



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:25 PM UTC

PDB ID : 6EL3 / pdb_00006el3
Title : Structure of Progesterone 5beta-Reductase from Arabidopsis thaliana in complex with NADP
Authors : Muller, Y.A.; Schmidt, K.; Egerer-Sieber, C.
Deposited on : 2017-09-27
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

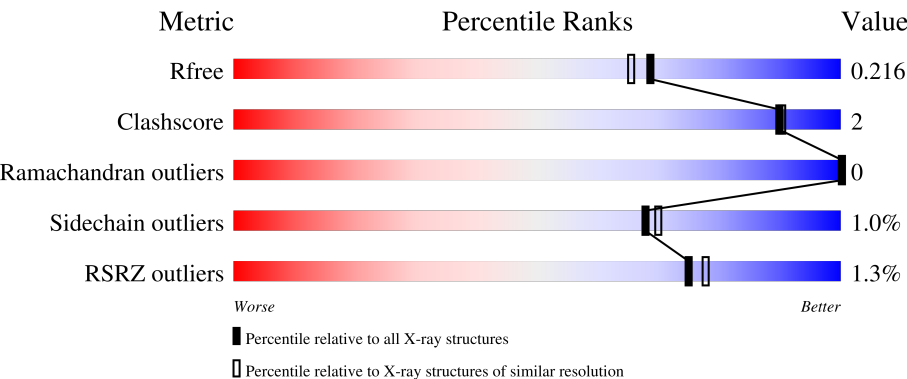
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	381	% 91% ...
2	B	381	% 92% ..
3	C	381	% 91% ..
4	D	381	2% 90% 6% .
5	E	381	% 91% ..

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Mol	Chain	Length	Quality of chain
6	F	381	% 89% 6% . .

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 20744 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 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	3	0
			2975	1925	484	550	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP Q9STX2
A	9	LYS	-	expression tag	UNP Q9STX2
A	10	HIS	-	expression tag	UNP Q9STX2
A	11	HIS	-	expression tag	UNP Q9STX2
A	12	HIS	-	expression tag	UNP Q9STX2
A	13	HIS	-	expression tag	UNP Q9STX2
A	14	HIS	-	expression tag	UNP Q9STX2
A	15	HIS	-	expression tag	UNP Q9STX2
A	16	GLN	-	expression tag	UNP Q9STX2

- Molecule 2 is a protein called 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	364	Total	C	N	O	S	0	1	0
			2965	1919	483	547	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	8	MET	-	initiating methionine	UNP Q9STX2
B	9	LYS	-	expression tag	UNP Q9STX2
B	10	HIS	-	expression tag	UNP Q9STX2
B	11	HIS	-	expression tag	UNP Q9STX2
B	12	HIS	-	expression tag	UNP Q9STX2
B	13	HIS	-	expression tag	UNP Q9STX2
B	14	HIS	-	expression tag	UNP Q9STX2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	HIS	-	expression tag	UNP Q9STX2
B	16	GLN	-	expression tag	UNP Q9STX2

- Molecule 3 is a protein called 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	364	Total	C	N	O	S	0	0	0
			2958	1914	483	545	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	MET	-	initiating methionine	UNP Q9STX2
C	9	LYS	-	expression tag	UNP Q9STX2
C	10	HIS	-	expression tag	UNP Q9STX2
C	11	HIS	-	expression tag	UNP Q9STX2
C	12	HIS	-	expression tag	UNP Q9STX2
C	13	HIS	-	expression tag	UNP Q9STX2
C	14	HIS	-	expression tag	UNP Q9STX2
C	15	HIS	-	expression tag	UNP Q9STX2
C	16	GLN	-	expression tag	UNP Q9STX2

- Molecule 4 is a protein called 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	364	Total	C	N	O	S	0	0	0
			2954	1910	483	545	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	8	MET	-	initiating methionine	UNP Q9STX2
D	9	LYS	-	expression tag	UNP Q9STX2
D	10	HIS	-	expression tag	UNP Q9STX2
D	11	HIS	-	expression tag	UNP Q9STX2
D	12	HIS	-	expression tag	UNP Q9STX2
D	13	HIS	-	expression tag	UNP Q9STX2
D	14	HIS	-	expression tag	UNP Q9STX2
D	15	HIS	-	expression tag	UNP Q9STX2
D	16	GLN	-	expression tag	UNP Q9STX2

- Molecule 5 is a protein called 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	364	Total	C	N	O	S	0	2	0
			2968	1920	483	549	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	8	MET	-	initiating methionine	UNP Q9STX2
E	9	LYS	-	expression tag	UNP Q9STX2
E	10	HIS	-	expression tag	UNP Q9STX2
E	11	HIS	-	expression tag	UNP Q9STX2
E	12	HIS	-	expression tag	UNP Q9STX2
E	13	HIS	-	expression tag	UNP Q9STX2
E	14	HIS	-	expression tag	UNP Q9STX2
E	15	HIS	-	expression tag	UNP Q9STX2
E	16	GLN	-	expression tag	UNP Q9STX2

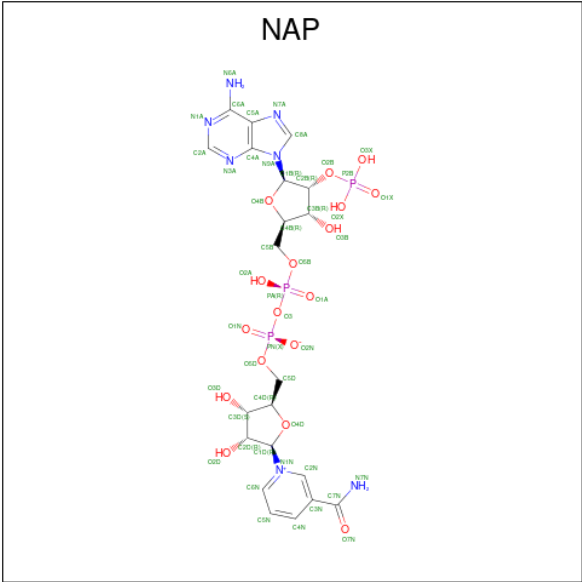
- Molecule 6 is a protein called 3-oxo-Delta(4,5)-steroid 5-beta-reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	364	Total	C	N	O	S	0	1	0
			2957	1911	483	547	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	8	MET	-	initiating methionine	UNP Q9STX2
F	9	LYS	-	expression tag	UNP Q9STX2
F	10	HIS	-	expression tag	UNP Q9STX2
F	11	HIS	-	expression tag	UNP Q9STX2
F	12	HIS	-	expression tag	UNP Q9STX2
F	13	HIS	-	expression tag	UNP Q9STX2
F	14	HIS	-	expression tag	UNP Q9STX2
F	15	HIS	-	expression tag	UNP Q9STX2
F	16	GLN	-	expression tag	UNP Q9STX2

- Molecule 7 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		
8	E	1	Total	Cl	0	0
			1	1		
8	F	1	Total	Cl	0	0
			1	1		

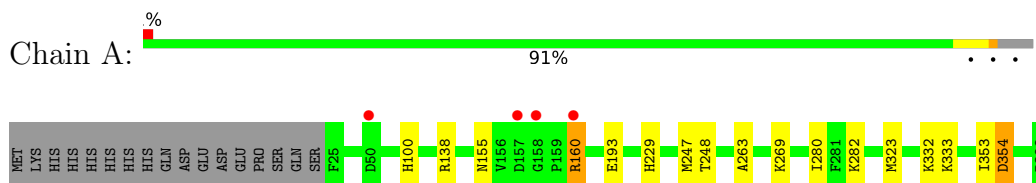
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	443	Total 443	O 443	0	0
9	B	450	Total 450	O 450	0	0
9	C	465	Total 465	O 465	0	0
9	D	440	Total 440	O 440	0	0
9	E	500	Total 500	O 500	0	0
9	F	375	Total 375	O 375	0	0

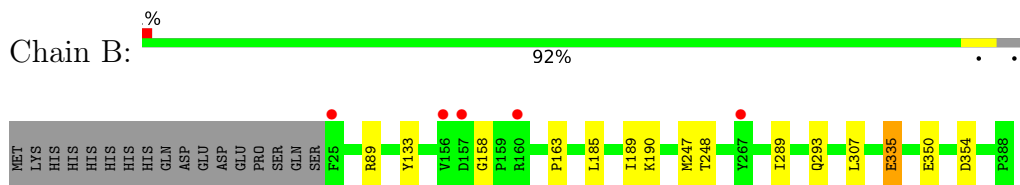
3 Residue-property plots [i](#)

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.

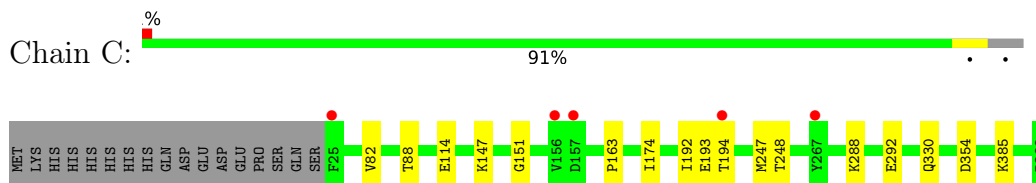
- Molecule 1: 3-oxo-Delta(4,5)-steroid 5-beta-reductase



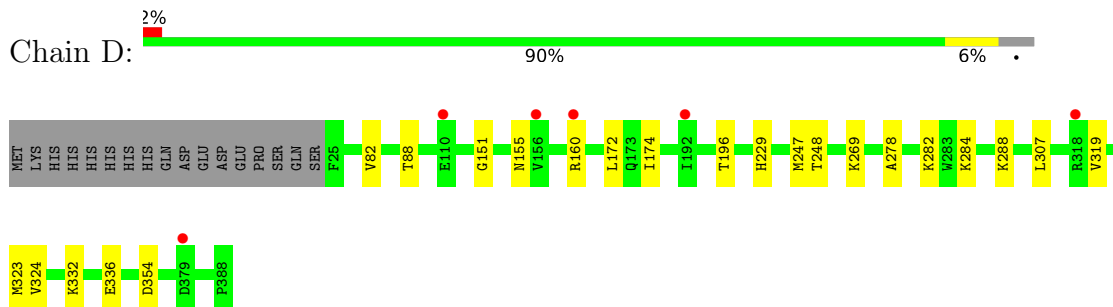
- Molecule 2: 3-oxo-Delta(4,5)-steroid 5-beta-reductase



- Molecule 3: 3-oxo-Delta(4,5)-steroid 5-beta-reductase



- Molecule 4: 3-oxo-Delta(4,5)-steroid 5-beta-reductase

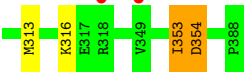
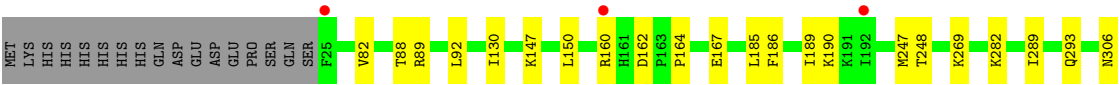
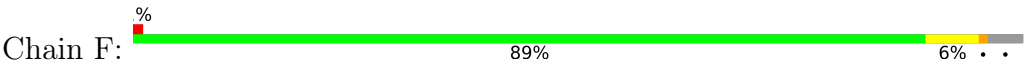


- Molecule 5: 3-oxo-Delta(4,5)-steroid 5-beta-reductase





● Molecule 6: 3-oxo-Delta(4,5)-steroid 5-beta-reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.46Å 94.86Å 313.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 1.90 46.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.90-1.90) 99.8 (46.90-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.168 , 0.213 0.173 , 0.216	Depositor DCC
R_{free} test set	2280 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20744	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.57% 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: MLY, CL, 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	A	0.47	1/2924 (0.0%)	0.71	0/3986
2	B	0.45	0/2897	0.69	2/3951 (0.1%)
3	C	0.50	0/2898	0.71	0/3951
4	D	0.48	0/2916	0.71	0/3973
5	E	0.49	1/2914 (0.0%)	0.69	0/3973
6	F	0.50	2/2933 (0.1%)	0.72	0/3995
All	All	0.48	4/17482 (0.0%)	0.71	2/23829 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	353	ILE	C-O	-6.23	1.17	1.24
5	E	354	ASP	C-O	-5.97	1.16	1.23
6	F	354	ASP	C-O	-5.96	1.16	1.23
1	A	354	ASP	C-O	-5.58	1.17	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	158	GLY	CA-C-N	5.48	125.45	120.03
2	B	158	GLY	C-N-CA	5.48	125.45	120.03

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	2975	0	2897	10	0
2	B	2965	0	2884	8	0
3	C	2958	0	2879	10	0
4	D	2954	0	2873	15	0
5	E	2968	0	2887	9	0
6	F	2957	0	2873	18	0
7	A	48	0	24	0	0
7	B	48	0	25	0	0
7	C	48	0	24	0	0
7	D	48	0	25	1	0
7	E	48	0	24	0	0
7	F	48	0	25	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	E	1	0	0	0	0
8	F	1	0	0	1	0
9	A	443	0	0	2	0
9	B	450	0	0	1	0
9	C	465	0	0	1	0
9	D	440	0	0	3	0
9	E	500	0	0	0	0
9	F	375	0	0	4	0
All	All	20744	0	17440	65	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 2.

