B-O2X	2.05	115.50	107.80
2	G	2406	NAP	O5B-C5B-C4B	-2.05	102.01	108.99
3	I	2508	ADQ	C2D-C3D-C4D	2.04	106.56	102.61
2	I	2408	NAP	O2N-PN-O3	2.03	112.77	107.27
3	F	2505	ADQ	O4'-C4'-C5'	-2.02	104.34	109.32
2	D	2403	NAP	O5B-C5B-C4B	-2.02	102.11	108.99
3	I	2508	ADQ	C6-C5-N7	2.02	135.99	132.09
2	A	2400	NAP	O3B-C3B-C2B	2.02	116.83	111.19
2	E	2404	NAP	O7N-C7N-N7N	2.02	125.53	122.62
3	B	2501	ADQ	O4'-C4'-C5'	-2.00	104.39	109.32

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
2	G	2406	NAP	C4B

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2400	NAP	C2B-C1B-N9A-C8A
2	B	2401	NAP	C2B-C1B-N9A-C8A
2	B	2401	NAP	C2B-C1B-N9A-C4A
2	C	2402	NAP	C2B-C1B-N9A-C8A
2	C	2402	NAP	C2B-C1B-N9A-C4A
2	D	2403	NAP	C2B-C1B-N9A-C8A
2	E	2404	NAP	C2B-C1B-N9A-C8A
2	E	2404	NAP	C5D-O5D-PN-O2N
2	F	2405	NAP	C2B-C1B-N9A-C8A
2	G	2406	NAP	C5D-O5D-PN-O3
2	G	2406	NAP	C5D-O5D-PN-O1N
2	G	2406	NAP	C5D-O5D-PN-O2N
2	H	2407	NAP	C2B-C1B-N9A-C8A
2	H	2407	NAP	C5D-O5D-PN-O3
2	H	2407	NAP	C5D-O5D-PN-O2N
2	I	2408	NAP	C5D-O5D-PN-O3
2	I	2408	NAP	C5D-O5D-PN-O2N
2	J	2409	NAP	C2B-C1B-N9A-C8A
3	A	2500	ADQ	PB-O3A-PA-O5D
3	B	2501	ADQ	C5D-O5D-PA-O1A
3	B	2501	ADQ	C5D-O5D-PA-O2A
3	B	2501	ADQ	C5D-O5D-PA-O3A
3	C	2502	ADQ	C5D-O5D-PA-O1A
3	C	2502	ADQ	C5D-O5D-PA-O2A
3	C	2502	ADQ	C5D-O5D-PA-O3A
3	D	2503	ADQ	C5D-O5D-PA-O1A
3	F	2505	ADQ	PA-O3A-PB-O3B
3	F	2505	ADQ	C5D-O5D-PA-O1A
3	H	2507	ADQ	C5D-O5D-PA-O1A
3	H	2507	ADQ	C5D-O5D-PA-O2A
3	H	2507	ADQ	O4D-C4D-C5D-O5D
3	H	2507	ADQ	C3D-C4D-C5D-O5D
3	I	2508	ADQ	C5D-O5D-PA-O1A
3	I	2508	ADQ	C5D-O5D-PA-O3A
3	J	2509	ADQ	C5D-O5D-PA-O2A
3	J	2509	ADQ	C5D-O5D-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	D	2503	ADQ	O5'-C5'-C6'-O6'
3	B	2501	ADQ	O5'-C5'-C6'-O6'
3	B	2501	ADQ	C4'-C5'-C6'-O6'
2	G	2406	NAP	O4B-C4B-C5B-O5B
3	D	2503	ADQ	O4D-C4D-C5D-O5D
3	E	2504	ADQ	O4D-C4D-C5D-O5D
2	A	2400	NAP	C2B-C1B-N9A-C4A
2	D	2403	NAP	C2B-C1B-N9A-C4A
2	E	2404	NAP	C2B-C1B-N9A-C4A
2	F	2405	NAP	C2B-C1B-N9A-C4A
2	G	2406	NAP	C2B-C1B-N9A-C4A
2	H	2407	NAP	C2B-C1B-N9A-C4A
2	I	2408	NAP	C2B-C1B-N9A-C4A
2	J	2409	NAP	C2B-C1B-N9A-C4A
2	G	2406	NAP	C2B-C1B-N9A-C8A
2	I	2408	NAP	C2B-C1B-N9A-C8A
2	G	2406	NAP	C3B-C4B-C5B-O5B
3	D	2503	ADQ	C3D-C4D-C5D-O5D
3	E	2504	ADQ	C3D-C4D-C5D-O5D
3	D	2503	ADQ	C4'-C5'-C6'-O6'
2	G	2406	NAP	C4B-C5B-O5B-PA
2	G	2406	NAP	PA-O3-PN-O2N
3	J	2509	ADQ	PB-O3A-PA-O1A
3	F	2505	ADQ	O4D-C4D-C5D-O5D
2	E	2404	NAP	C5D-O5D-PN-O3
2	E	2404	NAP	C5D-O5D-PN-O1N
2	G	2406	NAP	C5B-O5B-PA-O1A
2	H	2407	NAP	C5D-O5D-PN-O1N
2	I	2408	NAP	C5D-O5D-PN-O1N
3	D	2503	ADQ	C1'-O3B-PB-O3A
3	F	2505	ADQ	C5D-O5D-PA-O2A
3	H	2507	ADQ	C5D-O5D-PA-O3A
3	I	2508	ADQ	C5D-O5D-PA-O2A
2	E	2404	NAP	O4B-C4B-C5B-O5B
2	I	2408	NAP	O4B-C4B-C5B-O5B
3	D	2503	ADQ	PA-O3A-PB-O2B
3	C	2502	ADQ	PA-O3A-PB-O1B
2	C	2402	NAP	O4B-C4B-C5B-O5B
3	F	2505	ADQ	C3D-C4D-C5D-O5D
3	G	2506	ADQ	PB-O3A-PA-O1A
2	E	2404	NAP	C3B-C4B-C5B-O5B
2	I	2408	NAP	C3B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	J	2409	NAP	O4B-C4B-C5B-O5B
2	G	2406	NAP	PA-O3-PN-O1N
2	F	2405	NAP	O4B-C1B-N9A-C8A
2	G	2406	NAP	O4B-C1B-N9A-C8A
2	I	2408	NAP	O4B-C1B-N9A-C8A
2	H	2407	NAP	O4B-C4B-C5B-O5B
3	I	2508	ADQ	O4D-C4D-C5D-O5D
2	A	2400	NAP	C2B-O2B-P2B-O3X
2	J	2409	NAP	C2B-O2B-P2B-O2X
2	D	2403	NAP	O4B-C1B-N9A-C8A
2	E	2404	NAP	O4B-C1B-N9A-C8A
2	H	2407	NAP	O4B-C1B-N9A-C8A
2	J	2409	NAP	O4B-C1B-N9A-C8A
3	A	2500	ADQ	PB-O3A-PA-O2A
3	C	2502	ADQ	PB-O3A-PA-O2A
3	D	2503	ADQ	PA-O3A-PB-O1B
3	J	2509	ADQ	PB-O3A-PA-O2A

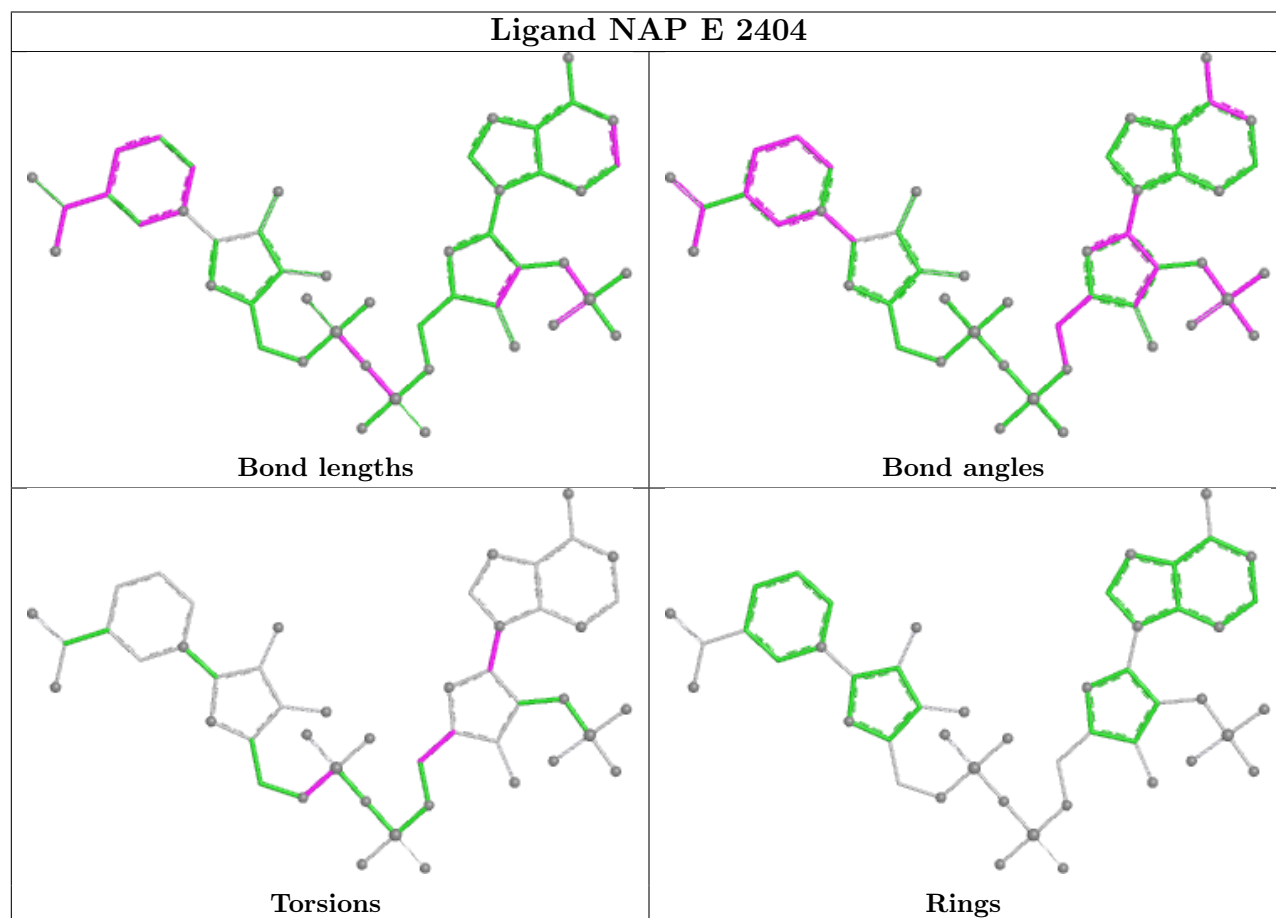
There are no ring outliers.

