



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 12:24 AM EDT

PDB ID : 6E07
Title : Crystal structure of Canton G6PD in complex with structural NADP
Authors : Rahighi, S.; Mochly-Rosen, D.; Wakatsuki, S.
Deposited on : 2018-07-06
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

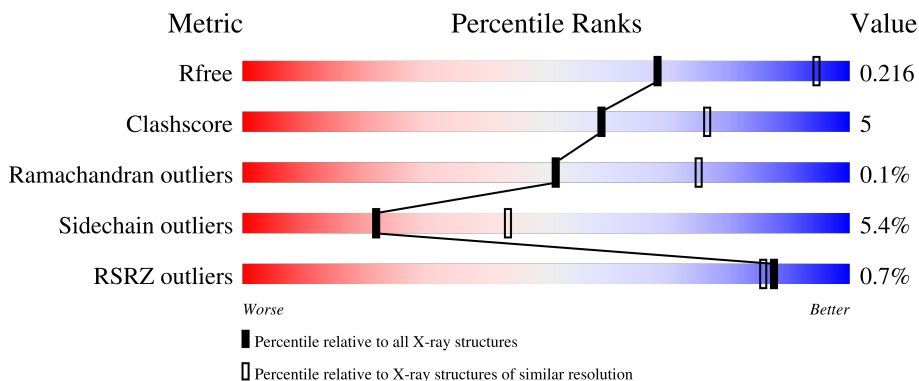
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	515	 83% 10% • 6%
1	C	515	 85% 9% 5%
1	F	515	 83% 10% • 6%
1	L	515	 79% 12% • 6%
1	N	515	 80% 13% • 6%

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Mol	Chain	Length	Quality of chain
1	Q	515	 % 81% 10% • • 5%
1	T	515	 % 80% 13% • 6%
1	W	515	 % 80% 13% • 6%

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
4	GOL	C	605	-	-	-	X
4	GOL	F	607	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32689 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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	486	3943	2518	683	722	20	0	0	0
1	C	487	3952	2524	685	723	20	0	0	0
1	F	486	3943	2518	683	722	20	0	0	0
1	N	486	3943	2518	683	722	20	0	0	0
1	Q	487	3953	2524	686	723	20	0	0	0
1	T	486	3943	2518	683	722	20	0	0	0
1	W	486	3943	2518	683	722	20	0	0	0
1	B	485	3934	2513	681	720	20	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	459	LEU	ARG	engineered mutation	UNP P11413
C	459	LEU	ARG	engineered mutation	UNP P11413
F	459	LEU	ARG	engineered mutation	UNP P11413
N	459	LEU	ARG	engineered mutation	UNP P11413
Q	459	LEU	ARG	engineered mutation	UNP P11413
T	459	LEU	ARG	engineered mutation	UNP P11413
W	459	LEU	ARG	engineered mutation	UNP P11413
B	459	LEU	ARG	engineered mutation	UNP P11413

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	L	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	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	Q	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	T	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	W	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		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	L	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	N	1	Total	O	P	0	0
			5	4	1		
3	Q	1	Total	O	P	0	0
			5	4	1		
3	T	1	Total	O	P	0	0
			5	4	1		
3	W	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	N	1	Total C O 6 3 3	0	0
4	Q	1	Total C O 6 3 3	0	0
4	Q	1	Total C O 6 3 3	0	0
4	T	1	Total C O 6 3 3	0	0
4	T	1	Total C O 6 3 3	0	0
4	W	1	Total C O 6 3 3	0	0
4	W	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	103	Total O 103 103	0	0
5	C	79	Total O 79 79	0	0
5	F	101	Total O 101 101	0	0
5	N	38	Total O 38 38	0	0

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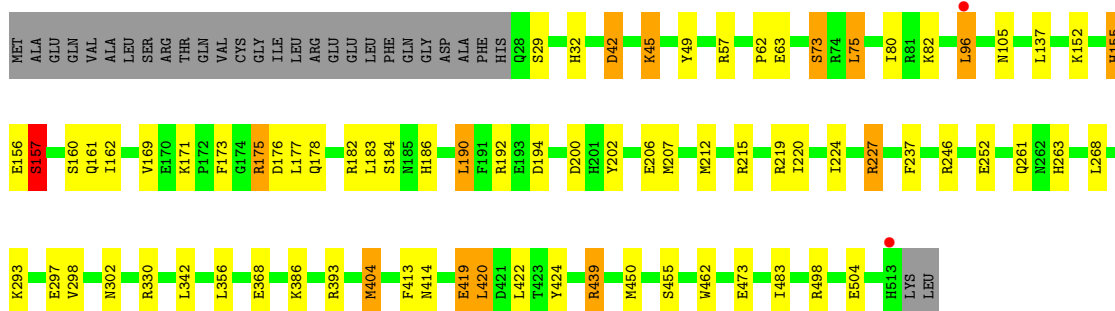
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	Q	66	Total 66	O 66	0	0
5	T	63	Total 63	O 63	0	0
5	W	52	Total 52	O 52	0	0
5	B	35	Total 35	O 35	0	0

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.

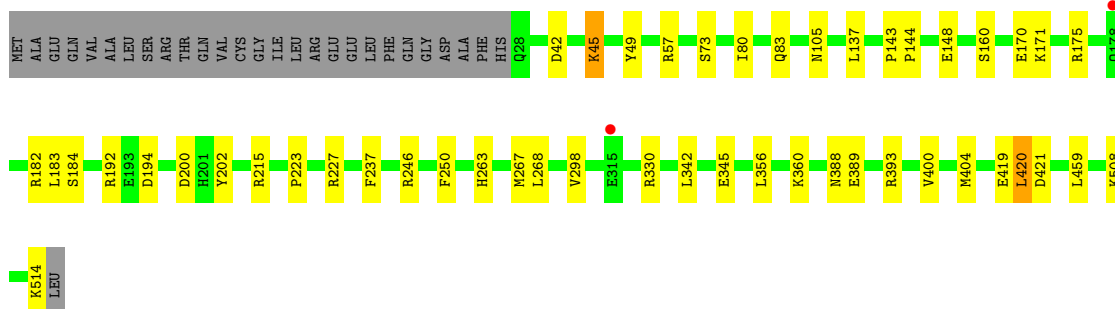
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain L: 




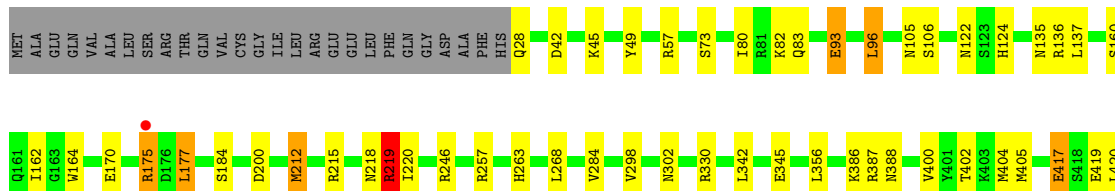
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain C: 



- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain F: 





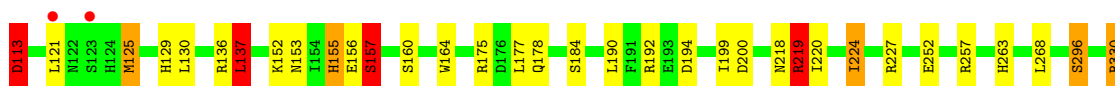
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain N: 80% 13% 6%



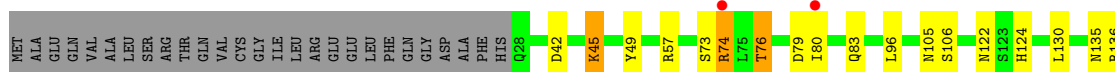
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain Q: 81% 10% 5%



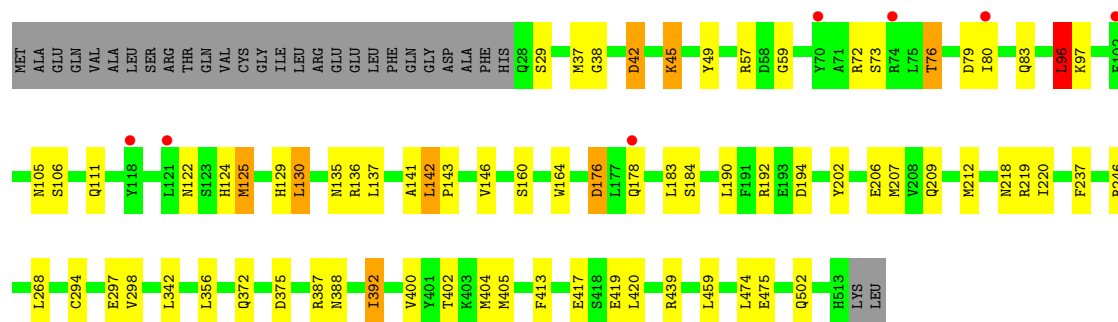
- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain T: 80% 13% 6%

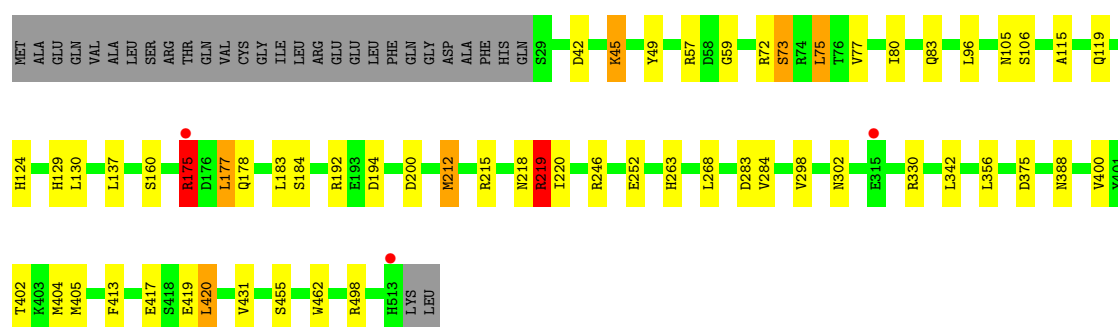
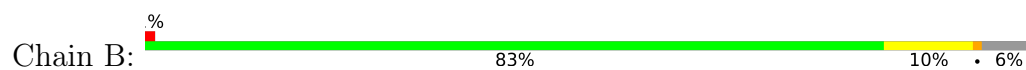


- Molecule 1: Glucose-6-phosphate 1-dehydrogenase

Chain W: 80% 13% 6%



- Molecule 1: Glucose-6-phosphate 1-dehydrogenase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.12Å 206.25Å 211.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.60 49.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.01-2.60) 100.0 (49.26-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0216	Depositor
R, R_{free}	0.187 , 0.211 0.194 , 0.216	Depositor DCC
R_{free} test set	8556 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtrriage
Anisotropy	0.154	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.003 for -h,l,k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32689	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: PO4, GOL, NAP

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	B	0.76	4/4030 (0.1%)	0.86	7/5453 (0.1%)
1	C	0.72	0/4048	0.86	7/5476 (0.1%)
1	F	0.75	1/4039 (0.0%)	0.87	16/5465 (0.3%)
1	L	0.79	4/4039 (0.1%)	0.91	12/5465 (0.2%)
1	N	0.71	1/4039 (0.0%)	0.85	7/5465 (0.1%)
1	Q	0.78	5/4050 (0.1%)	0.91	14/5480 (0.3%)
1	T	0.70	2/4039 (0.0%)	0.82	9/5465 (0.2%)
1	W	0.70	1/4039 (0.0%)	0.85	8/5465 (0.1%)
All	All	0.74	18/32323 (0.1%)	0.87	80/43734 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	L	0	1
1	Q	0	2
1	W	0	1
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	SER	CB-OG	-8.81	1.30	1.42
1	Q	296	SER	CB-OG	7.44	1.51	1.42
1	L	455	SER	CB-OG	-7.22	1.32	1.42
1	T	455	SER	CB-OG	-6.97	1.33	1.42
1	B	417	GLU	CD-OE1	6.53	1.32	1.25
1	Q	417	GLU	CD-OE2	6.14	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	345	GLU	CD-OE2	6.03	1.32	1.25
1	Q	417	GLU	CD-OE1	5.93	1.32	1.25
1	Q	29	SER	CB-OG	-5.83	1.34	1.42
1	F	417	GLU	CD-OE1	5.63	1.31	1.25
1	L	473	GLU	CD-OE1	5.35	1.31	1.25
1	L	252	GLU	CD-OE1	5.33	1.31	1.25
1	N	417	GLU	CD-OE1	5.19	1.31	1.25
1	T	368	GLU	CD-OE1	5.17	1.31	1.25
1	B	417	GLU	CD-OE2	5.12	1.31	1.25
1	W	294	CYS	CB-SG	-5.11	1.73	1.81
1	L	368	GLU	CD-OE1	5.04	1.31	1.25
1	B	252	GLU	CD-OE2	5.04	1.31	1.25

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	ASP	CB-CG-OD1	-10.98	108.42	118.30
1	W	219	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	Q	42	ASP	CB-CG-OD1	9.74	127.07	118.30
1	C	42	ASP	CB-CG-OD1	9.71	127.03	118.30
1	N	42	ASP	CB-CG-OD1	9.48	126.83	118.30
1	T	219	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	L	157	SER	N-CA-C	7.87	132.24	111.00
1	L	42	ASP	CB-CG-OD1	7.81	125.33	118.30
1	Q	157	SER	N-CA-C	7.72	131.85	111.00
1	Q	112	TYR	N-CA-C	-7.51	90.72	111.00
1	L	176	ASP	CB-CG-OD1	7.44	125.00	118.30
1	F	219	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	N	42	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	Q	257	ARG	CG-CD-NE	-7.42	96.23	111.80
1	W	130	LEU	CB-CG-CD1	7.39	123.57	111.00
1	B	212	MET	CG-SD-CE	-7.05	88.92	100.20
1	Q	42	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	B	219	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	Q	125	MET	CG-SD-CE	6.97	111.35	100.20
1	F	257	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	Q	96	LEU	CB-CG-CD1	6.89	122.72	111.00
1	B	219	ARG	CG-CD-NE	-6.85	97.42	111.80
1	W	219	ARG	CG-CD-NE	-6.79	97.54	111.80
1	F	212	MET	CG-SD-CE	-6.73	89.43	100.20
1	N	219	ARG	CG-CD-NE	-6.73	97.67	111.80
1	F	177	LEU	CB-CG-CD2	6.70	122.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	219	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	W	125	MET	CG-SD-CE	6.59	110.75	100.20
1	L	439	ARG	CG-CD-NE	6.46	125.37	111.80
1	F	219	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	Q	137	LEU	CA-CB-CG	6.35	129.91	115.30
1	B	215	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	T	219	ARG	CG-CD-NE	-6.23	98.71	111.80
1	Q	219	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	L	215	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	F	345	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	F	474	LEU	CB-CG-CD2	5.99	121.18	111.00
1	C	267	MET	CG-SD-CE	5.97	109.75	100.20
1	W	130	LEU	CB-CG-CD2	-5.75	101.23	111.00
1	B	175	ARG	CB-CA-C	5.71	121.82	110.40
1	F	96	LEU	CB-CG-CD1	5.66	120.62	111.00
1	N	257	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	F	215	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	C	459	LEU	CB-CG-CD1	-5.60	101.47	111.00
1	C	330	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	Q	156	GLU	N-CA-C	-5.58	95.94	111.00
1	L	450	MET	CG-SD-CE	-5.56	91.31	100.20
1	T	282	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	Q	219	ARG	CG-CD-NE	-5.52	100.20	111.80
1	F	219	ARG	CG-CD-NE	-5.51	100.22	111.80
1	F	474	LEU	CA-CB-CG	5.50	127.95	115.30
1	N	74	ARG	CG-CD-NE	5.50	123.35	111.80
1	F	387	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	L	176	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	T	267	MET	CG-SD-CE	5.37	108.78	100.20
1	F	257	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	Q	113	ASP	N-CA-CB	5.29	120.11	110.60
1	W	42	ASP	N-CA-CB	5.28	120.11	110.60
1	F	93	GLU	CA-CB-CG	5.27	125.00	113.40
1	T	330	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	215	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	W	96	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	393	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	T	450	MET	CG-SD-CE	5.19	108.50	100.20
1	B	42	ASP	N-CA-CB	5.18	119.93	110.60
1	T	219	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	L	156	GLU	N-CA-C	-5.16	97.07	111.00
1	T	42	ASP	N-CA-CB	5.16	119.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	257	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	177	LEU	CB-CG-CD2	5.12	119.71	111.00
1	N	215	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	F	42	ASP	N-CA-CB	5.12	119.81	110.60
1	F	493	ASP	CB-CG-OD1	5.11	122.90	118.30
1	L	227	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	N	219	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	W	176	ASP	CB-CG-OD2	5.04	122.83	118.30
1	Q	330	ARG	N-CA-C	5.03	124.57	111.00
1	T	458	LEU	CA-CB-CG	5.03	126.86	115.30
1	L	393	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	L	96	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	59	GLY	Peptide
1	L	155	HIS	Peptide
1	Q	155	HIS	Peptide
1	Q	199	ILE	Peptide
1	W	59	GLY	Peptide