All (65) 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:193:GLU:HG3	5:E:79:GLN:HE22	1.52	0.73
4:D:155:ASN:O	4:D:160:ARG:NH2	2.21	0.73
3:C:193:GLU:HG2	3:C:194:THR:HG23	1.72	0.72
4:D:151:GLY:HA3	4:D:174:ILE:HD11	1.74	0.69
1:A:155:ASN:O	1:A:160:ARG:NH2	2.27	0.68
2:B:247:MET:HE3	2:B:248:THR:H	1.58	0.68
5:E:163:PRO:HG2	6:F:282:MLY:HH22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:185:LEU:O	6:F:189:ILE:HG12	2.09	0.53
6:F:186:PHE:O	6:F:190:LYS:HG3	2.08	0.53
3:C:151:GLY:HA3	3:C:174:ILE:HD11	1.91	0.53
1:A:280:ILE:HD12	1:A:353:ILE:HD13	1.91	0.51
1:A:247:MET:HE3	1:A:248:THR:H	1.76	0.50
4:D:247:MET:HE3	4:D:248:THR:H	1.76	0.50
2:B:89:ARG:NH2	2:B:133:TYR:OH	2.45	0.49
6:F:160:ARG:NH2	9:F:518:HOH:O	2.46	0.49
6:F:92:LEU:HB3	6:F:130:ILE:HD11	1.95	0.49
6:F:150:LEU:HD22	6:F:160:ARG:HH21	1.77	0.49
1:A:229:HIS:CG	1:A:323:MET:HG2	2.49	0.48
3:C:247:MET:HE3	3:C:248:THR:H	1.79	0.48
6:F:247:MET:HE3	6:F:248:THR:H	1.78	0.47
3:C:163:PRO:HG2	4:D:282:MLY:HH22	1.96	0.47
2:B:335:GLU:H	2:B:335:GLU:CD	2.20	0.47
4:D:229:HIS:CG	4:D:323:MET:HG2	2.51	0.46
5:E:282:MLY:HH23	6:F:162:ASP:OD1	2.15	0.46
4:D:336:GLU:HB3	9:D:769:HOH:O	2.15	0.46
4:D:288:MLY:HH22	4:D:288:MLY:HD2	1.77	0.46
1:A:100:HIS:CD2	1:A:263:ALA:HB1	2.51	0.46
6:F:167:GLU:O	9:F:501:HOH:O	2.20	0.45
4:D:324:VAL:HG11	4:D:332:LYS:HG2	1.99	0.45
3:C:82:VAL:HA	3:C:88:THR:CG2	2.46	0.44
3:C:288:MLY:HE3	3:C:292:GLU:OE2	2.17	0.44
3:C:114:GLU:OE1	9:C:501:HOH:O	2.21	0.44
5:E:245:GLY:HA3	5:E:350:GLU:HG3	2.00	0.44
1:A:282:MLY:HH22	2:B:163:PRO:HG2	1.98	0.43
4:D:247:MET:HG3	9:D:677:HOH:O	2.17	0.43
6:F:313:MET:HE1	6:F:316:MLY:HH22	2.01	0.43
6:F:247:MET:HG3	9:F:621:HOH:O	2.18	0.43
5:E:247:MET:HE3	5:E:248:THR:H	1.84	0.43
5:E:288:MLY:HH13	5:E:288:MLY:HD3	1.63	0.43
6:F:147:MLY:HE3	8:F:402:CL:CL	2.56	0.43
1:A:138:ARG:NH1	9:A:502:HOH:O	2.24	0.43
4:D:82:VAL:HA	4:D:88:THR:CG2	2.49	0.42
6:F:89:ARG:NH1	9:F:513:HOH:O	2.42	0.42
6:F:150:LEU:HD22	6:F:160:ARG:NH2	2.34	0.42
2:B:289:ILE:O	2:B:293:GLN:HG2	2.18	0.42
4:D:196:THR:OG1	4:D:269:LYS:HD2	2.19	0.42
6:F:306:ASN:OD1	6:F:306:ASN:N	2.51	0.42
2:B:247:MET:HG3	9:B:706:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:330:GLN:HG2	3:C:385:LYS:HB2	2.02	0.42
5:E:164:PRO:HA	5:E:353:ILE:O	2.20	0.42
6:F:164:PRO:HA	6:F:353:ILE:O	2.19	0.42
3:C:147:MLY:HD2	3:C:147:MLY:HH22	1.87	0.42
4:D:319:VAL:O	4:D:323:MET:HG3	2.20	0.42
5:E:89:ARG:NH1	5:E:133:TYR:OH	2.53	0.42
4:D:82:VAL:HG22	7:D:401:NAP:N1A	2.34	0.42
4:D:278:ALA:HB2	9:D:527:HOH:O	2.20	0.41
3:C:147:MLY:HB3	3:C:147:MLY:HE3	1.81	0.41
2:B:185:LEU:O	2:B:189:ILE:HG12	2.21	0.41
4:D:284:MLY:HH13	4:D:284:MLY:HD2	1.72	0.41
6:F:82:VAL:HA	6:F:88:THR:CG2	2.51	0.41
6:F:289:ILE:O	6:F:293:GLN:HG2	2.21	0.41
1:A:332:LYS:HG2	9:A:797:HOH:O	2.20	0.41
2:B:335:GLU:OE1	2:B:335:GLU:N	2.52	0.40
1:A:269:MLY:HH22	1:A:269:MLY:HD3	1.70	0.40
5:E:284:MLY:HD3	5:E:284:MLY:HH22	1.67	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	321/381 (84%)	311 (97%)	10 (3%)	0	100	100
6	F	353/381 (93%)	343 (97%)	10 (3%)	0	100	100
All	All	674/762 (88%)	654 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/321 (96%)	304 (99%)	3 (1%)	68	70
2	B	304/320 (95%)	299 (98%)	5 (2%)	55	54
3	C	304/321 (95%)	302 (99%)	2 (1%)	76	78
4	D	306/323 (95%)	303 (99%)	3 (1%)	68	70
5	E	306/321 (95%)	303 (99%)	3 (1%)	68	70
6	F	308/324 (95%)	306 (99%)	2 (1%)	78	81
All	All	1835/1930 (95%)	1817 (99%)	18 (1%)	68	70