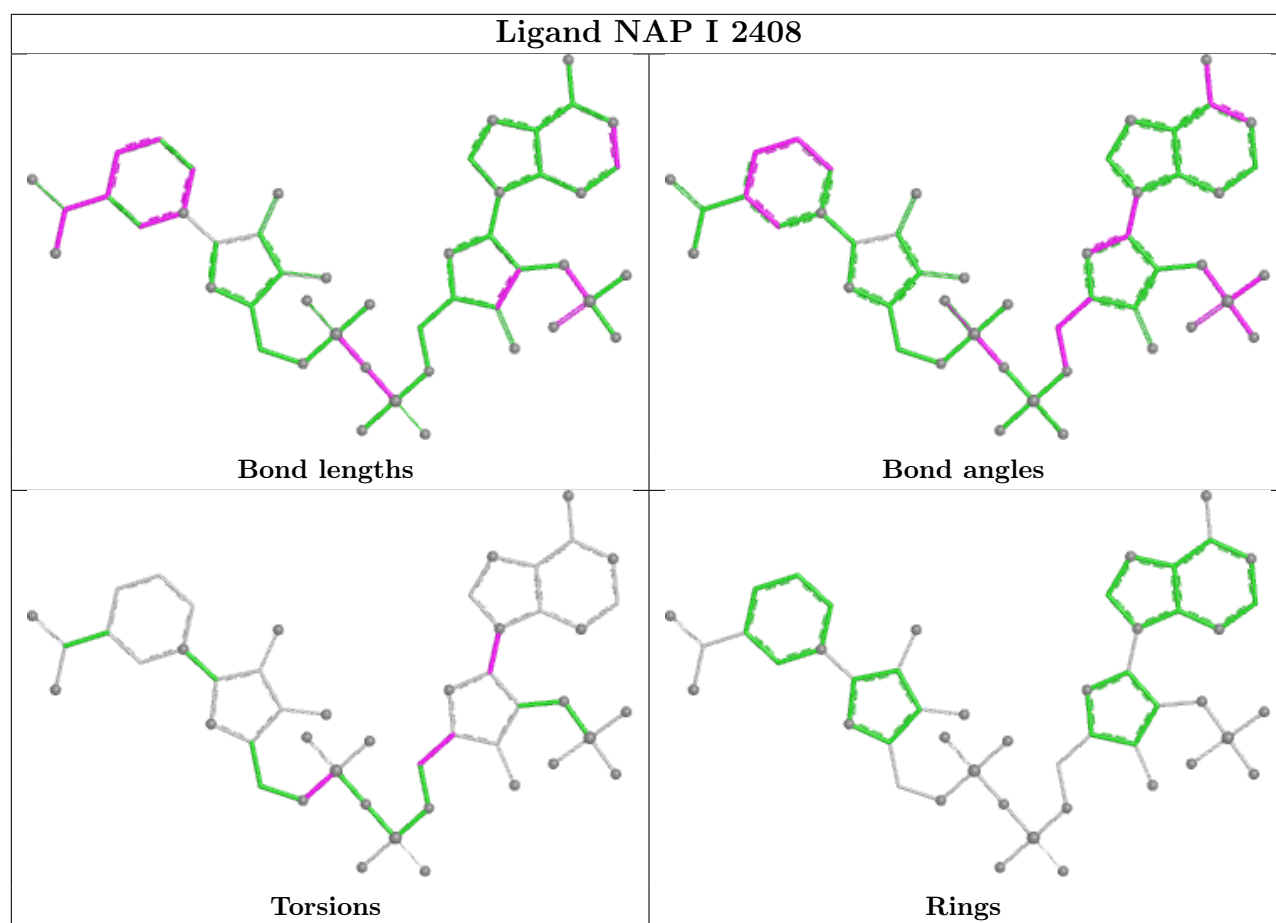
15 monomers are involved in 25 short contacts:

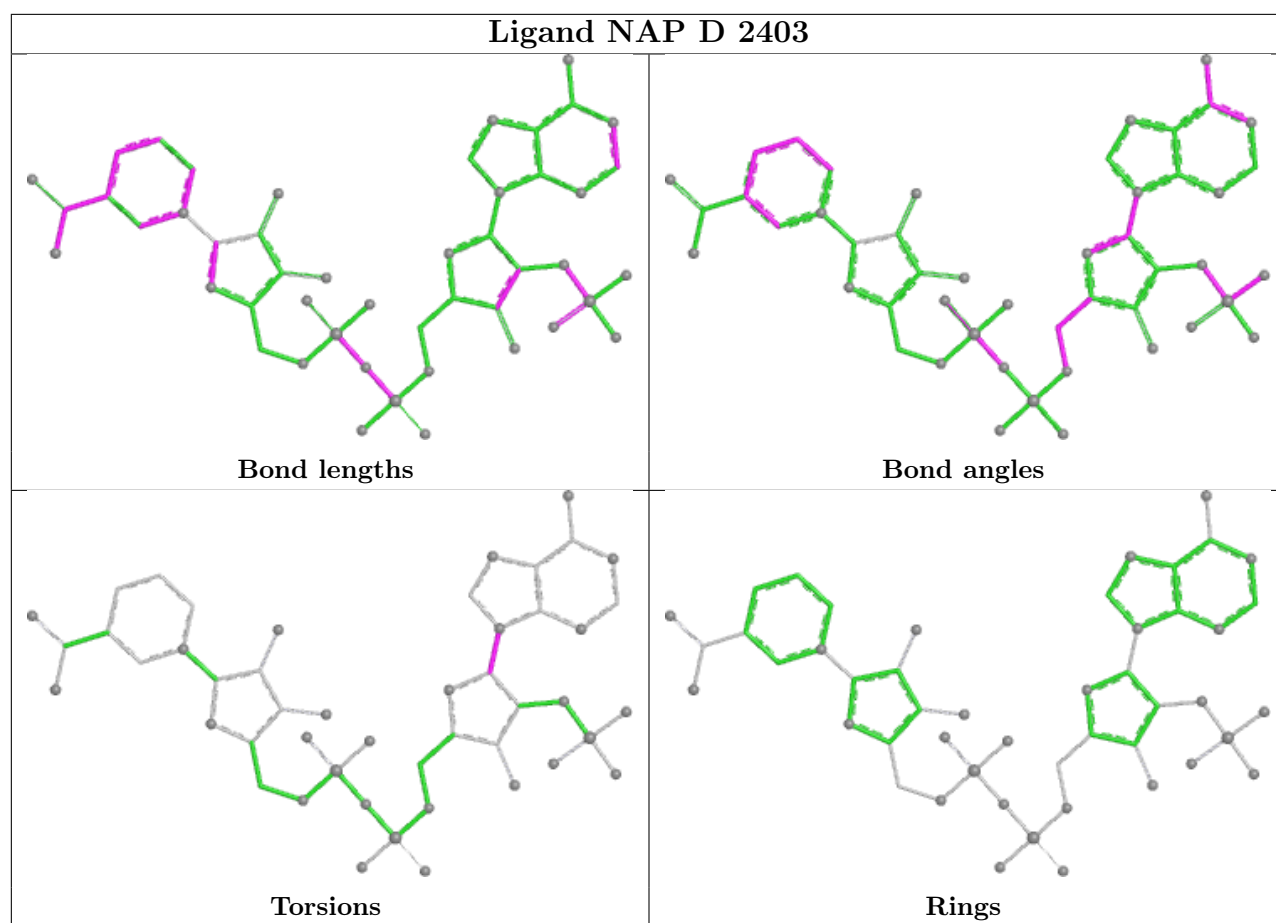
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2404	NAP	1	0
2	I	2408	NAP	1	0
2	B	2401	NAP	1	0
3	D	2503	ADQ	1	0
3	A	2500	ADQ	3	0
2	G	2406	NAP	1	0
3	C	2502	ADQ	2	0
3	H	2507	ADQ	1	0
3	I	2508	ADQ	3	0
3	B	2501	ADQ	2	0
2	H	2407	NAP	1	0
2	A	2400	NAP	1	0
2	F	2405	NAP	1	0
3	F	2505	ADQ	3	0
3	E	2504	ADQ	3	0