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	B	3934	0	3876	40	0
1	C	3952	0	3897	22	0
1	F	3943	0	3884	38	0
1	L	3943	0	3884	45	0
1	N	3943	0	3884	52	0
1	Q	3953	0	3891	51	0
1	T	3943	0	3884	40	0
1	W	3943	0	3884	59	0
2	B	48	0	25	2	0
2	C	48	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	48	0	25	0	0
2	L	48	0	25	0	0
2	N	48	0	25	1	0
2	Q	48	0	25	0	0
2	T	48	0	25	1	0
2	W	48	0	25	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	F	5	0	0	0	0
3	L	5	0	0	0	0
3	N	5	0	0	0	0
3	Q	5	0	0	0	0
3	T	5	0	0	0	0
3	W	5	0	0	0	0
4	B	6	0	8	0	0
4	C	24	0	32	4	0
4	F	30	0	40	1	0
4	L	42	0	56	1	0
4	N	36	0	48	3	0
4	Q	12	0	16	1	0
4	T	12	0	16	1	0
4	W	12	0	16	0	0
5	B	35	0	0	2	0
5	C	79	0	0	0	0
5	F	101	0	0	1	0
5	L	103	0	0	3	0
5	N	38	0	0	2	0
5	Q	66	0	0	1	0
5	T	63	0	0	6	0
5	W	52	0	0	0	0
All	All	32689	0	31516	300	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 5.