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	160	ARG
1	A	333	LYS
1	A	354	ASP
2	B	190	LYS
2	B	307	LEU
2	B	335	GLU
2	B	350	GLU
2	B	354	ASP
3	C	192	ILE
3	C	354	ASP
4	D	172	LEU
4	D	307	LEU
4	D	354	ASP
5	E	307	LEU
5	E	314	LYS
5	E	354	ASP
6	F	269	LYS
6	F	354	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	330	GLN
1	A	371	ASN
2	B	79	GLN
2	B	327	ASN
3	C	79	GLN
3	C	181	GLN
3	C	371	ASN
4	D	371	ASN
5	E	79	GLN
5	E	371	ASN
6	F	293	GLN
6	F	371	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	MLY	A	269	1	9,10,11	0.64	0	6,11,13	0.69	0
2	MLY	B	147	2	9,10,11	0.45	0	6,11,13	0.91	0
1	MLY	A	382	1	9,10,11	0.54	0	6,11,13	0.83	0
6	MLY	F	147	6	9,10,11	0.42	0	6,11,13	0.93	0
2	MLY	B	91	2	9,10,11	0.56	0	6,11,13	0.62	0
1	MLY	A	240	1	9,10,11	0.61	0	6,11,13	0.54	0
3	MLY	C	316	3	9,10,11	0.59	0	6,11,13	0.73	0
5	MLY	E	316	5	9,10,11	0.55	0	6,11,13	0.73	0
5	MLY	E	191	5	9,10,11	0.62	0	6,11,13	0.63	0
2	MLY	B	382	2	9,10,11	0.53	0	6,11,13	0.76	0
5	MLY	E	91	5	9,10,11	0.50	0	6,11,13	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MLY	B	284	2	9,10,11	0.59	0	6,11,13	0.80	0
5	MLY	E	228	5	9,10,11	0.50	0	6,11,13	0.82	0
1	MLY	A	316	1	9,10,11	0.52	0	6,11,13	0.71	0
5	MLY	E	288	5	9,10,11	0.52	0	6,11,13	0.91	0
1	MLY	A	241	1	9,10,11	0.53	0	6,11,13	0.97	0
6	MLY	F	282	6	9,10,11	0.60	0	6,11,13	0.83	0
6	MLY	F	288	6	9,10,11	0.57	0	6,11,13	0.76	0
4	MLY	D	382	4	9,10,11	0.55	0	6,11,13	0.79	0
2	MLY	B	240	2	9,10,11	0.53	0	6,11,13	0.93	0
3	MLY	C	382	3	9,10,11	0.58	0	6,11,13	0.92	0
4	MLY	D	240	4	9,10,11	0.52	0	6,11,13	0.64	0
6	MLY	F	382	6	9,10,11	0.52	0	6,11,13	0.85	0
2	MLY	B	57	2	9,10,11	0.70	0	6,11,13	0.86	0
3	MLY	C	282	3	9,10,11	0.42	0	6,11,13	0.82	0
4	MLY	D	288	4	9,10,11	0.53	0	6,11,13	0.72	0
5	MLY	E	57	5	9,10,11	0.59	0	6,11,13	0.68	0
3	MLY	C	228	3	9,10,11	0.47	0	6,11,13	0.90	0
4	MLY	D	147	4	9,10,11	0.39	0	6,11,13	0.88	0
2	MLY	B	325	2	9,10,11	0.45	0	6,11,13	0.62	0
5	MLY	E	284	5	9,10,11	0.68	0	6,11,13	1.03	0
3	MLY	C	147	3	9,10,11	0.42	0	6,11,13	0.93	0
2	MLY	B	191	2	9,10,11	0.59	0	6,11,13	0.76	0
2	MLY	B	332	2	9,10,11	0.53	0	6,11,13	0.94	0
2	MLY	B	288	2	9,10,11	0.44	0	6,11,13	0.82	0
3	MLY	C	332	3	9,10,11	0.60	0	6,11,13	0.72	0
4	MLY	D	282	4	9,10,11	0.50	0	6,11,13	0.93	0
5	MLY	E	282	5	9,10,11	0.54	0	6,11,13	0.61	0
2	MLY	B	385	2	9,10,11	0.55	0	6,11,13	0.80	0
1	MLY	A	191	1	9,10,11	0.55	0	6,11,13	0.66	0
3	MLY	C	57	3	9,10,11	0.53	0	6,11,13	0.98	0
3	MLY	C	314	3	9,10,11	0.67	0	6,11,13	0.67	0
6	MLY	F	57	6	9,10,11	0.59	0	6,11,13	0.82	0
1	MLY	A	282	1	9,10,11	0.51	0	6,11,13	0.78	0
5	MLY	E	147	5	9,10,11	0.39	0	6,11,13	0.91	0
6	MLY	F	240	6	9,10,11	0.48	0	6,11,13	0.73	0
2	MLY	B	316	2	9,10,11	0.48	0	6,11,13	0.61	0
1	MLY	A	288	1	9,10,11	0.49	0	6,11,13	0.84	0
5	MLY	E	382	5	9,10,11	0.58	0	6,11,13	0.74	0
1	MLY	A	228	1	9,10,11	0.48	0	6,11,13	0.82	0
1	MLY	A	147	1	9,10,11	0.33	0	6,11,13	0.94	0
2	MLY	B	228	2	9,10,11	0.48	0	6,11,13	0.88	0
6	MLY	F	316	6	9,10,11	0.50	0	6,11,13	0.81	0
3	MLY	C	325	3	9,10,11	0.49	0	6,11,13	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	91	1	9,10,11	0.46	0	6,11,13	0.72	0
5	MLY	E	332	5	9,10,11	0.49	0	6,11,13	0.97	0
4	MLY	D	57	4	9,10,11	0.71	0	6,11,13	0.73	0
5	MLY	E	240	5	9,10,11	0.54	0	6,11,13	0.62	0
4	MLY	D	316	4	9,10,11	0.55	0	6,11,13	0.71	0
3	MLY	C	91	3	9,10,11	0.49	0	6,11,13	0.66	0
1	MLY	A	284	1	9,10,11	0.63	0	6,11,13	0.78	0
3	MLY	C	240	3	9,10,11	0.52	0	6,11,13	0.69	0
4	MLY	D	191	4	9,10,11	0.56	0	6,11,13	0.75	0
6	MLY	F	91	6	9,10,11	0.54	0	6,11,13	0.59	0
1	MLY	A	57	1	9,10,11	0.57	0	6,11,13	0.74	0
4	MLY	D	228	4	9,10,11	0.43	0	6,11,13	0.90	0
6	MLY	F	284	6	9,10,11	0.60	0	6,11,13	0.79	0
6	MLY	F	228	6	9,10,11	0.48	0	6,11,13	0.95	0
3	MLY	C	288	3	9,10,11	0.48	0	6,11,13	0.89	0
4	MLY	D	91	4	9,10,11	0.58	0	6,11,13	0.59	0
5	MLY	E	325	5	9,10,11	0.51	0	6,11,13	0.67	0
4	MLY	D	284	4	9,10,11	0.63	0	6,11,13	0.98	0
2	MLY	B	282	2	9,10,11	0.46	0	6,11,13	0.91	0
3	MLY	C	241	3	9,10,11	0.63	0	6,11,13	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	269	1	-	3/8/9/11	-
2	MLY	B	147	2	-	1/8/9/11	-
1	MLY	A	382	1	-	0/8/9/11	-
6	MLY	F	147	6	-	1/8/9/11	-
2	MLY	B	91	2	-	0/8/9/11	-
1	MLY	A	240	1	-	0/8/9/11	-
3	MLY	C	316	3	-	1/8/9/11	-
5	MLY	E	316	5	-	2/8/9/11	-
5	MLY	E	191	5	-	0/8/9/11	-
2	MLY	B	382	2	-	0/8/9/11	-
5	MLY	E	91	5	-	2/8/9/11	-
2	MLY	B	284	2	-	1/8/9/11	-
5	MLY	E	228	5	-	0/8/9/11	-
1	MLY	A	316	1	-	1/8/9/11	-
5	MLY	E	288	5	-	2/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	241	1	-	0/8/9/11	-
6	MLY	F	282	6	-	0/8/9/11	-
6	MLY	F	288	6	-	2/8/9/11	-
4	MLY	D	382	4	-	0/8/9/11	-
2	MLY	B	240	2	-	0/8/9/11	-
3	MLY	C	382	3	-	0/8/9/11	-
4	MLY	D	240	4	-	1/8/9/11	-
6	MLY	F	382	6	-	0/8/9/11	-
2	MLY	B	57	2	-	0/8/9/11	-
3	MLY	C	282	3	-	0/8/9/11	-
4	MLY	D	288	4	-	1/8/9/11	-
5	MLY	E	57	5	-	0/8/9/11	-
3	MLY	C	228	3	-	0/8/9/11	-
4	MLY	D	147	4	-	2/8/9/11	-
2	MLY	B	325	2	-	0/8/9/11	-
5	MLY	E	284	5	-	3/8/9/11	-
3	MLY	C	147	3	-	3/8/9/11	-
2	MLY	B	191	2	-	0/8/9/11	-
2	MLY	B	332	2	-	1/8/9/11	-
2	MLY	B	288	2	-	1/8/9/11	-
3	MLY	C	332	3	-	0/8/9/11	-
4	MLY	D	282	4	-	0/8/9/11	-
5	MLY	E	282	5	-	2/8/9/11	-
2	MLY	B	385	2	-	0/8/9/11	-
1	MLY	A	191	1	-	0/8/9/11	-
3	MLY	C	57	3	-	0/8/9/11	-
3	MLY	C	314	3	-	3/8/9/11	-
6	MLY	F	57	6	-	0/8/9/11	-
1	MLY	A	282	1	-	1/8/9/11	-
5	MLY	E	147	5	-	0/8/9/11	-
6	MLY	F	240	6	-	0/8/9/11	-
2	MLY	B	316	2	-	1/8/9/11	-
1	MLY	A	288	1	-	1/8/9/11	-
5	MLY	E	382	5	-	0/8/9/11	-
1	MLY	A	228	1	-	2/8/9/11	-
1	MLY	A	147	1	-	1/8/9/11	-
2	MLY	B	228	2	-	0/8/9/11	-
6	MLY	F	316	6	-	4/8/9/11	-
3	MLY	C	325	3	-	0/8/9/11	-
1	MLY	A	91	1	-	0/8/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MLY	E	332	5	-	0/8/9/11	-
4	MLY	D	57	4	-	0/8/9/11	-
5	MLY	E	240	5	-	0/8/9/11	-
4	MLY	D	316	4	-	1/8/9/11	-
3	MLY	C	91	3	-	2/8/9/11	-
1	MLY	A	284	1	-	0/8/9/11	-
3	MLY	C	240	3	-	0/8/9/11	-
4	MLY	D	191	4	-	0/8/9/11	-
6	MLY	F	91	6	-	2/8/9/11	-
1	MLY	A	57	1	-	0/8/9/11	-
4	MLY	D	228	4	-	0/8/9/11	-
6	MLY	F	284	6	-	0/8/9/11	-
6	MLY	F	228	6	-	1/8/9/11	-
3	MLY	C	288	3	-	1/8/9/11	-
4	MLY	D	91	4	-	2/8/9/11	-
5	MLY	E	325	5	-	0/8/9/11	-
4	MLY	D	284	4	-	1/8/9/11	-
2	MLY	B	282	2	-	0/8/9/11	-
3	MLY	C	241	3	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	282	MLY	O-C-CA-CB
1	A	316	MLY	O-C-CA-CB
2	B	284	MLY	O-C-CA-CB
2	B	316	MLY	O-C-CA-CB
3	C	91	MLY	C-CA-CB-CG
3	C	314	MLY	N-CA-CB-CG
3	C	314	MLY	C-CA-CB-CG
3	C	316	MLY	O-C-CA-CB
4	D	91	MLY	C-CA-CB-CG
4	D	316	MLY	O-C-CA-CB
5	E	284	MLY	C-CA-CB-CG
5	E	316	MLY	O-C-CA-CB
6	F	316	MLY	O-C-CA-CB
1	A	269	MLY	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
3	C	147	MLY	CG-CD-CE-NZ
6	F	228	MLY	CG-CD-CE-NZ
6	F	316	MLY	CD-CE-NZ-CH1
6	F	316	MLY	CD-CE-NZ-CH2
1	A	228	MLY	CD-CE-NZ-CH1
1	A	269	MLY	CD-CE-NZ-CH2
3	C	241	MLY	CD-CE-NZ-CH2
4	D	284	MLY	CD-CE-NZ-CH1
6	F	288	MLY	CD-CE-NZ-CH2
3	C	241	MLY	CG-CD-CE-NZ
3	C	147	MLY	CE-CD-CG-CB
2	B	332	MLY	CD-CE-NZ-CH2
1	A	269	MLY	CD-CE-NZ-CH1
3	C	241	MLY	CD-CE-NZ-CH1
5	E	282	MLY	CG-CD-CE-NZ
6	F	288	MLY	CG-CD-CE-NZ
5	E	282	MLY	CD-CE-NZ-CH2
3	C	288	MLY	CG-CD-CE-NZ
3	C	91	MLY	CA-CB-CG-CD
5	E	288	MLY	CE-CD-CG-CB
6	F	316	MLY	CA-CB-CG-CD
4	D	91	MLY	CA-CB-CG-CD
5	E	288	MLY	CG-CD-CE-NZ
2	B	288	MLY	CG-CD-CE-NZ
5	E	91	MLY	CA-CB-CG-CD
1	A	288	MLY	CG-CD-CE-NZ
6	F	91	MLY	CA-CB-CG-CD
4	D	147	MLY	C-CA-CB-CG
5	E	91	MLY	C-CA-CB-CG
6	F	91	MLY	C-CA-CB-CG
5	E	284	MLY	CD-CE-NZ-CH2
5	E	284	MLY	N-CA-CB-CG
4	D	288	MLY	CG-CD-CE-NZ
4	D	240	MLY	CG-CD-CE-NZ
4	D	147	MLY	CE-CD-CG-CB
3	C	314	MLY	CE-CD-CG-CB
1	A	147	MLY	C-CA-CB-CG
1	A	228	MLY	C-CA-CB-CG
2	B	147	MLY	C-CA-CB-CG
3	C	147	MLY	C-CA-CB-CG
6	F	147	MLY	C-CA-CB-CG
5	E	316	MLY	CA-CB-CG-CD

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	269	MLY	1	0
6	F	147	MLY	1	0
5	E	288	MLY	1	0
6	F	282	MLY	1	0
4	D	288	MLY	1	0
5	E	284	MLY	1	0
3	C	147	MLY	2	0
4	D	282	MLY	1	0
5	E	282	MLY	1	0
1	A	282	MLY	1	0
6	F	316	MLY	1	0
3	C	288	MLY	1	0
4	D	284	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAP	C	401	-	50,52,52	3.28	13 (26%)	71,80,80	1.83	15 (21%)
7	NAP	E	401	-	50,52,52	3.35	15 (30%)	71,80,80	1.84	17 (23%)
7	NAP	F	401	-	50,52,52	3.42	15 (30%)	71,80,80	1.81	15 (21%)
7	NAP	B	401	-	50,52,52	3.36	15 (30%)	71,80,80	1.86	15 (21%)
7	NAP	A	401	-	50,52,52	3.39	13 (26%)	71,80,80	1.83	17 (23%)
7	NAP	D	401	-	50,52,52	3.26	14 (28%)	71,80,80	1.81	17 (23%)

