



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:38 AM BST

PDB ID : 1UP7
Title : Structure of the 6-phospho-beta glucosidase from *Thermotoga maritima* at 2.4 Angstrom resolution in the tetragonal form with NAD and glucose-6-phosphate
Authors : Varrot, A.; Yip, V.L.; Withers, S.G.; Davies, G.J.
Deposited on : 2003-09-29
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

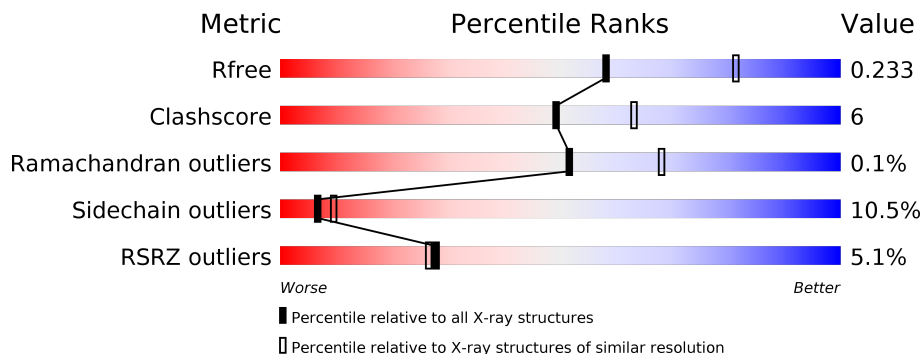
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	417	 4% 77% 18%
1	B	417	 5% 78% 16%
1	C	417	 2% 76% 19%
1	D	417	 4% 75% 20%
1	E	417	 8% 76% 18%
1	F	417	 6% 77% 19%

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Mol	Chain	Length	Quality of chain
1	G	417	<p>4% 78% 18% ..</p>
1	H	417	<p>6% 73% 22% ..</p>

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	G6P	A	1417	X	-	-	-
3	G6P	B	1417	X	-	-	-
3	G6P	C	1417	X	-	-	-
3	G6P	D	1417	X	-	-	-
3	G6P	E	1417	X	-	-	-
3	G6P	F	1417	X	-	-	-
3	G6P	G	1417	X	-	-	-
3	G6P	H	1417	X	-	-	-

2 Entry composition

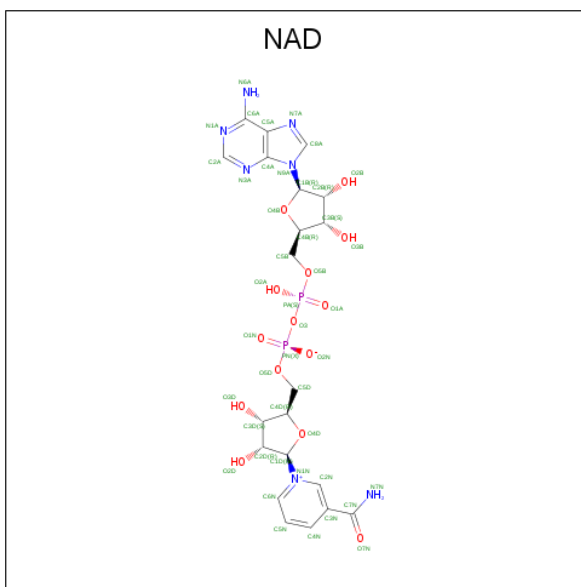
There are 5 unique types of molecules in this entry. The entry contains 27816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 6-PHOSPHO-BETA-GLUCOSIDASE.

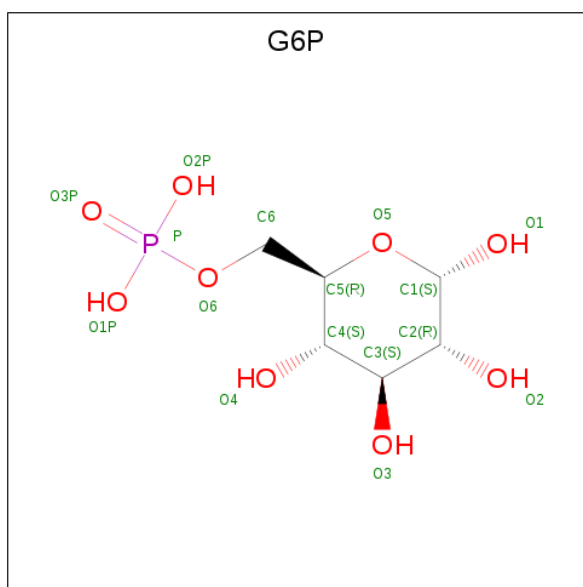
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	Total 3362	C 2166	N 563	O 624	S 9	10	0	0
1	B	409	Total 3318	C 2139	N 553	O 617	S 9	74	0	0
1	C	409	Total 3325	C 2144	N 553	O 618	S 10	26	1	0
1	D	409	Total 3317	C 2137	N 552	O 619	S 9	51	0	0
1	E	406	Total 3294	C 2124	N 548	O 613	S 9	154	0	0
1	F	411	Total 3333	C 2148	N 555	O 621	S 9	116	0	0
1	G	409	Total 3318	C 2139	N 553	O 617	S 9	77	0	0
1	H	407	Total 3300	C 2127	N 549	O 615	S 9	86	0	0

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is 6-O-phosphono-alpha-D-glucopyranose (three-letter code: G6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
3	A	1	Total 16	C 6	O 9	P 1	0	0
3	B	1	Total 16	C 6	O 9	P 1	0	0
3	C	1	Total 16	C 6	O 9	P 1	0	0
3	D	1	Total 16	C 6	O 9	P 1	0	0
3	E	1	Total 16	C 6	O 9	P 1	0	0
3	F	1	Total 16	C 6	O 9	P 1	0	0
3	G	1	Total 16	C 6	O 9	P 1	0	0
3	H	1	Total 16	C 6	O 9	P 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

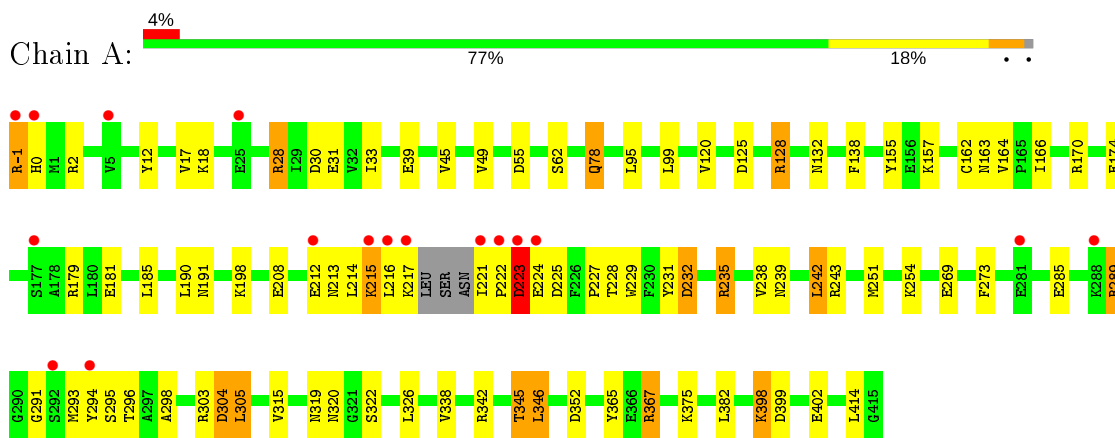
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	149	Total	O	0	0
			149	149		
5	B	103	Total	O	0	0
			103	103		
5	C	108	Total	O	0	0
			108	108		
5	D	91	Total	O	0	0
			91	91		
5	E	78	Total	O	0	0
			78	78		
5	F	83	Total	O	0	0
			83	83		
5	G	81	Total	O	0	0
			81	81		
5	H	66	Total	O	0	0
			66	66		

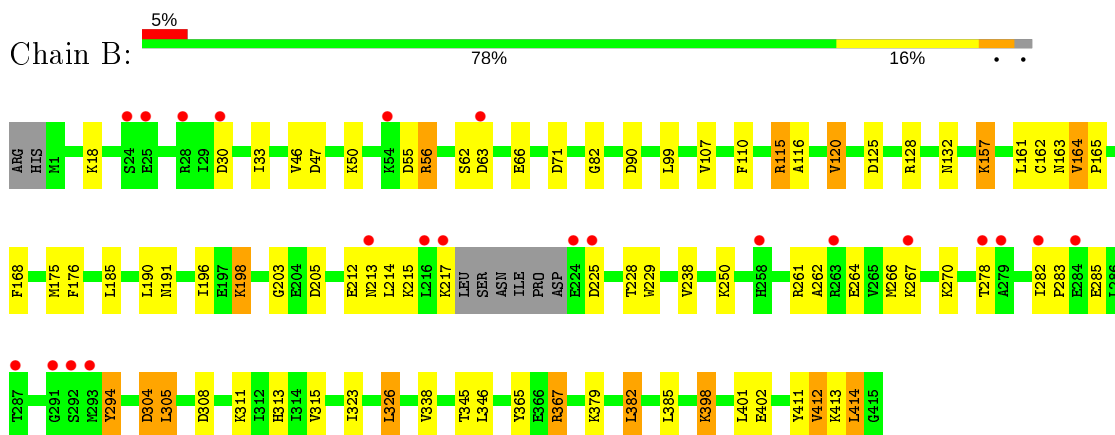
3 Residue-property plots [i](#)

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.

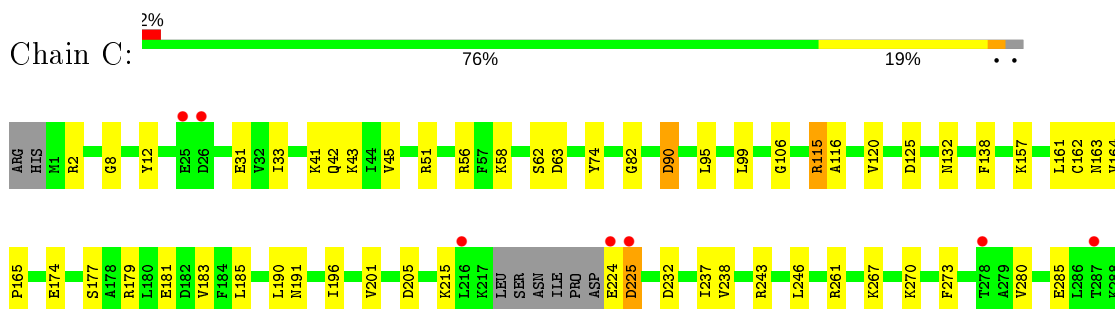
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

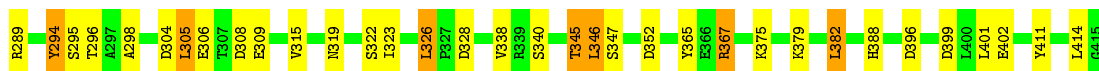


- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

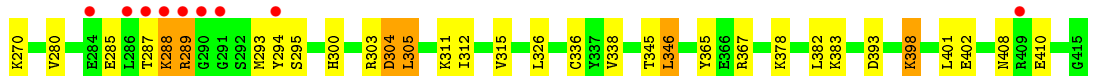
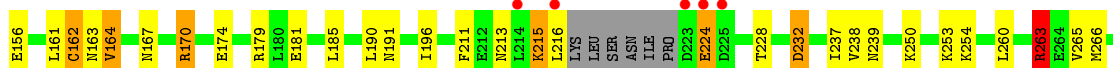
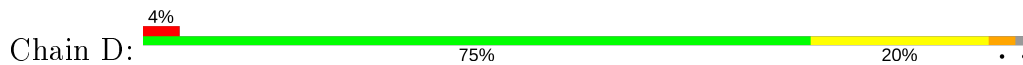


- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

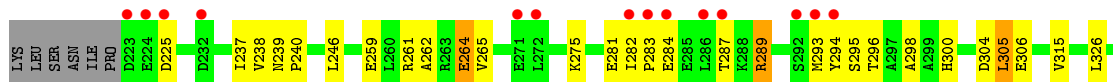
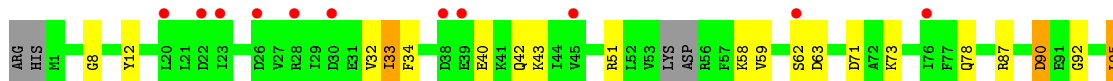
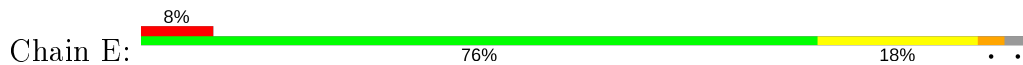




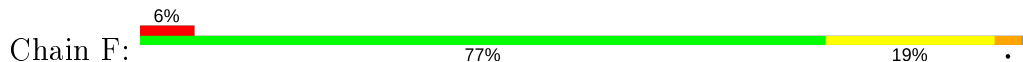
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE




- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

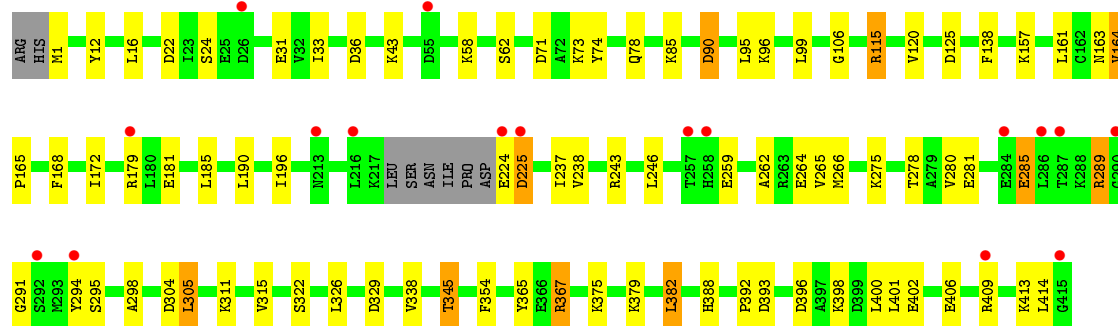


- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE




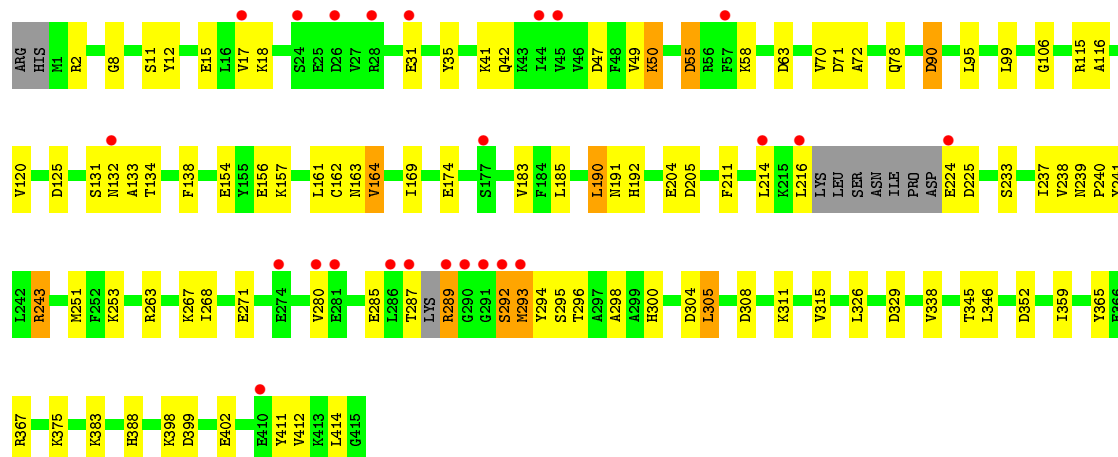
- Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain G:  4% 78% 18%



• Molecule 1: 6-PHOSPHO-BETA-GLUCOSIDASE

Chain H:  6% 73% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.13Å 178.13Å 278.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.40 19.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.96-2.40) 98.3 (19.96-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.41Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.199 , 0.240 0.196 , 0.233	Depositor DCC
R_{free} test set	16459 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtrriage
Anisotropy	0.222	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27816	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.65% 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: G6P, SO4, NAD