All (300) 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:F:218:ASN:HD21	1:W:405:MET:H	1.12	0.96
1:N:325:ASP:OD1	1:N:327:THR:HG22	1.67	0.93
1:N:405:MET:H	1:B:218:ASN:HD21	1.16	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:218:ASN:HD21	1:T:405:MET:H	1.15	0.93
1:F:405:MET:H	1:W:218:ASN:HD21	1.17	0.92
1:N:218:ASN:HD21	1:B:405:MET:H	1.15	0.92
1:Q:405:MET:H	1:T:218:ASN:HD21	1.17	0.91
1:L:175:ARG:HB3	1:Q:178:GLN:HE22	1.38	0.87
1:W:405:MET:HE1	1:W:417:GLU:CG	2.06	0.84
1:W:372:GLN:HE22	1:W:502:GLN:H	1.24	0.84
1:T:357:ARG:HD2	5:T:737:HOH:O	1.80	0.81
1:W:207:MET:HB3	1:W:392:ILE:CD1	2.10	0.81
1:Q:137:LEU:HD23	1:Q:164:TRP:CZ3	2.16	0.80
1:W:176:ASP:OD1	1:W:178:GLN:HG2	1.80	0.80
1:N:176:ASP:OD1	1:N:178:GLN:HG3	1.81	0.79
1:W:37:MET:C	1:W:142:LEU:HD11	2.03	0.79
1:W:405:MET:HE1	1:W:417:GLU:HG3	1.66	0.77
1:W:405:MET:CE	1:W:417:GLU:HG2	2.17	0.75
1:L:175:ARG:HB3	1:Q:178:GLN:NE2	2.03	0.74
1:W:45:LYS:HD3	1:W:83:GLN:HG2	1.69	0.74
1:W:405:MET:HE1	1:W:417:GLU:HG2	1.70	0.73
1:L:414:ASN:OD1	5:L:701:HOH:O	2.10	0.69
1:Q:70:TYR:CD1	1:Q:121:LEU:HD12	2.28	0.69
1:W:37:MET:O	1:W:142:LEU:CD1	2.41	0.69
1:B:115:ALA:O	1:B:119:GLN:HG2	1.93	0.68
1:N:218:ASN:HD21	1:B:405:MET:N	1.90	0.68
1:Q:218:ASN:HD21	1:T:405:MET:N	1.89	0.68
1:N:266:GLN:HE22	1:N:288:LYS:NZ	1.92	0.68
1:T:45:LYS:HD2	1:T:83:GLN:HG2	1.75	0.68
1:T:438:GLU:OE1	5:T:701:HOH:O	2.12	0.67
1:Q:129:HIS:CD2	1:Q:130:LEU:HD12	2.30	0.67
1:Q:137:LEU:HD23	1:Q:164:TRP:HZ3	1.56	0.67
2:T:601:NAP:N7A	5:T:702:HOH:O	2.28	0.66
1:F:218:ASN:HD21	1:W:405:MET:N	1.89	0.65
1:C:148:GLU:OE1	1:C:182:ARG:NH1	2.26	0.65
1:Q:218:ASN:ND2	1:T:405:MET:H	1.92	0.65
1:Q:388:ASN:HD22	1:T:220:ILE:H	1.43	0.65
1:B:302:ASN:ND2	1:B:498:ARG:HH22	1.95	0.65
1:F:405:MET:N	1:W:218:ASN:HD21	1.91	0.64
1:F:220:ILE:H	1:W:388:ASN:HD22	1.44	0.64
1:N:302:ASN:ND2	1:N:498:ARG:HH22	1.96	0.64
1:W:96:LEU:HD13	1:W:97:LYS:N	2.12	0.64
1:N:218:ASN:ND2	1:B:405:MET:H	1.92	0.64
1:L:182:ARG:NH2	1:Q:252:GLU:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ARG:HH22	4:C:606:GOL:H2	1.64	0.63
1:W:38:GLY:HA3	1:W:142:LEU:HD12	1.80	0.63
1:L:227:ARG:NH2	4:L:603:GOL:H2	2.14	0.62
1:L:73:SER:HB2	1:L:75:LEU:CD1	2.29	0.62
1:F:302:ASN:ND2	1:F:498:ARG:HH22	1.98	0.62
1:B:177:LEU:HD13	1:B:462:TRP:HB3	1.82	0.62
2:B:601:NAP:N1A	5:B:701:HOH:O	2.30	0.62
1:N:388:ASN:HD22	1:B:220:ILE:H	1.46	0.61
1:N:220:ILE:H	1:B:388:ASN:HD22	1.48	0.61
1:F:218:ASN:ND2	1:W:405:MET:H	1.91	0.61
1:T:249:TYR:HB2	5:T:747:HOH:O	2.01	0.61
1:W:474:LEU:HD23	1:W:475:GLU:HG3	1.82	0.61
2:N:601:NAP:H2A	5:N:730:HOH:O	2.00	0.61
1:Q:405:MET:N	1:T:218:ASN:HD21	1.95	0.61
1:L:386:LYS:HG3	1:L:504:GLU:OE1	2.00	0.61
1:W:372:GLN:NE2	1:W:387:ARG:HH11	1.99	0.60
1:T:201:HIS:ND1	5:T:704:HOH:O	2.32	0.60
1:F:474:LEU:HD13	1:F:475:GLU:HG3	1.83	0.60
1:B:177:LEU:HD13	1:B:462:TRP:CB	2.30	0.59
1:F:212:MET:HE3	1:F:284:VAL:HG13	1.82	0.59
1:L:302:ASN:ND2	1:L:498:ARG:HH22	1.99	0.59
1:N:80:ILE:HD11	1:N:107:TYR:CD2	2.38	0.59
1:W:122:ASN:ND2	1:W:136:ARG:HH12	2.01	0.59
1:Q:375:ASP:O	1:T:219:ARG:NH1	2.36	0.59
1:L:73:SER:HB2	1:L:75:LEU:HD13	1.83	0.59
1:F:405:MET:H	1:W:218:ASN:ND2	1.95	0.59
1:N:227:ARG:NH2	4:N:605:GOL:H2	2.19	0.58
1:W:37:MET:O	1:W:142:LEU:HD11	2.03	0.58
1:N:135:ASN:HD22	1:N:164:TRP:H	1.52	0.58
1:F:220:ILE:H	1:W:388:ASN:ND2	2.02	0.58
1:W:135:ASN:HD22	1:W:164:TRP:H	1.51	0.58
1:N:388:ASN:ND2	1:B:220:ILE:H	2.01	0.57
1:N:405:MET:N	1:B:218:ASN:HD21	1.94	0.57
1:F:212:MET:HE3	1:F:284:VAL:CG1	2.34	0.57
1:W:207:MET:HB3	1:W:392:ILE:HD11	1.85	0.57
1:F:135:ASN:HD22	1:F:164:TRP:H	1.51	0.57
1:T:135:ASN:HD22	1:T:164:TRP:H	1.52	0.57
1:T:122:ASN:ND2	1:T:136:ARG:HH12	2.03	0.57
1:L:175:ARG:CB	1:Q:178:GLN:HE22	2.14	0.56
1:W:38:GLY:N	1:W:142:LEU:HD11	2.21	0.56
1:C:200:ASP:OD1	1:C:263:HIS:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:388:ASN:ND2	1:T:220:ILE:H	2.03	0.56
1:Q:405:MET:H	1:T:218:ASN:ND2	1.96	0.56
1:Q:200:ASP:OD1	1:Q:263:HIS:HD2	1.89	0.56
1:W:392:ILE:O	1:W:392:ILE:HG13	2.06	0.56
1:F:122:ASN:ND2	1:F:136:ARG:HH12	2.03	0.56
1:Q:73:SER:HB2	1:Q:75:LEU:CD1	2.35	0.56
1:W:76:THR:HG23	1:W:79:ASP:OD2	2.06	0.56
1:W:38:GLY:HA3	1:W:142:LEU:CD1	2.37	0.55
1:N:220:ILE:H	1:B:388:ASN:ND2	2.03	0.55
1:B:212:MET:HE3	1:B:284:VAL:HG13	1.89	0.55
1:T:207:MET:HE3	1:T:424:TYR:CE2	2.42	0.55
1:L:200:ASP:OD1	1:L:263:HIS:HD2	1.90	0.55
1:L:32:HIS:CD2	1:L:62:PRO:HG2	2.42	0.55
1:N:72:ARG:O	1:N:74:ARG:NH1	2.39	0.55
1:L:207:MET:HE3	1:L:424:TYR:CE2	2.42	0.55
1:Q:73:SER:HB2	1:Q:75:LEU:HD13	1.87	0.55
1:T:200:ASP:OD1	1:T:263:HIS:HD2	1.89	0.55
1:W:372:GLN:HE21	1:W:387:ARG:HH11	1.54	0.55
1:F:388:ASN:HD22	1:W:220:ILE:H	1.53	0.54
1:L:206:GLU:HG3	1:L:207:MET:HE2	1.89	0.54
1:L:220:ILE:H	1:C:388:ASN:HD22	1.55	0.54
1:L:420:LEU:HB3	1:C:420:LEU:HB3	1.88	0.54
1:W:209:GLN:NE2	1:W:439:ARG:HD3	2.21	0.54
1:F:200:ASP:OD1	1:F:263:HIS:HD2	1.90	0.54
1:C:45:LYS:HD2	1:C:83:GLN:HG2	1.89	0.54
1:N:207:MET:HE3	1:N:424:TYR:CE2	2.43	0.54
1:N:200:ASP:OD1	1:N:263:HIS:HD2	1.90	0.54
1:Q:220:ILE:H	1:T:388:ASN:HD22	1.54	0.54
1:L:504:GLU:OE2	5:L:702:HOH:O	2.18	0.54
1:B:73:SER:HB2	1:B:75:LEU:CD1	2.38	0.54
1:T:76:THR:HG23	1:T:79:ASP:OD2	2.08	0.53
1:F:219:ARG:NH1	1:W:375:ASP:O	2.41	0.53
1:N:420:LEU:HB3	1:B:420:LEU:HB3	1.89	0.53
1:C:227:ARG:HH12	4:C:606:GOL:H2	1.72	0.53
1:N:266:GLN:HE22	1:N:288:LYS:HZ3	1.54	0.53
1:F:386:LYS:HB2	1:F:405:MET:HE1	1.91	0.53
1:B:200:ASP:OD1	1:B:263:HIS:HD2	1.92	0.53
1:F:45:LYS:HD2	1:F:83:GLN:HG2	1.91	0.53
1:Q:404:MET:HE2	1:Q:419:GLU:HA	1.90	0.53
1:Q:34:PHE:CD1	1:Q:137:LEU:HD12	2.44	0.52
1:F:405:MET:HE2	1:F:417:GLU:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:405:MET:H	1:B:218:ASN:ND2	1.97	0.52
1:B:212:MET:HE3	1:B:284:VAL:CG1	2.40	0.52
1:W:207:MET:HB3	1:W:392:ILE:HD12	1.90	0.52
1:T:175:ARG:NH2	1:T:252:GLU:HB3	2.24	0.51
1:F:175:ARG:HD3	1:F:175:ARG:N	2.25	0.51
1:N:227:ARG:HH22	4:N:605:GOL:H2	1.75	0.51
1:B:73:SER:HB2	1:B:75:LEU:HD13	1.93	0.51
1:F:49:TYR:CZ	1:F:80:ILE:HD13	2.46	0.51
1:Q:49:TYR:CZ	1:Q:80:ILE:HD13	2.46	0.51
1:W:143:PRO:O	1:W:146:VAL:HG22	2.09	0.51
1:W:49:TYR:CZ	1:W:80:ILE:HD13	2.46	0.51
1:L:161:GLN:C	1:L:162:ILE:HD12	2.31	0.51
1:Q:137:LEU:HD21	1:Q:444:VAL:HG12	1.92	0.51
1:B:45:LYS:HD2	1:B:83:GLN:HG2	1.93	0.51
1:C:49:TYR:CZ	1:C:80:ILE:HD13	2.46	0.50
1:B:49:TYR:CZ	1:B:80:ILE:HD13	2.47	0.50
1:L:49:TYR:CZ	1:L:80:ILE:HD13	2.46	0.50
1:W:142:LEU:CD1	1:W:142:LEU:N	2.73	0.50
1:N:161:GLN:C	1:N:162:ILE:HD12	2.31	0.50
1:Q:227:ARG:NH2	4:Q:603:GOL:H2	2.27	0.50
1:Q:219:ARG:NH1	1:T:375:ASP:O	2.45	0.50
1:Q:34:PHE:HD1	1:Q:137:LEU:HD12	1.75	0.50
1:Q:155:HIS:HD2	1:Q:190:LEU:HB3	1.77	0.50
1:L:155:HIS:CG	1:L:155:HIS:O	2.62	0.50
1:L:483:ILE:HG13	1:F:162:ILE:HD11	1.93	0.49
1:L:293:LYS:NZ	1:B:283:ASP:OD1	2.45	0.49
1:T:49:TYR:CZ	1:T:80:ILE:HD13	2.47	0.49
1:L:206:GLU:OE1	1:L:439:ARG:NH2	2.44	0.49
1:Q:45:LYS:HD2	1:Q:83:GLN:HG2	1.95	0.49
1:N:135:ASN:ND2	1:N:164:TRP:H	2.11	0.49
1:N:155:HIS:CD2	1:N:190:LEU:HD22	2.48	0.49
1:F:386:LYS:H	1:F:405:MET:CE	2.26	0.49
1:N:219:ARG:NH1	1:B:375:ASP:O	2.45	0.49
1:W:405:MET:CE	1:W:417:GLU:CG	2.80	0.49
1:N:222:GLY:HA2	4:N:606:GOL:H11	1.95	0.49
1:N:91:THR:HG22	1:N:94:GLU:CD	2.34	0.48
1:Q:177:LEU:HD13	1:Q:462:TRP:HB3	1.95	0.48
1:T:74:ARG:HD2	1:T:74:ARG:O	2.14	0.48
1:Q:137:LEU:HD23	1:Q:164:TRP:CH2	2.49	0.48
1:Q:404:MET:HE3	1:Q:418:SER:HB3	1.95	0.47
1:W:135:ASN:ND2	1:W:164:TRP:H	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:GLU:HG3	5:L:767:HOH:O	2.13	0.47
1:C:202:TYR:HH	1:C:237:PHE:HE1	1.60	0.47
1:F:388:ASN:ND2	1:W:220:ILE:H	2.12	0.47
1:Q:508:LYS:HA	1:Q:508:LYS:CE	2.45	0.47
1:T:268:LEU:C	1:T:268:LEU:HD23	2.35	0.47
1:L:206:GLU:HG3	1:L:207:MET:CE	2.45	0.47
1:C:389:GLU:OE2	4:C:605:GOL:H2	2.14	0.47
1:Q:153:ASN:O	1:Q:157:SER:OG	2.28	0.47
1:Q:220:ILE:H	1:T:388:ASN:ND2	2.13	0.47
1:Q:439:ARG:HG3	5:Q:737:HOH:O	2.14	0.47
1:Q:508:LYS:HA	1:Q:508:LYS:HE2	1.97	0.47
2:B:601:NAP:O1N	2:B:601:NAP:O5B	2.33	0.47
1:C:45:LYS:HB2	1:C:83:GLN:HE21	1.79	0.47
1:W:206:GLU:OE1	1:W:439:ARG:NH2	2.48	0.47
1:F:135:ASN:ND2	1:F:164:TRP:H	2.12	0.47
1:N:409:PRO:HB2	1:B:431:VAL:HG11	1.97	0.47
1:Q:268:LEU:C	1:Q:268:LEU:HD23	2.35	0.47
1:T:135:ASN:ND2	1:T:164:TRP:H	2.12	0.46
1:B:77:VAL:HG22	5:B:725:HOH:O	2.15	0.46
1:L:178:GLN:O	1:L:182:ARG:HG3	2.14	0.46
1:L:261:GLN:NE2	1:L:462:TRP:CH2	2.84	0.46
1:L:404:MET:HE2	1:L:419:GLU:HA	1.96	0.46
1:F:302:ASN:HD22	1:F:498:ARG:HH22	1.63	0.46
1:N:248:GLY:H	1:N:327:THR:HG23	1.80	0.46
1:L:302:ASN:HD22	1:L:498:ARG:HH22	1.61	0.46
1:W:42:ASP:HB3	1:W:45:LYS:HE3	1.98	0.46
1:W:209:GLN:HE22	1:W:439:ARG:HD3	1.80	0.46
1:B:298:VAL:HG22	1:B:342:LEU:HD21	1.98	0.46
1:F:268:LEU:HD23	1:F:268:LEU:C	2.36	0.46
1:W:192:ARG:NH1	1:W:194:ASP:OD1	2.49	0.46
1:C:192:ARG:NH1	1:C:194:ASP:OD1	2.49	0.46
1:B:192:ARG:NH1	1:B:194:ASP:OD1	2.49	0.46
1:B:129:HIS:ND1	1:B:130:LEU:HD12	2.31	0.46
1:N:80:ILE:CD1	1:N:107:TYR:CD2	2.99	0.45
1:L:224:ILE:CD1	1:C:223:PRO:HG2	2.47	0.45
1:N:268:LEU:C	1:N:268:LEU:HD23	2.36	0.45
1:L:192:ARG:NH1	1:L:194:ASP:OD1	2.49	0.45
1:Q:402:THR:HG22	1:Q:420:LEU:HB2	1.97	0.45
1:C:227:ARG:NH2	4:C:606:GOL:H2	2.31	0.45
1:T:192:ARG:NH1	1:T:194:ASP:OD1	2.49	0.45
1:W:202:TYR:HH	1:W:237:PHE:HE2	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LEU:C	1:C:268:LEU:HD23	2.36	0.45
1:T:298:VAL:HG22	1:T:342:LEU:HD21	1.99	0.45
1:L:220:ILE:H	1:C:388:ASN:ND2	2.15	0.45
1:N:330:ARG:NE	1:N:330:ARG:HA	2.32	0.45
1:B:268:LEU:C	1:B:268:LEU:HD23	2.36	0.45
1:F:405:MET:CE	1:F:417:GLU:HG2	2.46	0.45
1:Q:192:ARG:NH1	1:Q:194:ASP:OD1	2.50	0.44
1:W:268:LEU:HD23	1:W:268:LEU:C	2.37	0.44
1:W:72:ARG:HG2	1:W:111:GLN:OE1	2.17	0.44
1:Q:121:LEU:O	1:Q:121:LEU:HD23	2.17	0.44
1:L:75:LEU:CD1	1:L:75:LEU:N	2.80	0.44
1:Q:507:TYR:O	1:Q:508:LYS:HE3	2.17	0.44
1:C:298:VAL:HG22	1:C:342:LEU:HD21	2.00	0.44
1:L:75:LEU:HD13	1:L:75:LEU:N	2.33	0.44
1:L:169:VAL:HG12	1:L:173:PHE:HE1	1.82	0.44
1:N:91:THR:HG22	1:N:94:GLU:OE1	2.17	0.44
1:N:162:ILE:HD12	1:N:162:ILE:N	2.32	0.44
1:T:167:ILE:O	1:T:167:ILE:HG12	2.18	0.44
1:F:330:ARG:HA	1:F:330:ARG:NE	2.33	0.44
1:B:356:LEU:N	1:B:356:LEU:HD12	2.33	0.44
1:L:202:TYR:HH	1:L:237:PHE:HE2	1.64	0.43
1:L:268:LEU:C	1:L:268:LEU:HD23	2.39	0.43
1:N:72:ARG:NH1	1:N:111:GLN:HG3	2.33	0.43
1:N:161:GLN:HB2	1:N:162:ILE:HD12	2.00	0.43
1:N:171:LYS:HB3	5:N:702:HOH:O	2.18	0.43
1:L:356:LEU:N	1:L:356:LEU:HD12	2.33	0.43
1:N:375:ASP:O	1:B:219:ARG:NH1	2.49	0.43
1:L:162:ILE:HD12	1:L:162:ILE:N	2.33	0.43
1:N:95:LYS:HE2	1:N:95:LYS:HA	2.01	0.43
1:Q:75:LEU:CD1	1:Q:75:LEU:N	2.81	0.43
1:W:106:SER:OG	1:W:124:HIS:HE1	2.02	0.43
1:N:175:ARG:NH1	1:N:473:GLU:OE2	2.46	0.43
1:W:402:THR:HG22	1:W:420:LEU:HB2	2.00	0.43
1:N:206:GLU:HG3	1:N:207:MET:HE2	2.00	0.43
1:W:298:VAL:HG22	1:W:342:LEU:HD21	2.01	0.43
1:B:75:LEU:CD1	1:B:75:LEU:N	2.81	0.43
1:F:498:ARG:HD3	4:F:605:GOL:O3	2.19	0.43
1:N:203:LEU:HD21	1:N:266:GLN:HE21	1.84	0.43
1:Q:356:LEU:HD12	1:Q:356:LEU:N	2.34	0.42
1:F:45:LYS:HB2	1:F:83:GLN:HE21	1.84	0.42
1:N:248:GLY:H	1:N:327:THR:CG2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:95:LYS:HE2	1:Q:95:LYS:HA	2.01	0.42
1:W:125:MET:CE	1:W:136:ARG:HD3	2.50	0.42
1:B:75:LEU:HD13	1:B:75:LEU:N	2.34	0.42
1:N:146:VAL:HG13	1:N:150:VAL:HG23	2.02	0.42
1:Q:224:ILE:CD1	1:T:220:ILE:HA	2.48	0.42
1:F:356:LEU:N	1:F:356:LEU:HD12	2.34	0.42
1:Q:37:MET:HE1	1:Q:121:LEU:HD11	2.00	0.42
1:T:106:SER:OG	1:T:124:HIS:HE1	2.03	0.42
1:L:422:LEU:HB2	1:C:420:LEU:HD12	2.02	0.42
1:Q:155:HIS:CG	1:Q:155:HIS:O	2.73	0.42
1:B:175:ARG:CZ	1:B:175:ARG:HB3	2.50	0.42
1:F:402:THR:HG22	1:F:420:LEU:HB2	2.01	0.42
1:F:463:ARG:HD3	5:F:724:HOH:O	2.19	0.42
1:W:129:HIS:CD2	1:W:130:LEU:HD13	2.54	0.42
1:W:142:LEU:N	1:W:142:LEU:HD13	2.35	0.42
1:Q:125:MET:CE	1:Q:136:ARG:HD3	2.49	0.42
1:T:206:GLU:HG3	1:T:207:MET:HE2	2.01	0.42
1:W:356:LEU:N	1:W:356:LEU:HD12	2.35	0.42
1:L:42:ASP:HA	1:L:45:LYS:HG2	2.02	0.42
1:Q:75:LEU:HD13	1:Q:75:LEU:N	2.35	0.41
1:T:122:ASN:HD22	1:T:136:ARG:HH12	1.68	0.41
1:T:356:LEU:HD12	1:T:356:LEU:N	2.35	0.41
1:W:141:ALA:C	1:W:142:LEU:CD1	2.88	0.41
1:L:186:HIS:O	1:L:190:LEU:HD22	2.20	0.41
1:T:285:ARG:O	1:T:289:VAL:HG23	2.21	0.41
1:L:177:LEU:HD12	1:L:462:TRP:HB2	2.01	0.41
1:T:470:HIS:HB2	5:T:741:HOH:O	2.20	0.41
1:C:143:PRO:HA	1:C:144:PRO:HD3	1.98	0.41
1:C:170:GLU:HG3	1:C:171:LYS:HD2	2.02	0.41
1:N:106:SER:OG	1:N:124:HIS:HE1	2.03	0.41
1:N:248:GLY:N	1:N:327:THR:HG23	2.36	0.41
1:F:106:SER:OG	1:F:124:HIS:HE1	2.03	0.41
1:F:298:VAL:HG22	1:F:342:LEU:HD21	2.03	0.41
1:L:175:ARG:CZ	1:L:175:ARG:HB2	2.51	0.41
1:C:250:PHE:CE2	1:C:360:LYS:HE2	2.55	0.41
1:F:220:ILE:HG23	1:W:388:ASN:HD22	1.86	0.41
1:T:45:LYS:HB2	1:T:83:GLN:HE21	1.86	0.41
1:T:227:ARG:HH12	4:T:603:GOL:H12	1.86	0.41
1:C:356:LEU:HD12	1:C:356:LEU:N	2.36	0.41
1:B:402:THR:HG22	1:B:420:LEU:HB2	2.03	0.41
1:N:356:LEU:HD12	1:N:356:LEU:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:37:MET:O	1:W:142:LEU:HD13	2.20	0.40
1:N:302:ASN:HD21	1:N:498:ARG:HH22	1.64	0.40
1:T:402:THR:HG22	1:T:420:LEU:HB2	2.02	0.40
1:W:122:ASN:HD22	1:W:136:ARG:HH12	1.69	0.40
1:B:129:HIS:CE1	1:B:130:LEU:CD1	3.04	0.40
1:N:43:LEU:HD21	1:N:170:GLU:HG3	2.02	0.40
1:L:298:VAL:HG22	1:L:342:LEU:HD21	2.04	0.40
1:N:220:ILE:HG23	1:B:388:ASN:HD22	1.87	0.40
1:B:106:SER:OG	1:B:124:HIS:HE1	2.05	0.40
1:B:212:MET:CE	1:B:284:VAL:HG13	2.51	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	B	483/515 (94%)	469 (97%)	14 (3%)	0	100	100
1	C	485/515 (94%)	472 (97%)	13 (3%)	0	100	100
1	F	484/515 (94%)	471 (97%)	13 (3%)	0	100	100
1	L	484/515 (94%)	463 (96%)	19 (4%)	2 (0%)	34	57
1	N	484/515 (94%)	469 (97%)	15 (3%)	0	100	100
1	Q	485/515 (94%)	469 (97%)	14 (3%)	2 (0%)	34	57
1	T	484/515 (94%)	471 (97%)	13 (3%)	0	100	100
1	W	484/515 (94%)	467 (96%)	16 (3%)	1 (0%)	47	71
All	All	3873/4120 (94%)	3751 (97%)	117 (3%)	5 (0%)	51	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	157	SER
1	Q	113	ASP
1	Q	157	SER
1	L	171	LYS
1	W	29	SER

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	B	425/450 (94%)	404 (95%)	21 (5%)	25	48
1	C	427/450 (95%)	410 (96%)	17 (4%)	31	57
1	F	426/450 (95%)	406 (95%)	20 (5%)	26	50
1	L	426/450 (95%)	402 (94%)	24 (6%)	21	42
1	N	426/450 (95%)	398 (93%)	28 (7%)	16	33
1	Q	427/450 (95%)	403 (94%)	24 (6%)	21	42
1	T	426/450 (95%)	398 (93%)	28 (7%)	16	33
1	W	426/450 (95%)	405 (95%)	21 (5%)	25	48
All	All	3409/3600 (95%)	3226 (95%)	183 (5%)	22	44