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

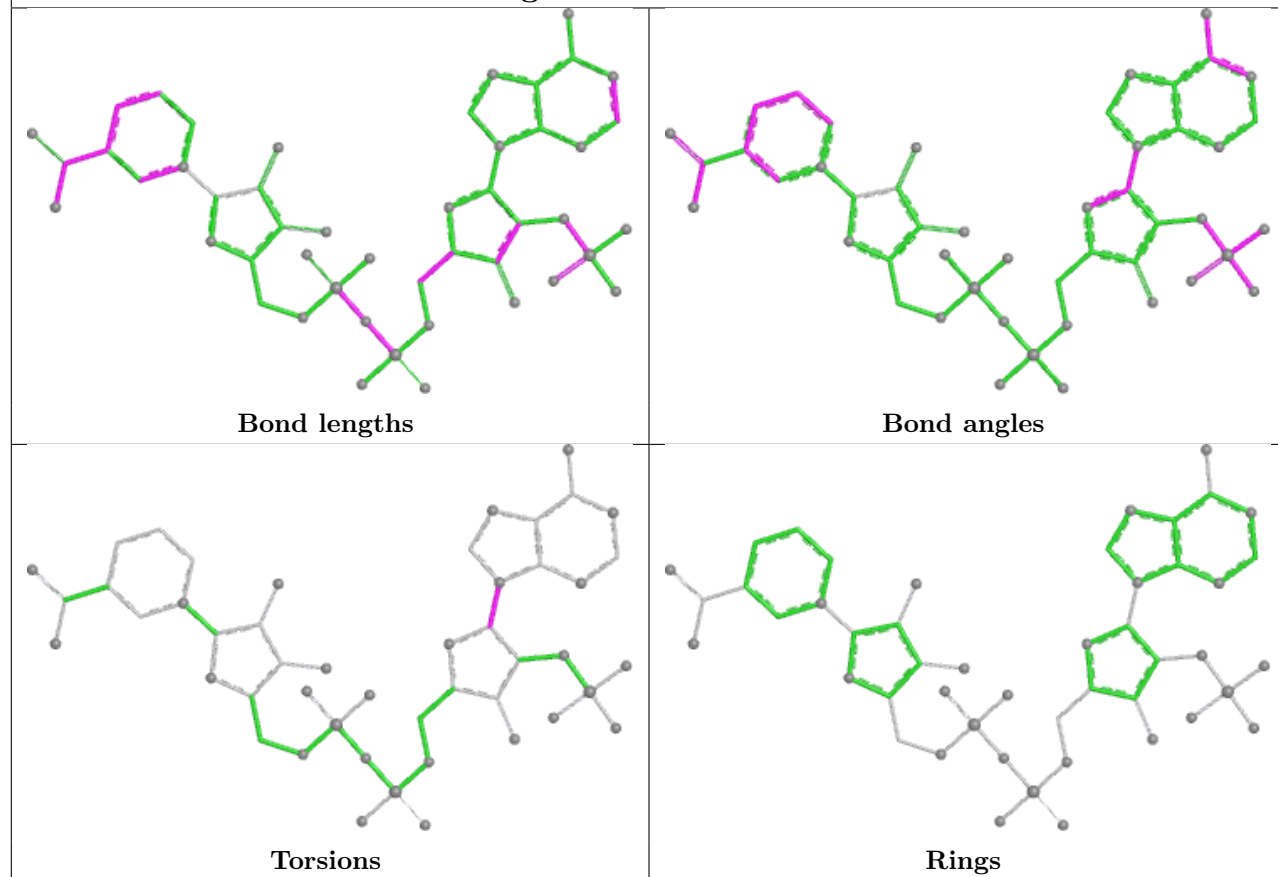
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