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	0.74	0/3429	0.88	10/4620 (0.2%)
1	B	0.65	0/3383	0.86	12/4557 (0.3%)
1	C	0.68	0/3391	0.90	15/4567 (0.3%)
1	D	0.74	1/3382 (0.0%)	0.87	11/4557 (0.2%)
1	E	0.68	4/3357 (0.1%)	0.85	12/4521 (0.3%)
1	F	0.53	0/3399	0.79	11/4579 (0.2%)
1	G	0.60	0/3383	0.83	13/4557 (0.3%)
1	H	0.57	1/3364 (0.0%)	0.78	12/4532 (0.3%)
All	All	0.65	6/27088 (0.0%)	0.85	96/36490 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	51	ARG	CZ-NH1	23.24	1.63	1.33
1	D	51	ARG	NE-CZ	8.03	1.43	1.33
1	E	51	ARG	NE-CZ	7.98	1.43	1.33
1	E	59	VAL	CB-CG2	6.38	1.66	1.52
1	H	50	LYS	CB-CG	5.79	1.68	1.52
1	E	51	ARG	CZ-NH2	5.72	1.40	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	ARG	NE-CZ-NH2	-21.85	109.37	120.30
1	C	115	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	E	51	ARG	NE-CZ-NH1	12.39	126.50	120.30
1	C	225	ASP	CB-CG-OD2	8.93	126.34	118.30
1	G	115	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	F	304	ASP	CB-CG-OD2	8.35	125.81	118.30
1	B	115	ARG	NE-CZ-NH2	-7.66	116.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	304	ASP	CB-CG-OD2	7.45	125.01	118.30
1	C	115	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	304	ASP	CB-CG-OD2	7.19	124.77	118.30
1	C	90	ASP	CB-CG-OD2	7.18	124.76	118.30
1	D	304	ASP	CB-CG-OD2	7.06	124.65	118.30
1	B	225	ASP	CB-CG-OD2	7.03	124.62	118.30
1	B	308	ASP	CB-CG-OD2	6.95	124.56	118.30
1	H	225	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	263	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	G	329	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	304	ASP	CB-CG-OD2	6.66	124.29	118.30
1	G	22	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	115	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	30	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	352	ASP	CB-CG-OD2	6.37	124.03	118.30
1	G	125	ASP	CB-CG-OD2	6.34	124.01	118.30
1	G	396	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	367	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	E	51	ARG	CD-NE-CZ	-6.16	114.97	123.60
1	G	367	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	H	63	ASP	CB-CG-OD2	6.12	123.81	118.30
1	G	304	ASP	CB-CG-OD2	6.09	123.78	118.30
1	E	115	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	H	304	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	47	ASP	CB-CG-OD2	6.01	123.71	118.30
1	E	225	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	63	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	367	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	C	63	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	63	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	125	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	367	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	G	90	ASP	CB-CG-OD2	5.84	123.55	118.30
1	C	396	ASP	CB-CG-OD2	5.84	123.55	118.30
1	D	393	ASP	CB-CG-OD2	5.81	123.53	118.30
1	F	396	ASP	CB-CG-OD2	5.78	123.50	118.30
1	C	328	ASP	CB-CG-OD2	5.74	123.47	118.30
1	D	55	ASP	CB-CG-OD2	5.72	123.45	118.30
1	F	329	ASP	CB-CG-OD2	5.68	123.41	118.30
1	F	308	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	55	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	396	ASP	CB-CG-OD2	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	179	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	H	308	ASP	CB-CG-OD2	5.61	123.35	118.30
1	H	352	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	232	ASP	CB-CG-OD2	5.60	123.34	118.30
1	G	115	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	F	125	ASP	CB-CG-OD2	5.57	123.31	118.30
1	F	393	ASP	CB-CG-OD2	5.53	123.28	118.30
1	C	232	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	225	ASP	CB-CG-OD2	5.49	123.24	118.30
1	F	30	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	125	ASP	CB-CG-OD2	5.47	123.22	118.30
1	H	90	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	38	ASP	CB-CG-OD2	5.45	123.21	118.30
1	E	329	ASP	CB-CG-OD1	5.45	123.20	118.30
1	D	263	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	H	329	ASP	CB-CG-OD2	5.42	123.17	118.30
1	F	71	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	55	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	308	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	399	ASP	CB-CG-OD2	5.37	123.13	118.30
1	H	205	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	125	ASP	CB-CG-OD2	5.32	123.09	118.30
1	H	125	ASP	CB-CG-OD2	5.31	123.08	118.30
1	G	71	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	367	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	30	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	205	ASP	CB-CG-OD2	5.26	123.03	118.30
1	E	304	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	223	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	205	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	125	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	55	ASP	CB-CG-OD2	5.18	122.96	118.30
1	C	399	ASP	CB-CG-OD2	5.16	122.94	118.30
1	G	36	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	223	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	26	ASP	CB-CG-OD2	5.14	122.92	118.30
1	G	393	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	367	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	71	ASP	CB-CG-OD2	5.13	122.91	118.30
1	E	90	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	232	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	71	ASP	CB-CG-OD2	5.06	122.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	63	ASP	CB-CG-OD2	5.05	122.85	118.30
1	G	225	ASP	CB-CG-OD2	5.04	122.84	118.30
1	H	47	ASP	CB-CG-OD2	5.03	122.83	118.30
1	H	71	ASP	CB-CG-OD2	5.03	122.82	118.30
1	D	26	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3362	0	3397	53	0
1	B	3318	0	3355	38	0
1	C	3325	0	3363	40	0
1	D	3317	0	3346	51	0
1	E	3294	0	3322	43	0
1	F	3333	0	3367	35	0
1	G	3318	0	3355	29	0
1	H	3300	0	3328	48	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	1	0
2	F	44	0	26	2	0
2	G	44	0	26	0	0
2	H	44	0	26	0	0
3	A	16	0	11	0	0
3	B	16	0	11	0	0
3	C	16	0	11	0	0
3	D	16	0	11	2	0
3	E	16	0	11	0	0
3	F	16	0	11	0	0
3	G	16	0	11	0	0
3	H	16	0	11	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	A	149	0	0	2	0
5	B	103	0	0	1	0
5	C	108	0	0	0	0
5	D	91	0	0	1	0
5	E	78	0	0	0	0
5	F	83	0	0	1	0
5	G	81	0	0	1	0
5	H	66	0	0	0	0
All	All	27816	0	27129	313	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 6.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HH11	1:A:235:ARG:HG2	0.97	1.07
1:H:162:CYS:HB2	1:H:191:ASN:ND2	1.80	0.96
1:A:235:ARG:NH1	1:A:235:ARG:HG2	1.76	0.92
1:E:162:CYS:HB2	1:E:191:ASN:HD21	1.34	0.91
1:B:398:LYS:O	1:B:402:GLU:HG3	1.72	0.87
1:H:162:CYS:HB2	1:H:191:ASN:HD21	1.34	0.87
1:B:305:LEU:HD13	1:B:338:VAL:HG13	1.58	0.83
1:A:346:LEU:HD12	1:D:346:LEU:CD1	2.08	0.82
1:D:48:PHE:HA	1:D:51:ARG:CZ	2.10	0.81
1:A:346:LEU:CD1	1:D:346:LEU:CD1	2.59	0.80
1:D:162:CYS:CB	1:D:191:ASN:HD21	1.97	0.77
1:E:346:LEU:HD12	1:H:346:LEU:HD12	1.66	0.77
1:H:162:CYS:CB	1:H:191:ASN:ND2	2.48	0.76
1:H:162:CYS:CB	1:H:191:ASN:HD21	1.99	0.75
1:A:345:THR:HG22	5:A:2106:HOH:O	1.85	0.75
1:C:8:GLY:HA3	1:C:42:GLN:HE21	1.51	0.75
1:A:162:CYS:CB	1:A:191:ASN:HD21	2.01	0.74
1:A:235:ARG:HH11	1:A:235:ARG:CG	1.89	0.73
1:A:162:CYS:HB2	1:A:191:ASN:HD21	1.54	0.73
1:G:90:ASP:OD1	1:G:115:ARG:NH2	2.22	0.72
1:E:162:CYS:HB2	1:E:191:ASN:ND2	2.05	0.72
1:D:2:ARG:HG3	1:D:31:GLU:HG3	1.70	0.71
1:E:33:ILE:HD11	1:E:62:SER:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ARG:HG2	1:B:56:ARG:HH11	1.54	0.70
1:B:346:LEU:HD23	1:C:346:LEU:HD12	1.73	0.70
1:D:162:CYS:HB2	1:D:191:ASN:HD21	1.56	0.70
1:F:138:PHE:HZ	1:F:298:ALA:HB2	1.57	0.70
1:E:162:CYS:CB	1:E:191:ASN:HD21	2.05	0.69
1:C:2:ARG:HG3	1:C:31:GLU:HG3	1.75	0.69
1:F:8:GLY:HA3	1:F:42:GLN:HE21	1.58	0.68
1:A:212:GLU:HA	1:A:215:LYS:HD3	1.77	0.67
1:A:295:SER:OG	1:A:296:THR:N	2.26	0.67
1:G:179:ARG:NH1	1:G:181:GLU:OE2	2.28	0.67
1:D:8:GLY:HA3	1:D:42:GLN:HE21	1.60	0.67
1:G:90:ASP:CG	1:G:115:ARG:HH22	1.98	0.67
1:D:163:ASN:HB3	1:D:294:TYR:CD1	2.30	0.66
1:C:90:ASP:CG	1:C:115:ARG:HH22	1.98	0.66
1:C:90:ASP:OD1	1:C:115:ARG:NH2	2.24	0.66
1:E:346:LEU:CD1	1:H:346:LEU:HD12	2.26	0.66
1:D:48:PHE:HA	1:D:51:ARG:NH2	2.11	0.65
1:E:259:GLU:OE1	1:E:264:GLU:HG2	1.97	0.65
1:H:70:VAL:O	1:H:131:SER:HB3	1.97	0.64
1:A:166:ILE:HG12	1:A:293:MET:HE3	1.78	0.64
1:A:346:LEU:HD12	1:D:346:LEU:HD13	1.78	0.64
1:F:289:ARG:NH2	2:F:1416:NAD:O1N	2.29	0.64
1:D:16:LEU:HA	1:D:295:SER:HB3	1.78	0.64
1:H:138:PHE:HZ	1:H:298:ALA:HB2	1.64	0.63
1:A:179:ARG:NH1	1:A:181:GLU:OE2	2.33	0.62
1:B:90:ASP:OD1	1:B:115:ARG:NH2	2.33	0.61
1:H:90:ASP:OD1	1:H:115:ARG:NH2	2.33	0.61
1:D:162:CYS:CB	1:D:191:ASN:ND2	2.64	0.61
1:E:87:ARG:NH1	1:E:265:VAL:HG21	2.16	0.61
1:H:163:ASN:HB3	1:H:294:TYR:CD1	2.36	0.61
1:A:269:GLU:O	1:A:273:PHE:HD2	1.84	0.60
1:H:296:THR:HG22	1:H:300:HIS:CE1	2.36	0.60
1:E:90:ASP:OD1	1:E:115:ARG:NH2	2.34	0.60
1:B:262:ALA:O	1:B:266:MET:HG3	2.01	0.60
1:F:138:PHE:CZ	1:F:298:ALA:HB2	2.35	0.60
1:H:138:PHE:CZ	1:H:298:ALA:HB2	2.36	0.60
1:E:296:THR:HG23	1:E:300:HIS:CE1	2.36	0.60
1:A:215:LYS:HG2	1:A:228:THR:HG23	1.83	0.59
1:E:87:ARG:HD3	1:E:262:ALA:CB	2.32	0.59
1:D:12:TYR:OH	1:D:289:ARG:HB3	2.02	0.59
1:B:164:VAL:HG22	1:B:165:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:17:VAL:HG11	1:H:49:VAL:HG13	1.85	0.59
1:E:87:ARG:HD3	1:E:262:ALA:HB2	1.84	0.59
1:C:163:ASN:HB3	1:C:294:TYR:CD1	2.38	0.59
1:F:12:TYR:OH	1:F:289:ARG:HB3	2.03	0.59
1:D:263:ARG:HD3	5:D:2049:HOH:O	2.01	0.59
1:A:162:CYS:CB	1:A:191:ASN:ND2	2.66	0.59
1:B:162:CYS:HB2	1:B:191:ASN:ND2	2.17	0.59
1:G:259:GLU:OE1	1:G:264:GLU:HG2	2.03	0.59
1:D:33:ILE:HD11	1:D:62:SER:HB2	1.86	0.58
1:E:346:LEU:CD1	1:H:346:LEU:CD1	2.82	0.58
1:B:82:GLY:HA2	1:B:411:TYR:CZ	2.39	0.58
1:H:305:LEU:HD13	1:H:338:VAL:HG13	1.86	0.57
1:H:292:SER:O	1:H:293:MET:HB2	2.03	0.57
1:C:305:LEU:HD13	1:C:338:VAL:HG13	1.86	0.57
1:D:300:HIS:HD2	1:D:303:ARG:NH2	2.02	0.57
1:D:48:PHE:HA	1:D:51:ARG:NH1	2.19	0.57
1:A:305:LEU:HD13	1:A:338:VAL:HG13	1.85	0.57
1:D:303:ARG:HD2	1:D:304:ASP:OD1	2.05	0.57
1:D:46:VAL:HG12	1:D:50:LYS:HE3	1.87	0.57
1:C:319:ASN:O	1:C:345:THR:HG21	2.06	0.56
1:B:56:ARG:NH1	1:B:56:ARG:HG2	2.18	0.56
1:G:33:ILE:HD11	1:G:62:SER:HB2	1.87	0.56
1:A:45:VAL:CG2	1:A:273:PHE:HE1	2.18	0.56
1:C:322:SER:HB2	1:C:345:THR:HG23	1.87	0.56
1:H:240:PRO:O	1:H:243:ARG:HG2	2.06	0.55
1:D:164:VAL:HG21	1:D:239:ASN:ND2	2.22	0.55
1:E:90:ASP:CG	1:E:115:ARG:HH22	2.10	0.55
1:E:170:ARG:O	1:E:174:GLU:HG3	2.06	0.55
1:C:382:LEU:HD13	1:C:401:LEU:HD22	1.89	0.55
1:E:116:ALA:O	1:E:120:VAL:HG13	2.07	0.55
1:F:82:GLY:HA3	1:F:115:ARG:HD3	1.89	0.55
1:B:305:LEU:HD13	1:B:338:VAL:CG1	2.35	0.54
1:C:179:ARG:NH1	1:C:181:GLU:OE2	2.39	0.54
1:F:262:ALA:O	1:F:266:MET:HG3	2.07	0.54
1:D:305:LEU:HD13	1:D:338:VAL:HG13	1.90	0.54
1:C:295:SER:OG	1:C:296:THR:N	2.40	0.54
1:B:132:ASN:O	1:B:157:LYS:NZ	2.42	0.53
1:H:12:TYR:OH	1:H:289:ARG:HB3	2.07	0.53
1:A:17:VAL:HG11	1:A:49:VAL:HG13	1.91	0.53
1:F:382:LEU:HD13	1:F:401:LEU:HD22	1.90	0.53
1:B:90:ASP:CG	1:B:115:ARG:HH22	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:LEU:HD13	1:C:401:LEU:CD2	2.38	0.53
1:D:224:GLU:OE2	1:D:254:LYS:HE3	2.09	0.53
1:G:305:LEU:HD13	1:G:338:VAL:HG13	1.91	0.53
1:D:294:TYR:HE1	3:D:1417:G6P:H3	1.73	0.53
1:D:382:LEU:HD21	1:D:398:LYS:HA	1.90	0.53
1:E:8:GLY:HA3	1:E:42:GLN:HE21	1.73	0.53
1:F:224:GLU:HB3	1:F:243:ARG:HH11	1.74	0.52
1:F:80:ARG:NH2	2:F:1416:NAD:O1N	2.40	0.52
1:F:292:SER:O	1:F:293:MET:HB2	2.09	0.52
1:F:163:ASN:HB3	1:F:294:TYR:CD1	2.45	0.52
1:H:240:PRO:O	1:H:243:ARG:CG	2.58	0.52
1:H:268:ILE:HG21	1:H:289:ARG:HG2	1.92	0.52
1:F:82:GLY:HA2	1:F:411:TYR:CZ	2.45	0.52
1:G:73:LYS:HG2	1:G:74:TYR:CE2	2.44	0.52
1:A:303:ARG:HD2	1:A:304:ASP:OD1	2.10	0.51
1:H:78:GLN:O	1:H:78:GLN:HG2	2.11	0.51
1:F:211:PHE:O	1:F:215:LYS:HD2	2.09	0.51
1:A:398:LYS:HD2	1:B:229:TRP:CD1	2.45	0.51
1:E:78:GLN:O	1:E:78:GLN:HG2	2.10	0.51
1:F:179:ARG:NH2	1:F:181:GLU:OE2	2.44	0.51
1:G:1:MET:N	5:G:2001:HOH:O	2.43	0.51
1:A:319:ASN:O	1:A:345:THR:HG21	2.10	0.51
1:E:115:ARG:HG2	1:E:411:TYR:CB	2.41	0.51
1:G:168:PHE:CZ	1:G:172:ILE:HD11	2.46	0.50
1:G:16:LEU:HD22	1:G:78:GLN:OE1	2.11	0.50
1:H:90:ASP:CG	1:H:115:ARG:HH22	2.12	0.50
1:A:162:CYS:HB2	1:A:191:ASN:ND2	2.24	0.50
1:C:12:TYR:OH	1:C:289:ARG:HB3	2.12	0.50
1:G:16:LEU:HA	1:G:295:SER:HB2	1.93	0.50
1:C:162:CYS:HB2	1:C:191:ASN:ND2	2.27	0.50
1:E:12:TYR:OH	1:E:289:ARG:HB3	2.12	0.50
1:A:346:LEU:HD12	1:D:346:LEU:HD12	1.92	0.50
1:A:346:LEU:CD1	1:D:346:LEU:HD11	2.40	0.49
1:B:323:ILE:HG21	1:B:326:LEU:HD22	1.94	0.49
1:F:196:ILE:HB	1:F:237:ILE:HB	1.94	0.49
1:F:262:ALA:O	1:F:265:VAL:HG22	2.13	0.49
1:F:303:ARG:HD2	1:F:304:ASP:OD1	2.13	0.49
1:E:346:LEU:HD12	1:H:346:LEU:CD1	2.41	0.49
1:F:224:GLU:OE1	1:F:243:ARG:NH1	2.45	0.49
1:H:72:ALA:O	1:H:133:ALA:HB2	2.12	0.49
1:B:412:VAL:HG23	1:B:414:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:HD13	1:C:338:VAL:CG1	2.42	0.49
1:E:190:LEU:HD13	1:E:359:ILE:HG23	1.93	0.49
1:A:2:ARG:HG3	1:A:31:GLU:HG3	1.94	0.49
1:A:208:GLU:OE2	1:A:235:ARG:NH2	2.45	0.49
1:E:305:LEU:HD13	1:E:338:VAL:HG13	1.94	0.49
1:F:224:GLU:O	1:F:243:ARG:HD2	2.12	0.49
1:H:294:TYR:HE1	3:H:1417:G6P:H3	1.77	0.49
1:A:45:VAL:CG2	1:A:273:PHE:CE1	2.96	0.48
1:B:198:LYS:NZ	1:B:205:ASP:OD2	2.46	0.48
1:B:46:VAL:O	1:B:50:LYS:HG3	2.13	0.48
1:E:117:PHE:N	1:E:118:PRO:HD2	2.28	0.48
1:A:224:GLU:OE2	1:A:254:LYS:HE3	2.13	0.48
1:C:183:VAL:HG22	1:C:201:VAL:HG22	1.95	0.48
1:G:406:GLU:OE1	1:G:406:GLU:HA	2.13	0.48
1:F:284:GLU:O	1:F:287:THR:OG1	2.31	0.48
1:A:322:SER:HB2	1:A:345:THR:HG23	1.96	0.48
1:B:66:GLU:HB2	5:B:2008:HOH:O	2.13	0.48
1:A:138:PHE:CZ	1:A:298:ALA:HB2	2.48	0.48
1:F:295:SER:OG	1:F:296:THR:N	2.45	0.48
1:H:164:VAL:HG11	1:H:239:ASN:HD21	1.79	0.48
1:D:35:TYR:C	1:D:42:GLN:HE22	2.17	0.48
1:B:175:MET:HE2	1:B:176:PHE:CE2	2.48	0.48
1:C:164:VAL:HB	1:C:165:PRO:HD3	1.96	0.48
1:B:168:PHE:CE2	1:B:196:ILE:HD13	2.49	0.48
1:A:291:GLY:O	1:A:294:TYR:HD1	1.96	0.47
1:H:190:LEU:HD13	1:H:359:ILE:HG23	1.95	0.47
1:C:33:ILE:HD11	1:C:62:SER:HB2	1.96	0.47
1:G:291:GLY:O	1:G:294:TYR:HD2	1.97	0.47
1:F:310:GLY:HA2	1:F:339:ARG:HB2	1.96	0.47
1:C:41:LYS:HE2	1:C:273:PHE:CZ	2.49	0.47
1:E:162:CYS:CB	1:E:191:ASN:ND2	2.73	0.47
1:E:346:LEU:HD11	1:H:346:LEU:CD1	2.45	0.47
1:H:8:GLY:HA3	1:H:42:GLN:HE21	1.80	0.47
1:C:116:ALA:O	1:C:120:VAL:HG13	2.15	0.47
1:C:31:GLU:HB3	1:C:58:LYS:HB2	1.97	0.46
1:G:382:LEU:HD13	1:G:401:LEU:HD22	1.97	0.46
1:H:224:GLU:CG	1:H:251:MET:HE1	2.45	0.46
1:G:379:LYS:HB3	1:H:233:SER:HA	1.97	0.46
1:E:104:THR:HG22	1:E:140:ASN:HB3	1.96	0.46
1:A:164:VAL:HG21	1:A:239:ASN:ND2	2.31	0.46
1:B:285:GLU:HG3	1:B:285:GLU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:CYS:HB2	1:D:191:ASN:ND2	2.25	0.46
1:D:179:ARG:HH12	1:D:181:GLU:CD	2.19	0.46
1:A:320:ASN:ND2	5:A:2107:HOH:O	2.49	0.46
1:E:152:TYR:OH	1:E:367:ARG:HD2	2.14	0.46
1:A:78:GLN:O	1:A:78:GLN:CG	2.64	0.46
1:C:224:GLU:OE2	1:C:243:ARG:NH1	2.48	0.46
1:F:145:ILE:O	1:F:149:VAL:HG23	2.15	0.46
1:D:115:ARG:HD3	1:D:408:ASN:OD1	2.16	0.46
1:E:73:LYS:NZ	1:E:306:GLU:OE2	2.38	0.46
1:F:295:SER:HB3	5:F:2041:HOH:O	2.15	0.46
1:G:196:ILE:HB	1:G:237:ILE:HB	1.98	0.45
1:G:224:GLU:OE2	1:G:243:ARG:NH1	2.49	0.45
1:B:304:ASP:OD2	1:B:313:HIS:NE2	2.42	0.45
1:C:352:ASP:OD2	1:D:383:LYS:NZ	2.45	0.45
1:B:162:CYS:SG	1:B:191:ASN:ND2	2.90	0.45
1:D:398:LYS:HE3	1:D:398:LYS:HB2	1.40	0.45
1:F:161:LEU:HD12	1:F:161:LEU:HA	1.74	0.45
1:H:116:ALA:O	1:H:120:VAL:HG13	2.17	0.45
1:E:168:PHE:CE2	1:E:196:ILE:HD13	2.52	0.45
1:B:163:ASN:HB3	1:B:294:TYR:CD2	2.52	0.45
1:D:16:LEU:CA	1:D:295:SER:HB3	2.46	0.45
1:A:33:ILE:HD11	1:A:62:SER:HB2	1.99	0.45
1:F:382:LEU:HD21	1:F:398:LYS:HG3	1.99	0.45
1:G:12:TYR:OH	1:G:289:ARG:HB3	2.16	0.45
1:B:346:LEU:CD2	1:C:346:LEU:HD12	2.46	0.45
1:D:294:TYR:CE1	3:D:1417:G6P:H3	2.52	0.45
1:A:346:LEU:HD11	1:D:346:LEU:HD11	1.97	0.45
1:E:32:VAL:HG12	1:E:34:PHE:CE1	2.51	0.45
1:A:216:LEU:O	1:A:217:LYS:O	2.34	0.44
1:C:106:GLY:HA2	1:C:388:HIS:CE1	2.52	0.44
1:G:285:GLU:O	1:G:285:GLU:HG3	2.17	0.44
1:C:138:PHE:CZ	1:C:298:ALA:HB2	2.53	0.44
1:A:0:HIS:HA	1:A:30:ASP:OD2	2.18	0.44
1:A:238:VAL:HG22	1:A:242:LEU:HD23	2.00	0.44
1:B:346:LEU:HD23	1:C:346:LEU:CD1	2.46	0.44
1:D:73:LYS:HG2	1:D:74:TYR:CE2	2.52	0.44
1:B:116:ALA:O	1:B:120:VAL:HG13	2.18	0.44
1:D:287:THR:C	1:D:289:ARG:H	2.20	0.44
1:A:285:GLU:O	1:A:285:GLU:CG	2.65	0.44
1:D:287:THR:C	1:D:289:ARG:N	2.72	0.44
1:B:346:LEU:CD2	1:C:346:LEU:CD1	2.95	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:106:GLY:HA2	1:H:388:HIS:CE1	2.53	0.43
1:A:-1:ARG:HD3	1:A:28:ARG:HD3	1.99	0.43
1:B:33:ILE:HD11	1:B:62:SER:HB2	2.01	0.43
1:G:164:VAL:N	1:G:165:PRO:CD	2.81	0.43
1:H:115:ARG:HG2	1:H:411:TYR:HB3	2.00	0.43
1:H:211:PHE:CE1	1:H:237:ILE:HG13	2.53	0.43
1:E:282:ILE:HA	1:E:283:PRO:HD3	1.89	0.43
1:D:211:PHE:O	1:D:215:LYS:HD2	2.19	0.43
1:H:11:SER:OG	1:H:289:ARG:NH1	2.51	0.43
1:E:138:PHE:CZ	1:E:298:ALA:HB2	2.53	0.43
1:H:162:CYS:SG	1:H:164:VAL:HG12	2.59	0.43
1:D:196:ILE:HB	1:D:237:ILE:HB	2.01	0.43
1:F:179:ARG:HG2	1:F:182:ASP:OD2	2.18	0.43
1:A:138:PHE:HZ	1:A:298:ALA:HB2	1.84	0.43
1:D:17:VAL:HG11	1:D:49:VAL:HG13	2.01	0.43
1:E:284:GLU:O	1:E:287:THR:OG1	2.34	0.43
1:G:392:PRO:HG3	1:G:400:LEU:HD23	2.00	0.43
1:C:196:ILE:HB	1:C:237:ILE:HB	1.99	0.43
1:F:224:GLU:HG2	1:F:251:MET:CE	2.48	0.43
1:B:107:VAL:O	1:B:110:PHE:HB3	2.19	0.42
1:E:261:ARG:HA	1:E:264:GLU:HG3	2.01	0.42
1:G:163:ASN:HB3	1:G:294:TYR:CD2	2.53	0.42
1:H:169:ILE:HG23	1:H:183:VAL:HB	2.01	0.42
1:A:163:ASN:HB3	1:A:294:TYR:CD1	2.54	0.42
1:E:296:THR:CG2	1:E:300:HIS:CE1	3.02	0.42
1:F:116:ALA:O	1:F:120:VAL:HG13	2.20	0.42
1:A:224:GLU:HG2	1:A:251:MET:CE	2.48	0.42
1:E:149:VAL:HG22	1:E:153:LEU:HD12	2.02	0.42
1:H:224:GLU:HG3	1:H:251:MET:HE1	2.01	0.42
1:B:382:LEU:HD13	1:B:401:LEU:HD22	2.02	0.42
1:B:215:LYS:HD3	1:B:228:THR:HG23	2.00	0.42
1:A:214:LEU:HD23	1:A:231:TYR:CZ	2.55	0.42
1:A:285:GLU:HG3	1:A:285:GLU:O	2.20	0.42
1:C:74:TYR:OH	1:C:306:GLU:OE2	2.25	0.42
1:D:167:ASN:OD1	1:D:170:ARG:NH2	2.53	0.42
1:H:305:LEU:HD13	1:H:338:VAL:CG1	2.49	0.42
1:B:282:ILE:HA	1:B:283:PRO:HD3	1.86	0.42
1:E:78:GLN:HG3	2:E:1416:NAD:N7N	2.35	0.42
1:H:192:HIS:CD2	1:H:241:TYR:CE2	3.07	0.42
1:A:346:LEU:CD1	1:D:346:LEU:HD12	2.48	0.42
1:A:224:GLU:OE1	1:A:243:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:PHE:HB2	1:D:51:ARG:HH22	1.85	0.42
1:E:161:LEU:HA	1:E:161:LEU:HD12	1.90	0.42
1:A:128:ARG:HB2	1:A:155:TYR:CE1	2.55	0.42
1:C:379:LYS:HE3	1:D:232:ASP:HB3	2.02	0.41
1:B:215:LYS:HG2	1:B:228:THR:HG23	2.01	0.41
1:H:35:TYR:C	1:H:42:GLN:HE22	2.23	0.41
1:E:92:GLY:HA2	1:E:95:LEU:HD22	2.01	0.41
1:G:31:GLU:HB3	1:G:58:LYS:HB2	2.02	0.41
1:H:162:CYS:SG	1:H:163:ASN:N	2.93	0.41
1:B:203:GLY:HA3	1:C:340:SER:HB3	2.02	0.41
1:E:239:ASN:OD1	1:E:240:PRO:HD2	2.20	0.41
1:A:12:TYR:OH	1:A:289:ARG:HB3	2.21	0.41
1:C:323:ILE:HG21	1:C:326:LEU:HD22	2.02	0.41
1:E:106:GLY:HA2	1:E:388:HIS:CE1	2.55	0.41
1:F:291:GLY:O	1:F:294:TYR:HD1	2.02	0.41
1:G:106:GLY:HA2	1:G:388:HIS:CE1	2.55	0.41
1:B:261:ARG:HA	1:B:264:GLU:HG3	2.03	0.41
1:C:45:VAL:CG2	1:C:273:PHE:CE1	3.03	0.41
1:H:2:ARG:HG3	1:H:31:GLU:HG3	2.02	0.41
1:G:354:PHE:HB2	1:H:383:LYS:HE2	2.02	0.41
1:A:232:ASP:HB3	1:B:379:LYS:HE2	2.03	0.41
1:E:196:ILE:HB	1:E:237:ILE:HB	2.02	0.41
1:F:166:ILE:HD13	1:F:293:MET:SD	2.61	0.41
1:G:322:SER:HB2	1:G:345:THR:HG23	2.02	0.41
1:D:305:LEU:HD13	1:D:338:VAL:CG1	2.51	0.41
1:D:9:GLY:HA2	1:D:45:VAL:HG21	2.03	0.41
1:F:409:ARG:HE	1:F:409:ARG:HB2	1.56	0.41
1:G:138:PHE:CZ	1:G:298:ALA:HB2	2.56	0.41
1:H:134:THR:HA	1:H:157:LYS:HB3	2.01	0.41
1:H:294:TYR:CE1	3:H:1417:G6P:H3	2.55	0.41
1:A:227:PRO:HG2	1:A:229:TRP:CE2	2.56	0.40
1:C:162:CYS:HB2	1:C:191:ASN:HD21	1.86	0.40
1:C:82:GLY:HA2	1:C:411:TYR:CZ	2.56	0.40
1:D:312:ILE:HA	1:D:336:CYS:O	2.21	0.40
1:D:84:LEU:HB2	1:D:266:MET:HE2	2.04	0.40
1:G:262:ALA:O	1:G:266:MET:HG3	2.21	0.40
1:C:285:GLU:O	1:C:285:GLU:HG2	2.22	0.40
1:C:82:GLY:HA3	1:C:115:ARG:HD3	2.04	0.40
1:D:260:LEU:O	1:D:263:ARG:HB2	2.22	0.40
1:F:16:LEU:HA	1:F:295:SER:HB2	2.02	0.40
1:G:379:LYS:O	1:H:233:SER:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:LEU:HA	1:C:161:LEU:HD12	1.96	0.40
1:D:382:LEU:HG	1:D:401:LEU:HD22	2.04	0.40
1:F:261:ARG:HA	1:F:264:GLU:HG3	2.01	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	410/417 (98%)	402 (98%)	6 (2%)	2 (0%)	29	41
1	B	405/417 (97%)	400 (99%)	5 (1%)	0	100	100
1	C	406/417 (97%)	399 (98%)	7 (2%)	0	100	100
1	D	405/417 (97%)	397 (98%)	6 (2%)	2 (0%)	29	41
1	E	398/417 (95%)	392 (98%)	6 (2%)	0	100	100
1	F	407/417 (98%)	399 (98%)	8 (2%)	0	100	100
1	G	405/417 (97%)	397 (98%)	8 (2%)	0	100	100
1	H	401/417 (96%)	391 (98%)	10 (2%)	0	100	100
All	All	3237/3336 (97%)	3177 (98%)	56 (2%)	4 (0%)	51	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO
1	A	223	ASP
1	D	288	LYS
1	D	285	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/369 (99%)	330 (90%)	36 (10%)	8	11
1	B	361/369 (98%)	327 (91%)	34 (9%)	8	13
1	C	362/369 (98%)	329 (91%)	33 (9%)	9	14
1	D	361/369 (98%)	318 (88%)	43 (12%)	5	6
1	E	358/369 (97%)	327 (91%)	31 (9%)	10	15
1	F	363/369 (98%)	318 (88%)	45 (12%)	4	5
1	G	361/369 (98%)	325 (90%)	36 (10%)	7	11
1	H	359/369 (97%)	314 (88%)	45 (12%)	4	5
All	All	2891/2952 (98%)	2588 (90%)	303 (10%)	7	9