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	29	SER
1	L	45	LYS
1	L	57	ARG
1	L	63	GLU
1	L	73	SER
1	L	75	LEU
1	L	82	LYS
1	L	96	LEU
1	L	105	ASN
1	L	137	LEU
1	L	152	LYS

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Mol	Chain	Res	Type
1	L	157	SER
1	L	160	SER
1	L	175	ARG
1	L	183	LEU
1	L	184	SER
1	L	190	LEU
1	L	212	MET
1	L	246	ARG
1	L	330	ARG
1	L	404	MET
1	L	413	PHE
1	L	419	GLU
1	L	420	LEU
1	C	45	LYS
1	C	57	ARG
1	C	73	SER
1	C	105	ASN
1	C	137	LEU
1	C	160	SER
1	C	175	ARG
1	C	183	LEU
1	C	184	SER
1	C	246	ARG
1	C	345	GLU
1	C	400	VAL
1	C	404	MET
1	C	419	GLU
1	C	420	LEU
1	C	508	LYS
1	C	514	LYS
1	F	28	GLN
1	F	57	ARG
1	F	73	SER
1	F	82	LYS
1	F	93	GLU
1	F	96	LEU
1	F	105	ASN
1	F	137	LEU
1	F	160	SER
1	F	170	GLU
1	F	175	ARG
1	F	177	LEU

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Mol	Chain	Res	Type
1	F	184	SER
1	F	219	ARG
1	F	246	ARG
1	F	400	VAL
1	F	404	MET
1	F	419	GLU
1	F	432	LYS
1	F	474	LEU
1	N	29	SER
1	N	45	LYS
1	N	57	ARG
1	N	63	GLU
1	N	72	ARG
1	N	73	SER
1	N	91	THR
1	N	95	LYS
1	N	96	LEU
1	N	105	ASN
1	N	111	GLN
1	N	137	LEU
1	N	146	VAL
1	N	160	SER
1	N	170	GLU
1	N	179	SER
1	N	181	ASP
1	N	184	SER
1	N	212	MET
1	N	219	ARG
1	N	246	ARG
1	N	296	SER
1	N	400	VAL
1	N	404	MET
1	N	413	PHE
1	N	419	GLU
1	N	420	LEU
1	N	432	LYS
1	Q	45	LYS
1	Q	57	ARG
1	Q	73	SER
1	Q	75	LEU
1	Q	95	LYS
1	Q	96	LEU

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Mol	Chain	Res	Type
1	Q	105	ASN
1	Q	113	ASP
1	Q	137	LEU
1	Q	152	LYS
1	Q	160	SER
1	Q	175	ARG
1	Q	184	SER
1	Q	219	ARG
1	Q	224	ILE
1	Q	296	SER
1	Q	330	ARG
1	Q	376	VAL
1	Q	386	LYS
1	Q	400	VAL
1	Q	404	MET
1	Q	413	PHE
1	Q	419	GLU
1	Q	508	LYS
1	T	45	LYS
1	T	57	ARG
1	T	73	SER
1	T	74	ARG
1	T	76	THR
1	T	96	LEU
1	T	105	ASN
1	T	130	LEU
1	T	137	LEU
1	T	152	LYS
1	T	160	SER
1	T	167	ILE
1	T	171	LYS
1	T	176	ASP
1	T	183	LEU
1	T	184	SER
1	T	219	ARG
1	T	246	ARG
1	T	249	TYR
1	T	296	SER
1	T	330	ARG
1	T	397	ASN
1	T	400	VAL
1	T	404	MET

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Mol	Chain	Res	Type
1	T	413	PHE
1	T	414	ASN
1	T	419	GLU
1	T	459	LEU
1	W	45	LYS
1	W	57	ARG
1	W	73	SER
1	W	76	THR
1	W	96	LEU
1	W	105	ASN
1	W	137	LEU
1	W	142	LEU
1	W	160	SER
1	W	183	LEU
1	W	184	SER
1	W	190	LEU
1	W	212	MET
1	W	246	ARG
1	W	297	GLU
1	W	392	ILE
1	W	400	VAL
1	W	404	MET
1	W	413	PHE
1	W	419	GLU
1	W	459	LEU
1	B	45	LYS
1	B	57	ARG
1	B	72	ARG
1	B	73	SER
1	B	75	LEU
1	B	96	LEU
1	B	105	ASN
1	B	137	LEU
1	B	160	SER
1	B	175	ARG
1	B	178	GLN
1	B	183	LEU
1	B	184	SER
1	B	219	ARG
1	B	246	ARG
1	B	330	ARG
1	B	400	VAL

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Mol	Chain	Res	Type
1	B	404	MET
1	B	413	PHE
1	B	419	GLU
1	B	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	32	HIS
1	L	126	ASN
1	L	209	GLN
1	L	263	HIS
1	L	302	ASN
1	C	28	GLN
1	C	83	GLN
1	C	185	ASN
1	C	263	HIS
1	C	307	GLN
1	C	384	GLN
1	C	388	ASN
1	C	513	HIS
1	F	83	GLN
1	F	122	ASN
1	F	124	HIS
1	F	135	ASN
1	F	218	ASN
1	F	263	HIS
1	F	302	ASN
1	F	388	ASN
1	F	451	HIS
1	N	124	HIS
1	N	135	ASN
1	N	155	HIS
1	N	218	ASN
1	N	263	HIS
1	N	266	GLN
1	N	302	ASN
1	N	388	ASN
1	N	451	HIS
1	N	470	HIS
1	Q	28	GLN
1	Q	83	GLN

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Mol	Chain	Res	Type
1	Q	124	HIS
1	Q	126	ASN
1	Q	129	HIS
1	Q	155	HIS
1	Q	178	GLN
1	Q	218	ASN
1	Q	263	HIS
1	Q	307	GLN
1	Q	388	ASN
1	Q	451	HIS
1	T	83	GLN
1	T	122	ASN
1	T	124	HIS
1	T	126	ASN
1	T	135	ASN
1	T	218	ASN
1	T	263	HIS
1	T	307	GLN
1	T	388	ASN
1	T	451	HIS
1	W	122	ASN
1	W	124	HIS
1	W	126	ASN
1	W	135	ASN
1	W	209	GLN
1	W	218	ASN
1	W	372	GLN
1	W	384	GLN
1	W	388	ASN
1	W	451	HIS
1	B	124	HIS
1	B	133	GLN
1	B	218	ASN
1	B	263	HIS
1	B	302	ASN
1	B	307	GLN
1	B	384	GLN
1	B	388	ASN
1	B	451	HIS

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](#)

45 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
4	GOL	L	606	-	5,5,5	0.71	0	5,5,5	0.51	0
4	GOL	W	604	-	5,5,5	0.48	0	5,5,5	0.18	0
4	GOL	C	605	-	5,5,5	0.67	0	5,5,5	0.67	0
4	GOL	Q	603	-	5,5,5	0.95	0	5,5,5	1.22	0
4	GOL	L	605	-	5,5,5	0.16	0	5,5,5	0.44	0
2	NAP	T	601	-	45,52,52	1.00	5 (11%)	56,80,80	1.55	9 (16%)
2	NAP	L	601	-	45,52,52	1.06	4 (8%)	56,80,80	1.57	8 (14%)
2	NAP	B	601	-	45,52,52	1.05	3 (6%)	56,80,80	1.88	12 (21%)
4	GOL	N	606	-	5,5,5	0.59	0	5,5,5	0.76	0
2	NAP	Q	601	-	45,52,52	0.88	2 (4%)	56,80,80	1.57	11 (19%)
4	GOL	C	603	-	5,5,5	0.40	0	5,5,5	0.27	0
4	GOL	N	605	-	5,5,5	0.54	0	5,5,5	0.66	0
4	GOL	N	608	-	5,5,5	0.33	0	5,5,5	0.31	0
3	PO4	F	602	-	4,4,4	0.69	0	6,6,6	0.66	0
4	GOL	T	604	-	5,5,5	0.60	0	5,5,5	0.42	0
2	NAP	C	601	-	45,52,52	1.00	2 (4%)	56,80,80	1.54	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	C	604	-	5,5,5	0.43	0	5,5,5	0.36	0
3	PO4	N	602	-	4,4,4	0.78	0	6,6,6	0.81	0
3	PO4	W	602	-	4,4,4	0.59	0	6,6,6	1.03	0
4	GOL	Q	604	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	N	607	-	5,5,5	0.74	0	5,5,5	0.87	0
4	GOL	C	606	-	5,5,5	0.80	0	5,5,5	0.96	0
4	GOL	N	604	-	5,5,5	0.47	0	5,5,5	0.14	0
4	GOL	F	603	-	5,5,5	0.72	0	5,5,5	0.98	0
4	GOL	L	603	-	5,5,5	0.62	0	5,5,5	0.40	0
3	PO4	C	602	-	4,4,4	0.75	0	6,6,6	0.95	0
4	GOL	L	604	-	5,5,5	0.46	0	5,5,5	0.39	0
4	GOL	L	607	-	5,5,5	0.64	0	5,5,5	0.57	0
4	GOL	F	604	-	5,5,5	0.49	0	5,5,5	0.31	0
2	NAP	F	601	-	45,52,52	0.90	2 (4%)	56,80,80	1.43	8 (14%)
4	GOL	F	605	-	5,5,5	0.27	0	5,5,5	0.22	0
4	GOL	F	606	-	5,5,5	0.37	0	5,5,5	0.37	0
4	GOL	T	603	-	5,5,5	0.64	0	5,5,5	0.67	0
4	GOL	W	603	-	5,5,5	0.72	0	5,5,5	0.73	0
4	GOL	B	603	-	5,5,5	0.71	0	5,5,5	0.77	0
2	NAP	N	601	-	45,52,52	1.11	4 (8%)	56,80,80	1.67	11 (19%)
3	PO4	T	602	-	4,4,4	0.72	0	6,6,6	0.78	0
4	GOL	N	603	-	5,5,5	0.44	0	5,5,5	0.53	0
4	GOL	L	609	-	5,5,5	0.71	0	5,5,5	0.68	0
3	PO4	Q	602	-	4,4,4	0.82	0	6,6,6	0.51	0
4	GOL	L	608	-	5,5,5	0.48	0	5,5,5	0.55	0
3	PO4	B	602	-	4,4,4	0.75	0	6,6,6	0.72	0
4	GOL	F	607	-	5,5,5	0.61	0	5,5,5	0.31	0
3	PO4	L	602	-	4,4,4	0.67	0	6,6,6	0.79	0
2	NAP	W	601	-	45,52,52	0.83	1 (2%)	56,80,80	1.44	9 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	L	606	-	-	2/4/4/4	-
4	GOL	W	604	-	-	0/4/4/4	-
4	GOL	C	605	-	-	2/4/4/4	-
4	GOL	Q	603	-	-	2/4/4/4	-
4	GOL	L	605	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	T	601	-	-	5/31/67/67	0/5/5/5
2	NAP	L	601	-	-	3/31/67/67	0/5/5/5
2	NAP	B	601	-	-	7/31/67/67	0/5/5/5
4	GOL	N	606	-	-	2/4/4/4	-
2	NAP	Q	601	-	-	2/31/67/67	0/5/5/5
4	GOL	C	603	-	-	2/4/4/4	-
4	GOL	N	605	-	-	2/4/4/4	-
4	GOL	N	608	-	-	2/4/4/4	-
4	GOL	T	604	-	-	0/4/4/4	-
2	NAP	C	601	-	-	4/31/67/67	0/5/5/5
4	GOL	C	604	-	-	0/4/4/4	-
4	GOL	Q	604	-	-	3/4/4/4	-
4	GOL	N	607	-	-	2/4/4/4	-
4	GOL	C	606	-	-	1/4/4/4	-
4	GOL	N	604	-	-	2/4/4/4	-
4	GOL	F	603	-	-	4/4/4/4	-
4	GOL	L	603	-	-	0/4/4/4	-
4	GOL	L	607	-	-	3/4/4/4	-
4	GOL	L	604	-	-	1/4/4/4	-
4	GOL	F	604	-	-	1/4/4/4	-
2	NAP	F	601	-	-	5/31/67/67	0/5/5/5
4	GOL	F	605	-	-	2/4/4/4	-
4	GOL	F	606	-	-	2/4/4/4	-
4	GOL	T	603	-	-	3/4/4/4	-
4	GOL	W	603	-	-	2/4/4/4	-
4	GOL	B	603	-	-	2/4/4/4	-
2	NAP	N	601	-	-	2/31/67/67	0/5/5/5
4	GOL	N	603	-	-	4/4/4/4	-
4	GOL	L	609	-	-	2/4/4/4	-
4	GOL	L	608	-	-	2/4/4/4	-
4	GOL	F	607	-	-	0/4/4/4	-
2	NAP	W	601	-	-	7/31/67/67	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	NAP	O4B-C1B	3.32	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	601	NAP	C2A-N3A	3.10	1.37	1.32
2	N	601	NAP	O4B-C1B	3.08	1.45	1.41
2	N	601	NAP	C5A-C4A	2.92	1.48	1.40
2	L	601	NAP	O4D-C1D	2.80	1.45	1.41
2	B	601	NAP	C5A-C4A	2.76	1.48	1.40
2	T	601	NAP	C2A-N3A	2.62	1.36	1.32
2	T	601	NAP	O4D-C1D	2.60	1.44	1.41
2	N	601	NAP	O4D-C1D	2.55	1.44	1.41
2	B	601	NAP	P2B-O2B	2.51	1.64	1.59
2	B	601	NAP	O4B-C1B	2.30	1.44	1.41
2	C	601	NAP	C2A-N3A	2.28	1.35	1.32
2	T	601	NAP	C5A-C4A	2.26	1.46	1.40
2	F	601	NAP	C5A-C4A	2.21	1.46	1.40
2	L	601	NAP	O4B-C1B	2.17	1.44	1.41
2	Q	601	NAP	C2A-N3A	2.12	1.35	1.32
2	N	601	NAP	C2A-N3A	2.10	1.35	1.32
2	T	601	NAP	C4A-N3A	2.09	1.38	1.35
2	W	601	NAP	C5A-C4A	2.07	1.46	1.40
2	L	601	NAP	C5A-C4A	2.05	1.46	1.40
2	F	601	NAP	C2A-N3A	2.03	1.35	1.32
2	Q	601	NAP	C5A-C4A	2.02	1.46	1.40
2	T	601	NAP	O4B-C1B	2.01	1.43	1.41