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
7	NAP	C	401	-	-	6/35/67/67	0/5/5/5
7	NAP	E	401	-	-	10/35/67/67	0/5/5/5
7	NAP	F	401	-	-	10/35/67/67	0/5/5/5
7	NAP	B	401	-	-	9/35/67/67	0/5/5/5
7	NAP	A	401	-	-	8/35/67/67	0/5/5/5
7	NAP	D	401	-	-	7/35/67/67	0/5/5/5

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	401	NAP	O4D-C1D	15.29	1.61	1.40
7	E	401	NAP	O4D-C1D	14.91	1.60	1.40
7	A	401	NAP	O4D-C1D	14.68	1.60	1.40
7	B	401	NAP	O4D-C1D	14.62	1.60	1.40
7	C	401	NAP	O4D-C1D	14.44	1.59	1.40
7	D	401	NAP	O4D-C1D	14.27	1.59	1.40
7	A	401	NAP	C2B-C1B	-8.69	1.31	1.53
7	F	401	NAP	C2B-C1B	-8.39	1.32	1.53
7	B	401	NAP	C2B-C1B	-8.32	1.32	1.53
7	C	401	NAP	C2B-C1B	-8.18	1.33	1.53
7	C	401	NAP	O4B-C1B	8.05	1.60	1.42
7	E	401	NAP	O4B-C1B	8.04	1.60	1.42
7	D	401	NAP	C2B-C1B	-7.99	1.33	1.53
7	E	401	NAP	C2B-C1B	-7.96	1.33	1.53
7	B	401	NAP	O4B-C1B	7.95	1.60	1.42
7	A	401	NAP	O4B-C1B	7.93	1.60	1.42
7	D	401	NAP	O4B-C1B	7.91	1.60	1.42
7	F	401	NAP	O4B-C1B	7.91	1.60	1.42
7	B	401	NAP	O4B-C4B	-6.52	1.30	1.45
7	A	401	NAP	O4D-C4D	-6.45	1.30	1.45
7	F	401	NAP	C7N-N7N	6.37	1.44	1.33
7	A	401	NAP	O4B-C4B	-6.31	1.31	1.45
7	F	401	NAP	O4B-C4B	-6.20	1.31	1.45
7	C	401	NAP	O4B-C4B	-6.13	1.31	1.45
7	E	401	NAP	O4B-C4B	-6.12	1.31	1.45
7	D	401	NAP	C7N-N7N	6.09	1.44	1.33
7	B	401	NAP	C7N-N7N	6.02	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	401	NAP	O4B-C4B	-6.02	1.31	1.45
7	B	401	NAP	O4D-C4D	-6.02	1.31	1.45
7	E	401	NAP	O4D-C4D	-6.01	1.31	1.45
7	F	401	NAP	O4D-C4D	-5.94	1.31	1.45
7	D	401	NAP	O4D-C4D	-5.92	1.31	1.45
7	A	401	NAP	C7N-N7N	5.91	1.43	1.33
7	C	401	NAP	O4D-C4D	-5.74	1.32	1.45
7	E	401	NAP	C7N-N7N	5.53	1.43	1.33
7	C	401	NAP	C7N-N7N	5.41	1.42	1.33
7	E	401	NAP	C6A-N6A	4.10	1.44	1.34
7	A	401	NAP	C6A-N6A	4.02	1.44	1.34
7	C	401	NAP	C6A-N6A	3.98	1.44	1.34
7	B	401	NAP	C6A-N6A	3.92	1.44	1.34
7	D	401	NAP	C6A-N6A	3.85	1.44	1.34
7	F	401	NAP	C6A-N6A	3.82	1.44	1.34
7	B	401	NAP	C3N-C7N	3.60	1.56	1.50
7	A	401	NAP	C3N-C7N	3.27	1.55	1.50
7	E	401	NAP	O2D-C2D	3.19	1.50	1.43
7	C	401	NAP	O2D-C2D	3.17	1.50	1.43
7	F	401	NAP	C3N-C7N	3.14	1.55	1.50
7	D	401	NAP	O2D-C2D	3.08	1.50	1.43
7	B	401	NAP	O2D-C2D	3.07	1.50	1.43
7	A	401	NAP	O2D-C2D	3.02	1.50	1.43
7	F	401	NAP	O2D-C2D	2.99	1.50	1.43
7	C	401	NAP	C3N-C7N	2.95	1.55	1.50
7	D	401	NAP	C3N-C7N	2.78	1.54	1.50
7	E	401	NAP	C3N-C7N	2.75	1.54	1.50
7	E	401	NAP	C2A-N1A	2.71	1.38	1.33
7	A	401	NAP	O3B-C3B	-2.59	1.36	1.43
7	C	401	NAP	O3B-C3B	-2.58	1.36	1.43
7	B	401	NAP	C2N-N1N	2.55	1.37	1.35
7	E	401	NAP	O3B-C3B	-2.52	1.36	1.43
7	C	401	NAP	C2A-N1A	2.52	1.38	1.33
7	D	401	NAP	O3B-C3B	-2.36	1.37	1.43
7	F	401	NAP	O3D-C3D	-2.35	1.37	1.43
7	A	401	NAP	C2A-N3A	2.35	1.38	1.33
7	C	401	NAP	C2A-N3A	2.32	1.38	1.33
7	E	401	NAP	O3D-C3D	-2.31	1.37	1.43
7	B	401	NAP	C2A-N1A	2.30	1.38	1.33
7	F	401	NAP	O3B-C3B	-2.25	1.37	1.43
7	D	401	NAP	C2A-N1A	2.24	1.37	1.33
7	F	401	NAP	C8A-N7A	2.24	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	NAP	O3B-C3B	-2.24	1.37	1.43
7	E	401	NAP	C2A-N3A	2.22	1.37	1.33
7	C	401	NAP	C8A-N7A	2.21	1.35	1.31
7	E	401	NAP	C8A-N7A	2.21	1.35	1.31
7	F	401	NAP	C1B-N9A	-2.20	1.40	1.46
7	A	401	NAP	C2A-N1A	2.20	1.37	1.33
7	F	401	NAP	PN-O3	-2.19	1.57	1.59
7	B	401	NAP	C1B-N9A	-2.13	1.40	1.46
7	A	401	NAP	C2N-N1N	2.11	1.37	1.35
7	F	401	NAP	C2A-N1A	2.10	1.37	1.33
7	B	401	NAP	C5D-C4D	2.09	1.57	1.51
7	E	401	NAP	PN-O3	-2.09	1.57	1.59
7	D	401	NAP	C1B-N9A	-2.06	1.40	1.46
7	D	401	NAP	C2N-N1N	2.06	1.37	1.35
7	B	401	NAP	C8A-N7A	2.06	1.35	1.31
7	D	401	NAP	C8A-N7A	2.04	1.35	1.31

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	401	NAP	N3A-C2A-N1A	-5.87	119.69	128.58
7	E	401	NAP	C5A-C4A-N3A	-5.84	118.67	126.72
7	C	401	NAP	N3A-C2A-N1A	-5.75	119.88	128.58
7	C	401	NAP	C5A-C4A-N3A	-5.68	118.90	126.72
7	F	401	NAP	N3A-C2A-N1A	-5.65	120.03	128.58
7	B	401	NAP	N3A-C2A-N1A	-5.57	120.15	128.58
7	A	401	NAP	C5A-C4A-N3A	-5.48	119.18	126.72
7	B	401	NAP	C5A-C4A-N3A	-5.46	119.19	126.72
7	E	401	NAP	N3A-C2A-N1A	-5.37	120.45	128.58
7	F	401	NAP	C5A-C4A-N3A	-5.35	119.34	126.72
7	A	401	NAP	N3A-C2A-N1A	-5.29	120.57	128.58
7	D	401	NAP	C5A-C4A-N3A	-5.23	119.51	126.72
7	E	401	NAP	N6A-C6A-N1A	-4.83	107.62	118.38
7	B	401	NAP	N6A-C6A-N1A	-4.78	107.73	118.38
7	C	401	NAP	C4D-O4D-C1D	-4.59	105.72	109.92
7	F	401	NAP	N6A-C6A-N1A	-4.57	108.19	118.38
7	A	401	NAP	N6A-C6A-N1A	-4.54	108.26	118.38
7	A	401	NAP	N9A-C8A-N7A	-4.53	107.52	113.94
7	B	401	NAP	N9A-C8A-N7A	-4.52	107.53	113.94
7	D	401	NAP	N6A-C6A-N1A	-4.32	108.75	118.38
7	D	401	NAP	C4D-O4D-C1D	-4.27	106.02	109.92
7	B	401	NAP	C4D-O4D-C1D	-4.05	106.21	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	401	NAP	N9A-C8A-N7A	-4.05	108.19	113.94
7	C	401	NAP	N6A-C6A-N1A	-3.94	109.60	118.38
7	D	401	NAP	N9A-C8A-N7A	-3.86	108.46	113.94
7	F	401	NAP	C4D-O4D-C1D	-3.77	106.47	109.92
7	A	401	NAP	C4D-O4D-C1D	-3.73	106.51	109.92
7	C	401	NAP	N9A-C8A-N7A	-3.70	108.68	113.94
7	E	401	NAP	N9A-C8A-N7A	-3.68	108.71	113.94
7	C	401	NAP	N3A-C4A-N9A	3.66	133.40	127.17
7	B	401	NAP	C2A-N3A-C4A	3.65	120.75	111.83
7	A	401	NAP	N3A-C4A-N9A	3.65	133.37	127.17
7	E	401	NAP	C4D-O4D-C1D	-3.64	106.59	109.92
7	C	401	NAP	C2A-N3A-C4A	3.61	120.64	111.83
7	E	401	NAP	C5A-C6A-N6A	3.59	132.18	123.29
7	D	401	NAP	N3A-C4A-N9A	3.56	133.23	127.17
7	E	401	NAP	N3A-C4A-N9A	3.55	133.21	127.17
7	E	401	NAP	C2A-N3A-C4A	3.55	120.50	111.83
7	C	401	NAP	C6N-N1N-C2N	-3.52	118.89	121.88
7	D	401	NAP	C2A-N3A-C4A	3.51	120.41	111.83
7	F	401	NAP	C2A-N3A-C4A	3.49	120.36	111.83
7	F	401	NAP	N3A-C4A-N9A	3.48	133.09	127.17
7	B	401	NAP	C5A-C6A-N6A	3.45	131.83	123.29
7	B	401	NAP	N3A-C4A-N9A	3.43	133.00	127.17
7	A	401	NAP	C2A-N3A-C4A	3.40	120.12	111.83
7	A	401	NAP	C5A-C6A-N6A	3.34	131.55	123.29
7	A	401	NAP	C5A-N7A-C8A	3.31	108.66	103.45
7	F	401	NAP	C5A-C6A-N6A	3.30	131.47	123.29
7	B	401	NAP	C5A-N7A-C8A	3.26	108.58	103.45
7	E	401	NAP	C6N-N1N-C2N	-3.10	119.24	121.88
7	D	401	NAP	C5A-C6A-N6A	3.05	130.83	123.29
7	E	401	NAP	C5A-N7A-C8A	3.04	108.22	103.45
7	A	401	NAP	C4A-N9A-C1B	-2.99	119.63	126.63
7	F	401	NAP	C4A-N9A-C1B	-2.95	119.74	126.63
7	D	401	NAP	C4A-N9A-C1B	-2.83	120.02	126.63
7	C	401	NAP	C4A-N9A-C1B	-2.80	120.08	126.63
7	B	401	NAP	C4A-N9A-C1B	-2.79	120.10	126.63
7	F	401	NAP	C5A-N7A-C8A	2.77	107.80	103.45
7	A	401	NAP	C6N-N1N-C2N	-2.76	119.53	121.88
7	F	401	NAP	C6N-N1N-C2N	-2.74	119.55	121.88
7	E	401	NAP	C6A-C5A-C4A	2.69	120.85	117.18
7	C	401	NAP	C5A-C6A-N6A	2.68	129.92	123.29
7	B	401	NAP	C6N-N1N-C2N	-2.66	119.61	121.88
7	C	401	NAP	C5A-N7A-C8A	2.63	107.59	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	401	NAP	C6A-C5A-C4A	2.60	120.73	117.18
7	A	401	NAP	C6A-C5A-C4A	2.53	120.63	117.18
7	A	401	NAP	C4A-N9A-C8A	2.50	108.36	105.74
7	D	401	NAP	C6N-N1N-C2N	-2.50	119.75	121.88
7	D	401	NAP	C5A-N7A-C8A	2.44	107.29	103.45
7	C	401	NAP	C1B-N9A-C8A	2.44	132.51	127.09
7	E	401	NAP	C4A-C5A-N7A	-2.43	107.80	110.58
7	A	401	NAP	O2N-PN-O3	2.43	113.83	107.27
7	E	401	NAP	C4A-N9A-C1B	-2.37	121.08	126.63
7	B	401	NAP	C4A-C5A-N7A	-2.36	107.88	110.58
7	B	401	NAP	C4A-N9A-C8A	2.36	108.21	105.74
7	C	401	NAP	C2N-C3N-C4N	2.35	120.99	118.26
7	F	401	NAP	C1B-N9A-C8A	2.32	132.25	127.09
7	D	401	NAP	C4A-N9A-C8A	2.29	108.14	105.74
7	B	401	NAP	C6A-C5A-C4A	2.28	120.29	117.18
7	F	401	NAP	C6A-C5A-C4A	2.25	120.25	117.18
7	A	401	NAP	C4A-C5A-N7A	-2.25	108.01	110.58
7	D	401	NAP	C2N-C3N-C4N	2.23	120.85	118.26
7	E	401	NAP	C2N-C3N-C4N	2.22	120.84	118.26
7	A	401	NAP	C1B-N9A-C8A	2.21	132.00	127.09
7	A	401	NAP	C2N-C3N-C4N	2.17	120.78	118.26
7	F	401	NAP	C4A-N9A-C8A	2.16	108.01	105.74
7	E	401	NAP	O4B-C1B-C2B	-2.15	102.88	106.59
7	D	401	NAP	C1B-N9A-C8A	2.13	131.83	127.09
7	E	401	NAP	C1B-N9A-C8A	2.11	131.78	127.09
7	E	401	NAP	C5A-C4A-N9A	2.11	108.11	105.81
7	D	401	NAP	C6A-C5A-C4A	2.10	120.05	117.18
7	D	401	NAP	O4B-C1B-N9A	-2.07	104.12	108.09
7	D	401	NAP	C3N-C7N-N7N	2.06	120.28	117.74
7	B	401	NAP	C1B-N9A-C8A	2.06	131.67	127.09
7	C	401	NAP	C5B-C4B-C3B	-2.05	107.84	115.21
7	F	401	NAP	O4B-C1B-C2B	-2.02	103.11	106.59