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ARG
1	A	18	LYS
1	A	28	ARG
1	A	39	GLU
1	A	78	GLN
1	A	95	LEU
1	A	99	LEU
1	A	120	VAL
1	A	128	ARG
1	A	132	ASN
1	A	157	LYS
1	A	170	ARG
1	A	174	GLU
1	A	185	LEU
1	A	190	LEU
1	A	198	LYS
1	A	213	ASN
1	A	215	LYS
1	A	221	ILE

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Mol	Chain	Res	Type
1	A	223	ASP
1	A	235	ARG
1	A	242	LEU
1	A	289	ARG
1	A	305	LEU
1	A	315	VAL
1	A	326	LEU
1	A	342	ARG
1	A	345	THR
1	A	346	LEU
1	A	365	TYR
1	A	367	ARG
1	A	375	LYS
1	A	382	LEU
1	A	398	LYS
1	A	402	GLU
1	A	414	LEU
1	B	18	LYS
1	B	56	ARG
1	B	99	LEU
1	B	120	VAL
1	B	128	ARG
1	B	157	LYS
1	B	161	LEU
1	B	164	VAL
1	B	185	LEU
1	B	190	LEU
1	B	198	LYS
1	B	212	GLU
1	B	213	ASN
1	B	214	LEU
1	B	217	LYS
1	B	238	VAL
1	B	250	LYS
1	B	267	LYS
1	B	270	LYS
1	B	278	THR
1	B	294	TYR
1	B	305	LEU
1	B	311	LYS
1	B	315	VAL
1	B	326	LEU

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Mol	Chain	Res	Type
1	B	345	THR
1	B	365	TYR
1	B	367	ARG
1	B	382	LEU
1	B	385	LEU
1	B	398	LYS
1	B	412	VAL
1	B	413	LYS
1	B	414	LEU
1	C	43	LYS
1	C	51	ARG
1	C	56	ARG
1	C	95	LEU
1	C	99	LEU
1	C	132	ASN
1	C	157	LYS
1	C	174	GLU
1	C	177	SER
1	C	185	LEU
1	C	190	LEU
1	C	215	LYS
1	C	225	ASP
1	C	238	VAL
1	C	246	LEU
1	C	261	ARG
1	C	267	LYS
1	C	270	LYS
1	C	280	VAL
1	C	294	TYR
1	C	305	LEU
1	C	309	GLU
1	C	315	VAL
1	C	326	LEU
1	C	345	THR
1	C	346	LEU
1	C	347	SER
1	C	365	TYR
1	C	367	ARG
1	C	375	LYS
1	C	382	LEU
1	C	402	GLU
1	C	414	LEU

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Mol	Chain	Res	Type
1	D	24	SER
1	D	39	GLU
1	D	41	LYS
1	D	63	ASP
1	D	95	LEU
1	D	99	LEU
1	D	128	ARG
1	D	132	ASN
1	D	156	GLU
1	D	161	LEU
1	D	162	CYS
1	D	164	VAL
1	D	170	ARG
1	D	174	GLU
1	D	185	LEU
1	D	190	LEU
1	D	213	ASN
1	D	215	LYS
1	D	216	LEU
1	D	224	GLU
1	D	228	THR
1	D	238	VAL
1	D	250	LYS
1	D	253	LYS
1	D	263	ARG
1	D	265	VAL
1	D	270	LYS
1	D	280	VAL
1	D	288	LYS
1	D	289	ARG
1	D	293	MET
1	D	305	LEU
1	D	311	LYS
1	D	315	VAL
1	D	326	LEU
1	D	345	THR
1	D	346	LEU
1	D	365	TYR
1	D	367	ARG
1	D	378	LYS
1	D	398	LYS
1	D	402	GLU

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Mol	Chain	Res	Type
1	D	410	GLU
1	E	33	ILE
1	E	40	GLU
1	E	43	LYS
1	E	58	LYS
1	E	95	LEU
1	E	99	LEU
1	E	120	VAL
1	E	128	ARG
1	E	129	LYS
1	E	185	LEU
1	E	190	LEU
1	E	198	LYS
1	E	238	VAL
1	E	246	LEU
1	E	264	GLU
1	E	275	LYS
1	E	281	GLU
1	E	289	ARG
1	E	293	MET
1	E	294	TYR
1	E	295	SER
1	E	305	LEU
1	E	315	VAL
1	E	326	LEU
1	E	345	THR
1	E	346	LEU
1	E	367	ARG
1	E	375	LYS
1	E	398	LYS
1	E	402	GLU
1	E	414	LEU
1	F	1	MET
1	F	18	LYS
1	F	44	ILE
1	F	56	ARG
1	F	99	LEU
1	F	132	ASN
1	F	166	ILE
1	F	170	ARG
1	F	174	GLU
1	F	175	MET

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Mol	Chain	Res	Type
1	F	177	SER
1	F	179	ARG
1	F	185	LEU
1	F	190	LEU
1	F	208	GLU
1	F	212	GLU
1	F	215	LYS
1	F	223	ASP
1	F	233	SER
1	F	238	VAL
1	F	242	LEU
1	F	243	ARG
1	F	253	LYS
1	F	259	GLU
1	F	261	ARG
1	F	264	GLU
1	F	270	LYS
1	F	275	LYS
1	F	277	ARG
1	F	281	GLU
1	F	285	GLU
1	F	287	THR
1	F	293	MET
1	F	295	SER
1	F	311	LYS
1	F	315	VAL
1	F	326	LEU
1	F	346	LEU
1	F	365	TYR
1	F	367	ARG
1	F	382	LEU
1	F	398	LYS
1	F	402	GLU
1	F	406	GLU
1	F	414	LEU
1	G	24	SER
1	G	43	LYS
1	G	85	LYS
1	G	95	LEU
1	G	96	LYS
1	G	99	LEU
1	G	120	VAL

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Mol	Chain	Res	Type
1	G	157	LYS
1	G	161	LEU
1	G	164	VAL
1	G	185	LEU
1	G	190	LEU
1	G	225	ASP
1	G	238	VAL
1	G	246	LEU
1	G	265	VAL
1	G	275	LYS
1	G	278	THR
1	G	280	VAL
1	G	281	GLU
1	G	285	GLU
1	G	289	ARG
1	G	305	LEU
1	G	311	LYS
1	G	315	VAL
1	G	326	LEU
1	G	345	THR
1	G	365	TYR
1	G	367	ARG
1	G	375	LYS
1	G	382	LEU
1	G	398	LYS
1	G	402	GLU
1	G	409	ARG
1	G	413	LYS
1	G	414	LEU
1	H	15	GLU
1	H	18	LYS
1	H	41	LYS
1	H	50	LYS
1	H	55	ASP
1	H	58	LYS
1	H	95	LEU
1	H	99	LEU
1	H	132	ASN
1	H	154	GLU
1	H	156	GLU
1	H	161	LEU
1	H	164	VAL

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Mol	Chain	Res	Type
1	H	174	GLU
1	H	185	LEU
1	H	190	LEU
1	H	204	GLU
1	H	214	LEU
1	H	216	LEU
1	H	238	VAL
1	H	243	ARG
1	H	253	LYS
1	H	263	ARG
1	H	267	LYS
1	H	271	GLU
1	H	280	VAL
1	H	285	GLU
1	H	287	THR
1	H	289	ARG
1	H	292	SER
1	H	293	MET
1	H	295	SER
1	H	305	LEU
1	H	311	LYS
1	H	315	VAL
1	H	326	LEU
1	H	345	THR
1	H	365	TYR
1	H	367	ARG
1	H	375	LYS
1	H	398	LYS
1	H	399	ASP
1	H	402	GLU
1	H	412	VAL
1	H	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	191	ASN
1	A	300	HIS
1	A	320	ASN
1	B	132	ASN
1	B	320	ASN

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Mol	Chain	Res	Type
1	C	42	GLN
1	C	213	ASN
1	D	42	GLN
1	D	191	ASN
1	D	300	HIS
1	D	320	ASN
1	E	42	GLN
1	E	191	ASN
1	E	300	HIS
1	E	320	ASN
1	F	42	GLN
1	F	213	ASN
1	F	320	ASN
1	G	320	ASN
1	H	42	GLN
1	H	300	HIS
1	H	320	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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
3	G6P	H	1417	-	16,16,16	0.46	0	24,24,24	0.99	1 (4%)
2	NAD	B	1416	-	42,48,48	1.85	3 (7%)	50,73,73	1.25	5 (10%)
2	NAD	A	1416	-	42,48,48	1.85	5 (11%)	50,73,73	1.40	7 (14%)
2	NAD	D	1416	-	42,48,48	1.81	3 (7%)	50,73,73	1.24	4 (8%)
2	NAD	C	1416	-	42,48,48	1.80	3 (7%)	50,73,73	1.26	4 (8%)
2	NAD	F	1416	-	42,48,48	1.75	3 (7%)	50,73,73	1.30	4 (8%)
2	NAD	E	1416	-	42,48,48	1.77	3 (7%)	50,73,73	1.37	4 (8%)
2	NAD	H	1416	-	42,48,48	1.69	3 (7%)	50,73,73	1.25	4 (8%)
2	NAD	G	1416	-	42,48,48	1.80	3 (7%)	50,73,73	1.34	6 (12%)
3	G6P	A	1417	-	16,16,16	0.71	0	24,24,24	1.20	2 (8%)
3	G6P	C	1417	-	16,16,16	0.70	0	24,24,24	1.12	1 (4%)
3	G6P	G	1417	-	16,16,16	0.64	0	24,24,24	1.02	2 (8%)
3	G6P	D	1417	-	16,16,16	0.44	0	24,24,24	0.92	0
4	SO4	C	1418	-	4,4,4	0.61	0	6,6,6	0.38	0
3	G6P	F	1417	-	16,16,16	0.51	0	24,24,24	1.00	2 (8%)
4	SO4	A	1418	-	4,4,4	0.37	0	6,6,6	0.54	0
3	G6P	E	1417	-	16,16,16	0.56	0	24,24,24	0.83	0
3	G6P	B	1417	-	16,16,16	0.46	0	24,24,24	0.70	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
3	G6P	H	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
2	NAD	B	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	A	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	D	1416	-	-	11/26/62/62	0/5/5/5
2	NAD	C	1416	-	-	10/26/62/62	0/5/5/5
2	NAD	F	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	E	1416	-	-	5/26/62/62	0/5/5/5
2	NAD	H	1416	-	-	7/26/62/62	0/5/5/5
2	NAD	G	1416	-	-	9/26/62/62	0/5/5/5
3	G6P	A	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	G	1417	-	1/1/6/6	5/6/26/26	0/1/1/1
3	G6P	D	1417	-	1/1/6/6	2/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	G6P	F	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	C	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	E	1417	-	1/1/6/6	2/6/26/26	0/1/1/1
3	G6P	B	1417	-	1/1/6/6	2/6/26/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1416	NAD	O7N-C7N	9.70	1.42	1.24
2	G	1416	NAD	O7N-C7N	9.49	1.42	1.24
2	D	1416	NAD	O7N-C7N	9.49	1.42	1.24
2	A	1416	NAD	O7N-C7N	9.30	1.42	1.24
2	C	1416	NAD	O7N-C7N	9.17	1.41	1.24
2	E	1416	NAD	O7N-C7N	9.10	1.41	1.24
2	F	1416	NAD	O7N-C7N	9.08	1.41	1.24
2	H	1416	NAD	O7N-C7N	8.89	1.41	1.24
2	C	1416	NAD	C2A-N3A	4.16	1.38	1.32
2	E	1416	NAD	C2A-N3A	3.93	1.38	1.32
2	B	1416	NAD	C2A-N3A	3.90	1.38	1.32
2	G	1416	NAD	C2A-N3A	3.78	1.38	1.32
2	D	1416	NAD	C2A-N3A	3.74	1.38	1.32
2	A	1416	NAD	C2A-N3A	3.57	1.37	1.32
2	F	1416	NAD	C2A-N3A	3.55	1.37	1.32
2	H	1416	NAD	C2A-N3A	3.33	1.37	1.32
2	B	1416	NAD	C2A-N1A	2.99	1.39	1.33
2	E	1416	NAD	C2A-N1A	2.87	1.39	1.33
2	C	1416	NAD	C2A-N1A	2.74	1.39	1.33
2	A	1416	NAD	C2A-N1A	2.69	1.38	1.33
2	D	1416	NAD	C2A-N1A	2.68	1.38	1.33
2	A	1416	NAD	C2N-N1N	2.61	1.38	1.35
2	F	1416	NAD	C2A-N1A	2.57	1.38	1.33
2	G	1416	NAD	C2A-N1A	2.46	1.38	1.33
2	H	1416	NAD	C2A-N1A	2.28	1.38	1.33
2	A	1416	NAD	PN-O2N	-2.17	1.45	1.55