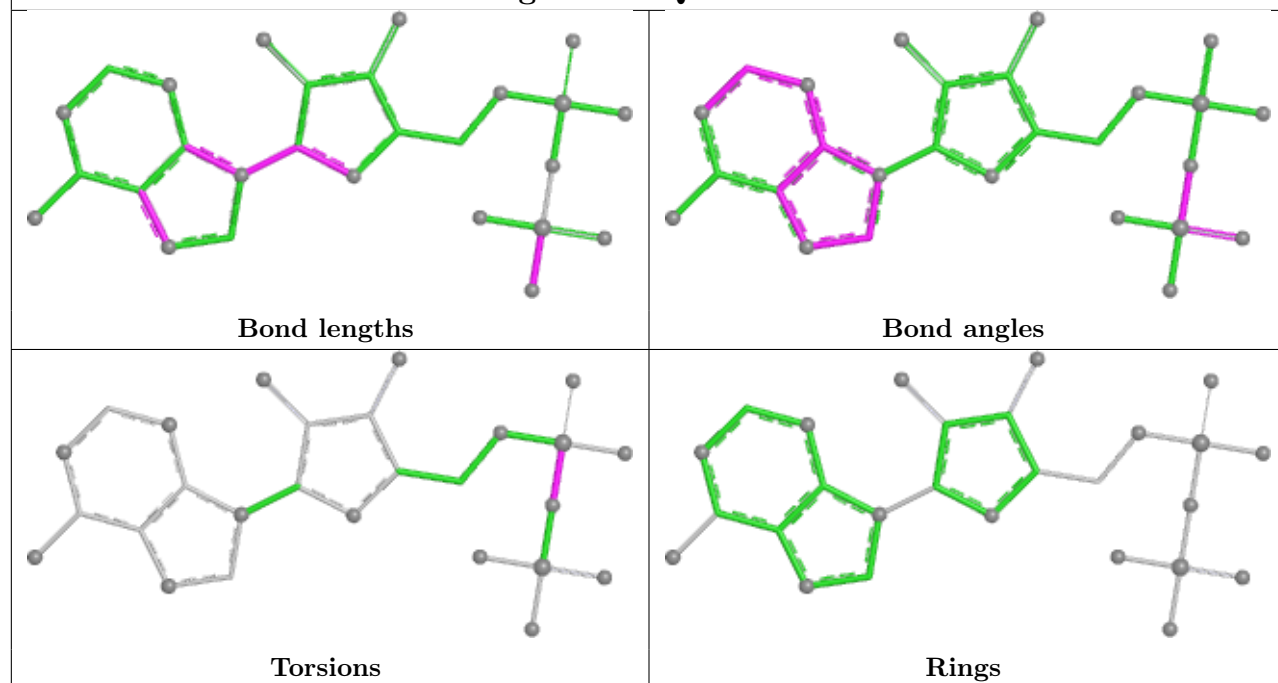




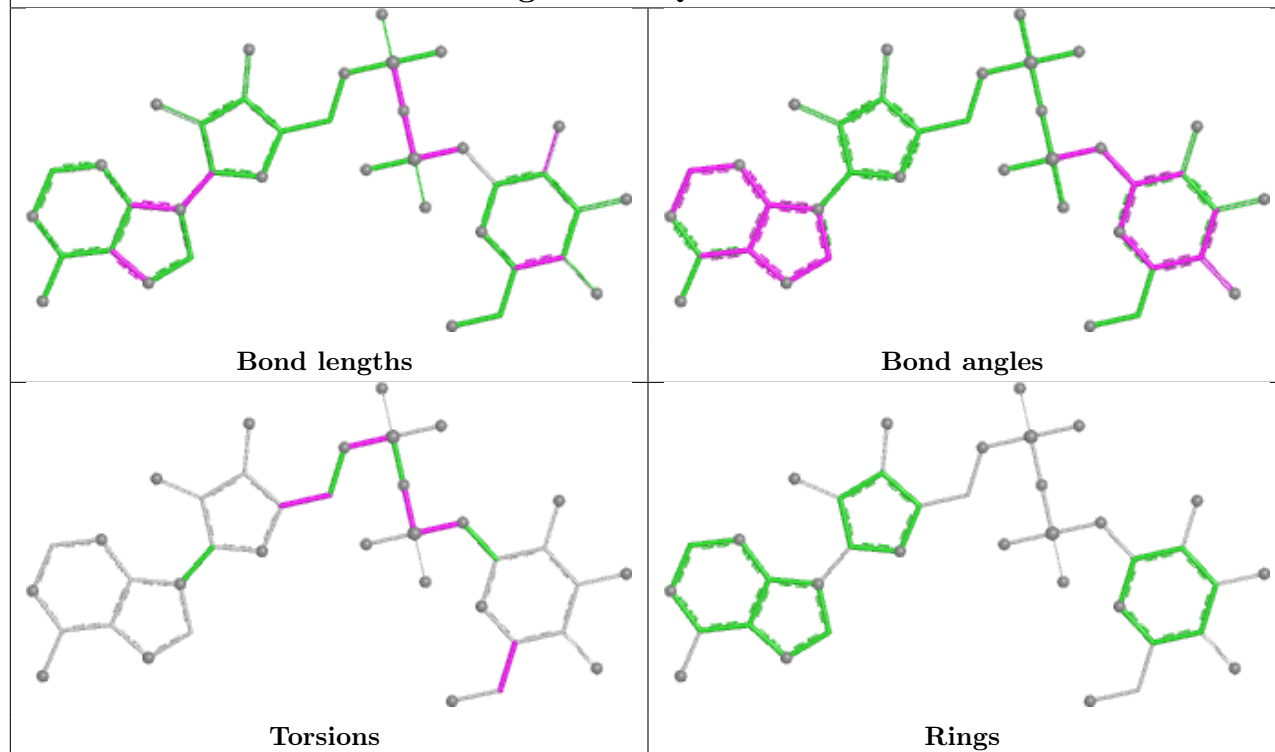
Ligand NAP B 2401



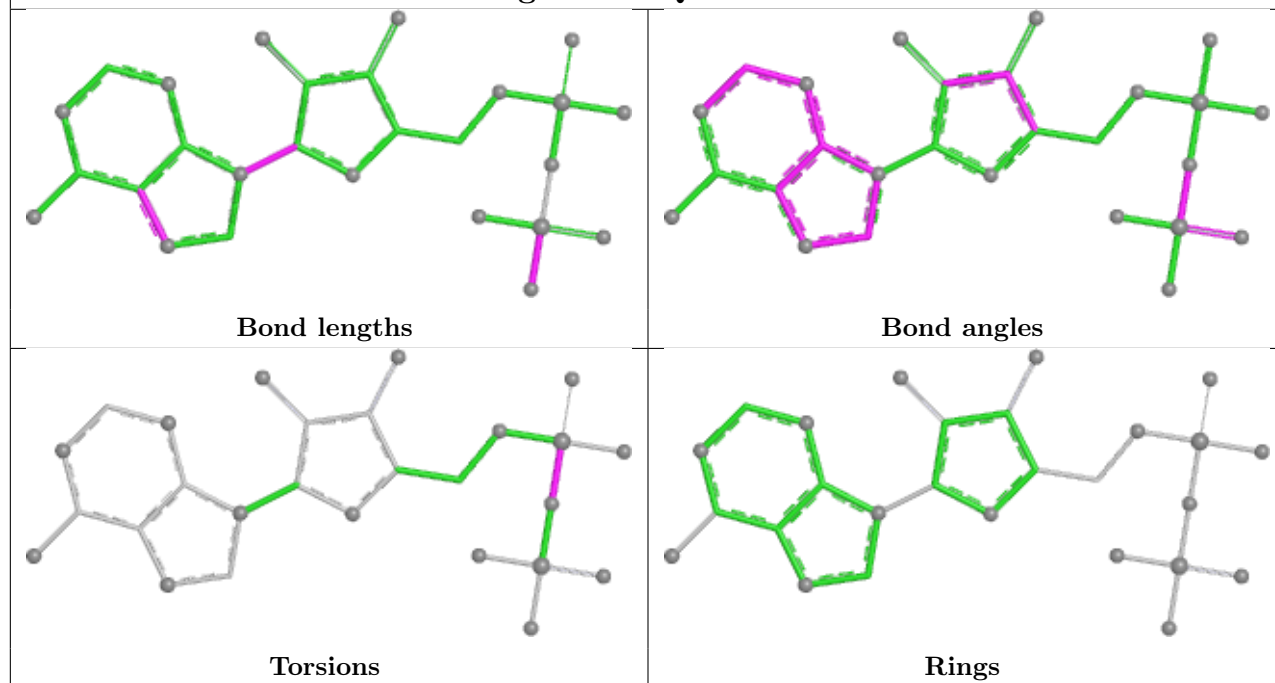
Ligand ADQ G 2506



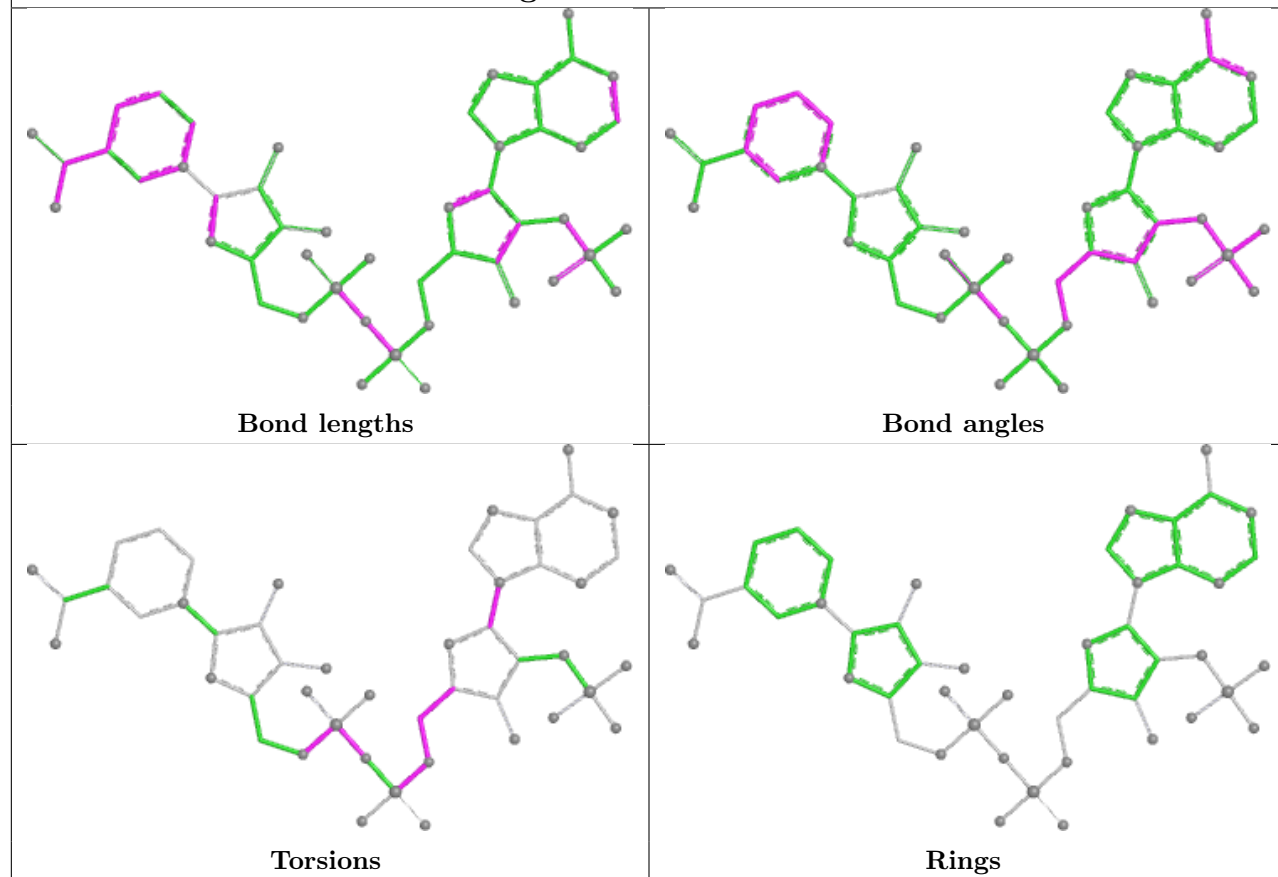
Ligand ADQ D 2503



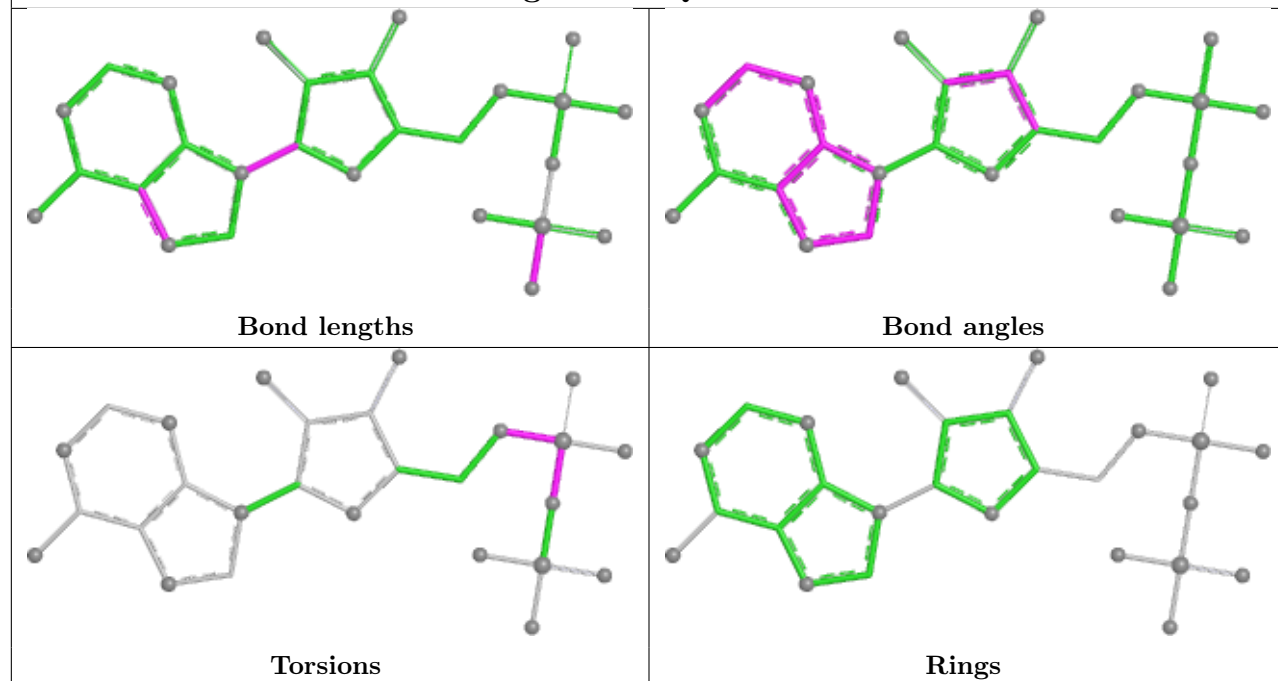