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	401	NAP	C5D-O5D-PN-O3
7	A	401	NAP	C5D-O5D-PN-O2N
7	A	401	NAP	O4D-C1D-N1N-C2N
7	B	401	NAP	C5D-O5D-PN-O3
7	B	401	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
7	B	401	NAP	C5D-O5D-PN-O2N
7	B	401	NAP	O4D-C1D-N1N-C2N
7	C	401	NAP	C5D-O5D-PN-O3
7	C	401	NAP	C5D-O5D-PN-O1N
7	C	401	NAP	C5D-O5D-PN-O2N
7	C	401	NAP	O4D-C1D-N1N-C2N
7	D	401	NAP	C5D-O5D-PN-O3
7	D	401	NAP	C5D-O5D-PN-O2N
7	D	401	NAP	O4D-C1D-N1N-C2N
7	E	401	NAP	C5D-O5D-PN-O3
7	E	401	NAP	C5D-O5D-PN-O1N
7	E	401	NAP	C5D-O5D-PN-O2N
7	E	401	NAP	O4D-C1D-N1N-C2N
7	F	401	NAP	C5D-O5D-PN-O3
7	F	401	NAP	C5D-O5D-PN-O2N
7	F	401	NAP	O4D-C1D-N1N-C2N
7	F	401	NAP	O4D-C1D-N1N-C6N
7	E	401	NAP	C1B-C2B-O2B-P2B
7	D	401	NAP	C1B-C2B-O2B-P2B
7	E	401	NAP	C3B-C2B-O2B-P2B
7	D	401	NAP	C3B-C2B-O2B-P2B
7	A	401	NAP	C5D-O5D-PN-O1N
7	D	401	NAP	C5D-O5D-PN-O1N
7	F	401	NAP	C5D-O5D-PN-O1N
7	A	401	NAP	C2D-C1D-N1N-C6N
7	B	401	NAP	C2D-C1D-N1N-C6N
7	E	401	NAP	C2D-C1D-N1N-C6N
7	F	401	NAP	C2D-C1D-N1N-C6N
7	B	401	NAP	C1B-C2B-O2B-P2B
7	F	401	NAP	C1B-C2B-O2B-P2B
7	B	401	NAP	C3B-C2B-O2B-P2B
7	F	401	NAP	C3B-C2B-O2B-P2B
7	A	401	NAP	O4D-C1D-N1N-C6N
7	B	401	NAP	O4D-C1D-N1N-C6N
7	C	401	NAP	O4D-C1D-N1N-C6N
7	D	401	NAP	O4D-C1D-N1N-C6N
7	E	401	NAP	O4D-C1D-N1N-C6N
7	F	401	NAP	O4B-C4B-C5B-O5B
7	A	401	NAP	C1B-C2B-O2B-P2B
7	C	401	NAP	C1B-C2B-O2B-P2B
7	E	401	NAP	PN-O3-PA-O2A
7	A	401	NAP	C3B-C2B-O2B-P2B

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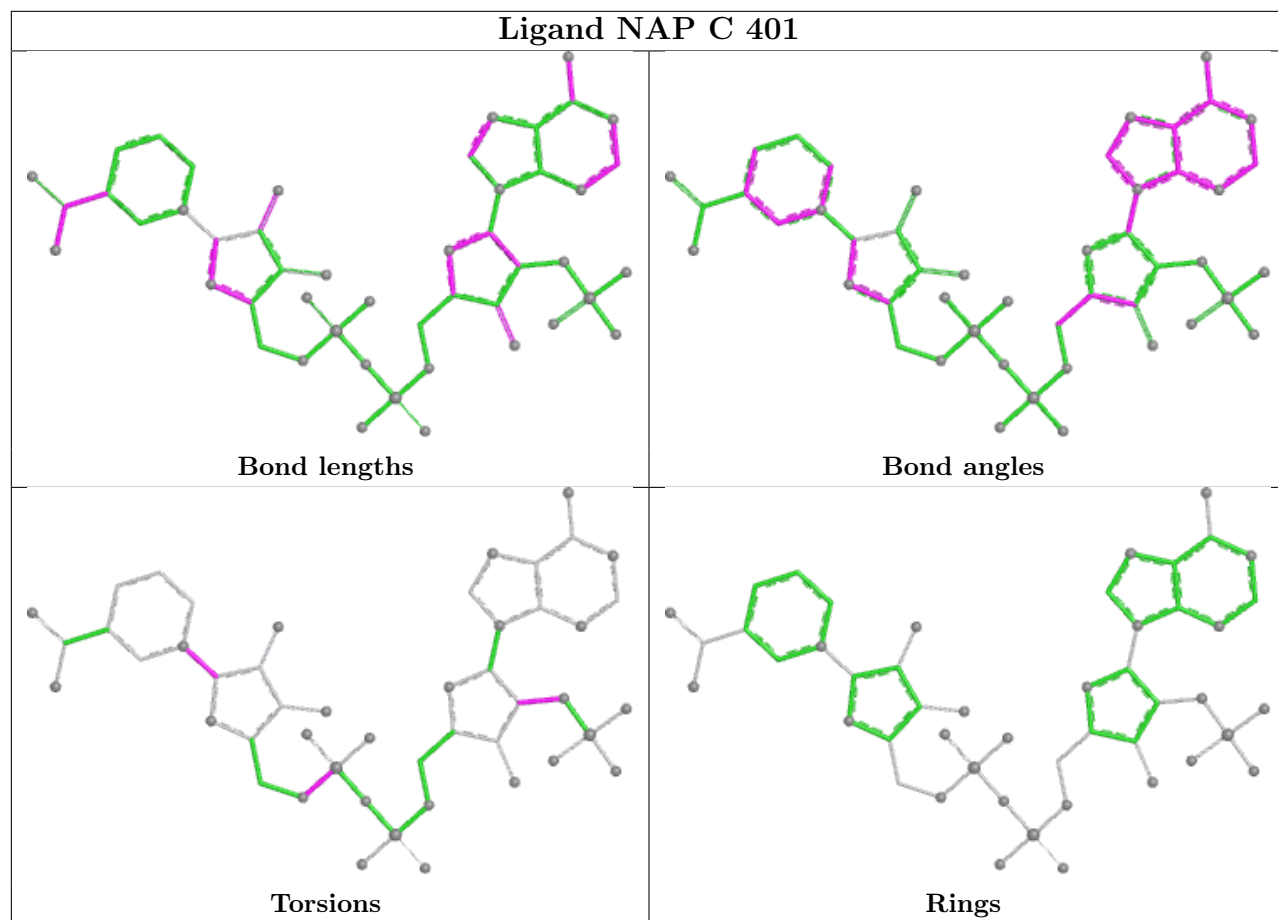
Mol	Chain	Res	Type	Atoms
7	B	401	NAP	PN-O3-PA-O2A
7	E	401	NAP	O4B-C4B-C5B-O5B
7	F	401	NAP	C3B-C4B-C5B-O5B