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1416	NAD	N3A-C2A-N1A	-6.15	119.07	128.68
2	F	1416	NAD	N3A-C2A-N1A	-5.95	119.37	128.68
2	G	1416	NAD	N3A-C2A-N1A	-5.91	119.44	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1416	NAD	N3A-C2A-N1A	-5.77	119.66	128.68
2	E	1416	NAD	N3A-C2A-N1A	-5.72	119.74	128.68
2	A	1416	NAD	N3A-C2A-N1A	-5.71	119.76	128.68
2	B	1416	NAD	N3A-C2A-N1A	-5.65	119.86	128.68
2	D	1416	NAD	N3A-C2A-N1A	-5.31	120.38	128.68
2	E	1416	NAD	PN-O3-PA	-3.77	119.88	132.83
3	A	1417	G6P	O2P-P-O6	3.14	115.09	106.73
2	F	1416	NAD	PN-O3-PA	-2.95	122.69	132.83
2	A	1416	NAD	C1B-N9A-C4A	-2.89	121.56	126.64
2	G	1416	NAD	O4B-C1B-C2B	-2.79	102.84	106.93
2	E	1416	NAD	O4B-C1B-C2B	-2.70	102.98	106.93
2	H	1416	NAD	O4B-C1B-C2B	-2.66	103.05	106.93
3	H	1417	G6P	O5-C5-C4	2.64	114.48	109.69
2	A	1416	NAD	O7N-C7N-C3N	2.53	122.66	119.63
2	B	1416	NAD	PN-O3-PA	-2.51	124.21	132.83
2	C	1416	NAD	C1B-N9A-C4A	-2.51	122.23	126.64
2	G	1416	NAD	O7N-C7N-C3N	2.51	122.64	119.63
2	H	1416	NAD	PN-O3-PA	-2.43	124.48	132.83
2	F	1416	NAD	C3D-C2D-C1D	2.38	104.57	100.98
2	A	1416	NAD	O4B-C1B-C2B	-2.34	103.51	106.93
2	G	1416	NAD	PN-O3-PA	-2.33	124.84	132.83
3	C	1417	G6P	O2-C2-C1	2.29	114.48	109.16
2	H	1416	NAD	O5D-C5D-C4D	2.25	116.74	108.99
2	D	1416	NAD	C3D-C2D-C1D	2.24	104.35	100.98
2	D	1416	NAD	C4A-C5A-N7A	-2.22	107.08	109.40
2	C	1416	NAD	C3N-C7N-N7N	2.21	120.41	117.75
2	A	1416	NAD	O7N-C7N-N7N	-2.20	119.45	122.58
3	G	1417	G6P	P-O6-C6	2.19	124.34	118.30
2	D	1416	NAD	O4B-C1B-C2B	-2.19	103.72	106.93
2	A	1416	NAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	B	1416	NAD	C3D-C2D-C1D	2.14	104.21	100.98
2	G	1416	NAD	O3B-C3B-C4B	-2.12	104.93	111.05
2	B	1416	NAD	O7N-C7N-C3N	2.10	122.15	119.63
3	F	1417	G6P	O5-C5-C4	2.08	113.47	109.69
3	G	1417	G6P	O2P-P-O6	2.04	112.15	106.73
2	B	1416	NAD	O4B-C1B-C2B	-2.04	103.95	106.93
2	E	1416	NAD	C6N-N1N-C2N	-2.04	120.12	121.97
3	F	1417	G6P	C3-C4-C5	2.03	113.86	110.24
2	F	1416	NAD	O2N-PN-O1N	2.02	122.20	112.24
3	A	1417	G6P	C4-C3-C2	-2.01	107.31	110.82
2	A	1416	NAD	C3D-C2D-C1D	2.01	104.00	100.98
2	G	1416	NAD	O2N-PN-O1N	2.01	122.16	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1416	NAD	O2N-PN-O1N	2.00	122.14	112.24

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	H	1417	G6P	C1
3	A	1417	G6P	C1
3	G	1417	G6P	C1
3	D	1417	G6P	C1
3	F	1417	G6P	C1
3	C	1417	G6P	C1
3	E	1417	G6P	C1
3	B	1417	G6P	C1

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1417	G6P	C4-C5-C6-O6
3	H	1417	G6P	O5-C5-C6-O6
2	D	1416	NAD	C5B-O5B-PA-O1A
2	D	1416	NAD	C5B-O5B-PA-O2A
2	D	1416	NAD	PN-O3-PA-O5B
2	D	1416	NAD	C5D-O5D-PN-O2N
2	C	1416	NAD	PA-O3-PN-O5D
2	C	1416	NAD	C5D-O5D-PN-O2N
2	F	1416	NAD	O4D-C4D-C5D-O5D
2	H	1416	NAD	C5D-O5D-PN-O2N
2	G	1416	NAD	PA-O3-PN-O5D
3	A	1417	G6P	C4-C5-C6-O6
3	A	1417	G6P	O5-C5-C6-O6
3	G	1417	G6P	C4-C5-C6-O6
3	G	1417	G6P	O5-C5-C6-O6
3	G	1417	G6P	C6-O6-P-O1P
3	G	1417	G6P	C6-O6-P-O2P
3	D	1417	G6P	C4-C5-C6-O6
3	D	1417	G6P	O5-C5-C6-O6
3	F	1417	G6P	C4-C5-C6-O6
3	F	1417	G6P	O5-C5-C6-O6
3	C	1417	G6P	C4-C5-C6-O6
3	C	1417	G6P	O5-C5-C6-O6
3	E	1417	G6P	C4-C5-C6-O6
3	E	1417	G6P	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	B	1417	G6P	C4-C5-C6-O6
3	B	1417	G6P	O5-C5-C6-O6
2	F	1416	NAD	C3D-C4D-C5D-O5D
2	E	1416	NAD	C3D-C4D-C5D-O5D
2	C	1416	NAD	C2N-C3N-C7N-O7N
2	C	1416	NAD	O4D-C4D-C5D-O5D
2	C	1416	NAD	C3D-C4D-C5D-O5D
2	E	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	C3D-C4D-C5D-O5D
2	C	1416	NAD	C4N-C3N-C7N-O7N
2	C	1416	NAD	C2N-C3N-C7N-N7N
2	C	1416	NAD	C4N-C3N-C7N-N7N
2	H	1416	NAD	C3D-C4D-C5D-O5D
2	H	1416	NAD	O4D-C4D-C5D-O5D
3	G	1417	G6P	C6-O6-P-O3P
2	B	1416	NAD	O4D-C4D-C5D-O5D
2	G	1416	NAD	C4N-C3N-C7N-O7N
2	F	1416	NAD	PA-O3-PN-O5D
2	E	1416	NAD	PA-O3-PN-O5D
2	H	1416	NAD	PA-O3-PN-O5D
2	G	1416	NAD	C4N-C3N-C7N-N7N
2	B	1416	NAD	C5B-O5B-PA-O3
2	D	1416	NAD	C5D-O5D-PN-O3
2	C	1416	NAD	C5B-O5B-PA-O3
2	F	1416	NAD	C5B-O5B-PA-O3
2	E	1416	NAD	C5B-O5B-PA-O3
2	G	1416	NAD	C5B-O5B-PA-O3
2	A	1416	NAD	C4N-C3N-C7N-O7N
2	B	1416	NAD	C3D-C4D-C5D-O5D
2	F	1416	NAD	O4B-C4B-C5B-O5B
2	G	1416	NAD	C2N-C3N-C7N-O7N
2	A	1416	NAD	C4N-C3N-C7N-N7N
2	D	1416	NAD	O4D-C4D-C5D-O5D
2	B	1416	NAD	PA-O3-PN-O2N
2	A	1416	NAD	PA-O3-PN-O2N
2	G	1416	NAD	C2N-C3N-C7N-N7N
2	D	1416	NAD	PA-O3-PN-O2N
2	D	1416	NAD	C3D-C4D-C5D-O5D
2	A	1416	NAD	C2N-C3N-C7N-O7N
2	A	1416	NAD	C2N-C3N-C7N-N7N
2	D	1416	NAD	C5B-O5B-PA-O3

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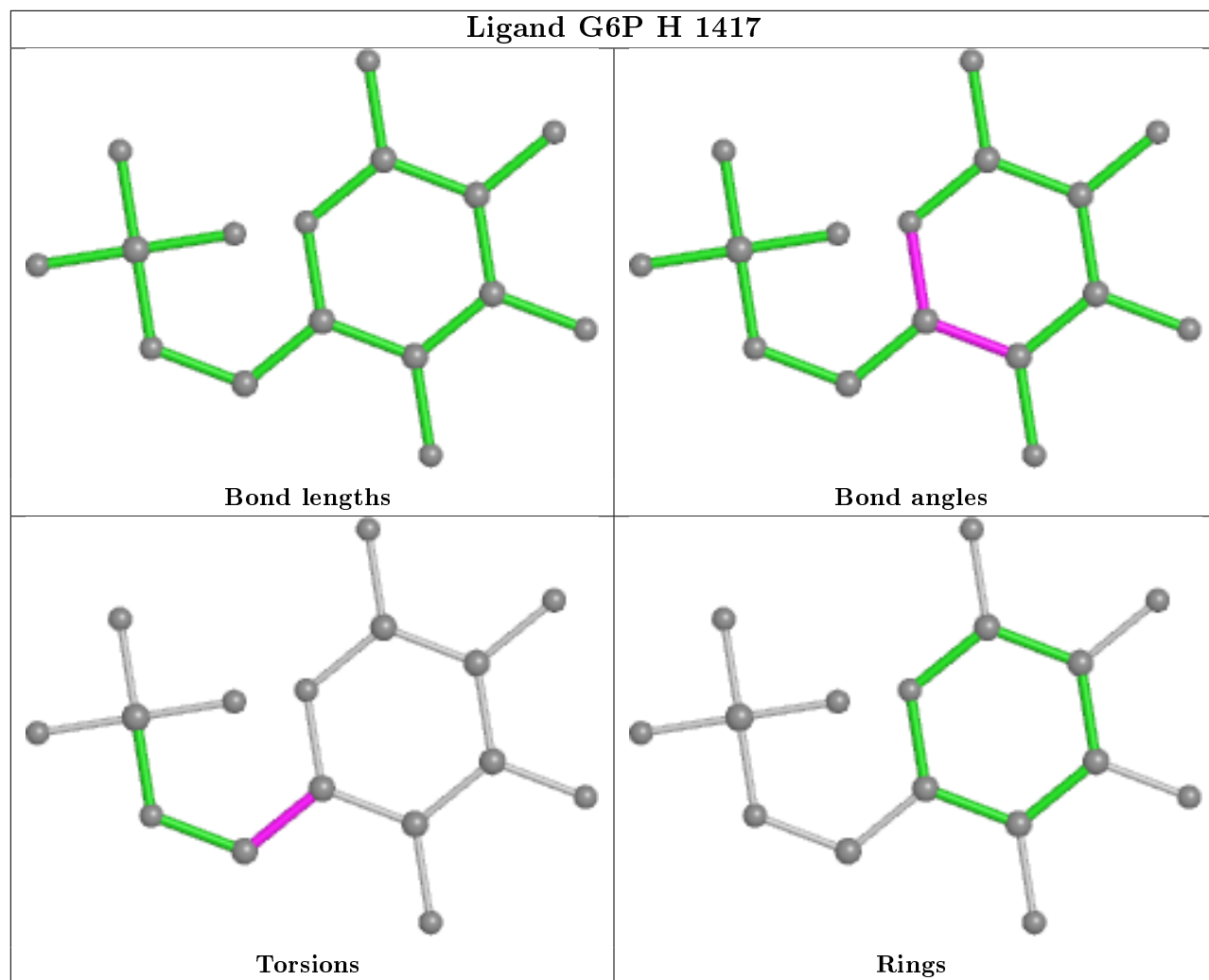
Mol	Chain	Res	Type	Atoms
2	H	1416	NAD	C5D-O5D-PN-O3
2	G	1416	NAD	C2D-C1D-N1N-C2N
2	E	1416	NAD	PN-O3-PA-O2A
2	H	1416	NAD	PA-O3-PN-O2N
2	D	1416	NAD	C4B-C5B-O5B-PA
2	B	1416	NAD	C5B-O5B-PA-O1A
2	D	1416	NAD	C5D-O5D-PN-O1N
2	C	1416	NAD	C5D-O5D-PN-O1N
2	H	1416	NAD	C5D-O5D-PN-O1N

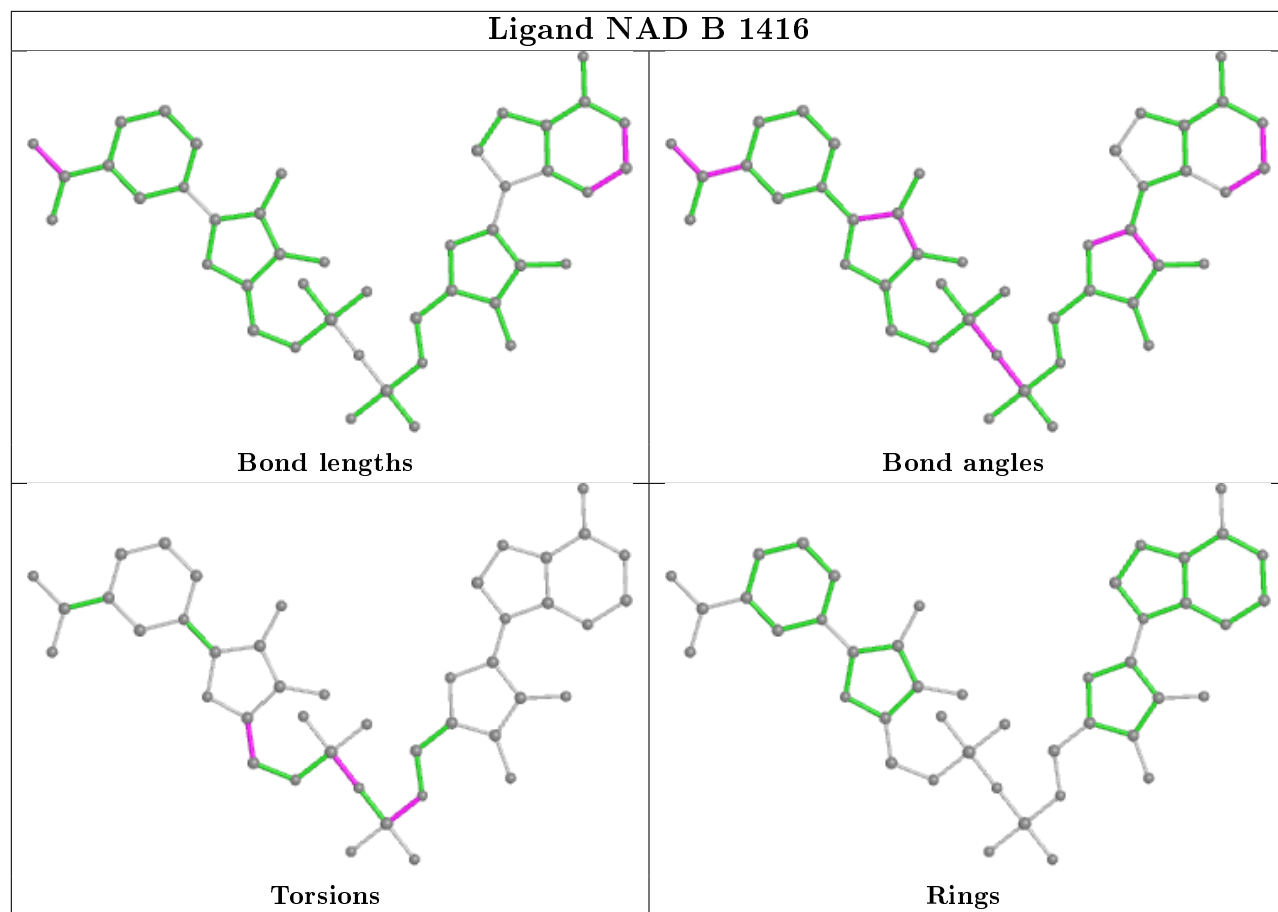
There are no ring outliers.

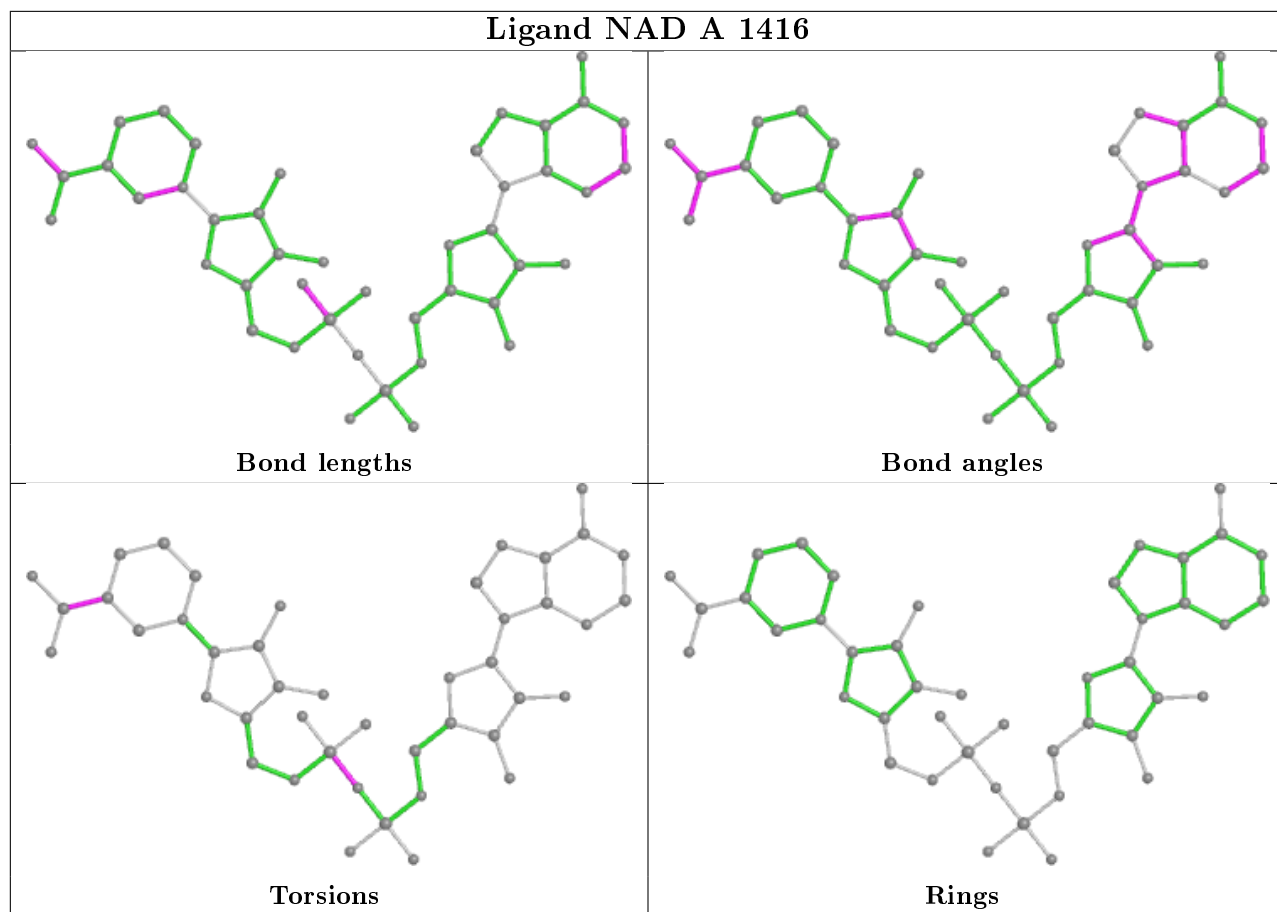
4 monomers are involved in 7 short contacts:

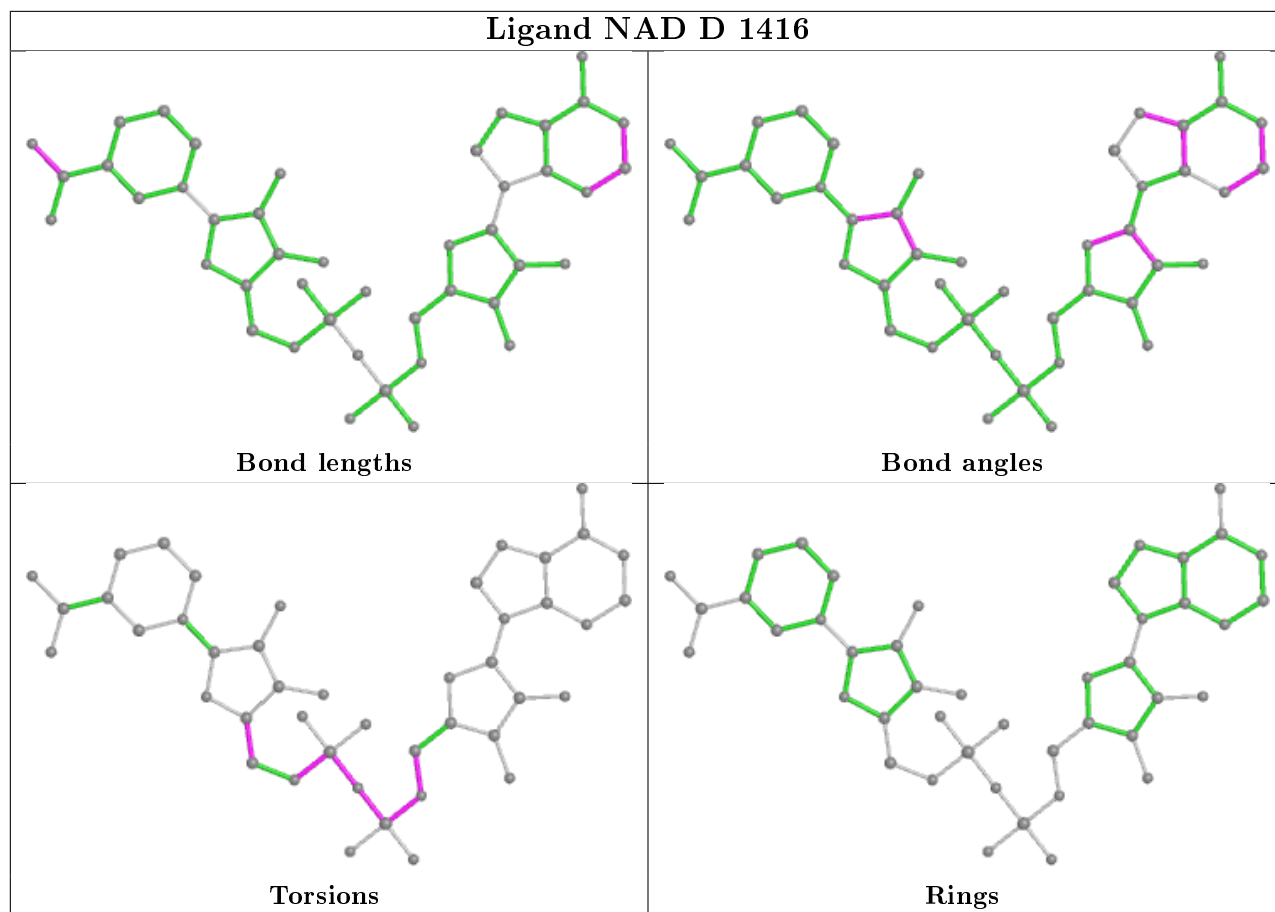
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1417	G6P	2	0
2	F	1416	NAD	2	0
2	E	1416	NAD	1	0
3	D	1417	G6P	2	0