Ligand ADQ A 2500



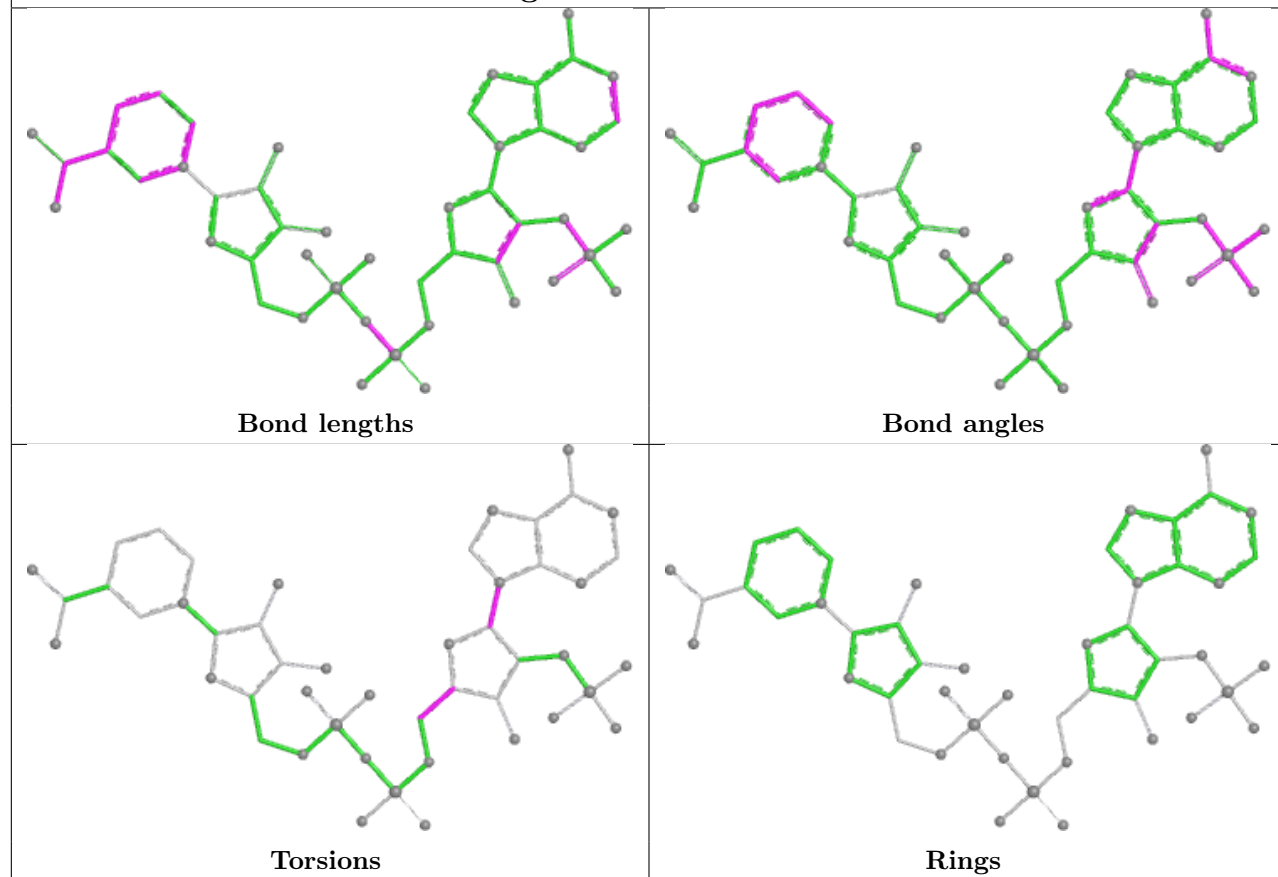
Ligand NAP G 2406



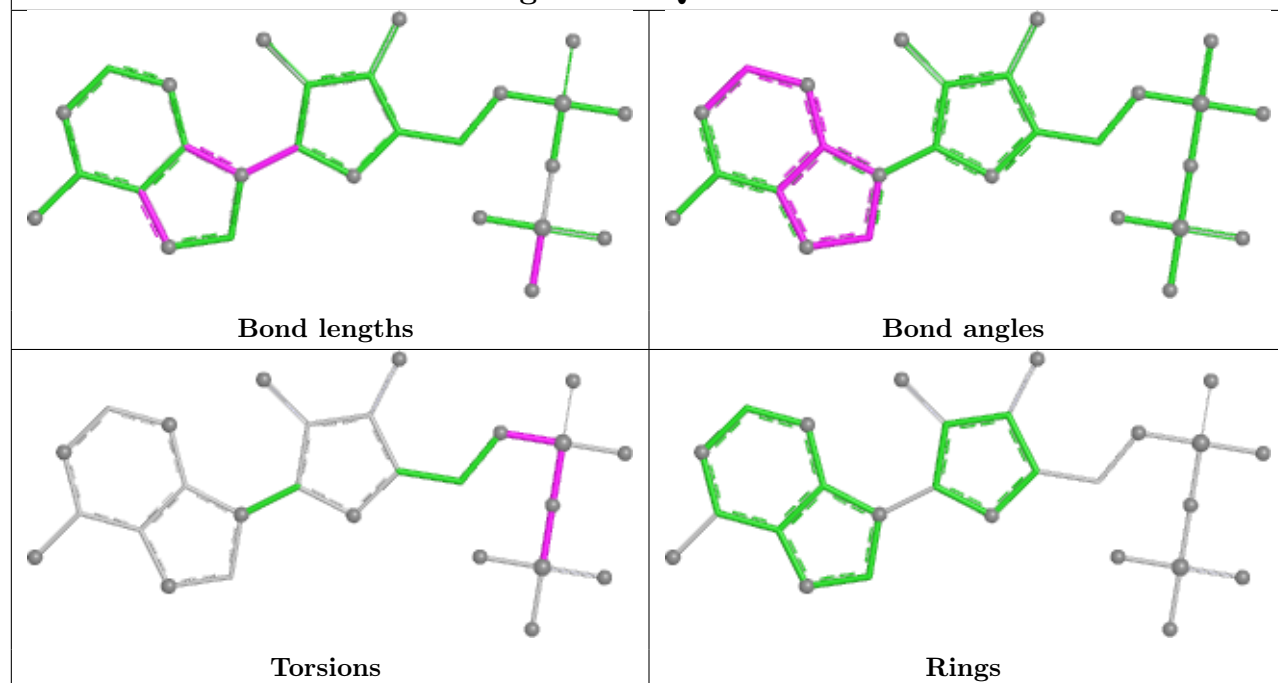
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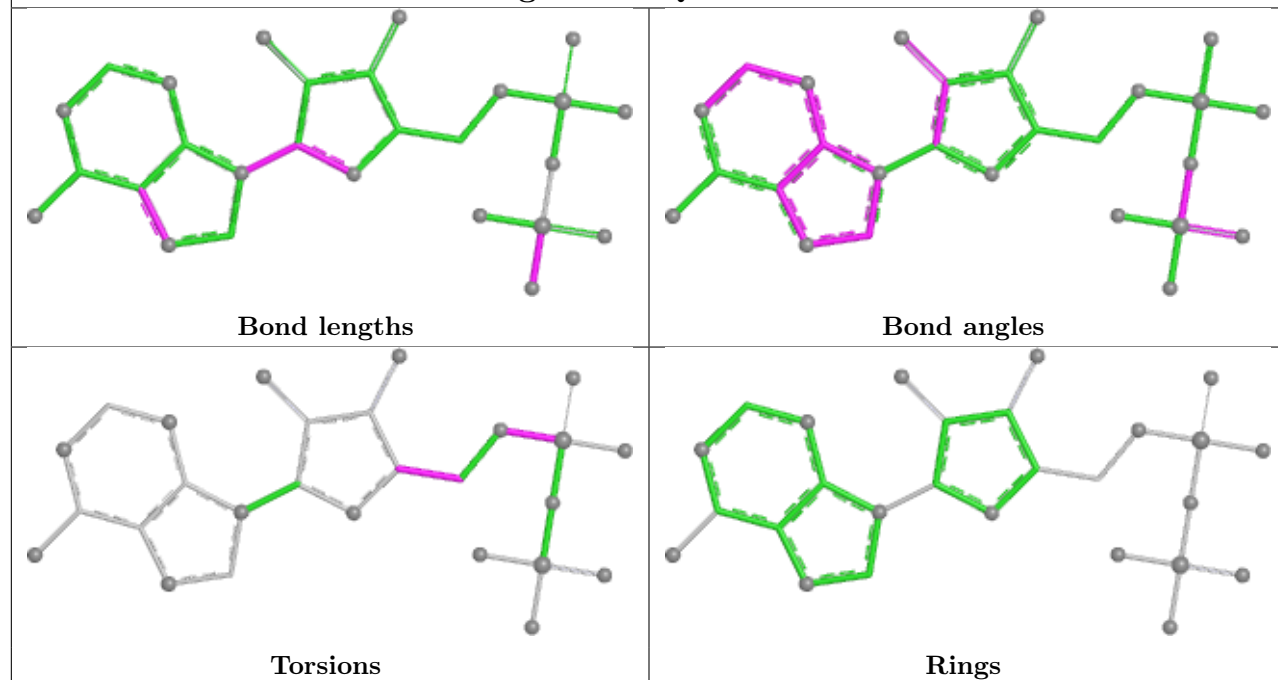
Ligand NAP C 2402