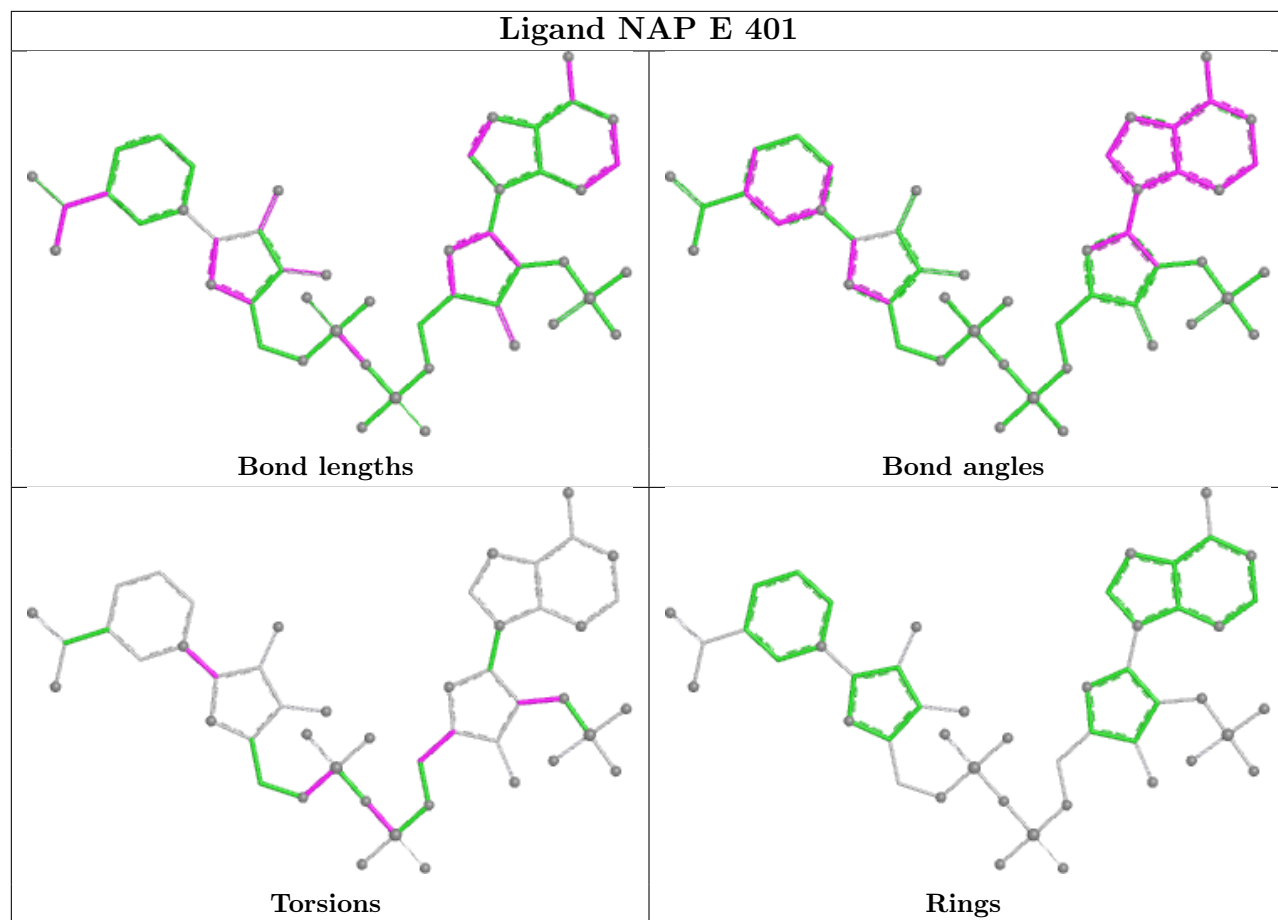
There are no ring outliers.

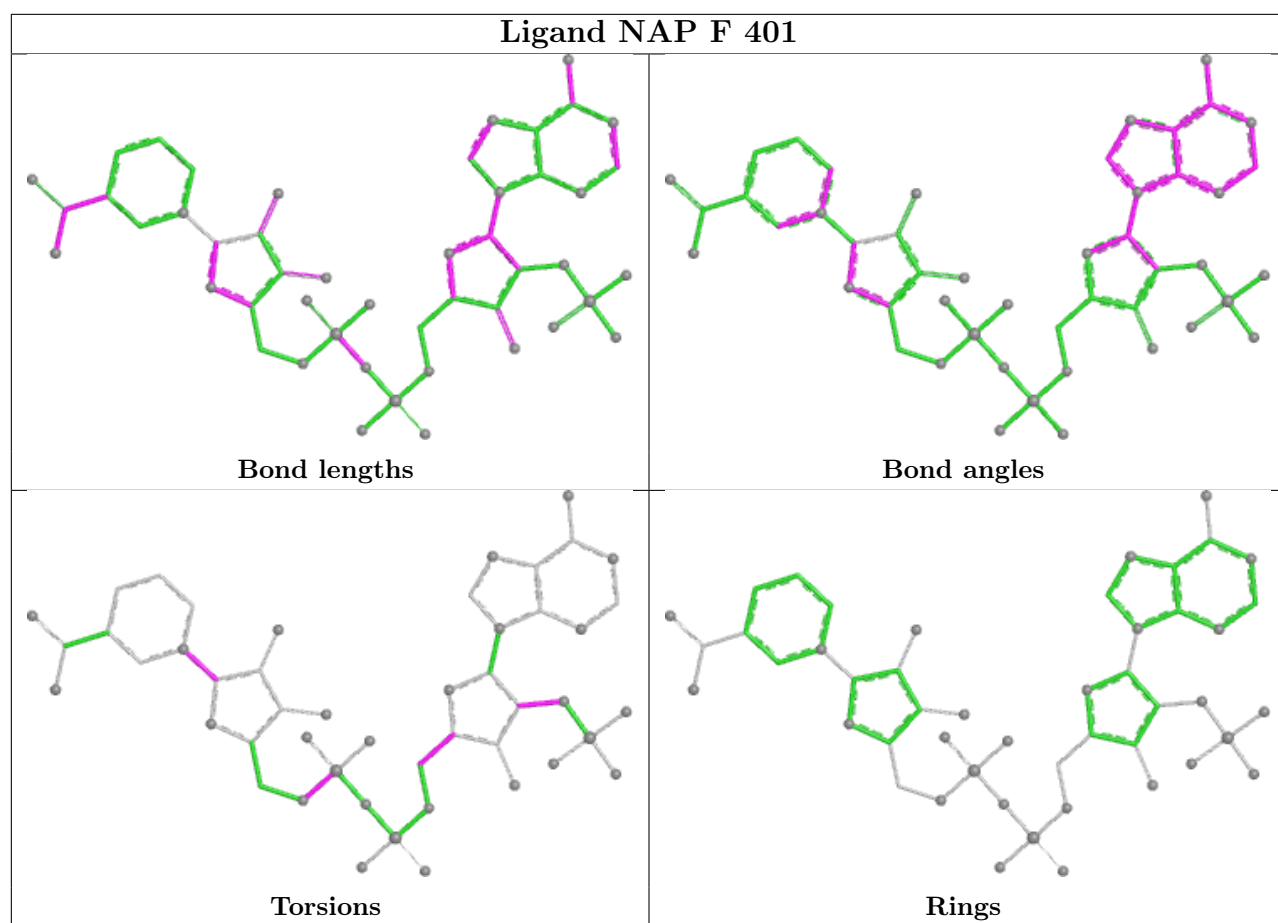
1 monomer is involved in 1 short contact:

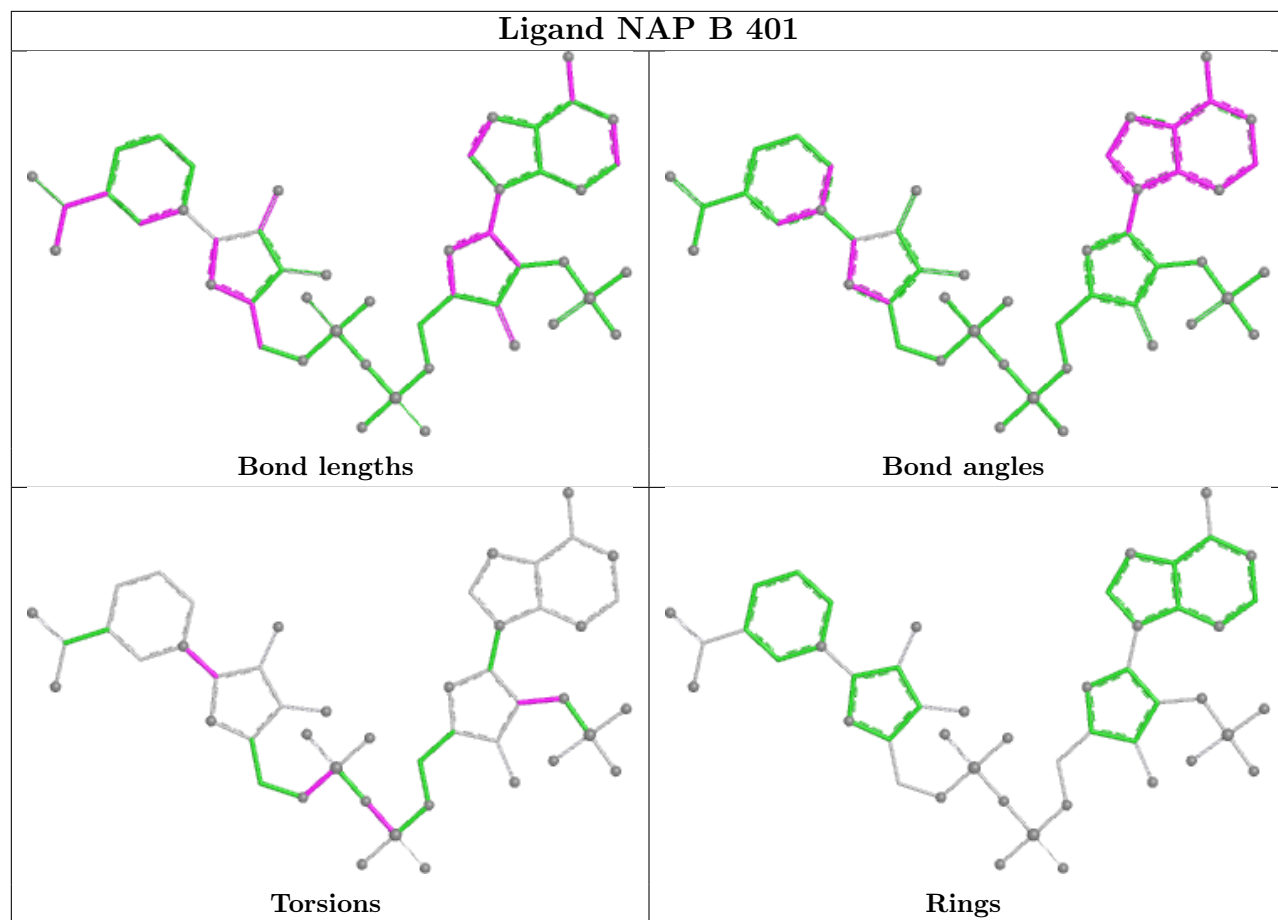
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	401	NAP	1	0