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAP	PN-O3-PA	-5.86	112.71	132.83
2	B	601	NAP	N6A-C6A-N1A	5.09	129.14	118.57
2	T	601	NAP	N3A-C2A-N1A	-5.07	120.76	128.68
2	C	601	NAP	N3A-C2A-N1A	-4.61	121.47	128.68
2	L	601	NAP	N3A-C2A-N1A	-4.55	121.57	128.68
2	T	601	NAP	C1B-N9A-C4A	-4.51	118.72	126.64
2	F	601	NAP	N3A-C2A-N1A	-4.50	121.64	128.68
2	Q	601	NAP	C3N-C7N-N7N	4.34	122.95	117.75
2	C	601	NAP	C3N-C7N-N7N	4.25	122.86	117.75
2	Q	601	NAP	N3A-C2A-N1A	-4.25	122.04	128.68
2	W	601	NAP	N3A-C2A-N1A	-4.21	122.10	128.68
2	B	601	NAP	C5A-C6A-N6A	-4.20	113.96	120.35
2	B	601	NAP	C4A-C5A-N7A	4.15	113.72	109.40
2	L	601	NAP	PN-O3-PA	-4.14	118.63	132.83
2	N	601	NAP	O4B-C1B-C2B	-4.04	99.58	106.59
2	B	601	NAP	N3A-C2A-N1A	-4.02	122.39	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAP	C3B-C2B-C1B	-4.00	95.38	102.89
2	N	601	NAP	N6A-C6A-N1A	3.91	126.68	118.57
2	T	601	NAP	C3N-C7N-N7N	3.81	122.32	117.75
2	F	601	NAP	C3N-C7N-N7N	3.69	122.18	117.75
2	W	601	NAP	C3N-C7N-N7N	3.62	122.09	117.75
2	N	601	NAP	PN-O3-PA	-3.59	120.51	132.83
2	N	601	NAP	C3N-C7N-N7N	3.57	122.04	117.75
2	F	601	NAP	C1B-N9A-C4A	-3.50	120.48	126.64
2	C	601	NAP	C1B-N9A-C4A	-3.48	120.53	126.64
2	Q	601	NAP	C1B-N9A-C4A	-3.42	120.64	126.64
2	W	601	NAP	C1B-N9A-C4A	-3.33	120.79	126.64
2	Q	601	NAP	O7N-C7N-N7N	-3.32	117.86	122.58
2	Q	601	NAP	PN-O3-PA	-3.30	121.50	132.83
2	L	601	NAP	C1B-N9A-C4A	-3.26	120.91	126.64
2	F	601	NAP	O3X-P2B-O2X	3.18	119.78	107.64
2	C	601	NAP	O3X-P2B-O2X	3.17	119.74	107.64
2	L	601	NAP	O3X-P2B-O2X	3.13	119.61	107.64
2	N	601	NAP	O3X-P2B-O2X	3.11	119.52	107.64
2	N	601	NAP	C5A-C6A-N6A	-3.08	115.67	120.35
2	N	601	NAP	N3A-C2A-N1A	-3.06	123.89	128.68
2	N	601	NAP	O7N-C7N-C3N	-3.06	115.97	119.63
2	F	601	NAP	PN-O3-PA	-3.05	122.34	132.83
2	C	601	NAP	PN-O3-PA	-3.02	122.47	132.83
2	N	601	NAP	C2N-C3N-C4N	2.94	121.60	118.26
2	B	601	NAP	C2A-N1A-C6A	2.91	123.73	118.75
2	T	601	NAP	O3X-P2B-O2X	2.88	118.63	107.64
2	C	601	NAP	O7N-C7N-N7N	-2.85	118.53	122.58
2	T	601	NAP	PN-O3-PA	-2.75	123.40	132.83
2	B	601	NAP	C3N-C7N-N7N	2.70	120.99	117.75
2	L	601	NAP	O2N-PN-O1N	2.70	125.58	112.24
2	W	601	NAP	PN-O3-PA	-2.70	123.57	132.83
2	W	601	NAP	O3X-P2B-O2X	2.64	117.74	107.64
2	N	601	NAP	C3B-C2B-C1B	-2.62	97.96	102.89
2	B	601	NAP	O4B-C4B-C5B	-2.53	101.05	109.37
2	T	601	NAP	O7N-C7N-N7N	-2.50	119.03	122.58
2	B	601	NAP	O2A-PA-O5B	-2.46	96.31	107.75
2	Q	601	NAP	N6A-C6A-N1A	2.46	123.68	118.57
2	C	601	NAP	C3B-C2B-C1B	-2.42	98.35	102.89
2	N	601	NAP	C5N-C4N-C3N	-2.36	117.55	120.34
2	F	601	NAP	C2A-N1A-C6A	2.35	122.77	118.75
2	B	601	NAP	O3X-P2B-O2X	2.34	116.56	107.64
2	F	601	NAP	N6A-C6A-N1A	2.33	123.42	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	601	NAP	O3X-P2B-O2X	2.33	116.53	107.64
2	Q	601	NAP	O2A-PA-O5B	-2.30	97.04	107.75
2	L	601	NAP	C5A-C6A-N6A	-2.29	116.86	120.35
2	T	601	NAP	C2A-N1A-C6A	2.29	122.67	118.75
2	W	601	NAP	O2N-PN-O1N	2.28	123.52	112.24
2	T	601	NAP	O3X-P2B-O2B	-2.27	95.84	105.99
2	W	601	NAP	C3D-C2D-C1D	2.25	104.37	100.98
2	L	601	NAP	O2A-PA-O1A	2.21	123.18	112.24
2	W	601	NAP	O2A-PA-O1A	2.21	123.18	112.24
2	W	601	NAP	C4A-C5A-N7A	-2.20	107.10	109.40
2	Q	601	NAP	O2A-PA-O1A	2.20	123.11	112.24
2	L	601	NAP	C3N-C7N-N7N	2.19	120.38	117.75
2	B	601	NAP	O2A-PA-O1A	2.13	122.79	112.24
2	Q	601	NAP	C3B-C2B-C1B	-2.12	98.90	102.89
2	F	601	NAP	O7N-C7N-N7N	-2.12	119.57	122.58
2	C	601	NAP	C5A-C6A-N6A	-2.11	117.15	120.35
2	C	601	NAP	O5B-C5B-C4B	2.05	116.05	108.99
2	T	601	NAP	N6A-C6A-N1A	2.05	122.82	118.57
2	Q	601	NAP	C5A-C6A-N6A	-2.01	117.30	120.35

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	601	NAP	PN-O3-PA-O5B
2	T	601	NAP	PN-O3-PA-O5B
2	W	601	NAP	PN-O3-PA-O5B
2	B	601	NAP	C5B-O5B-PA-O3
2	B	601	NAP	PN-O3-PA-O5B
4	L	606	GOL	O1-C1-C2-O2
4	L	606	GOL	O1-C1-C2-C3
4	L	607	GOL	O1-C1-C2-C3
4	L	609	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-C3
4	C	605	GOL	O1-C1-C2-C3
4	F	603	GOL	O1-C1-C2-O2
4	F	603	GOL	O1-C1-C2-C3
4	F	603	GOL	C1-C2-C3-O3
4	F	605	GOL	C1-C2-C3-O3
4	F	605	GOL	O2-C2-C3-O3
4	F	606	GOL	O1-C1-C2-C3
4	N	603	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	N	603	GOL	C1-C2-C3-O3
4	N	606	GOL	C1-C2-C3-O3
4	N	608	GOL	O1-C1-C2-C3
4	Q	603	GOL	O1-C1-C2-C3
4	Q	604	GOL	O1-C1-C2-C3
4	T	603	GOL	O1-C1-C2-C3
4	W	603	GOL	O1-C1-C2-C3
4	B	603	GOL	O1-C1-C2-C3
2	N	601	NAP	C3B-C2B-O2B-P2B
2	Q	601	NAP	C3B-C2B-O2B-P2B
2	B	601	NAP	C3B-C2B-O2B-P2B
4	L	607	GOL	O1-C1-C2-O2
4	N	606	GOL	O2-C2-C3-O3
2	C	601	NAP	C1B-C2B-O2B-P2B
2	T	601	NAP	C1B-C2B-O2B-P2B
2	L	601	NAP	C3B-C2B-O2B-P2B
2	C	601	NAP	C3B-C2B-O2B-P2B
2	F	601	NAP	C3B-C2B-O2B-P2B
2	T	601	NAP	C3B-C2B-O2B-P2B
2	W	601	NAP	C3B-C2B-O2B-P2B
4	L	608	GOL	O1-C1-C2-C3
4	N	604	GOL	O1-C1-C2-C3
4	N	607	GOL	O1-C1-C2-C3
2	L	601	NAP	C1B-C2B-O2B-P2B
2	F	601	NAP	C1B-C2B-O2B-P2B
2	W	601	NAP	C1B-C2B-O2B-P2B
4	L	609	GOL	O1-C1-C2-O2
4	C	603	GOL	O1-C1-C2-O2
4	C	605	GOL	O1-C1-C2-O2
4	F	603	GOL	O2-C2-C3-O3
4	Q	603	GOL	O1-C1-C2-O2
4	W	603	GOL	O1-C1-C2-O2
4	F	606	GOL	O1-C1-C2-O2
4	N	604	GOL	O1-C1-C2-O2
4	N	608	GOL	O1-C1-C2-O2
4	Q	604	GOL	O1-C1-C2-O2
4	T	603	GOL	O1-C1-C2-O2
4	B	603	GOL	O1-C1-C2-O2
4	N	603	GOL	O2-C2-C3-O3
2	L	601	NAP	PN-O3-PA-O5B
2	C	601	NAP	PN-O3-PA-O5B
2	N	601	NAP	PN-O3-PA-O5B

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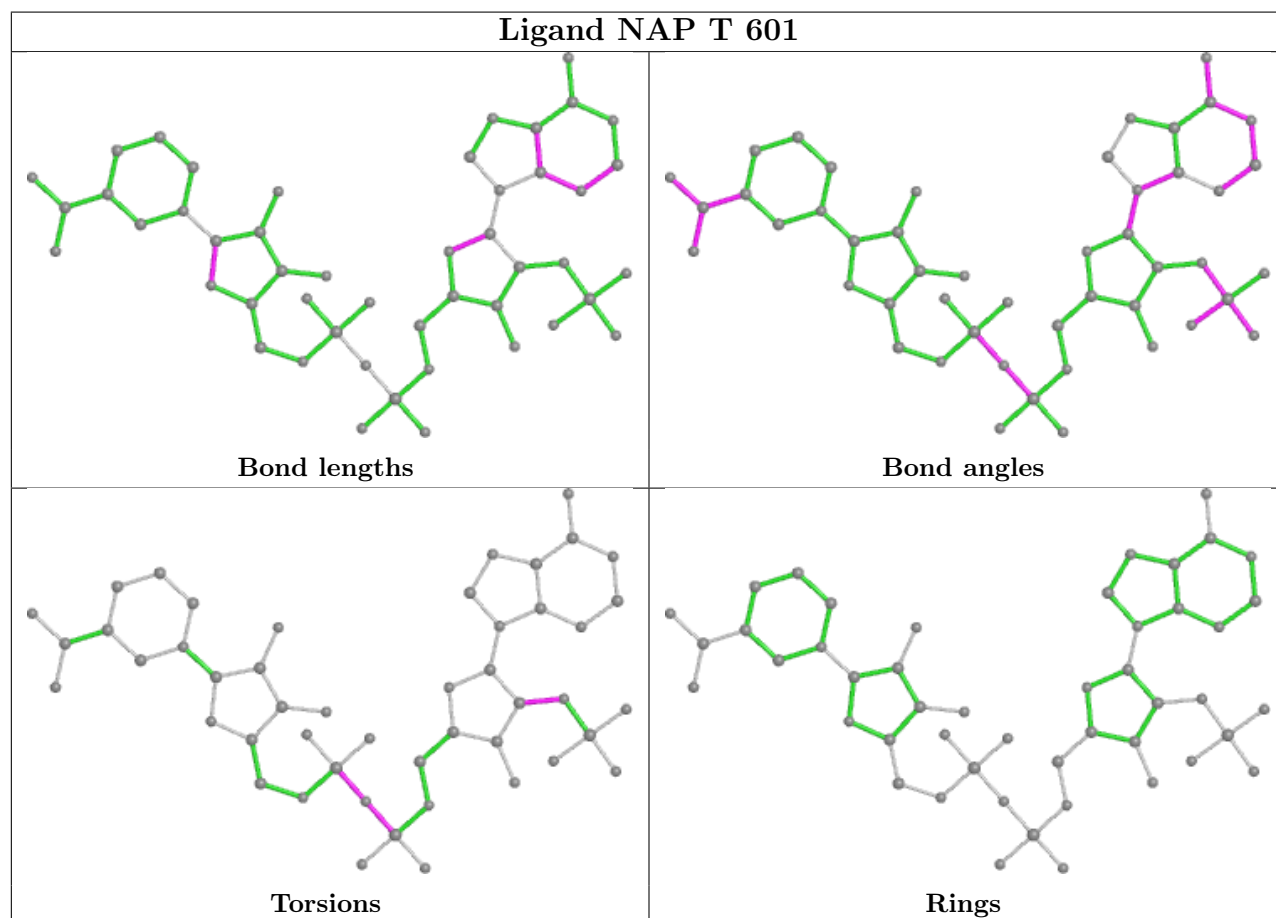
Mol	Chain	Res	Type	Atoms
4	L	608	GOL	O1-C1-C2-O2
4	F	604	GOL	O2-C2-C3-O3
4	N	607	GOL	O1-C1-C2-O2
2	C	601	NAP	PA-O3-PN-O1N
2	B	601	NAP	PA-O3-PN-O1N
4	N	605	GOL	O1-C1-C2-C3
2	B	601	NAP	C5B-O5B-PA-O2A
2	Q	601	NAP	C1B-C2B-O2B-P2B
2	W	601	NAP	PA-O3-PN-O1N
2	F	601	NAP	PA-O3-PN-O1N
2	T	601	NAP	PA-O3-PN-O1N
4	N	603	GOL	O1-C1-C2-O2
4	N	605	GOL	O1-C1-C2-O2
2	W	601	NAP	C2B-O2B-P2B-O1X
2	W	601	NAP	C2B-O2B-P2B-O3X
4	L	604	GOL	O2-C2-C3-O3
2	B	601	NAP	O4B-C4B-C5B-O5B
2	F	601	NAP	PA-O3-PN-O2N
2	T	601	NAP	PA-O3-PN-O2N
2	W	601	NAP	PA-O3-PN-O2N
2	B	601	NAP	PA-O3-PN-O2N
4	L	607	GOL	C1-C2-C3-O3
4	C	606	GOL	O1-C1-C2-C3
4	Q	604	GOL	C1-C2-C3-O3
4	T	603	GOL	O2-C2-C3-O3