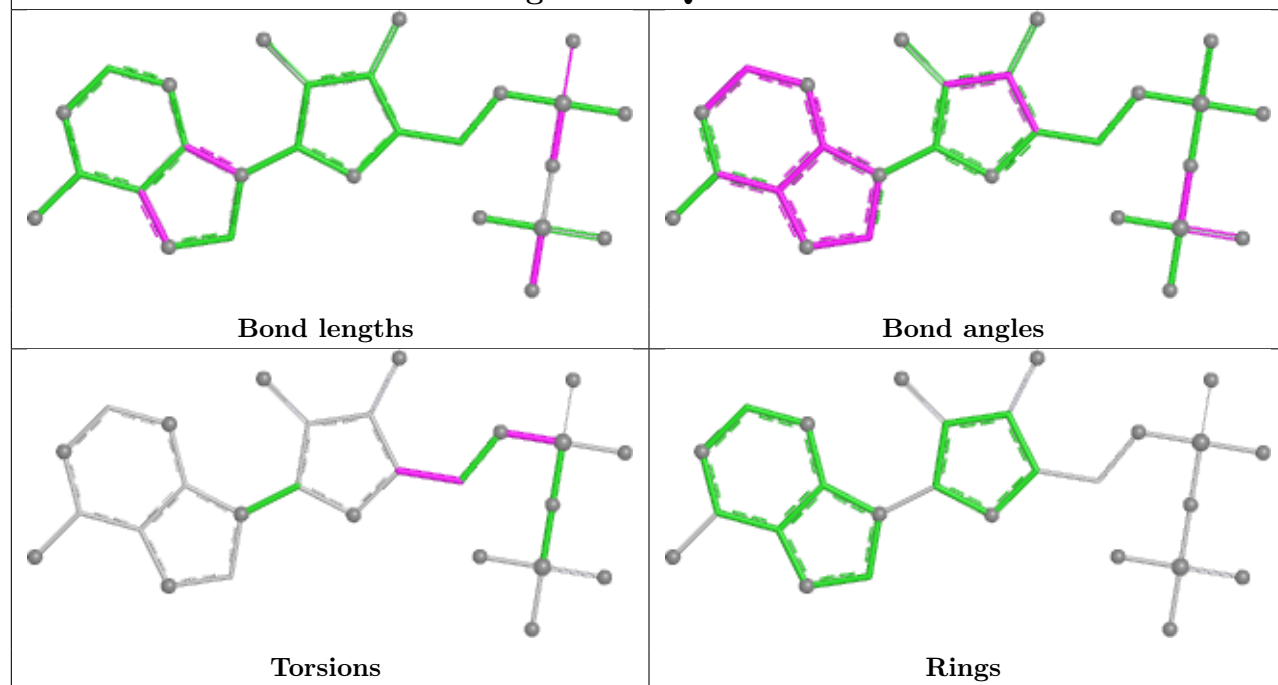
Ligand ADQ C 2502

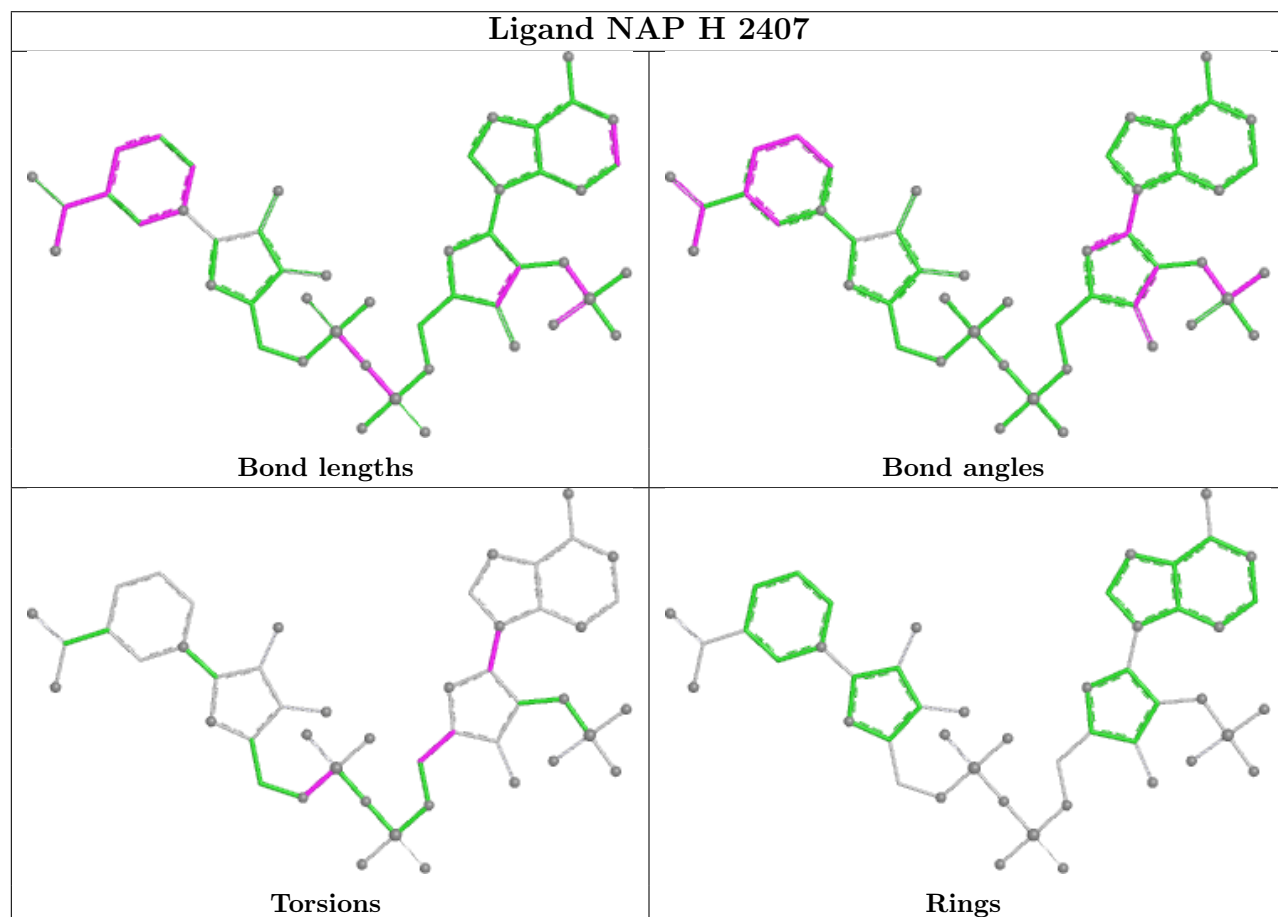
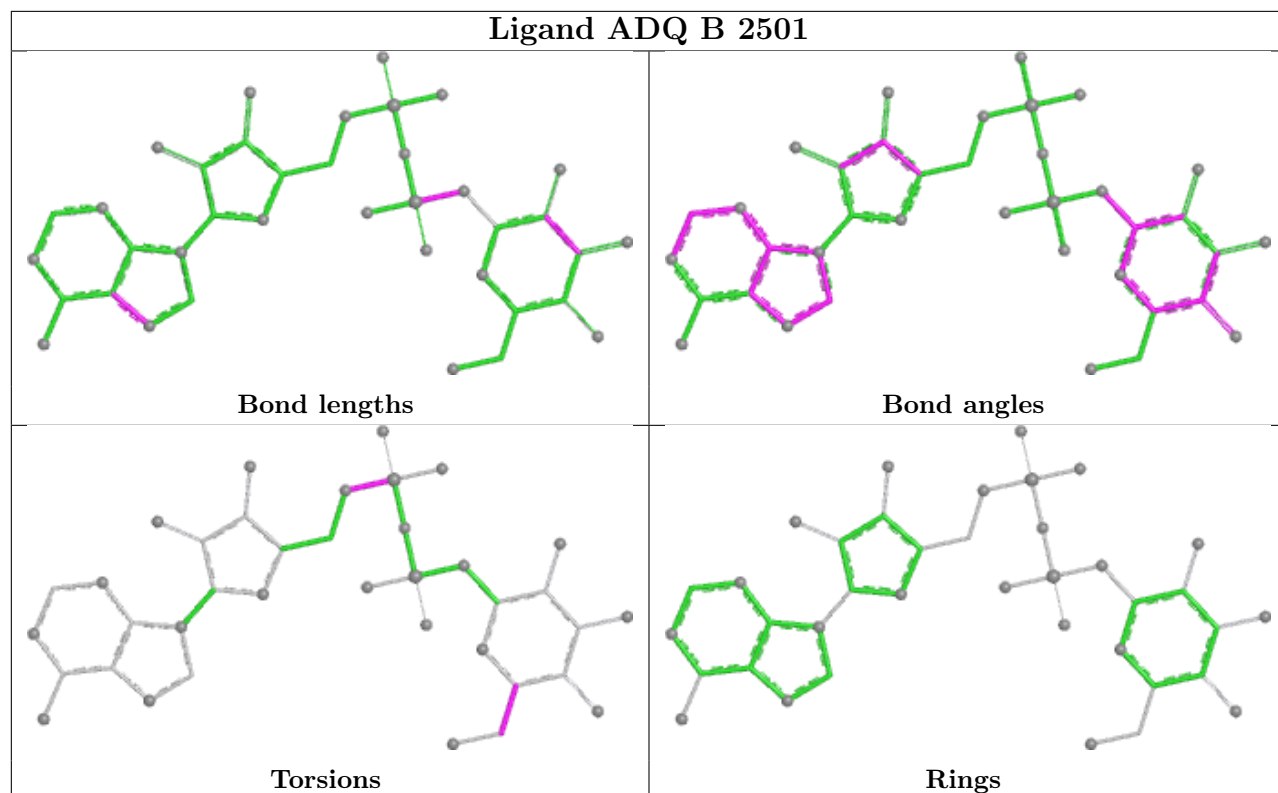