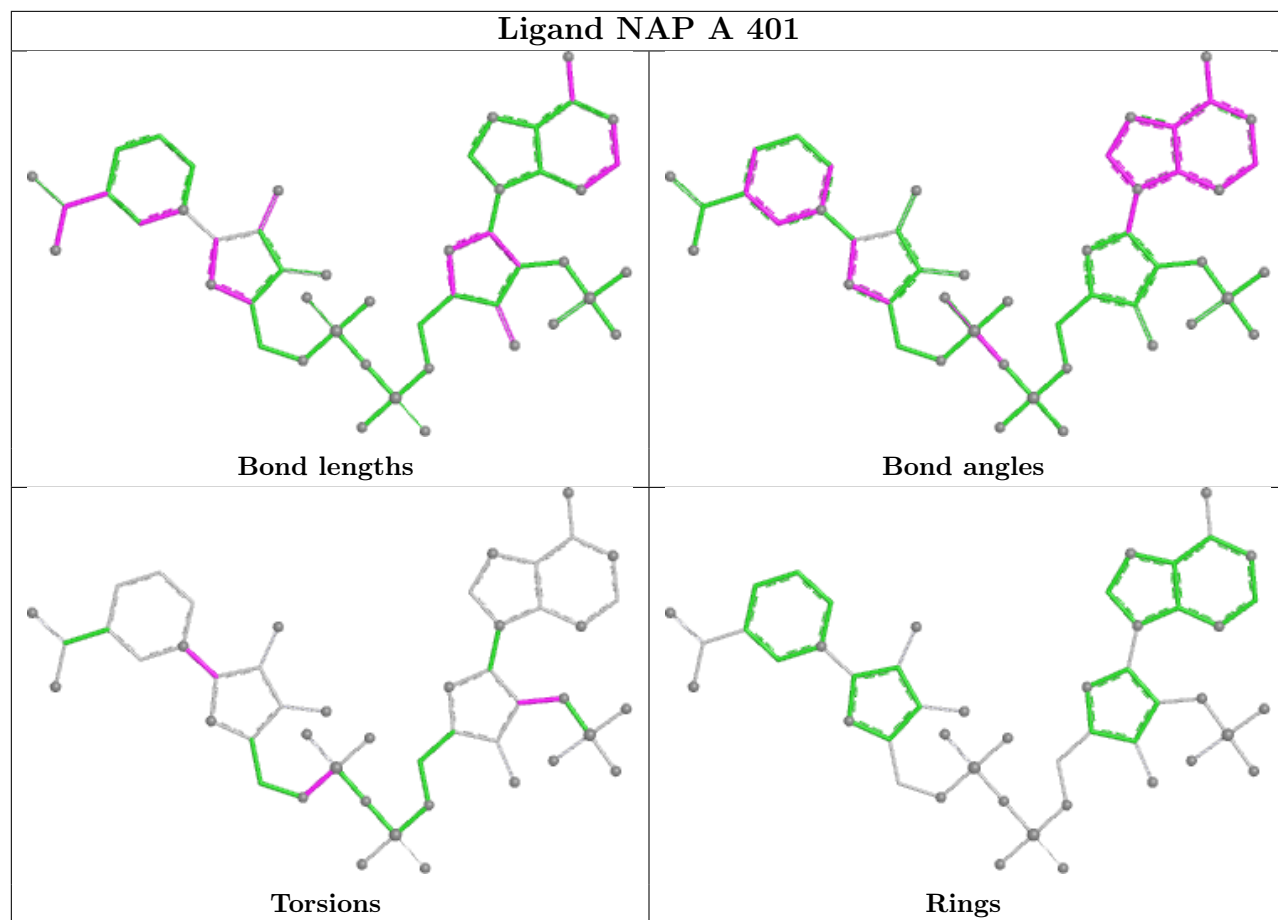
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

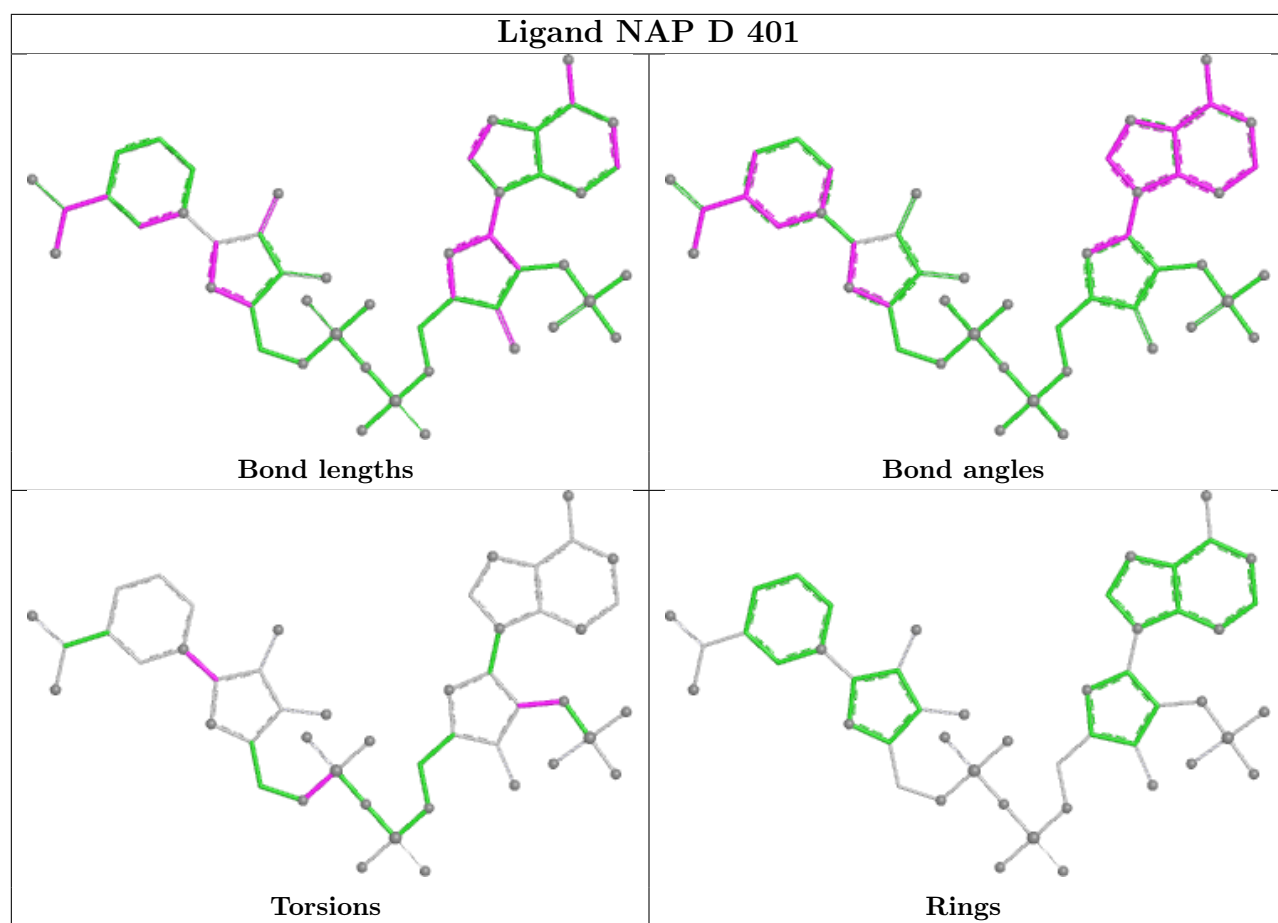












5.7 Other polymers [i](#)

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	A	351/381 (92%)	-0.32	4 (1%) 78 80	11, 20, 38, 61	3 (0%)
2	B	350/381 (91%)	-0.30	5 (1%) 73 76	14, 21, 36, 59	1 (0%)
3	C	351/381 (92%)	-0.33	5 (1%) 73 76	12, 20, 36, 56	0
4	D	353/381 (92%)	-0.31	6 (1%) 69 72	12, 20, 42, 59	0
5	E	351/381 (92%)	-0.41	2 (0%) 85 87	12, 19, 35, 49	2 (0%)
6	F	354/381 (92%)	-0.21	5 (1%) 73 76	14, 22, 42, 61	1 (0%)
All	All	2110/2286 (92%)	-0.31	27 (1%) 75 78	11, 20, 38, 61	7 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	267	TYR	4.2
1	A	157	ASP	4.0
3	C	156	VAL	3.1
3	C	157	ASP	3.0
4	D	192	ILE	3.0
2	B	157	ASP	2.9
2	B	25	PHE	2.9
2	B	267	TYR	2.8
1	A	160	ARG	2.8
6	F	318	ARG	2.7
4	D	110	GLU	2.5
6	F	160	ARG	2.4
6	F	192	ILE	2.4
1	A	50	ASP	2.3
3	C	194	THR	2.3
4	D	160	ARG	2.2
1	A	158	GLY	2.2
5	E	25	PHE	2.2
6	F	349	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	156	VAL	2.2
4	D	318	ARG	2.2
5	E	156	VAL	2.1
3	C	25	PHE	2.0
2	B	156	VAL	2.0
4	D	379	ASP	2.0
6	F	25	PHE	2.0
2	B	160	ARG	2.0

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

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	MLY	D	191	11/12	0.78	0.15	33,37,44,48	0
4	MLY	D	316	11/12	0.85	0.13	37,40,46,47	0
3	MLY	C	241	11/12	0.88	0.15	21,28,55,57	0
6	MLY	F	228	11/12	0.88	0.12	28,32,43,49	0
6	MLY	F	316	11/12	0.89	0.11	37,41,47,48	0
5	MLY	E	191	11/12	0.90	0.10	25,29,33,34	0
1	MLY	A	191	11/12	0.90	0.10	27,28,33,38	0
3	MLY	C	314	11/12	0.90	0.14	23,33,51,57	0
1	MLY	A	241	11/12	0.91	0.13	22,27,51,53	0
1	MLY	A	284	11/12	0.91	0.13	19,24,41,42	0
1	MLY	A	316	11/12	0.91	0.10	34,36,43,44	0
4	MLY	D	228	11/12	0.91	0.10	25,31,43,45	0
2	MLY	B	191	11/12	0.91	0.10	26,29,34,35	0
2	MLY	B	284	11/12	0.91	0.11	20,23,38,39	0
5	MLY	E	284	11/12	0.91	0.12	16,22,39,39	0
6	MLY	F	91	11/12	0.91	0.11	24,32,44,45	0
2	MLY	B	325	11/12	0.91	0.09	24,27,29,30	0
6	MLY	F	284	11/12	0.91	0.11	18,23,35,38	0
2	MLY	B	385	11/12	0.91	0.12	21,25,42,44	0
4	MLY	D	284	11/12	0.92	0.11	20,25,40,41	0
4	MLY	D	91	11/12	0.92	0.10	19,22,35,36	0
2	MLY	B	228	11/12	0.92	0.09	24,26,42,43	0
6	MLY	F	288	11/12	0.92	0.10	20,25,39,45	0
1	MLY	A	269	11/12	0.92	0.12	15,22,36,38	0
2	MLY	B	91	11/12	0.93	0.09	20,26,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	MLY	A	228	11/12	0.93	0.10	21,28,45,46	0
3	MLY	C	228	11/12	0.93	0.09	19,22,38,38	0
2	MLY	B	316	11/12	0.93	0.09	25,26,36,37	0
5	MLY	E	316	11/12	0.93	0.10	23,26,43,44	0
5	MLY	E	228	11/12	0.94	0.10	16,19,34,34	0
5	MLY	E	282	11/12	0.94	0.09	15,18,33,35	0
3	MLY	C	288	11/12	0.94	0.09	17,21,43,44	0
5	MLY	E	288	11/12	0.94	0.10	16,25,41,41	0
4	MLY	D	240	11/12	0.94	0.07	24,28,34,38	0
5	MLY	E	332	11/12	0.94	0.09	21,25,34,42	0
6	MLY	F	57	11/12	0.94	0.08	23,26,31,33	0
3	MLY	C	91	11/12	0.94	0.09	21,25,37,41	0
4	MLY	D	288	11/12	0.94	0.10	20,23,40,43	0
2	MLY	B	332	11/12	0.94	0.09	24,29,47,53	0
4	MLY	D	382	11/12	0.94	0.07	19,24,29,30	0
2	MLY	B	240	11/12	0.94	0.09	22,23,41,42	0
6	MLY	F	382	11/12	0.94	0.08	22,29,34,37	0
1	MLY	A	282	11/12	0.95	0.07	18,21,29,30	0
2	MLY	B	288	11/12	0.95	0.09	19,25,38,41	0
1	MLY	A	91	11/12	0.95	0.07	18,22,33,34	0
3	MLY	C	240	11/12	0.95	0.09	20,25,35,35	0
1	MLY	A	240	11/12	0.95	0.08	21,27,34,35	0
1	MLY	A	382	11/12	0.95	0.08	18,23,32,33	0
2	MLY	B	382	11/12	0.95	0.07	20,22,29,31	0
3	MLY	C	316	11/12	0.95	0.07	21,23,35,39	0
5	MLY	E	57	11/12	0.95	0.07	18,22,29,29	0
5	MLY	E	91	11/12	0.95	0.08	19,25,30,35	0
3	MLY	C	332	11/12	0.95	0.08	17,22,34,38	0
4	MLY	D	57	11/12	0.95	0.08	18,23,32,32	0
1	MLY	A	57	11/12	0.96	0.07	18,20,28,30	0
5	MLY	E	325	11/12	0.96	0.07	19,21,23,24	0
4	MLY	D	147	11/12	0.96	0.06	12,17,24,25	0
5	MLY	E	382	11/12	0.96	0.07	14,18,27,29	0
3	MLY	C	57	11/12	0.96	0.06	19,25,33,36	0
2	MLY	B	282	11/12	0.96	0.07	18,23,30,30	0
3	MLY	C	147	11/12	0.96	0.06	14,17,24,26	0
6	MLY	F	240	11/12	0.96	0.07	23,28,32,36	0
5	MLY	E	240	11/12	0.96	0.08	18,24,34,37	0
3	MLY	C	325	11/12	0.96	0.05	18,20,22,22	0
1	MLY	A	288	11/12	0.96	0.08	20,27,39,41	0
2	MLY	B	57	11/12	0.96	0.07	19,22,31,32	0
1	MLY	A	147	11/12	0.97	0.06	12,16,25,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MLY	F	282	11/12	0.97	0.06	18,22,27,32	0
5	MLY	E	147	11/12	0.97	0.06	13,15,24,24	0
3	MLY	C	382	11/12	0.97	0.06	14,18,28,30	0
4	MLY	D	282	11/12	0.97	0.06	15,21,28,30	0
3	MLY	C	282	11/12	0.97	0.07	13,19,29,30	0
6	MLY	F	147	11/12	0.98	0.05	14,18,24,26	0
2	MLY	B	147	11/12	0.98	0.05	14,16,25,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