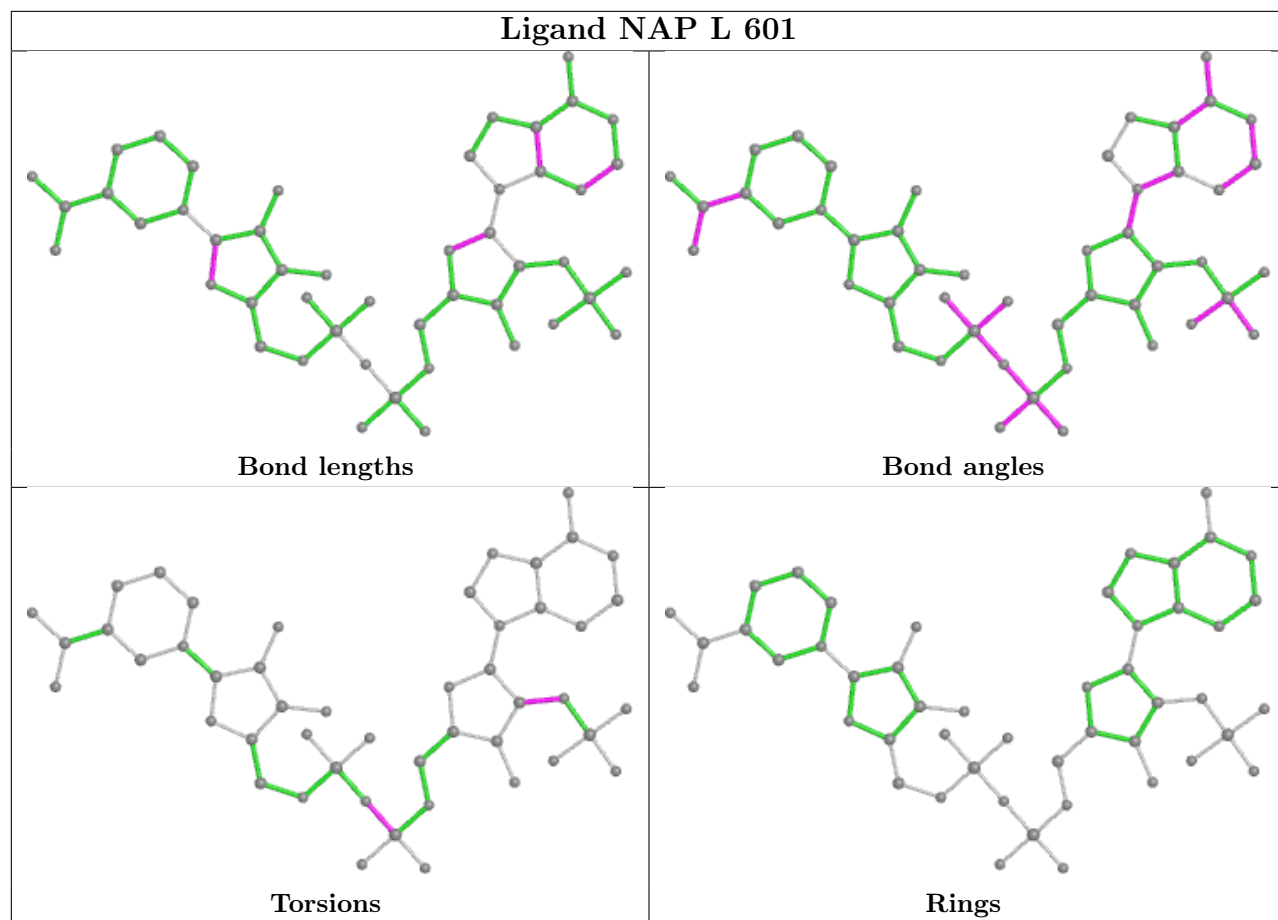
There are no ring outliers.

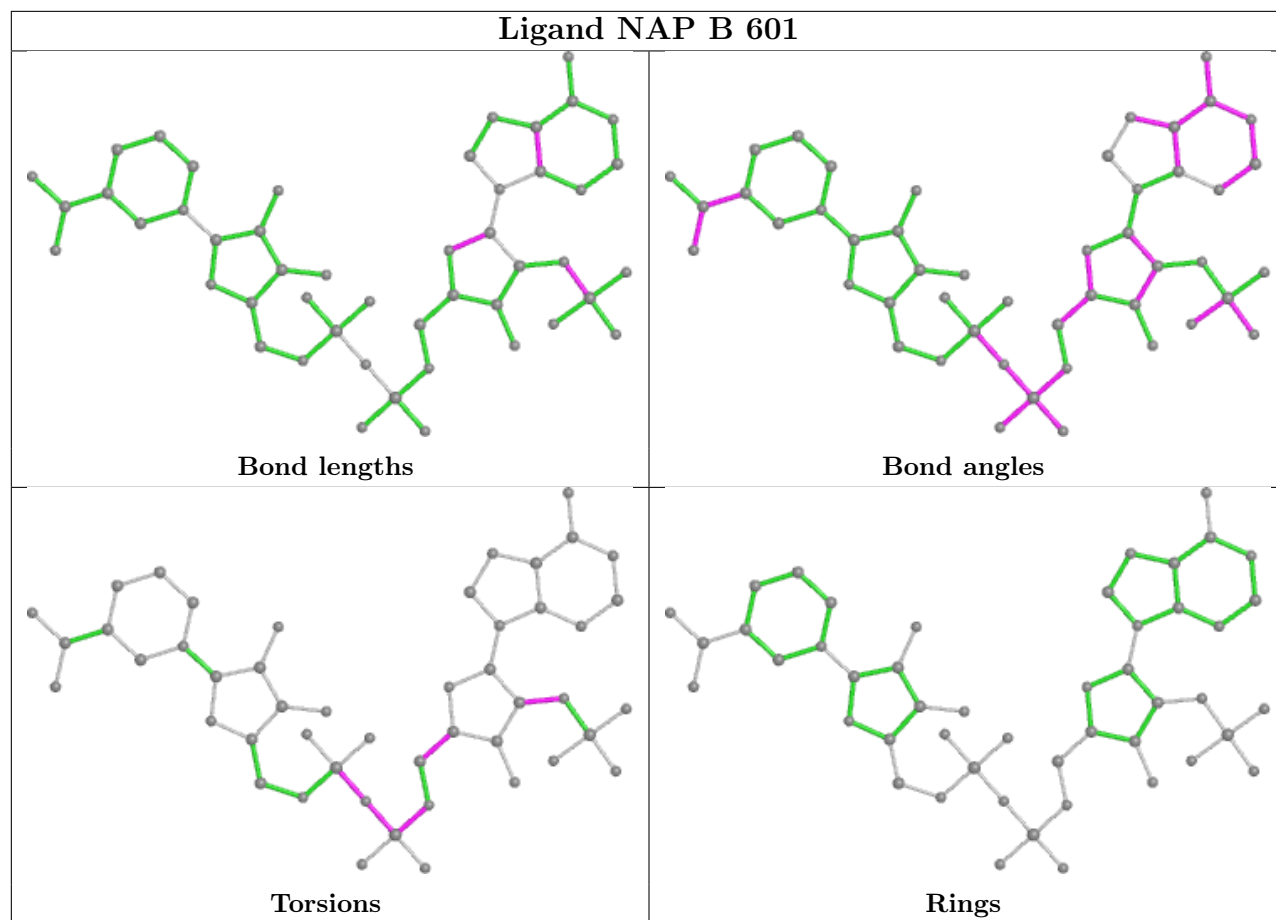
11 monomers are involved in 15 short contacts:

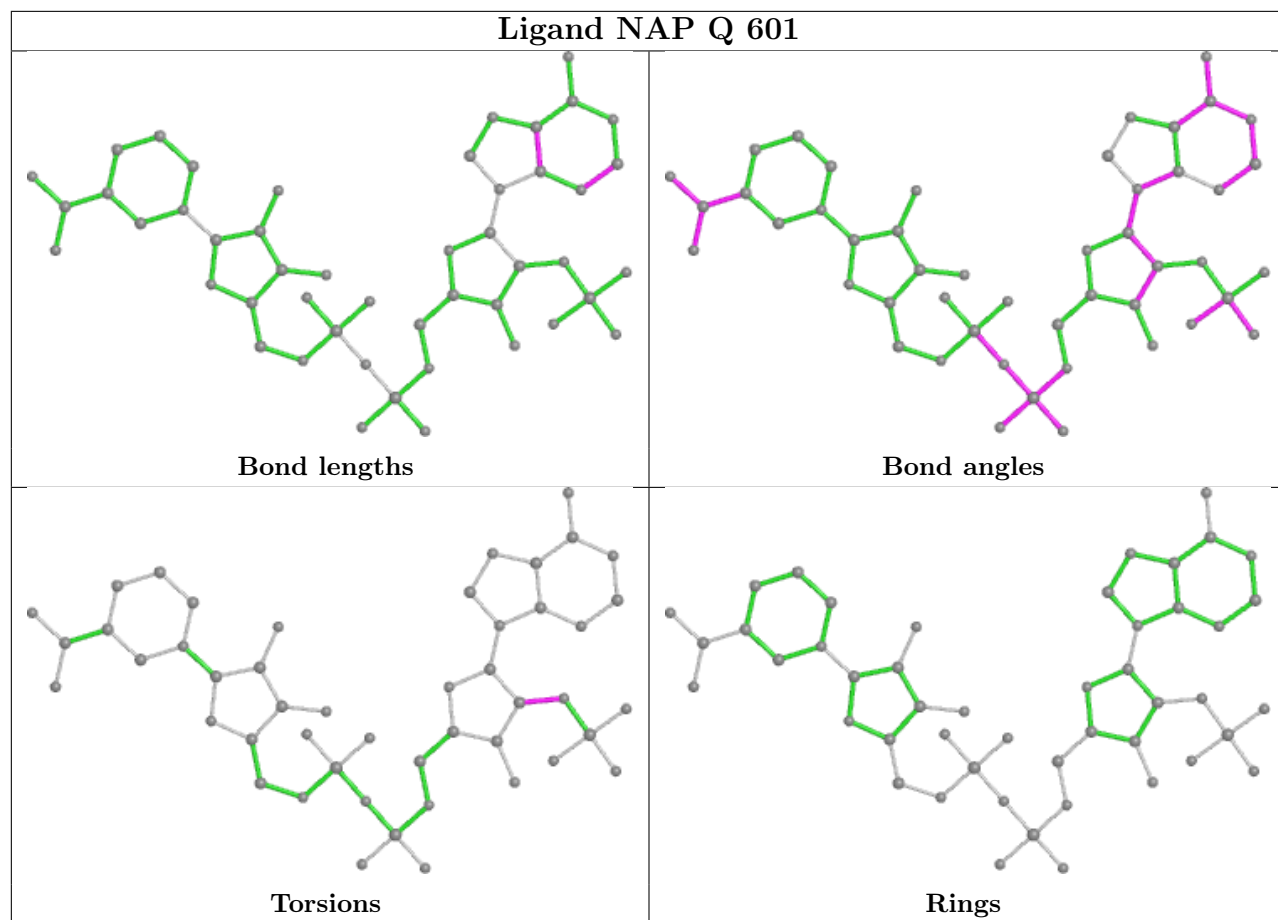
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	605	GOL	1	0
4	Q	603	GOL	1	0
2	T	601	NAP	1	0
2	B	601	NAP	2	0
4	N	606	GOL	1	0
4	N	605	GOL	2	0
4	C	606	GOL	3	0
4	L	603	GOL	1	0
4	F	605	GOL	1	0
4	T	603	GOL	1	0
2	N	601	NAP	1	0

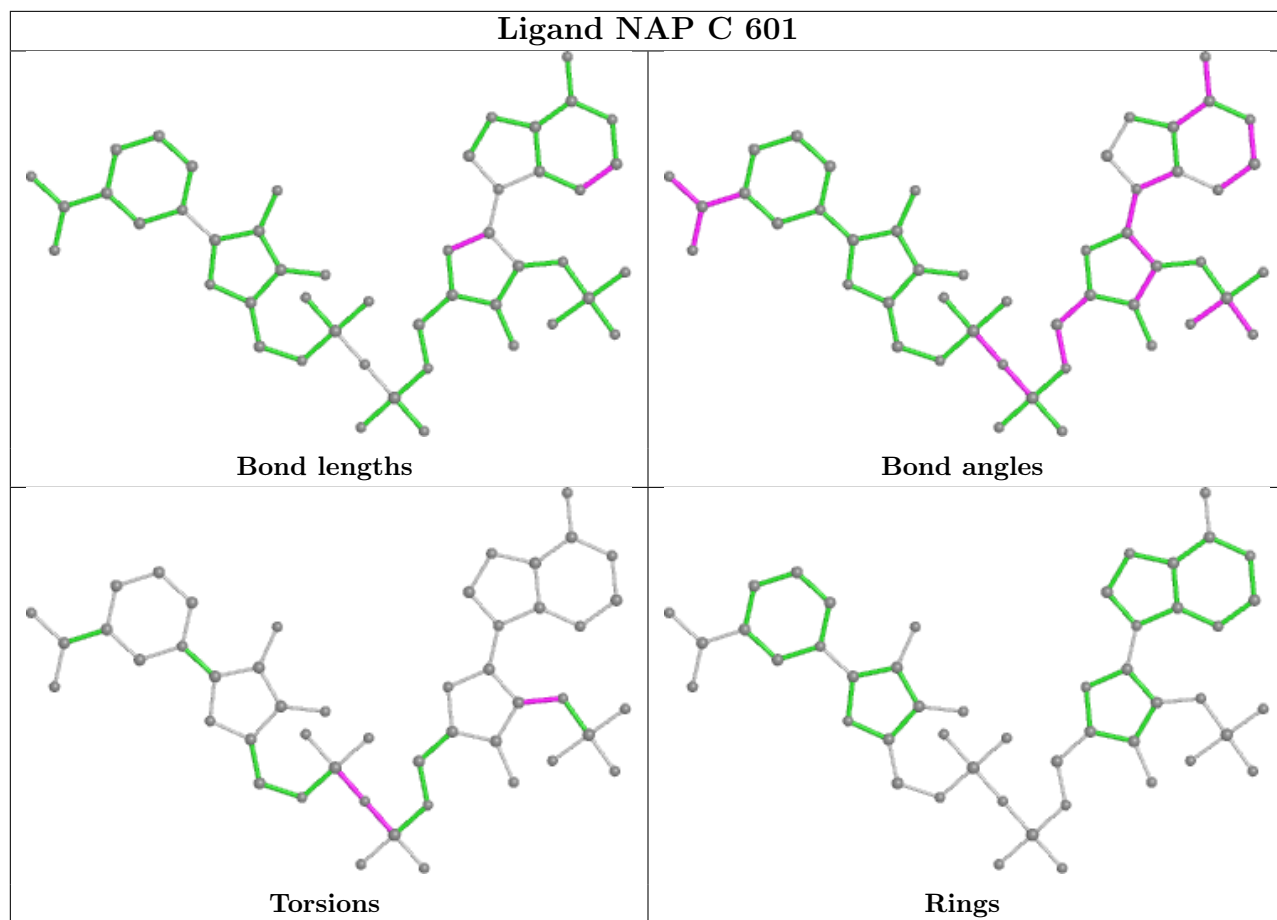
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