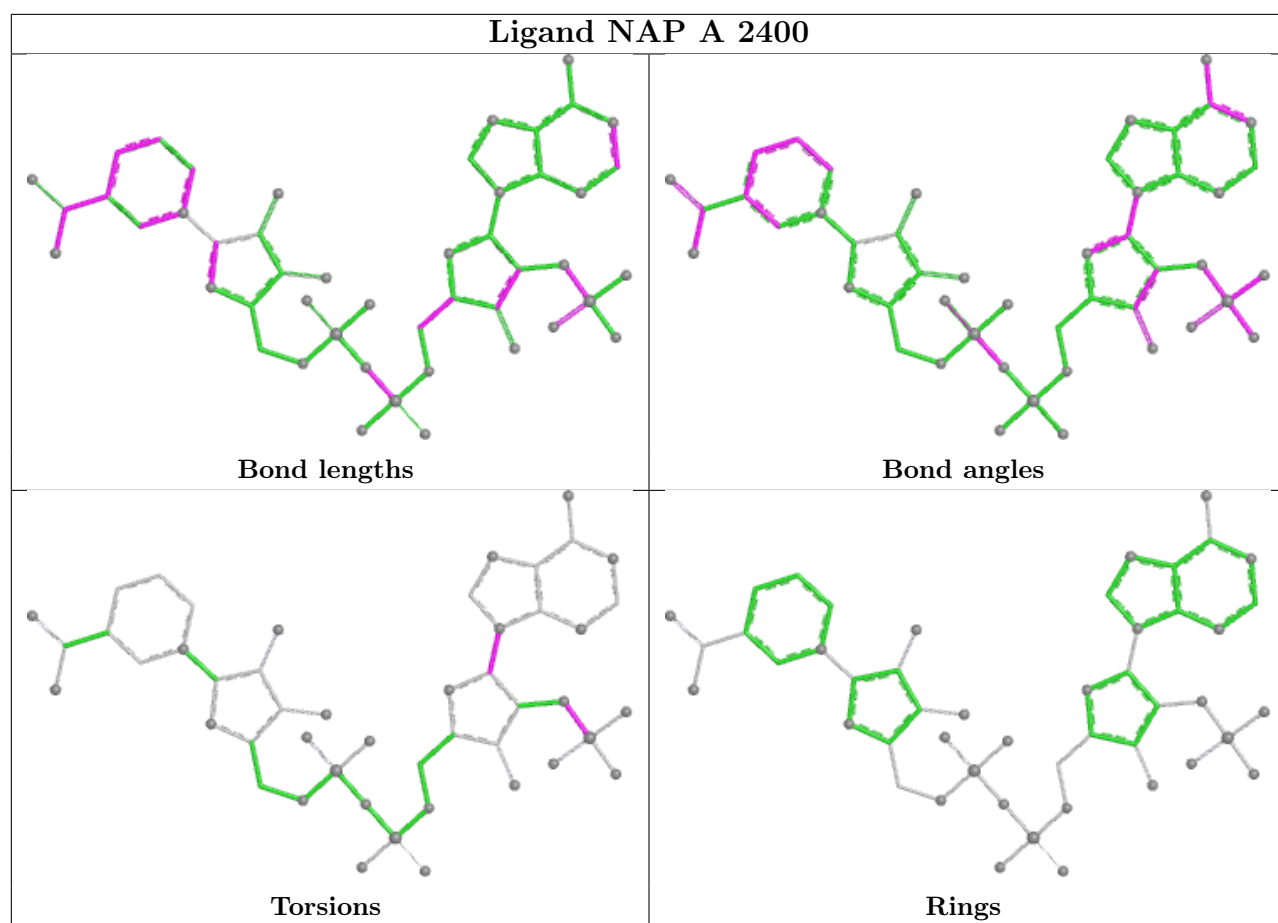
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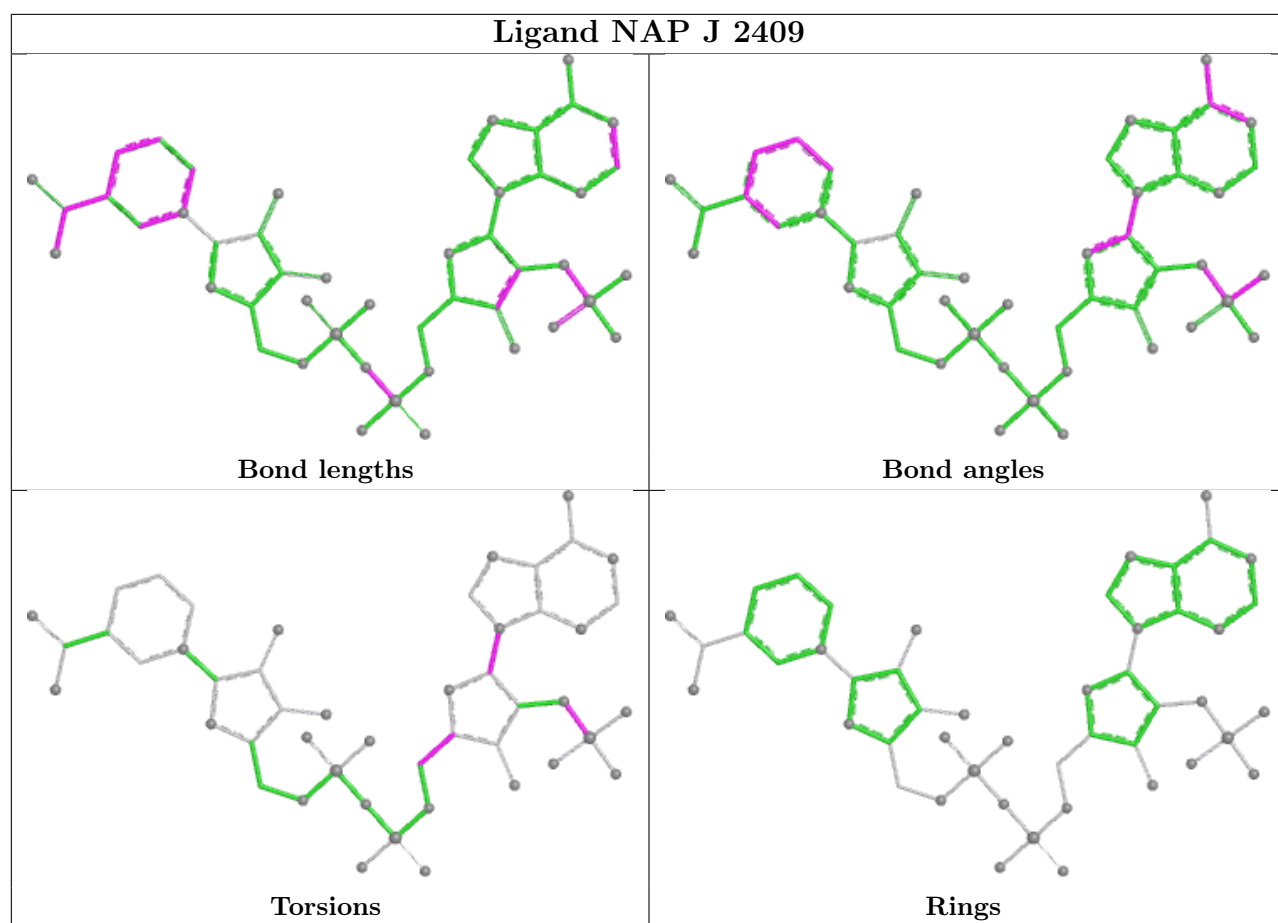