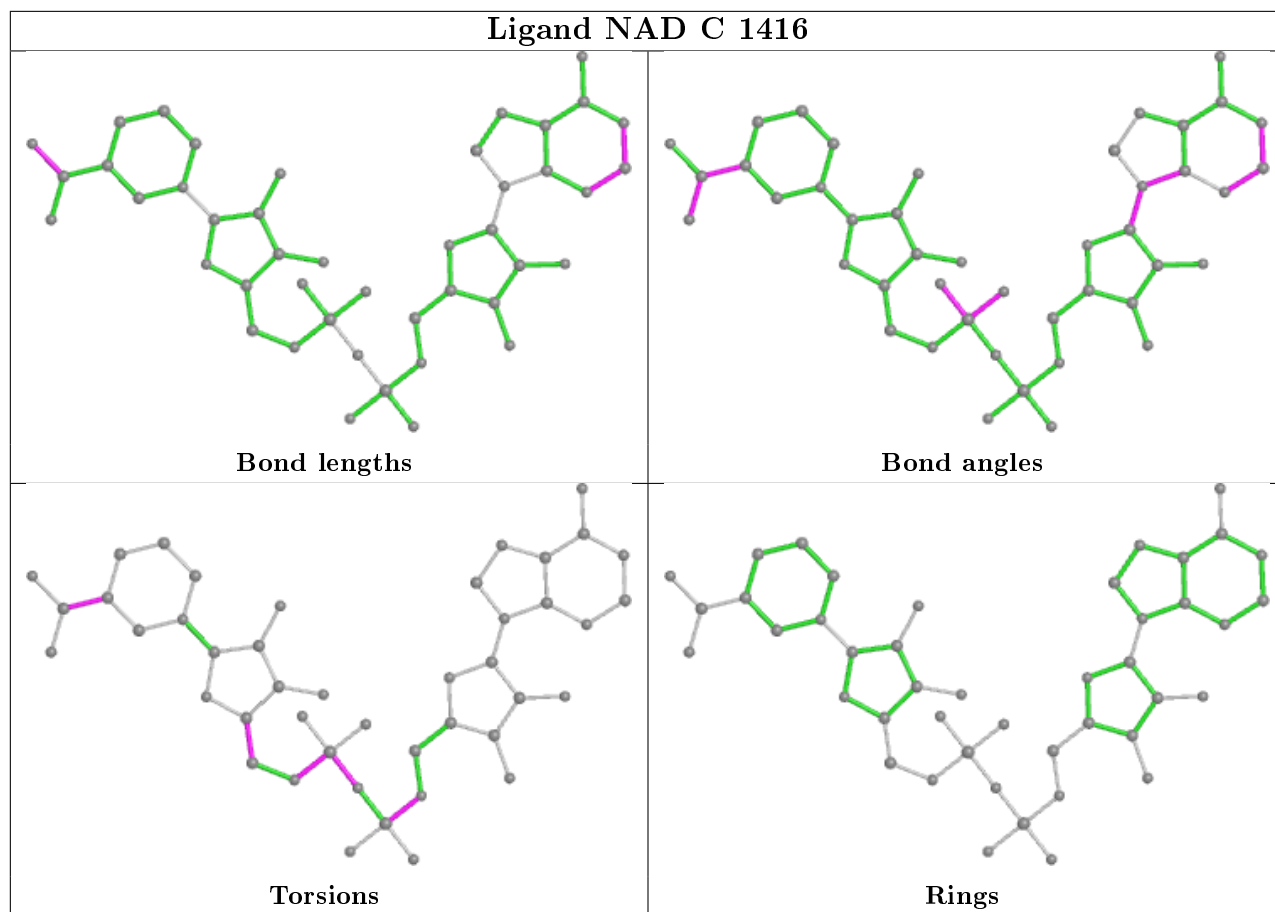
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