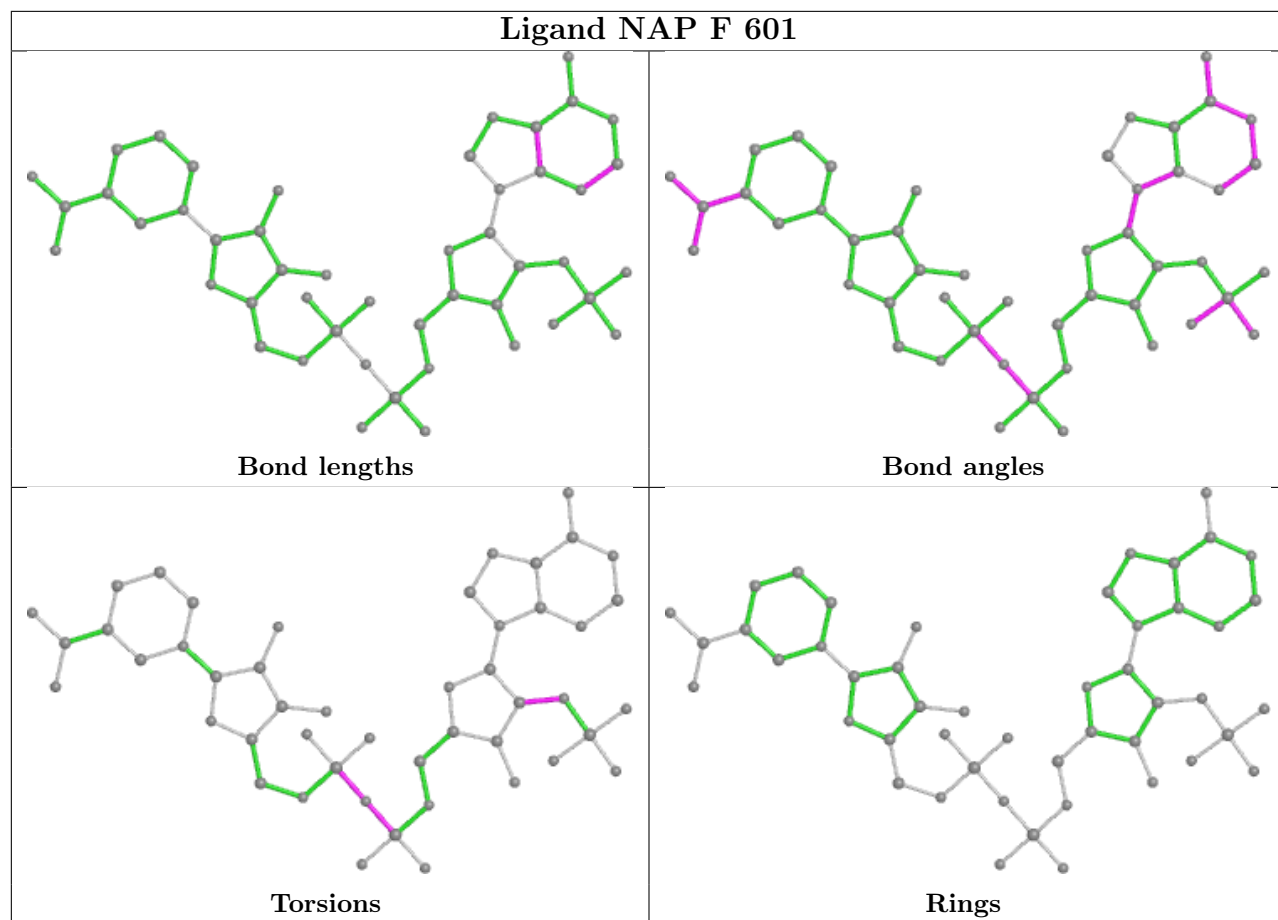


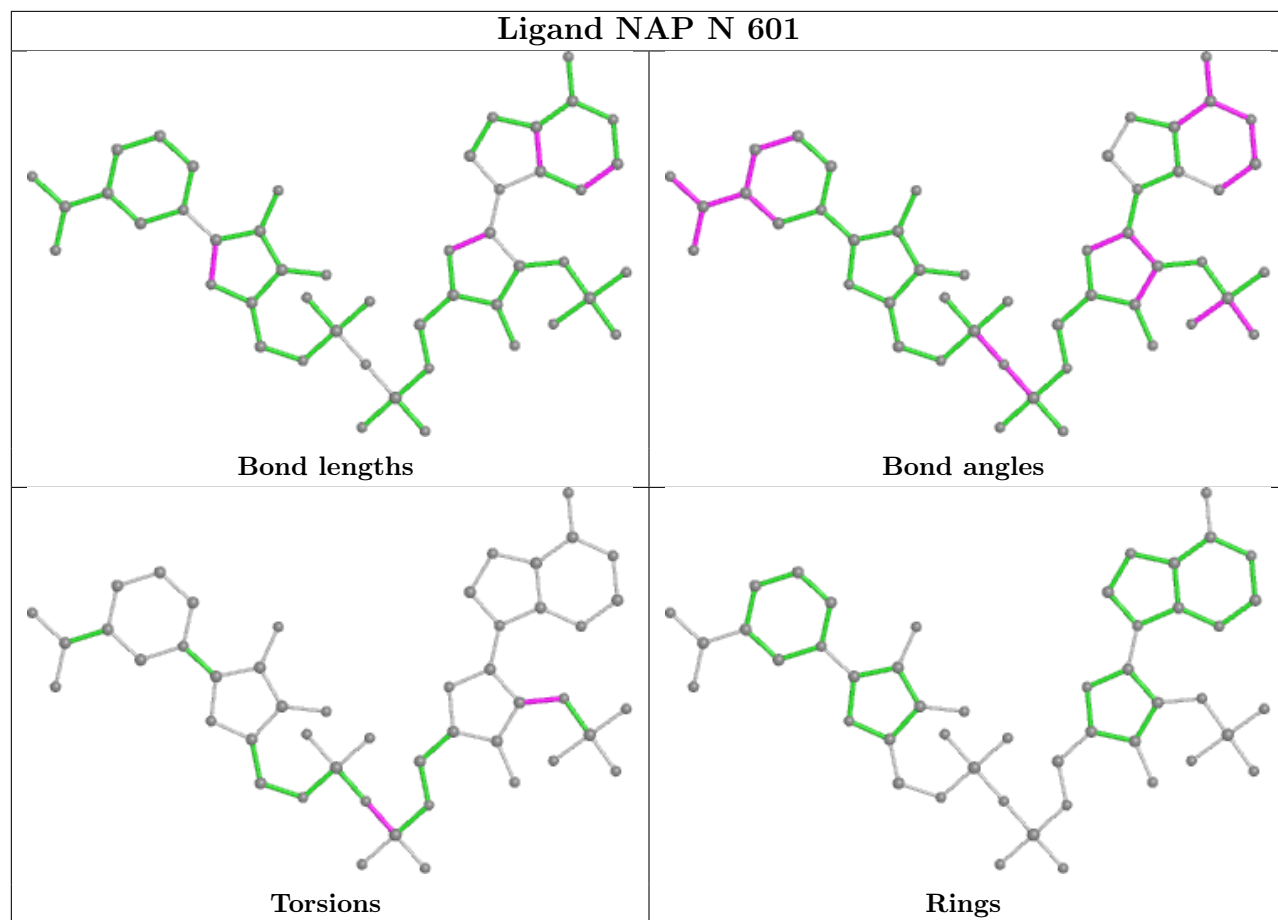


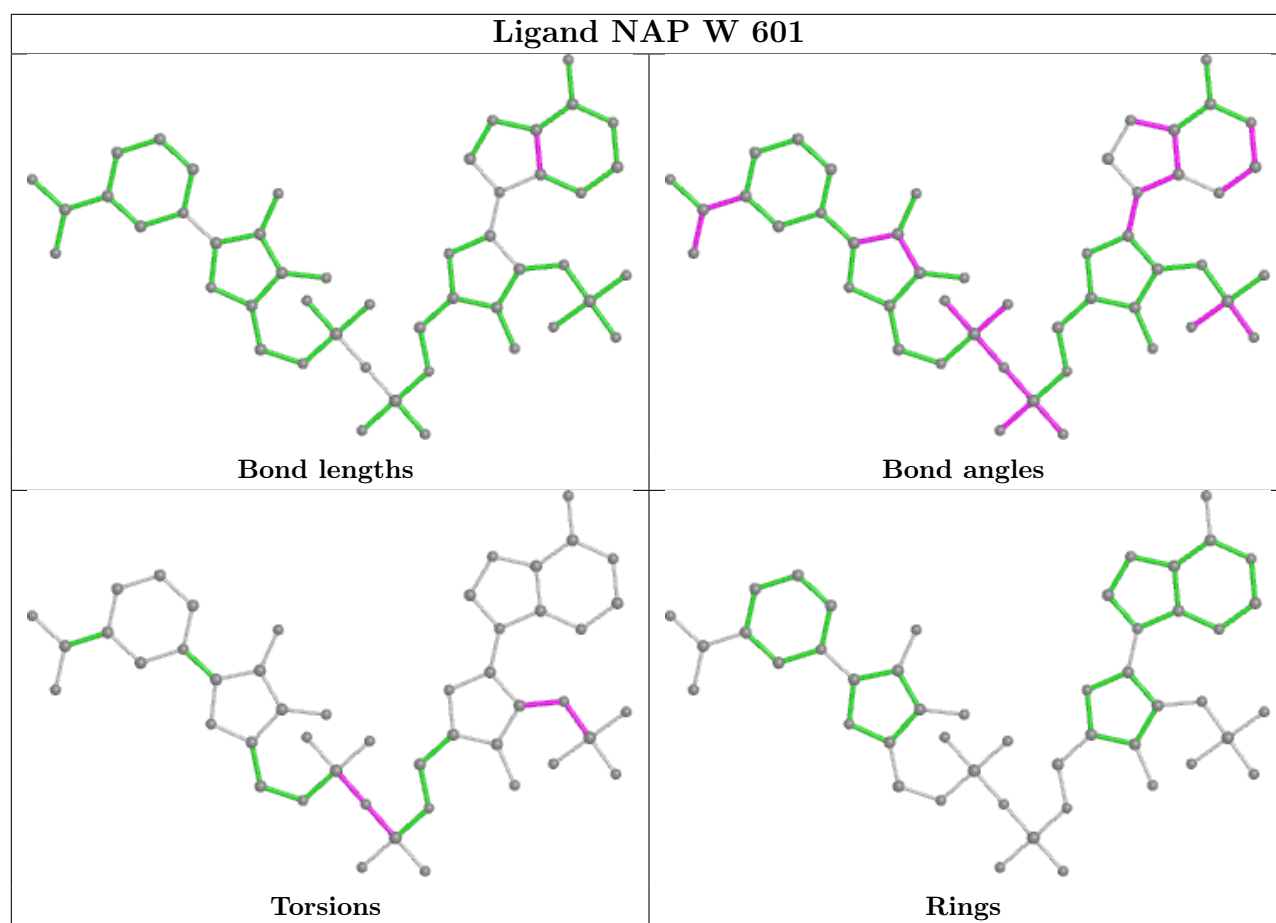












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	B	485/515 (94%)	-0.29	3 (0%) 89 88	30, 54, 91, 134	0
1	C	487/515 (94%)	-0.30	2 (0%) 92 91	29, 50, 91, 142	0
1	F	486/515 (94%)	-0.37	1 (0%) 95 95	32, 48, 82, 113	0
1	L	486/515 (94%)	-0.28	2 (0%) 92 91	27, 48, 102, 127	0
1	N	486/515 (94%)	-0.13	1 (0%) 95 95	30, 61, 96, 137	0
1	Q	487/515 (94%)	-0.18	5 (1%) 82 80	32, 53, 100, 126	0
1	T	486/515 (94%)	-0.10	5 (1%) 82 80	37, 63, 97, 129	0
1	W	486/515 (94%)	-0.04	7 (1%) 75 71	37, 65, 109, 133	0
All	All	3889/4120 (94%)	-0.21	26 (0%) 87 86	27, 55, 97, 142	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	178	GLN	4.8
1	Q	74	ARG	3.9
1	W	80	ILE	3.9
1	W	121	LEU	3.2
1	T	74	ARG	3.2
1	B	513	HIS	2.9
1	T	249	TYR	2.9
1	L	513	HIS	2.6
1	T	330	ARG	2.5
1	Q	108	VAL	2.5
1	N	92	PRO	2.4
1	W	178	GLN	2.4
1	C	315	GLU	2.4
1	W	102	PHE	2.4
1	L	96	LEU	2.3
1	T	80	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	175	ARG	2.3
1	B	175	ARG	2.2
1	B	315	GLU	2.2
1	T	176	ASP	2.2
1	Q	123	SER	2.1
1	W	70	TYR	2.1
1	W	118	TYR	2.1
1	Q	413	PHE	2.1
1	W	74	ARG	2.1
1	Q	121	LEU	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(Å ²)	Q<0.9
4	GOL	C	603	6/6	0.43	0.35	80,90,96,96	0
4	GOL	F	607	6/6	0.52	0.58	77,93,99,103	0
4	GOL	C	605	6/6	0.58	0.47	77,94,103,104	0
4	GOL	N	604	6/6	0.70	0.31	85,90,94,94	0
4	GOL	L	606	6/6	0.74	0.34	66,72,77,78	0
4	GOL	F	606	6/6	0.74	0.17	85,93,95,97	0
4	GOL	T	604	6/6	0.76	0.27	86,91,93,94	0
4	GOL	N	607	6/6	0.77	0.28	63,68,73,73	0
4	GOL	L	608	6/6	0.77	0.26	84,90,91,92	0
4	GOL	C	604	6/6	0.78	0.26	64,73,83,83	0
4	GOL	Q	604	6/6	0.79	0.29	61,70,72,73	0
3	PO4	L	602	5/5	0.79	0.20	90,96,101,112	0
3	PO4	W	602	5/5	0.80	0.20	90,94,96,106	0