Ligand ADQ I 2508

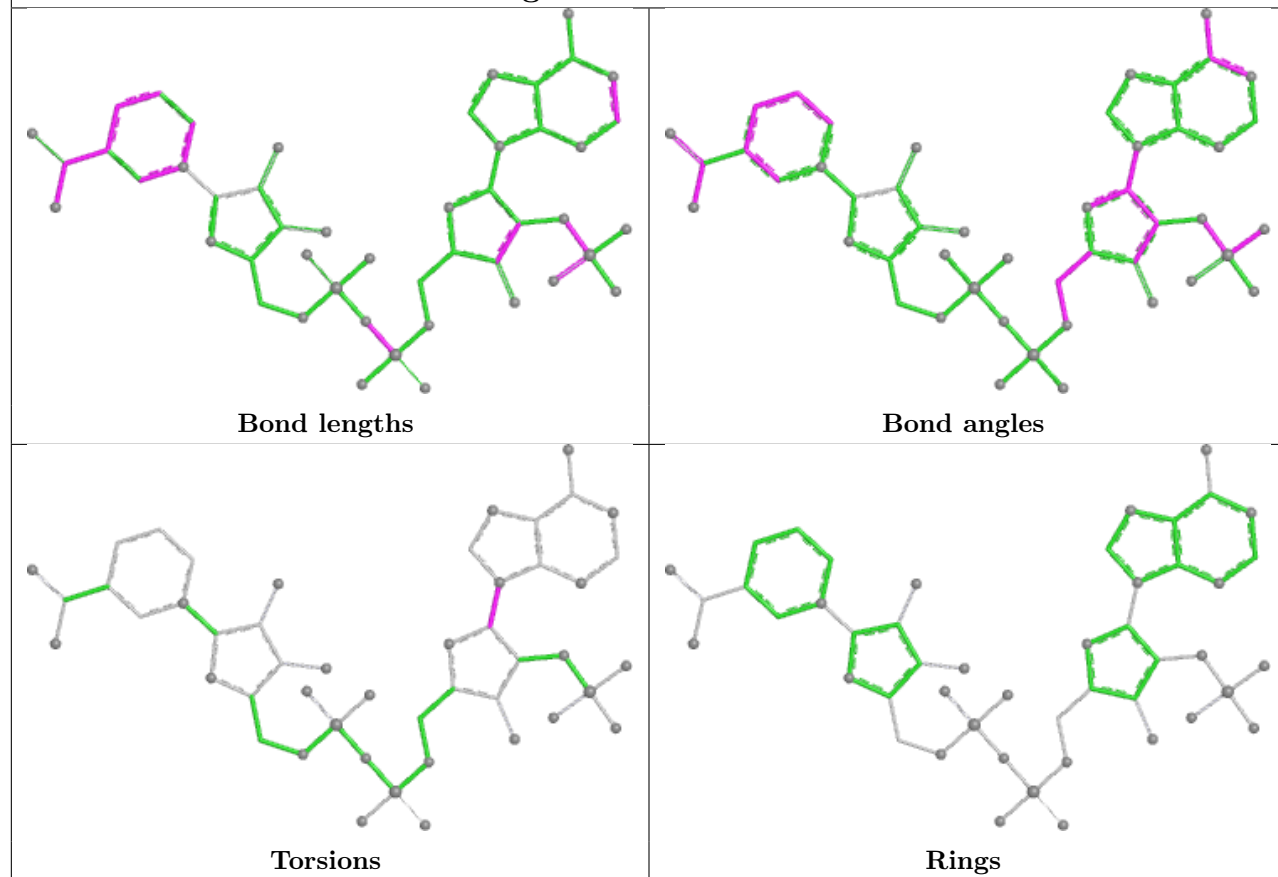




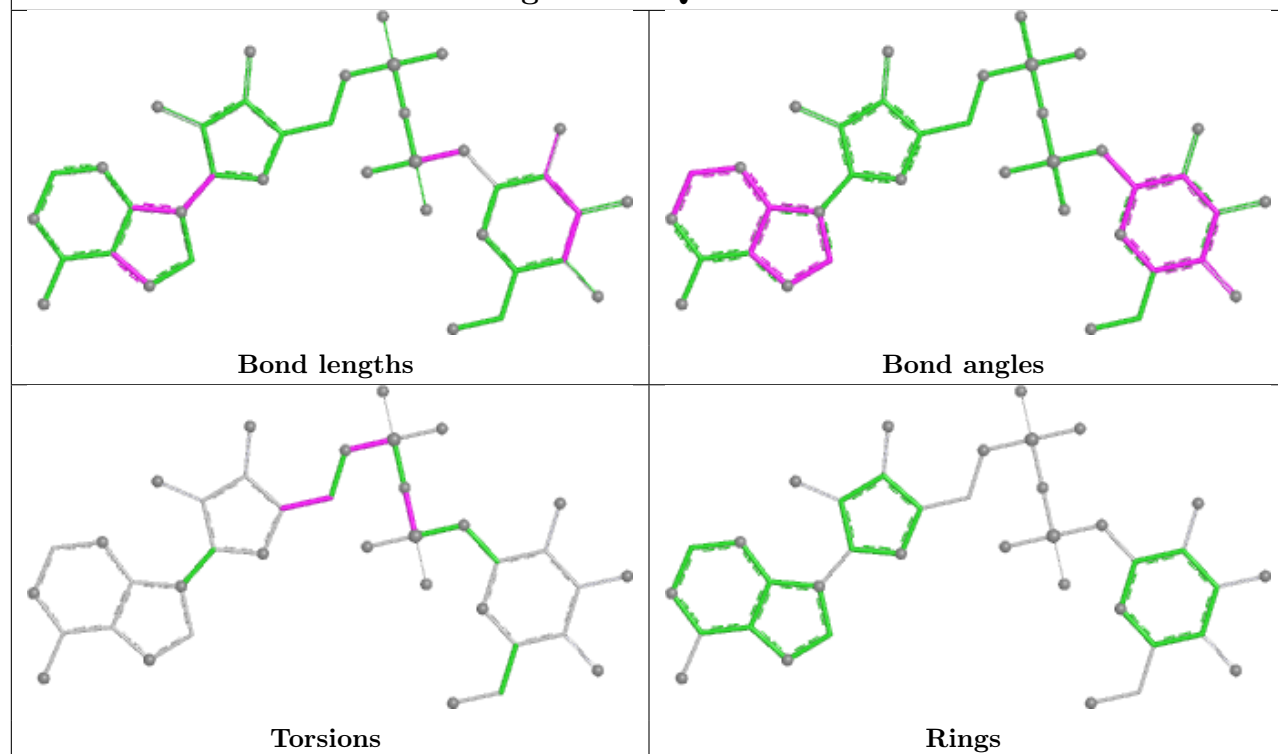


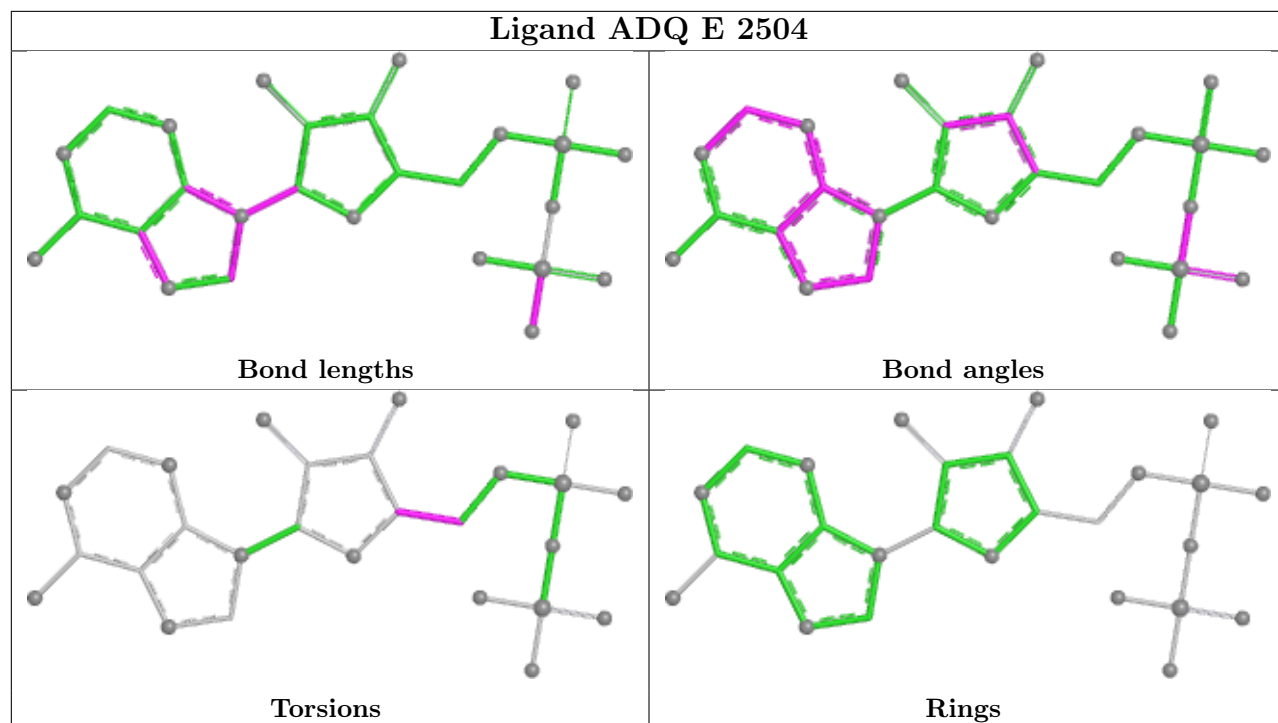


Ligand NAP F 2405



Ligand ADQ F 2505





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.