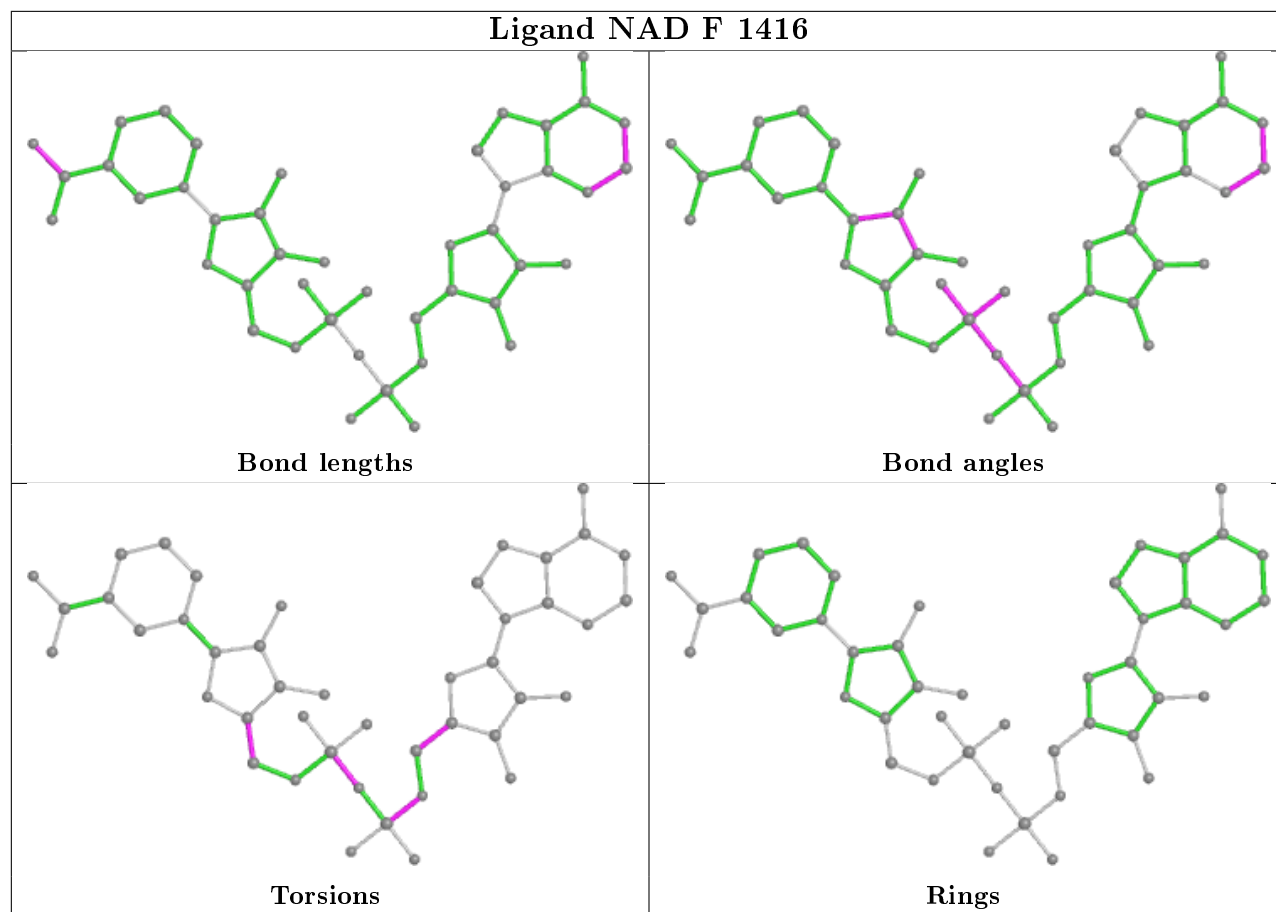


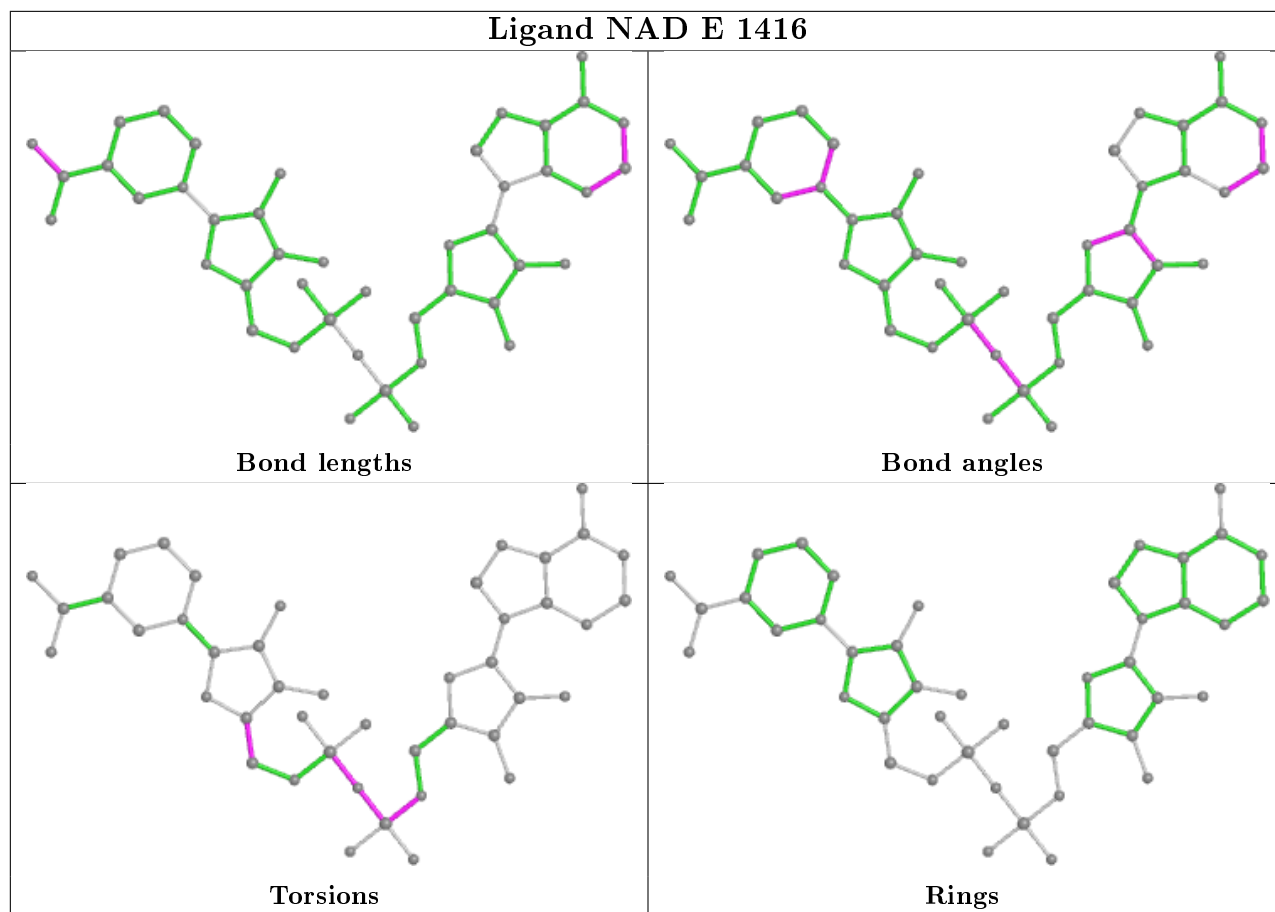


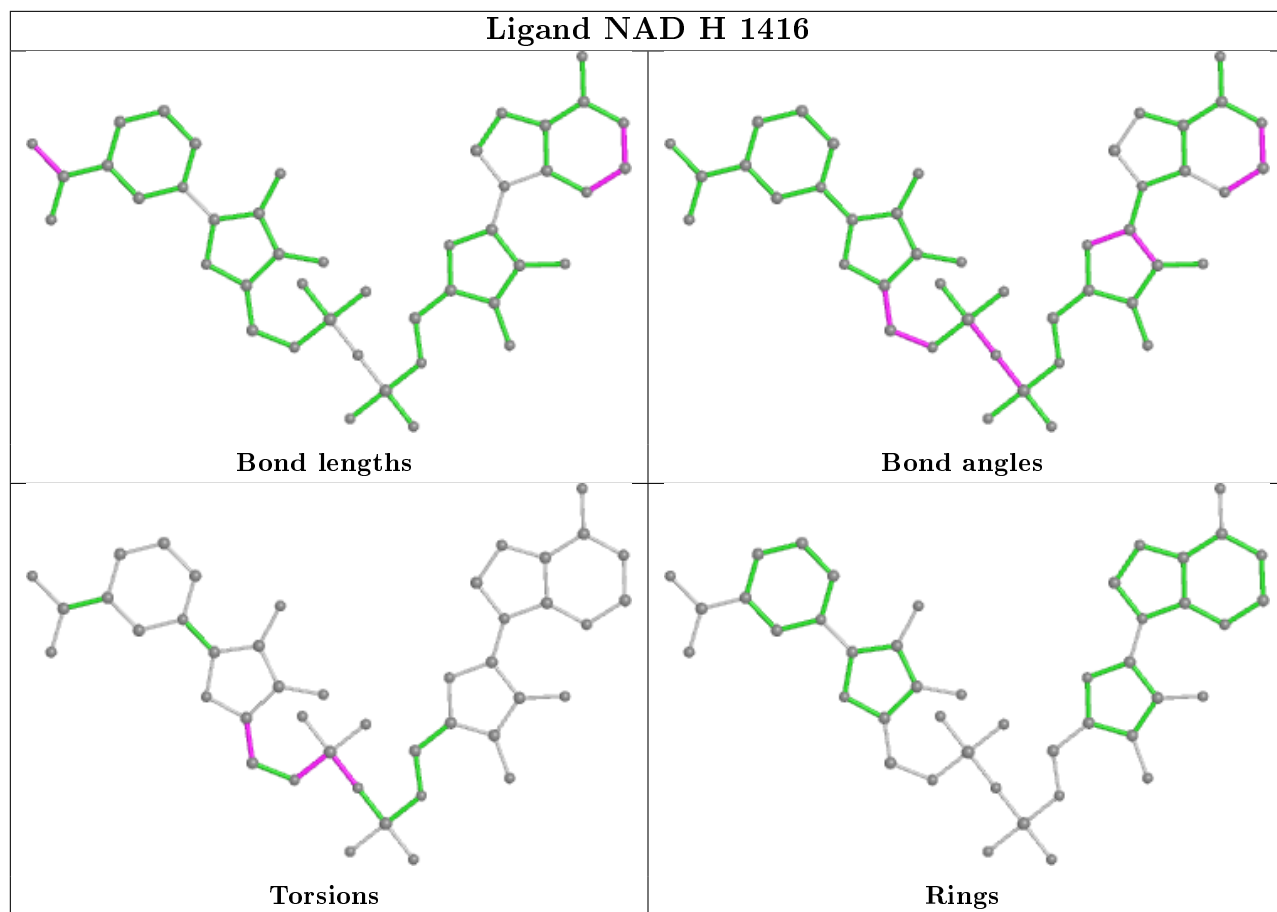


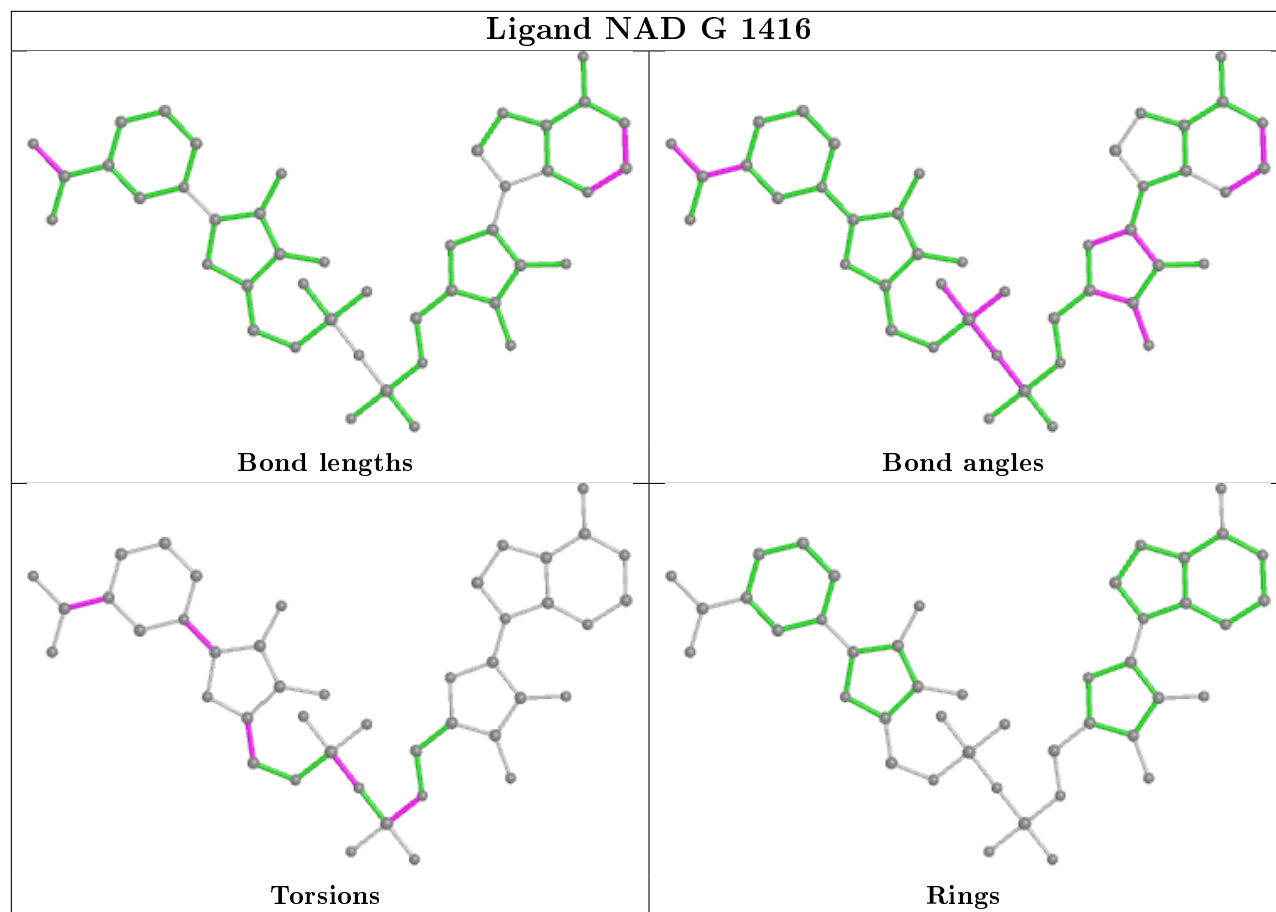


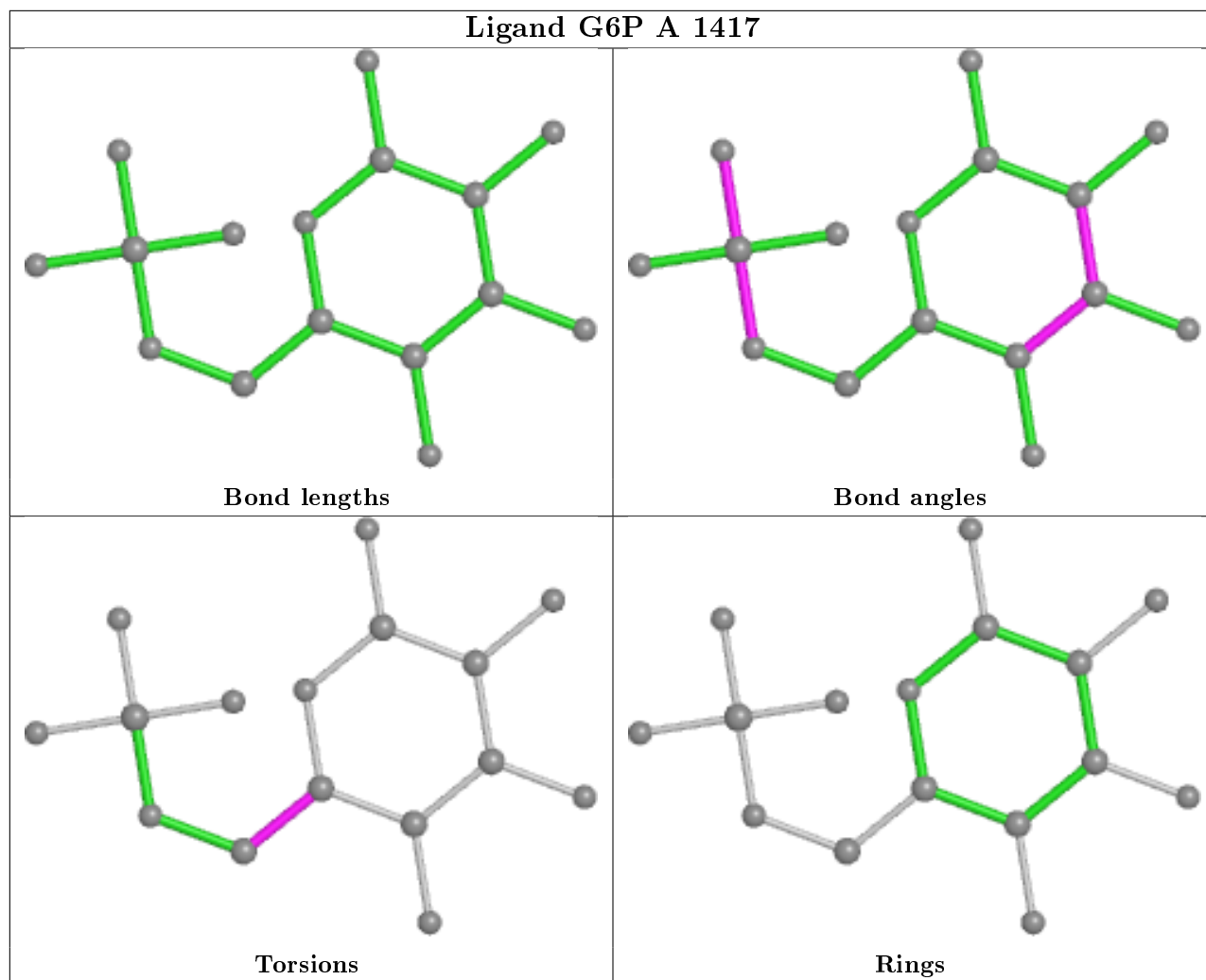


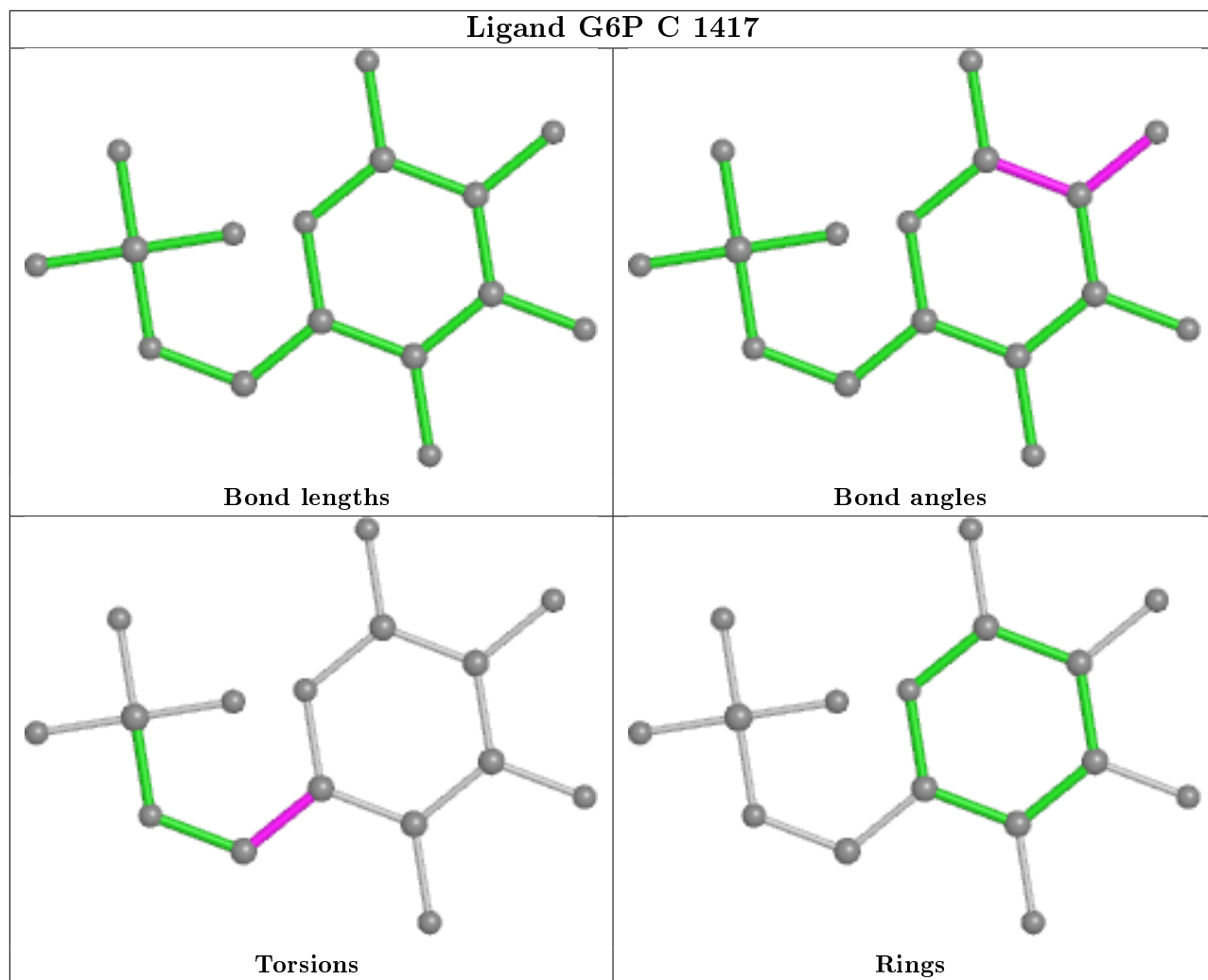


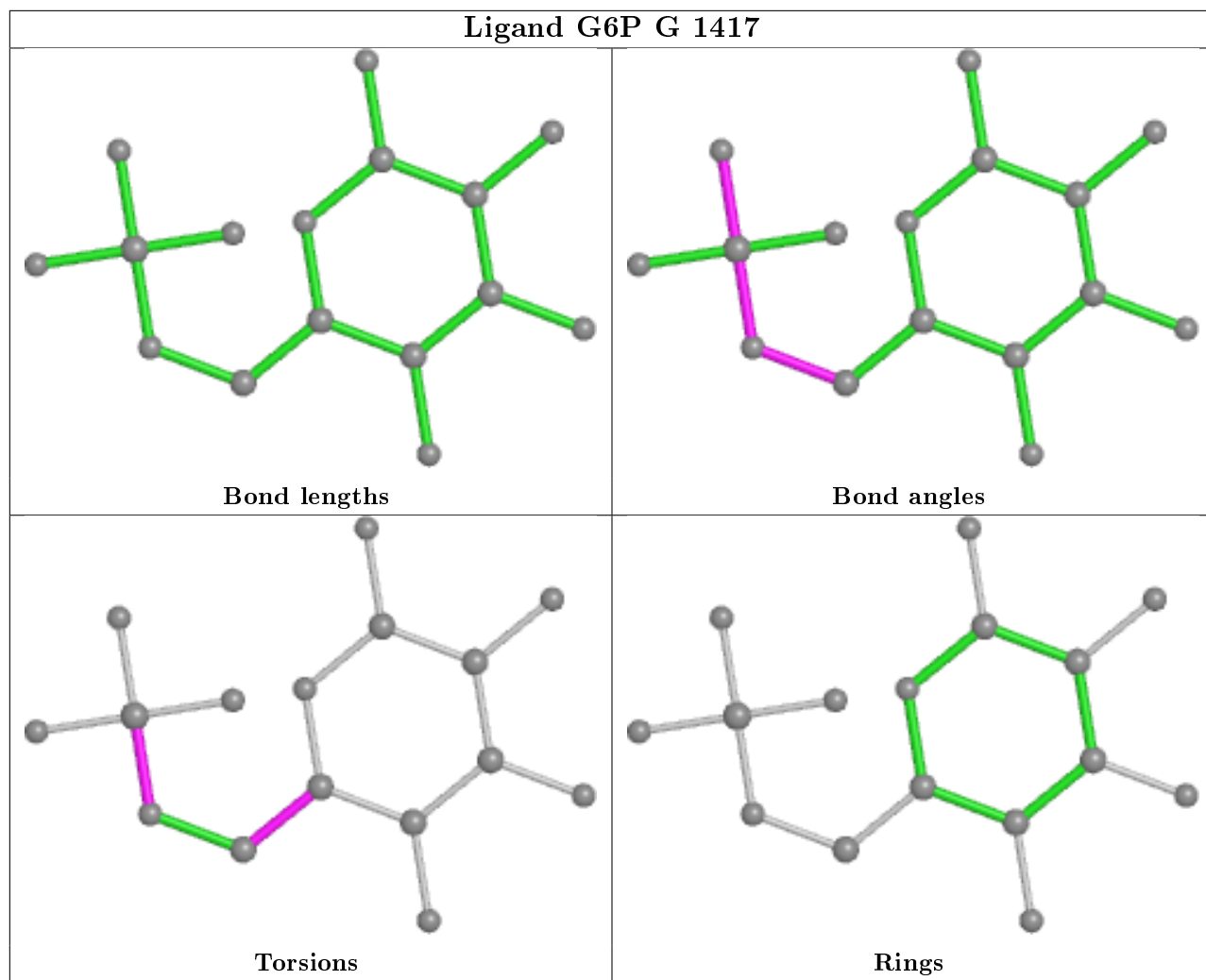


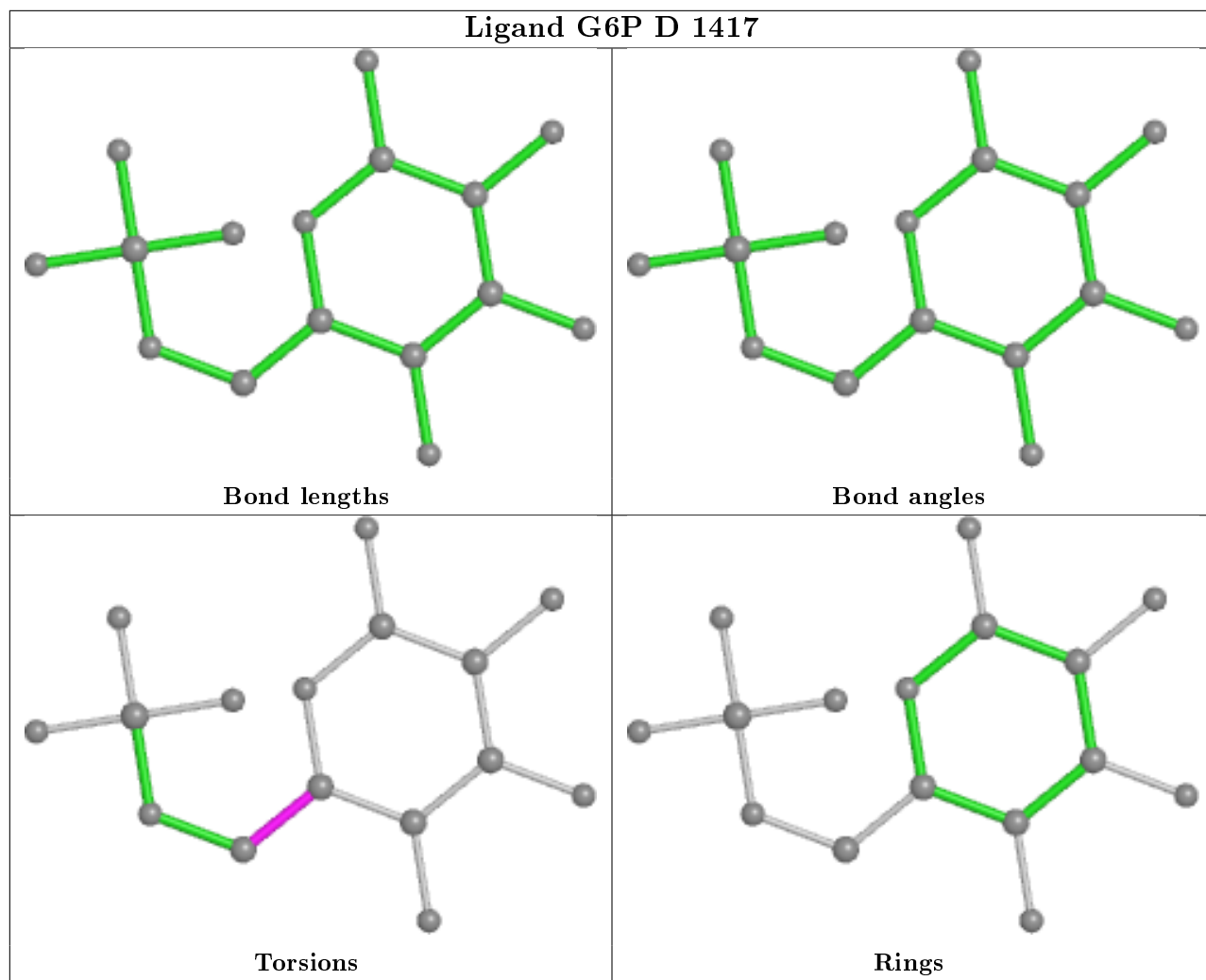


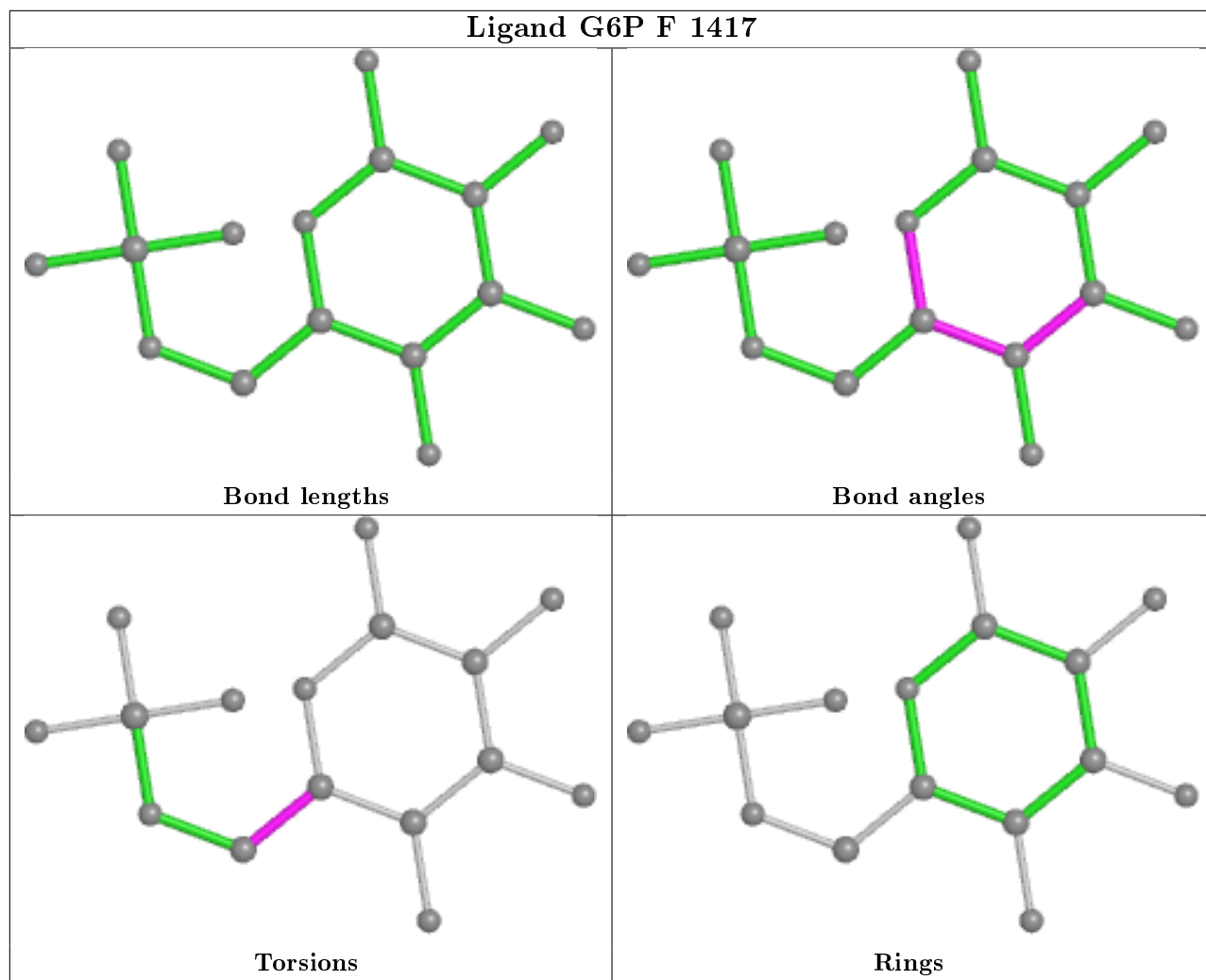


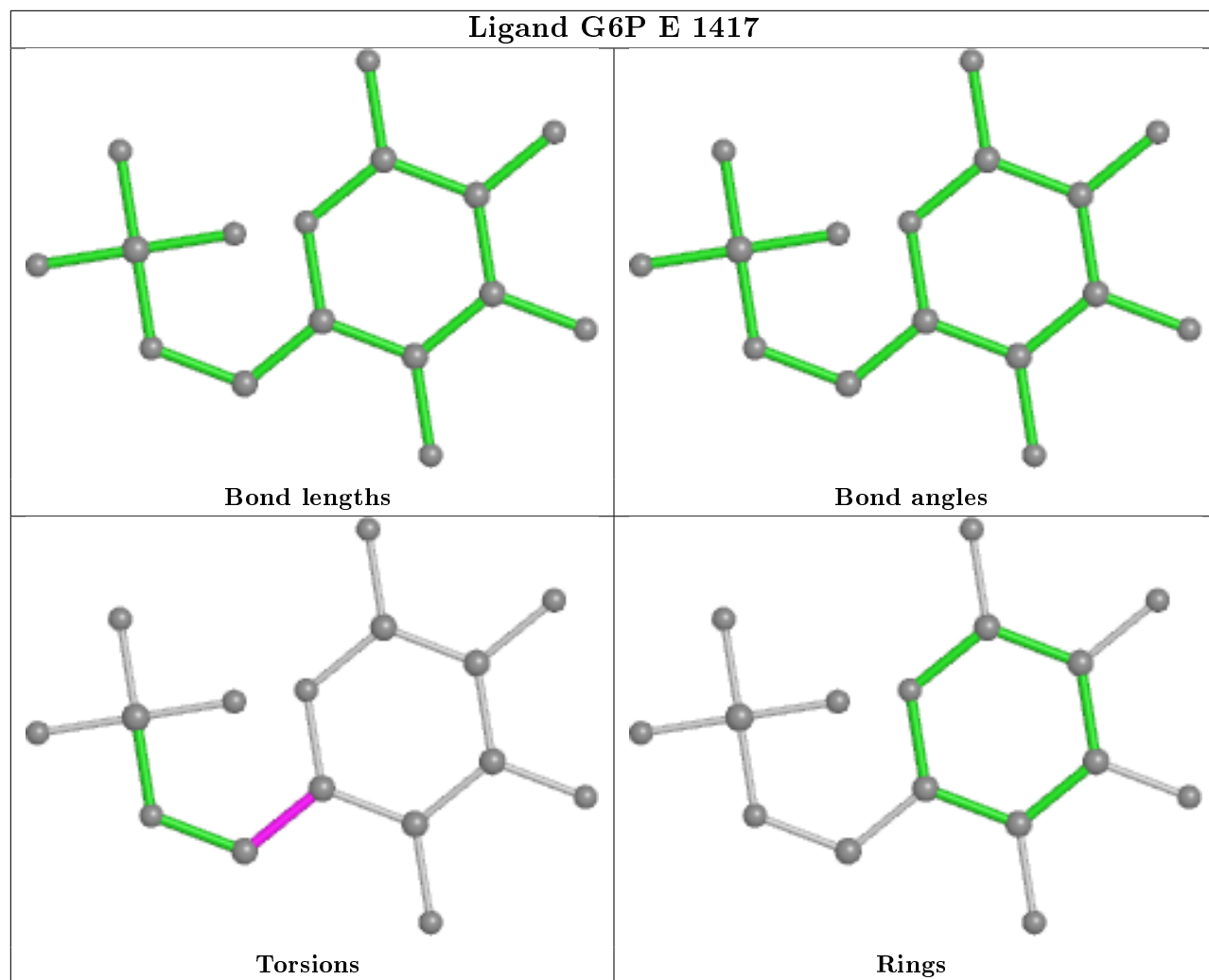


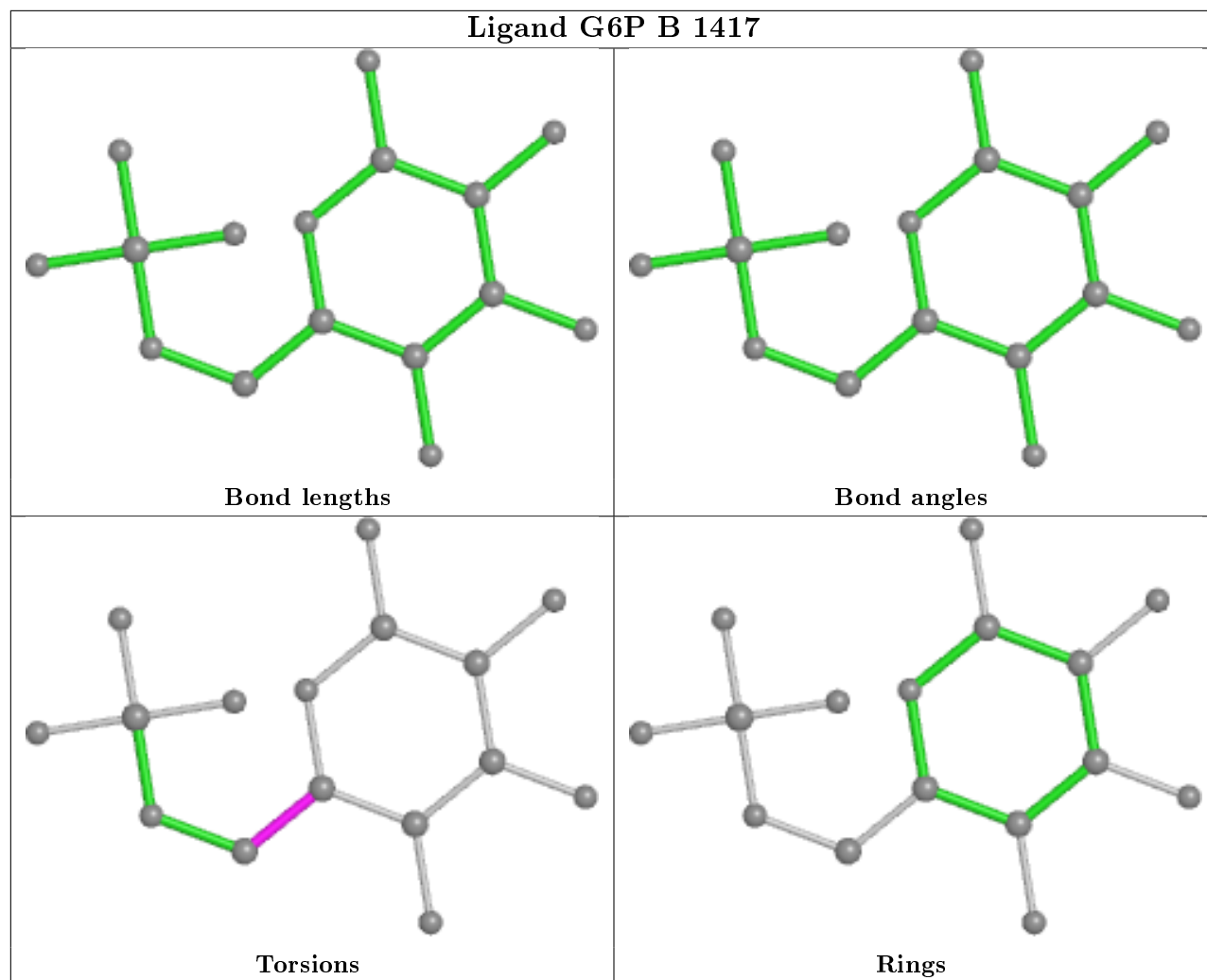












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/417 (99%)	-0.13	17 (4%) 37 36	13, 19, 26, 58	3 (0%)
1	B	409/417 (98%)	0.02	22 (5%) 25 24	12, 19, 25, 31	22 (5%)
1	C	409/417 (98%)	-0.20	7 (1%) 70 68	13, 19, 25, 31	13 (3%)
1	D	409/417 (98%)	-0.13	18 (4%) 34 33	13, 19, 27, 39	18 (4%)
1	E	406/417 (97%)	0.27	35 (8%) 10 9	13, 19, 24, 30	41 (10%)
1	F	411/417 (98%)	0.13	26 (6%) 20 18	13, 19, 25, 36	31 (7%)
1	G	409/417 (98%)	-0.12	17 (4%) 36 35	13, 19, 25, 30	22 (5%)
1	H	407/417 (97%)	0.02	24 (5%) 22 21	13, 19, 26, 36	25 (6%)
All	All	3274/3336 (98%)	-0.02	166 (5%) 28 26	12, 19, 25, 58	175 (5%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	6.9
1	F	216	LEU	5.8
1	A	222	PRO	5.8
1	D	223	ASP	5.7
1	F	222	PRO	5.3
1	A	223	ASP	5.1
1	E	293	MET	4.9
1	E	223	ASP	4.8
1	E	292	SER	4.8
1	E	287	THR	4.7
1	H	291	GLY	4.7
1	B	216	LEU	4.7
1	E	224	GLU	4.5
1	H	177	SER	4.4
1	G	224	GLU	4.3
1	F	224	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	287	THR	4.2
1	B	292	SER	4.1
1	E	294	TYR	4.1
1	E	213	ASN	4.1
1	C	216	LEU	4.0
1	A	216	LEU	4.0
1	B	278	THR	4.0
1	F	292	SER	3.9
1	C	278	THR	3.9
1	D	287	THR	3.9
1	G	287	THR	3.8
1	H	280	VAL	3.7
1	G	415	GLY	3.6
1	B	224	GLU	3.6
1	F	293	MET	3.6
1	A	-1	ARG	3.5
1	B	217	LYS	3.5
1	F	284	GLU	3.5
1	C	25	GLU	3.5
1	A	0	HIS	3.4
1	D	294	TYR	3.4
1	E	45	VAL	3.4
1	G	216	LEU	3.3
1	H	26	ASP	3.3
1	H	286	LEU	3.3
1	G	26	ASP	3.3
1	D	291	GLY	3.3
1	G	292	SER	3.3
1	D	26	ASP	3.2
1	H	224	GLU	3.2
1	E	272	LEU	3.2
1	E	38	ASP	3.2
1	B	225	ASP	3.2
1	D	290	GLY	3.2
1	B	213	ASN	3.1
1	F	217	LYS	3.1
1	D	286	LEU	3.1
1	F	290	GLY	3.1
1	F	287	THR	3.0
1	E	26	ASP	3.0
1	H	410	GLU	3.0
1	B	24	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	282	ILE	3.0
1	F	266	MET	2.9
1	A	288	LYS	2.9
1	E	163	ASN	2.9
1	H	214	LEU	2.9
1	C	225	ASP	2.8
1	F	213	ASN	2.8
1	H	24	SER	2.8
1	G	286	LEU	2.8
1	C	224	GLU	2.8
1	D	288	LYS	2.8
1	H	287	THR	2.8
1	E	286	LEU	2.8
1	B	54	LYS	2.7
1	E	216	LEU	2.7
1	H	290	GLY	2.7
1	E	173	ALA	2.7
1	D	55	ASP	2.7
1	A	294	TYR	2.7
1	F	288	LYS	2.7
1	E	22	ASP	2.7
1	F	223	ASP	2.7
1	E	169	ILE	2.7
1	G	409	ARG	2.7
1	H	289	ARG	2.6
1	A	177	SER	2.6
1	B	279	ALA	2.6
1	B	291	GLY	2.6
1	H	44	ILE	2.6
1	B	30	ASP	2.6
1	B	293	MET	2.6
1	H	281	GLU	2.6
1	B	28	ARG	2.6
1	E	30	ASP	2.5
1	F	409	ARG	2.5
1	A	25	GLU	2.5
1	C	26	ASP	2.5
1	F	71	ASP	2.5
1	F	259	GLU	2.5
1	E	225	ASP	2.5
1	G	284	GLU	2.5
1	H	274	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	167	ASN	2.5
1	G	294	TYR	2.5
1	G	213	ASN	2.5