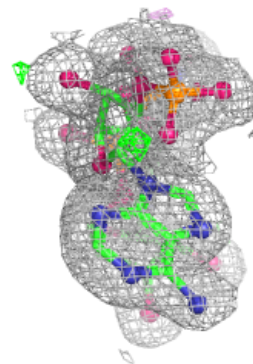
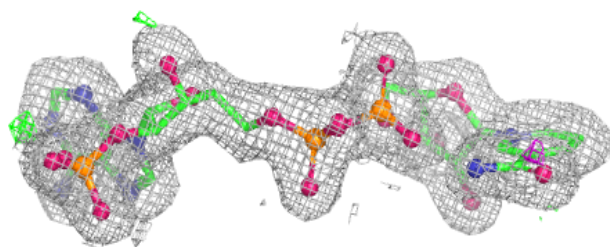
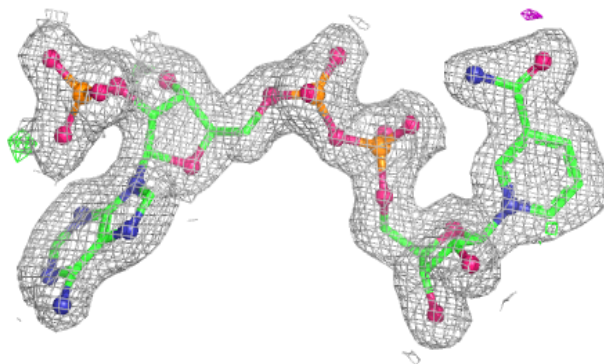
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	E	402	1/1	0.97	0.09	24,24,24,24	0
7	NAP	B	401	48/48	0.98	0.05	11,15,18,19	0
7	NAP	C	401	48/48	0.98	0.05	11,15,16,17	0
7	NAP	D	401	48/48	0.98	0.04	11,14,16,19	0
7	NAP	F	401	48/48	0.98	0.04	13,16,19,21	0
8	CL	B	402	1/1	0.98	0.06	25,25,25,25	0
8	CL	C	402	1/1	0.98	0.07	24,24,24,24	0
7	NAP	A	401	48/48	0.98	0.04	12,16,18,19	0
8	CL	A	402	1/1	0.99	0.06	23,23,23,23	0
8	CL	D	402	1/1	0.99	0.04	22,22,22,22	0
7	NAP	E	401	48/48	0.99	0.04	10,14,16,17	0
8	CL	F	402	1/1	0.99	0.05	24,24,24,24	0

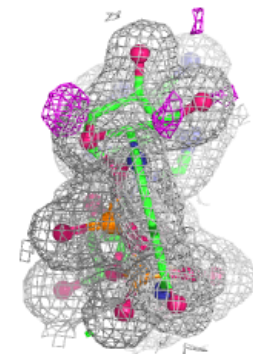
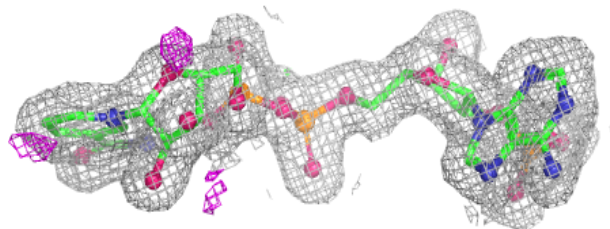
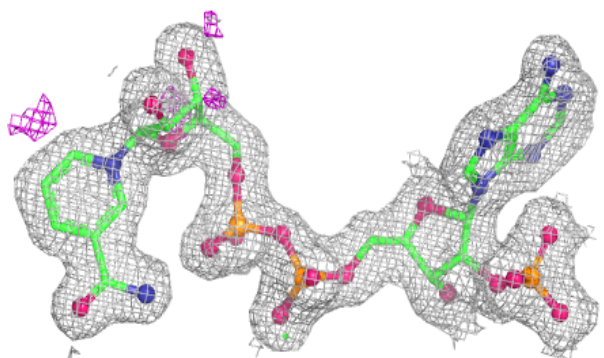
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP B 401:

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

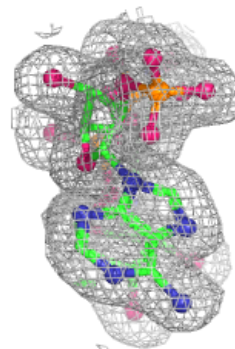
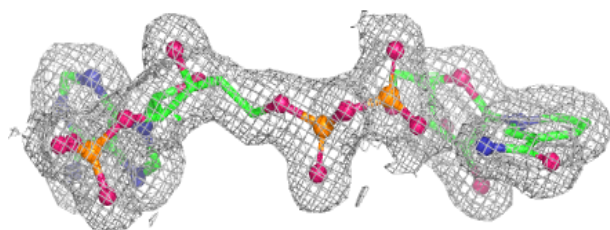
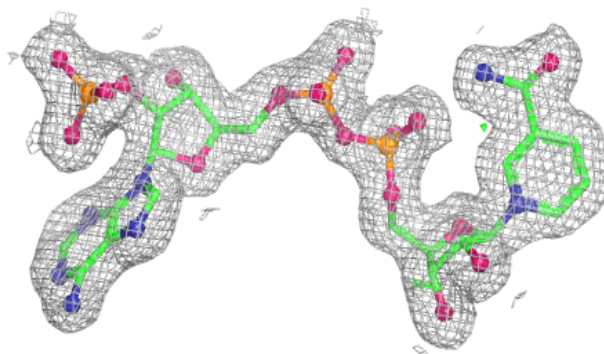
**Electron density around NAP C 401:**

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

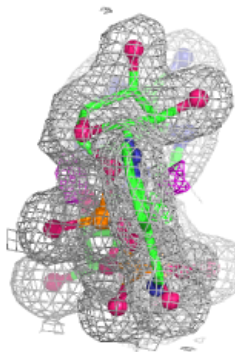
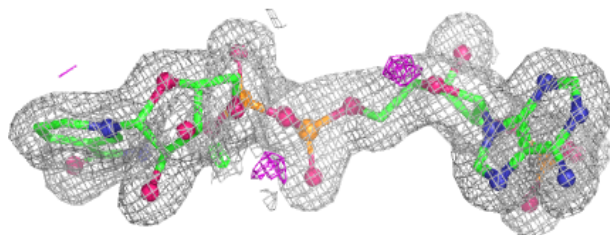
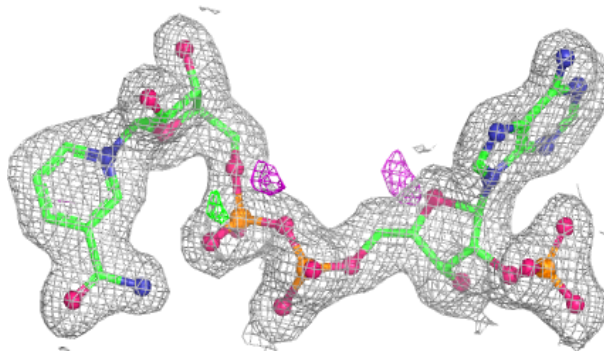


Electron density around NAP D 401:

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

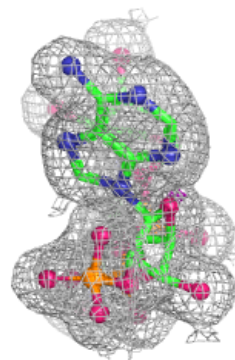
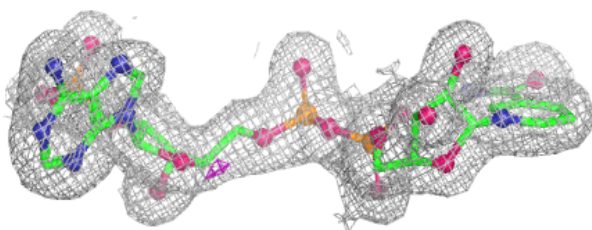
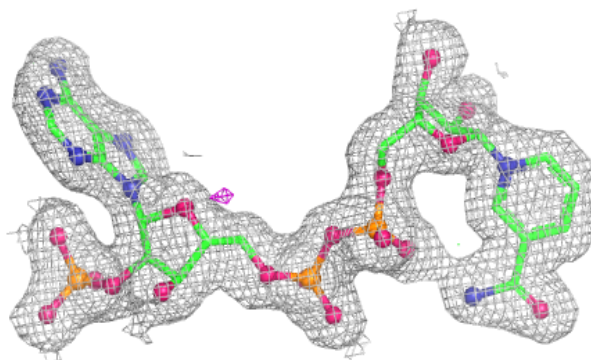
**Electron density around NAP F 401:**

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

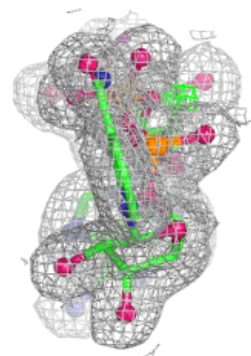
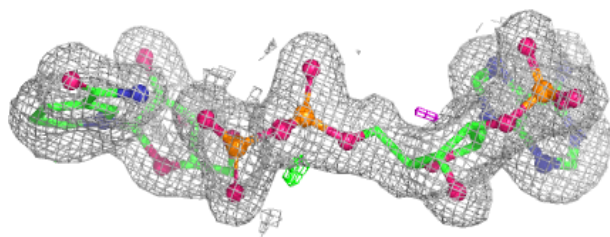
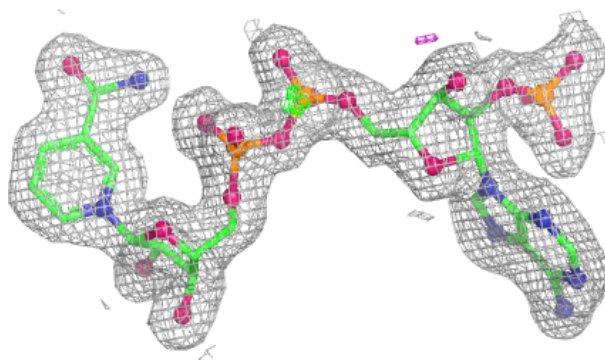


Electron density around NAP A 401:

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

**Electron density around NAP E 401:**

$2mF_o-DF_c$ (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.