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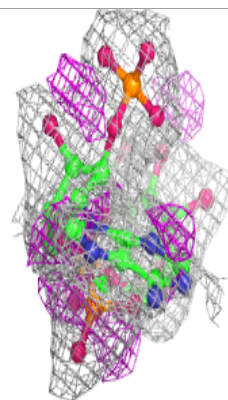
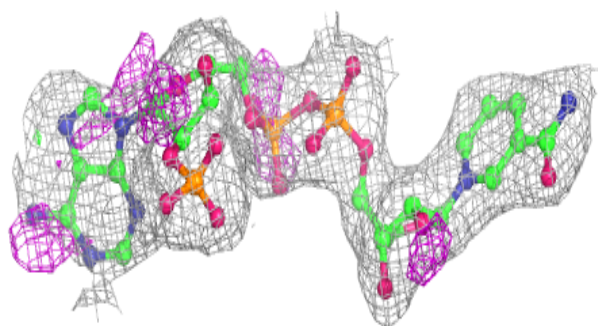
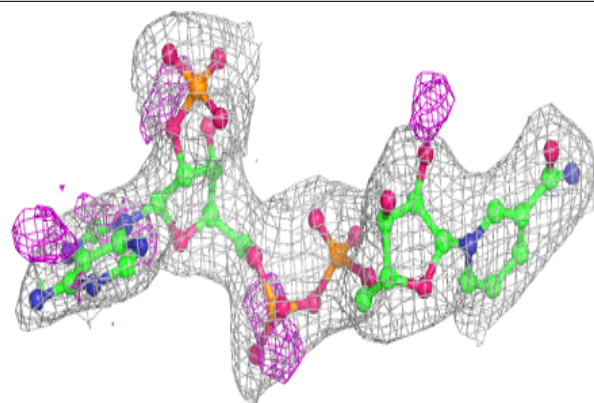
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	603	6/6	0.80	0.26	43,46,49,57	0
4	GOL	L	609	6/6	0.82	0.28	66,74,77,79	0
3	PO4	B	602	5/5	0.82	0.16	103,109,112,118	0
4	GOL	Q	603	6/6	0.82	0.22	41,45,47,51	0
3	PO4	C	602	5/5	0.83	0.19	87,88,89,102	0
4	GOL	W	604	6/6	0.84	0.45	75,78,79,80	0
4	GOL	N	603	6/6	0.84	0.29	64,67,72,74	0
4	GOL	L	607	6/6	0.85	0.28	59,65,67,67	0
3	PO4	T	602	5/5	0.86	0.14	88,91,98,103	0
4	GOL	F	604	6/6	0.86	0.23	58,66,70,70	0
3	PO4	N	602	5/5	0.87	0.14	77,84,92,95	0
4	GOL	N	606	6/6	0.87	0.35	68,72,77,81	0
4	GOL	W	603	6/6	0.87	0.17	46,54,54,63	0
4	GOL	L	604	6/6	0.87	0.23	65,75,79,82	0
4	GOL	F	605	6/6	0.87	0.28	69,78,82,91	0
4	GOL	C	606	6/6	0.88	0.24	38,41,50,53	0
4	GOL	L	603	6/6	0.89	0.21	43,47,50,52	0
3	PO4	Q	602	5/5	0.90	0.14	88,90,99,100	0
4	GOL	F	603	6/6	0.91	0.19	39,43,46,47	0
4	GOL	T	603	6/6	0.91	0.23	47,53,56,59	0
4	GOL	L	605	6/6	0.91	0.22	69,70,71,75	0
4	GOL	N	608	6/6	0.92	0.19	68,74,76,76	0
3	PO4	F	602	5/5	0.92	0.13	80,80,84,93	0
4	GOL	N	605	6/6	0.93	0.22	39,48,50,51	0
2	NAP	N	601	48/48	0.95	0.14	42,52,68,73	0
2	NAP	B	601	48/48	0.96	0.15	39,46,57,68	0
2	NAP	F	601	48/48	0.96	0.13	43,54,65,73	0
2	NAP	W	601	48/48	0.97	0.11	41,49,54,57	0
2	NAP	C	601	48/48	0.97	0.12	38,47,53,54	0
2	NAP	T	601	48/48	0.97	0.12	42,52,57,58	0
2	NAP	L	601	48/48	0.98	0.13	32,38,50,53	0
2	NAP	Q	601	48/48	0.98	0.12	34,42,54,54	0

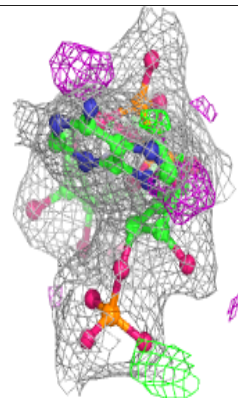
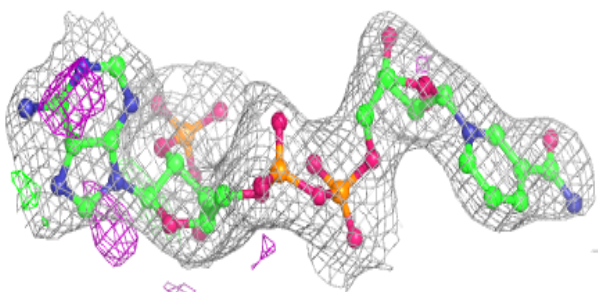
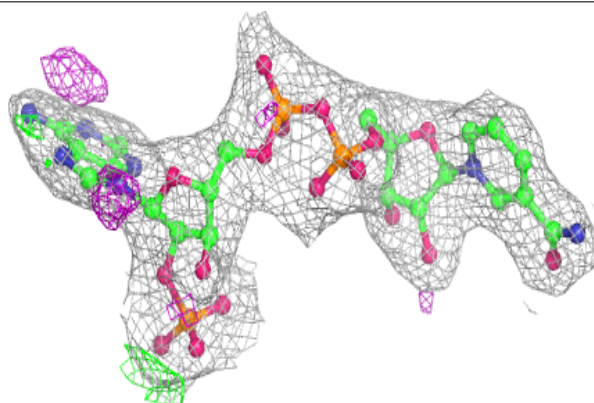
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP N 601:

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

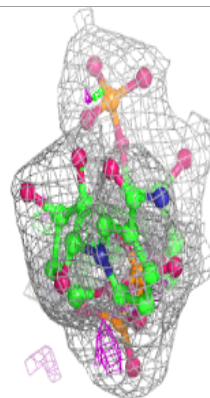
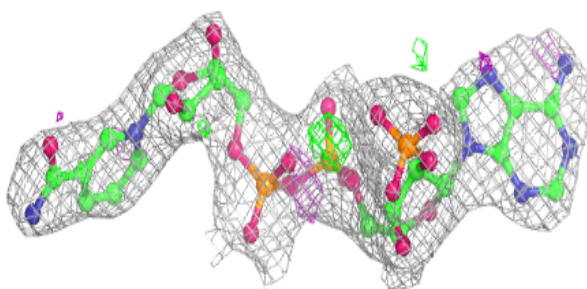
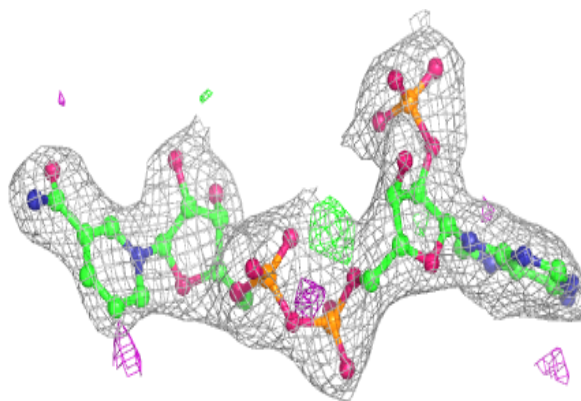
**Electron density around NAP B 601:**

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

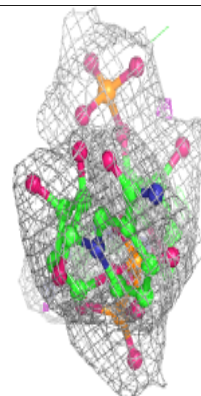
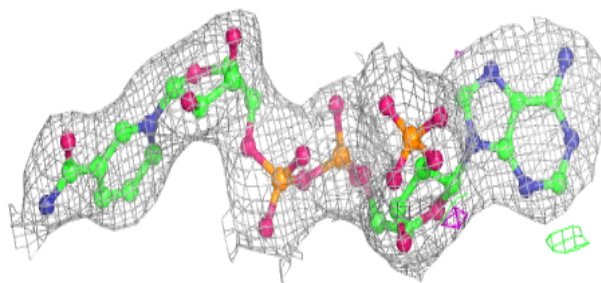
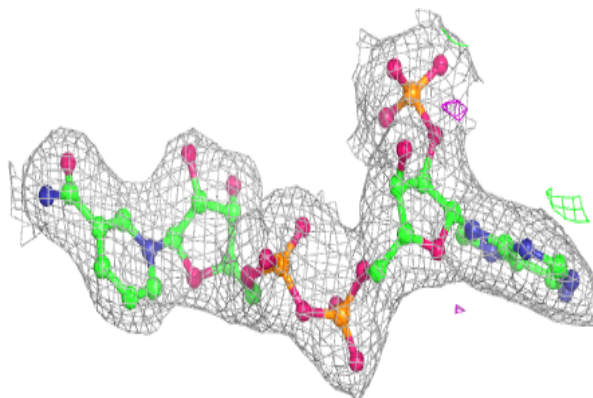


Electron density around NAP F 601:

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

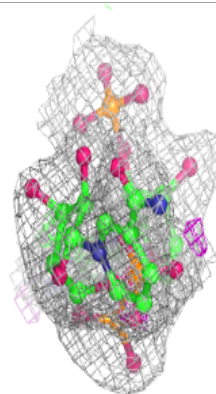
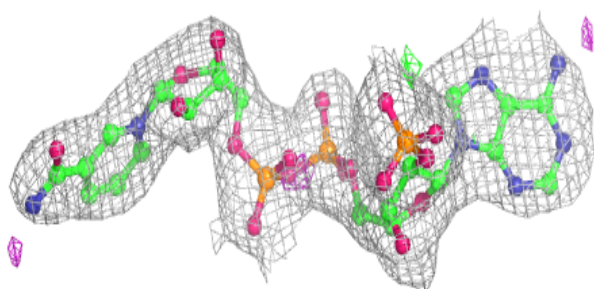
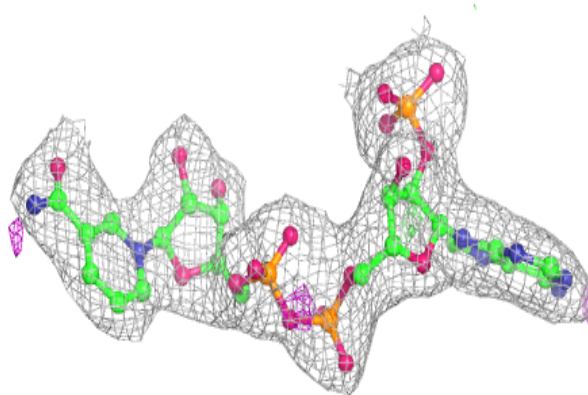
**Electron density around NAP W 601:**

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

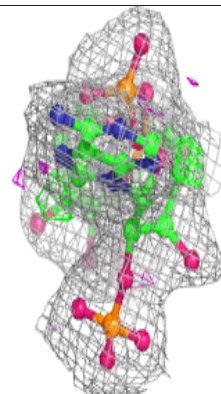
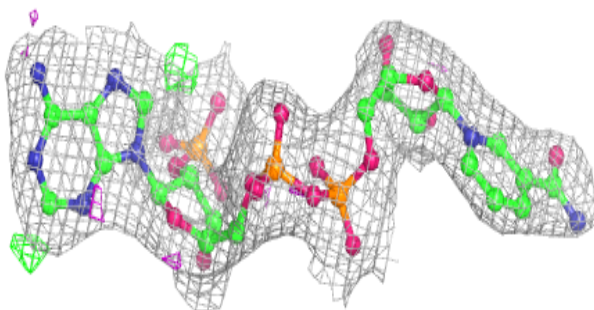
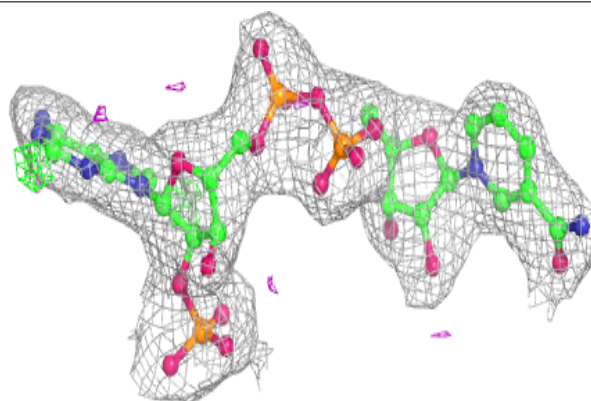


Electron density around NAP C 601:

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

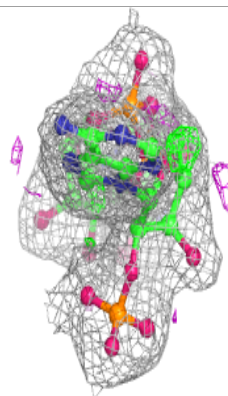
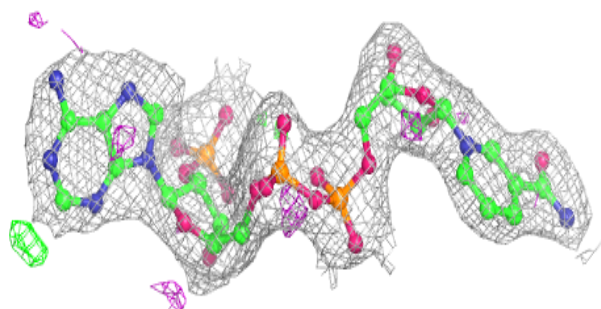
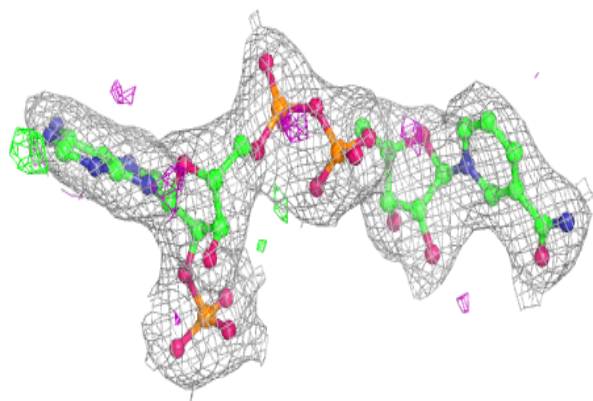
**Electron density around NAP T 601:**

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

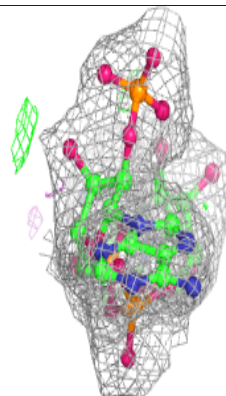
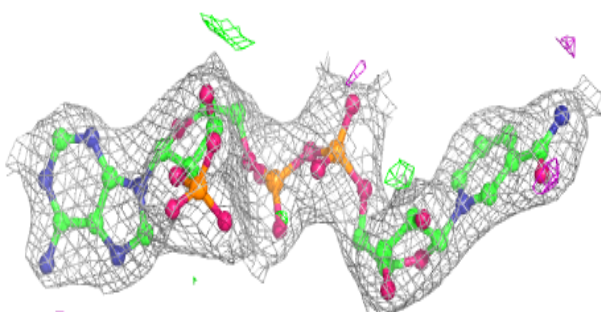
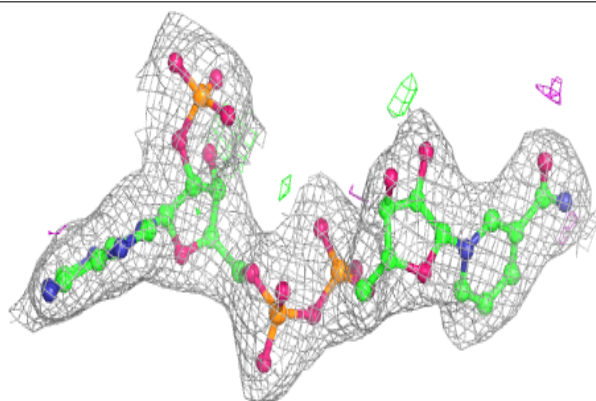


Electron density around NAP L 601:

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

**Electron density around NAP Q 601:**

$2mF_o-DF_c$ (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.