1	E	39	GLU	2.5
1	E	212	GLU	2.5
1	F	5	VAL	2.4
1	H	45	VAL	2.4
1	A	281	GLU	2.4
1	D	224	GLU	2.4
1	G	290	GLY	2.4
1	F	277	ARG	2.4
1	E	174	GLU	2.4
1	F	415	GLY	2.4
1	H	132	ASN	2.4
1	E	23	ILE	2.4
1	E	76	ILE	2.4
1	D	25	GLU	2.4
1	A	217	LYS	2.4
1	B	25	GLU	2.4
1	C	287	THR	2.4
1	G	225	ASP	2.4
1	D	24	SER	2.4
1	D	214	LEU	2.4
1	F	3	ILE	2.3
1	H	31	GLU	2.3
1	B	63	ASP	2.3
1	A	212	GLU	2.3
1	H	292	SER	2.3
1	A	215	LYS	2.3
1	F	286	LEU	2.3
1	G	258	HIS	2.3
1	G	179	ARG	2.3
1	A	292	SER	2.3
1	E	20	LEU	2.2
1	A	5	VAL	2.2
1	E	211	PHE	2.2
1	E	283	PRO	2.2
1	E	28	ARG	2.2
1	B	282	ILE	2.2
1	F	257	THR	2.2
1	G	257	THR	2.2
1	H	293	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	225	ASP	2.2
1	E	284	GLU	2.2
1	B	258	HIS	2.1
1	E	232	ASP	2.1
1	D	289	ARG	2.1
1	A	224	GLU	2.1
1	F	44	ILE	2.1
1	H	57	PHE	2.1
1	D	284	GLU	2.1
1	E	271	GLU	2.1
1	H	216	LEU	2.1
1	B	267	LYS	2.1
1	D	409	ARG	2.1
1	F	294	TYR	2.1
1	B	263	ARG	2.1
1	H	28	ARG	2.1
1	F	26	ASP	2.1
1	D	216	LEU	2.1
1	E	132	ASN	2.1
1	B	284	GLU	2.1
1	G	55	ASP	2.0
1	F	280	VAL	2.0
1	H	17	VAL	2.0
1	E	62	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

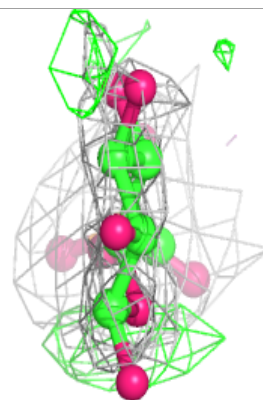
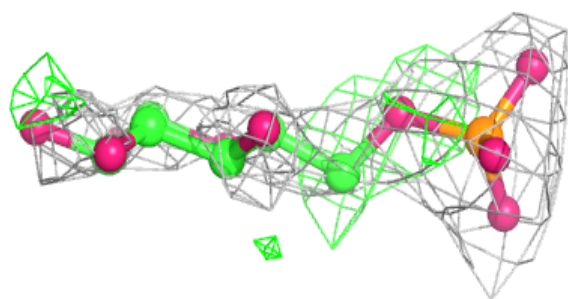
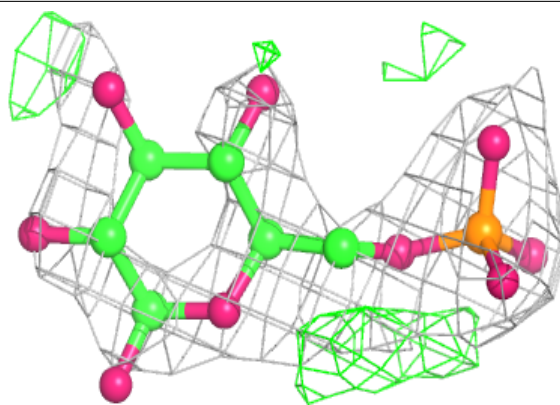
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	1418	5/5	0.81	0.25	57,59,61,62	0
3	G6P	E	1417	16/16	0.82	0.31	36,39,40,40	16
3	G6P	F	1417	16/16	0.83	0.31	47,52,54,55	16
4	SO4	C	1418	5/5	0.83	0.21	53,54,61,63	0
3	G6P	D	1417	16/16	0.85	0.27	43,47,48,49	16
3	G6P	H	1417	16/16	0.85	0.28	43,48,49,51	16
2	NAD	E	1416	44/44	0.87	0.30	31,33,39,41	44
3	G6P	G	1417	16/16	0.87	0.28	62,70,71,71	0
3	G6P	A	1417	16/16	0.90	0.24	46,58,60,60	0
2	NAD	F	1416	44/44	0.90	0.38	21,35,41,45	44
3	G6P	B	1417	16/16	0.91	0.32	37,42,45,45	16
2	NAD	H	1416	44/44	0.93	0.44	24,28,35,39	44
3	G6P	C	1417	16/16	0.93	0.30	58,69,71,71	0
2	NAD	B	1416	44/44	0.95	0.12	34,52,64,69	0
2	NAD	D	1416	44/44	0.96	0.11	31,44,54,55	0
2	NAD	G	1416	44/44	0.97	0.10	30,48,59,62	0
2	NAD	A	1416	44/44	0.98	0.09	21,35,49,52	0
2	NAD	C	1416	44/44	0.98	0.09	24,41,53,59	0

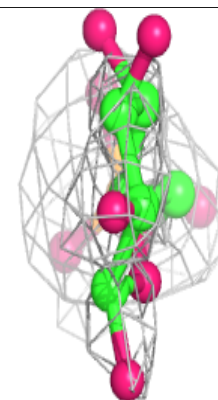
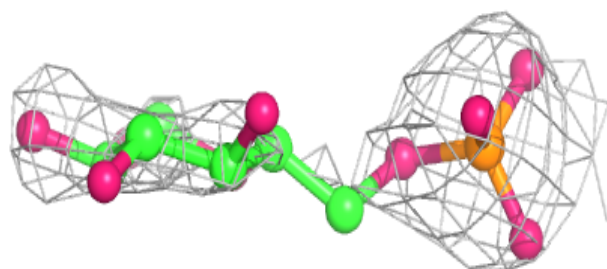
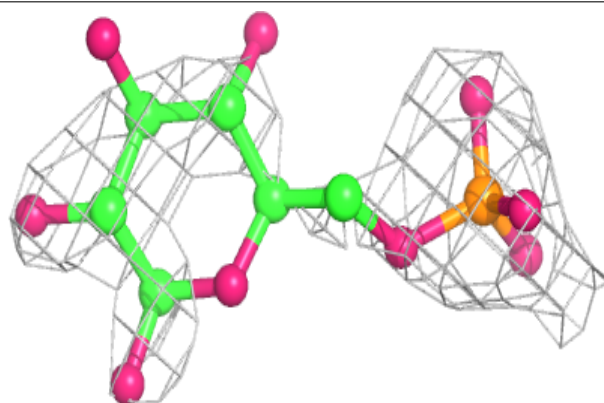
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G6P E 1417:

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

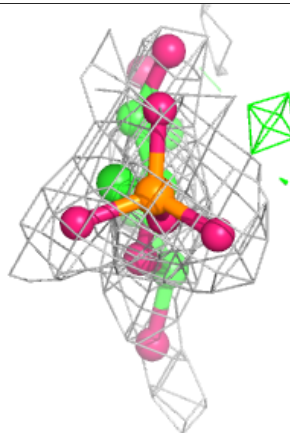
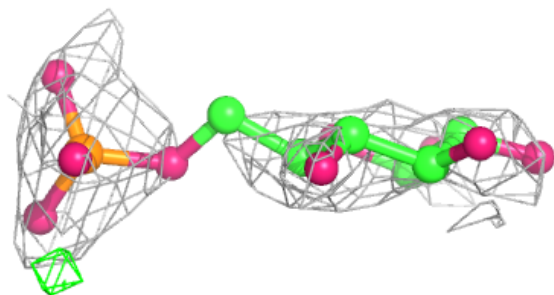
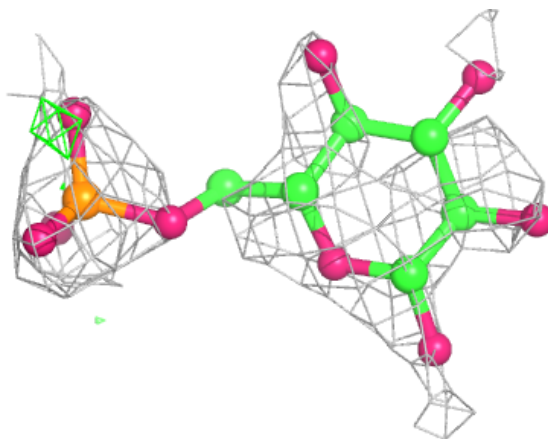
**Electron density around G6P F 1417:**

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

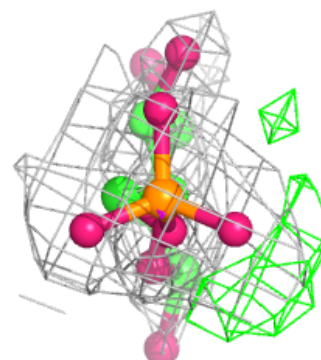
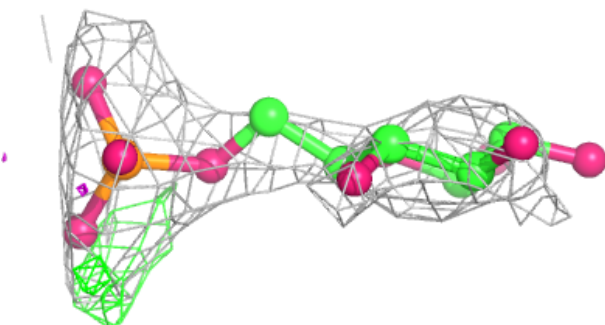
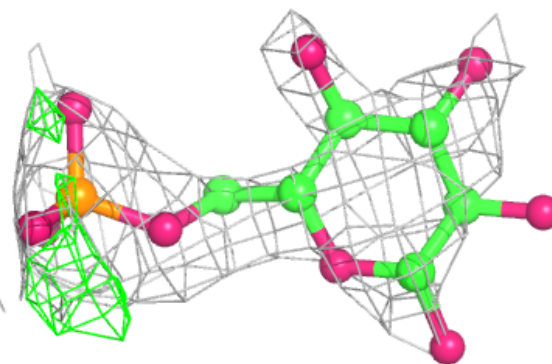


Electron density around G6P D 1417:

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

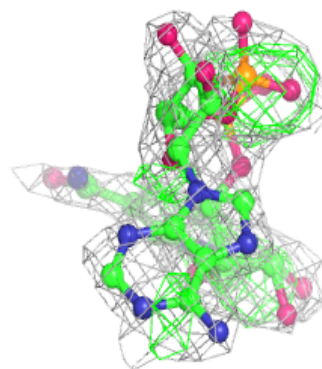
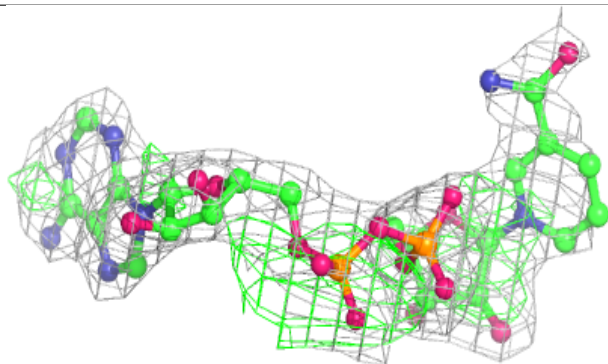
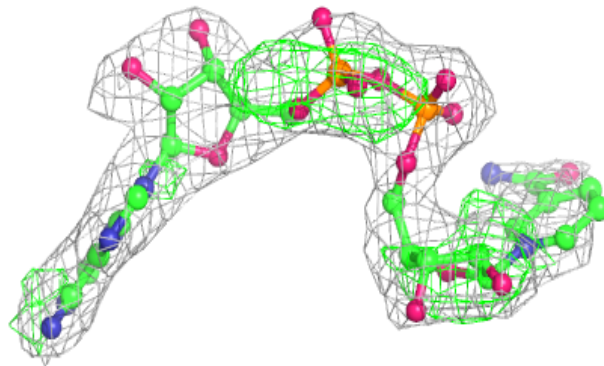
**Electron density around G6P H 1417:**

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



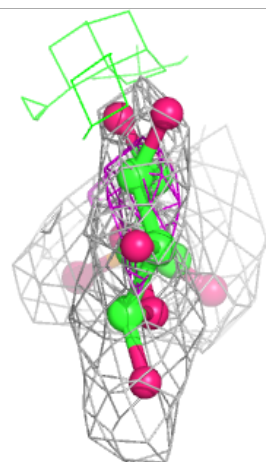
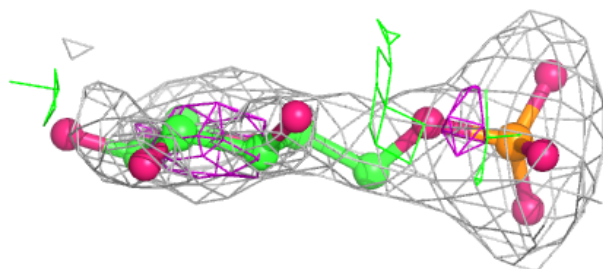
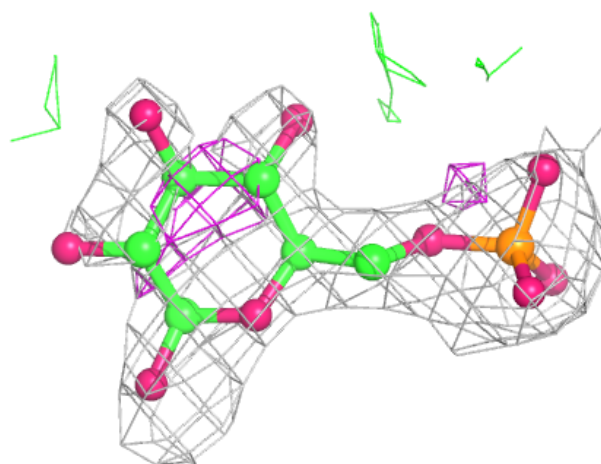
Electron density around NAD E 1416:

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



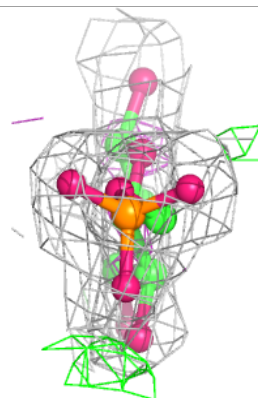
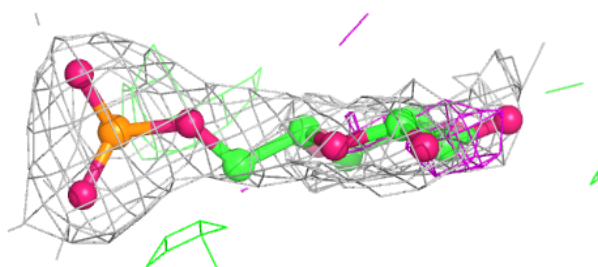
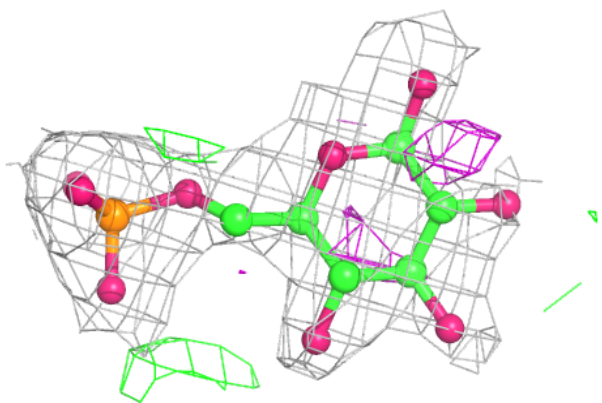
Electron density around G6P G 1417:

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

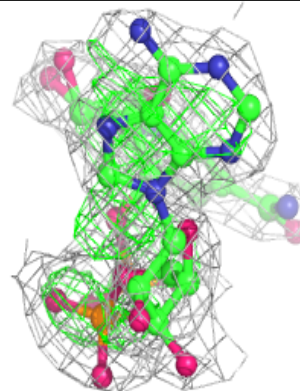
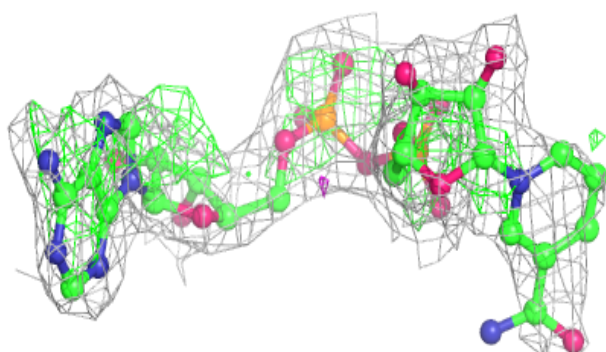
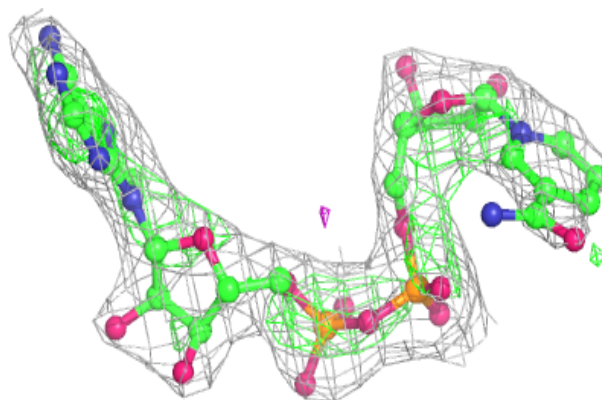


Electron density around G6P A 1417:

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

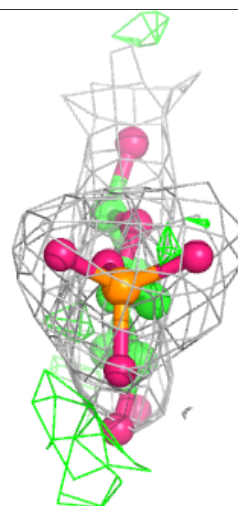
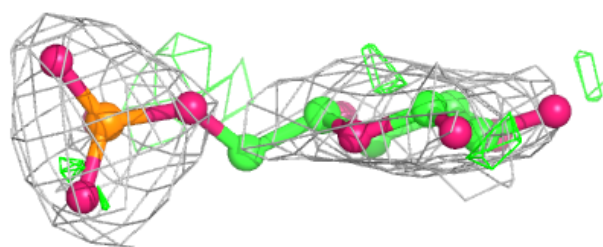
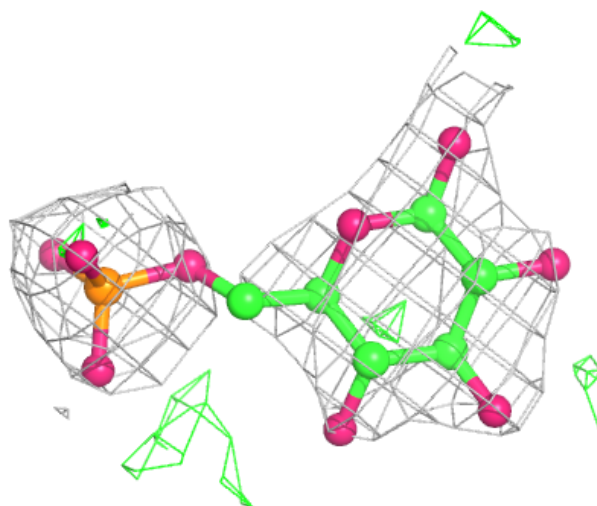
**Electron density around NAD F 1416:**

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



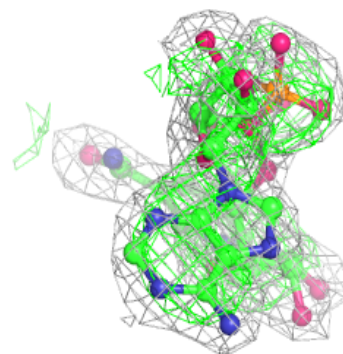
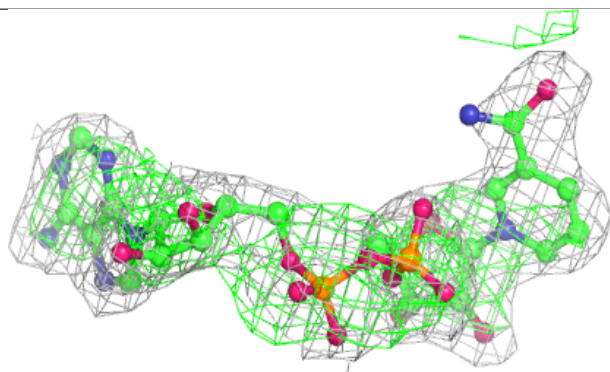
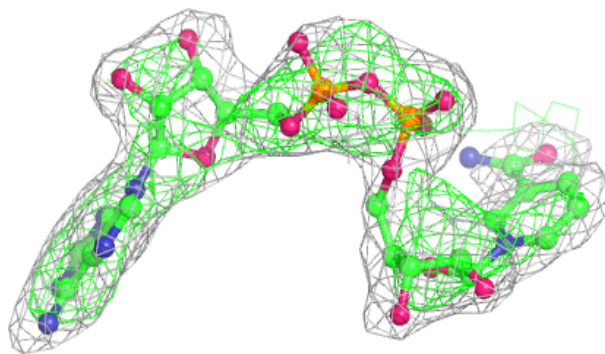
Electron density around G6P B 1417:

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

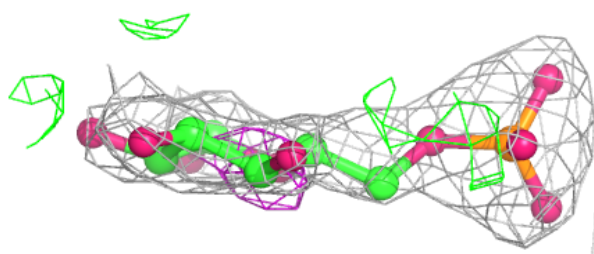
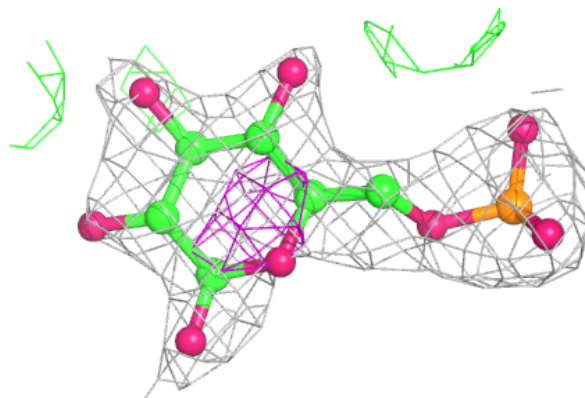


Electron density around NAD H 1416:

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

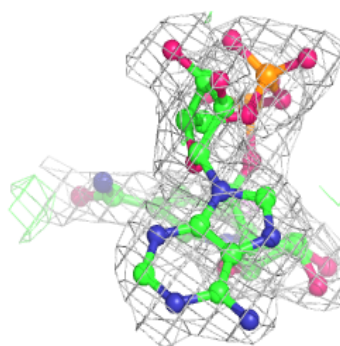
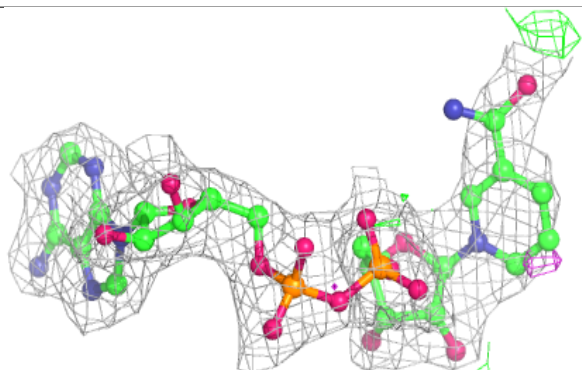
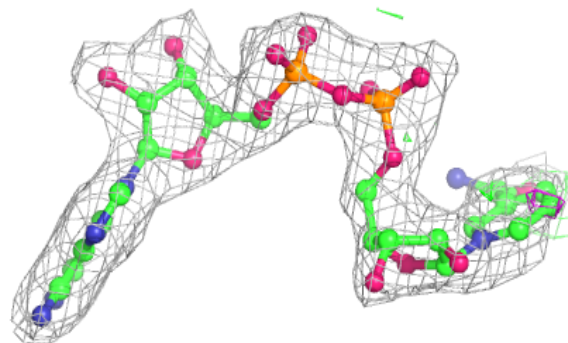
**Electron density around G6P C 1417:**

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

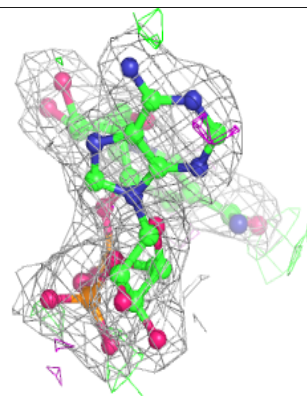
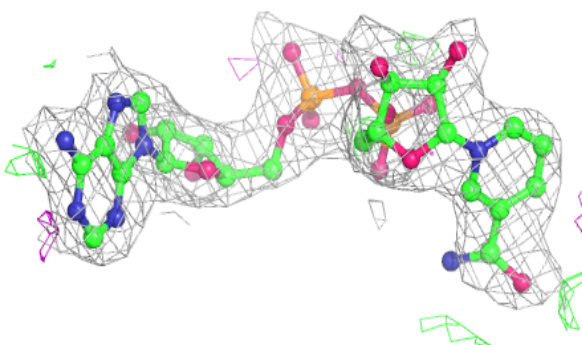
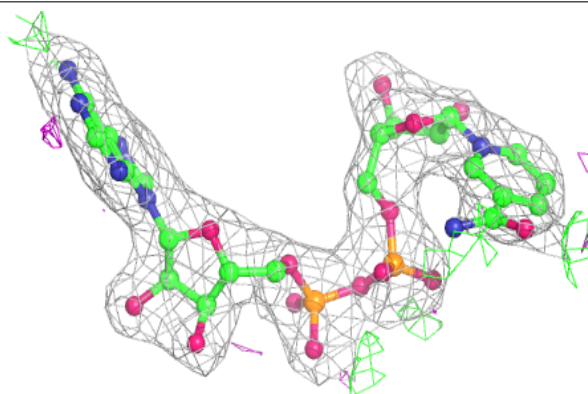


Electron density around NAD B 1416:

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

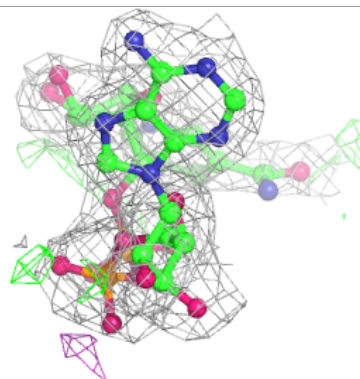
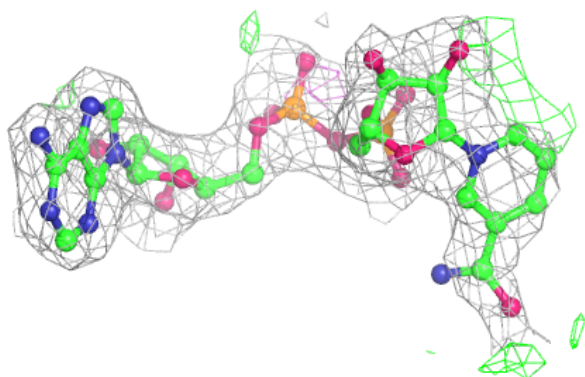
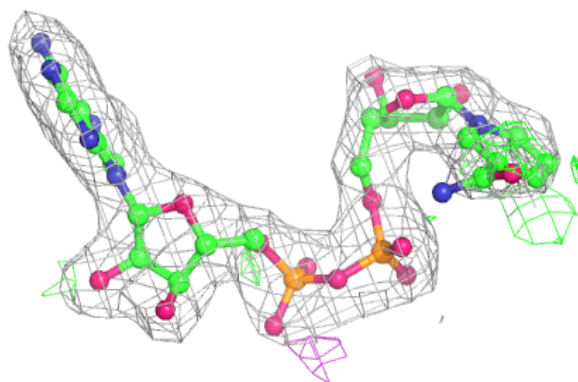
**Electron density around NAD D 1416:**

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

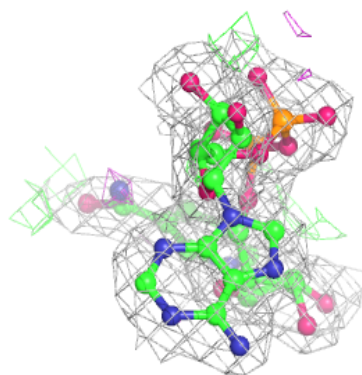
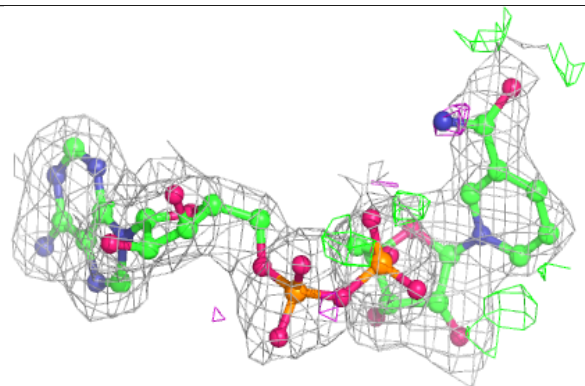
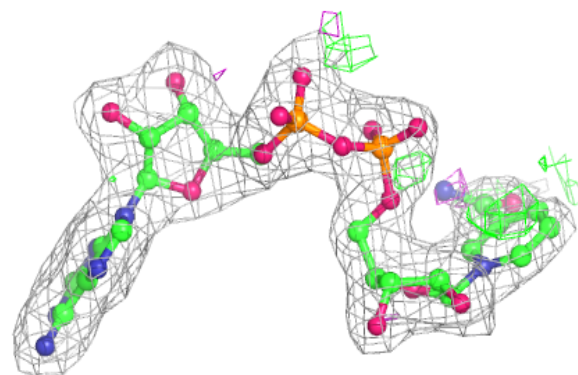


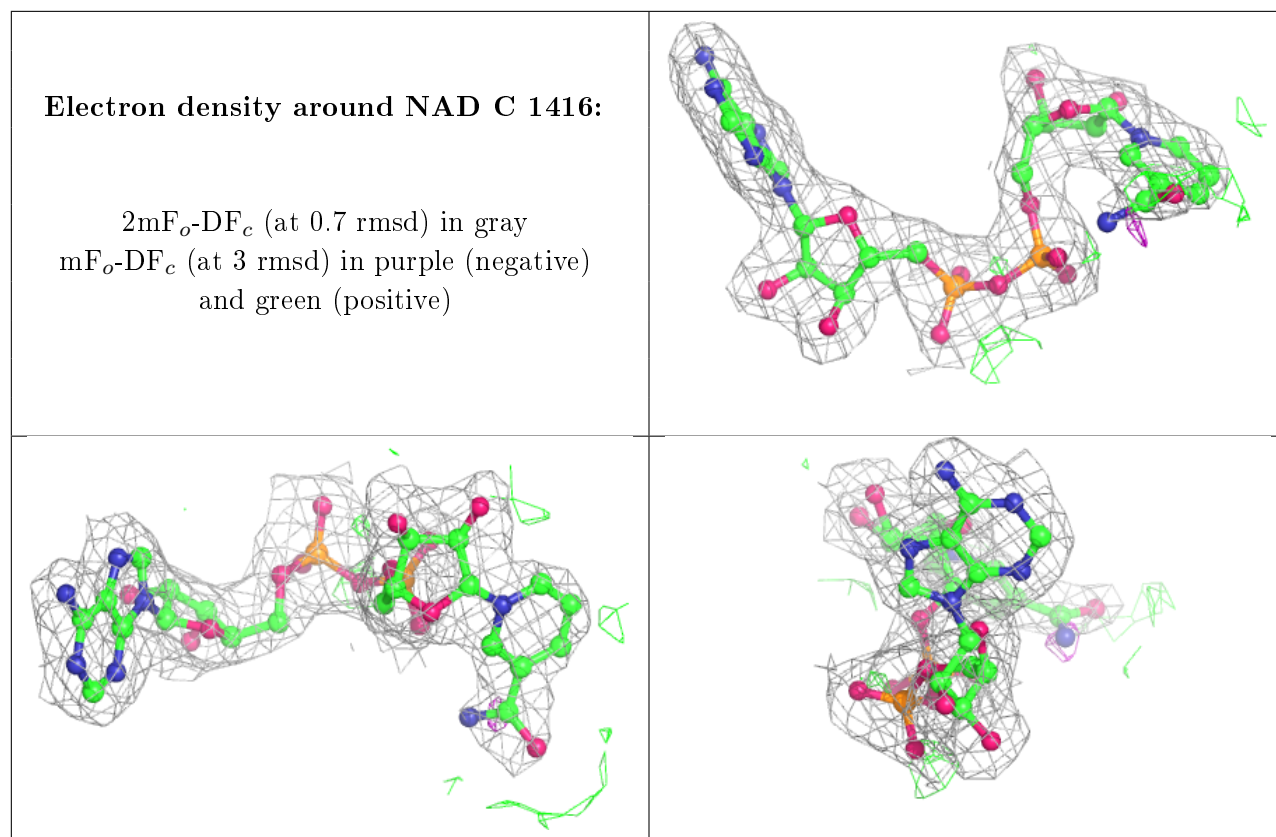
Electron density around NAD G 1416:

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

**Electron density around NAD A 1416:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.