



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:07 PM UTC

PDB ID : 8JFI / pdb_00008jfi
Title : Crystal structure of 3-oxoacyl-ACP reductase FabG in complex with NADP+ and 3-keto-hexanoyl-ACP from Helicobacter pylori
Authors : Zhou, J.S.; Zhang, L.
Deposited on : 2023-05-18
Resolution : 2.38 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:

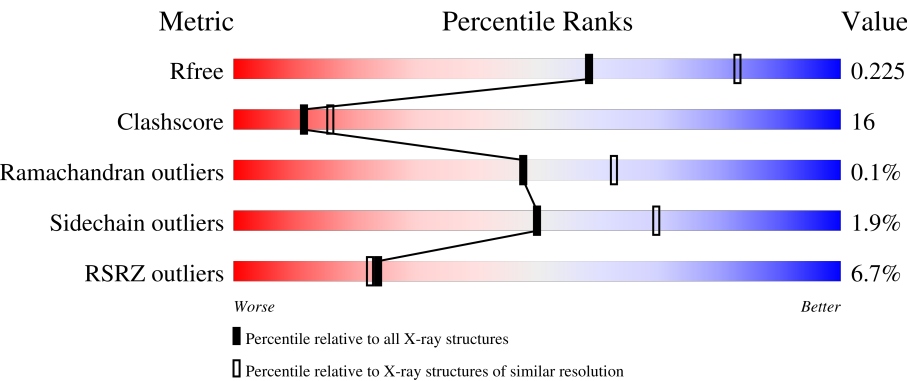
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	248	4% 75% 23% ..
1	B	248	4% 71% 22% ..
1	C	248	3% 62% 31% 5%
1	D	248	5% 67% 29% .
1	E	248	4% 64% 30% ..

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Mol	Chain	Length	Quality of chain
1	F	248	9%56%36%6%
2	G	75	24%35%45%13%
2	H	75	11%15%5%80%
2	I	75	7%5%88%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11923 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-oxoacyl-[acyl-carrier-protein] reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1875	1179	323	363	10			
1	B	237	Total	C	N	O	S	0	0	0
			1789	1128	309	343	9			
1	C	236	Total	C	N	O	S	0	0	0
			1782	1123	307	343	9			
1	D	237	Total	C	N	O	S	0	0	0
			1787	1126	308	344	9			
1	E	237	Total	C	N	O	S	0	0	0
			1790	1128	308	344	10			
1	F	233	Total	C	N	O	S	0	0	0
			1755	1106	304	336	9			

There are 6 discrepancies between the modelled and reference sequences:

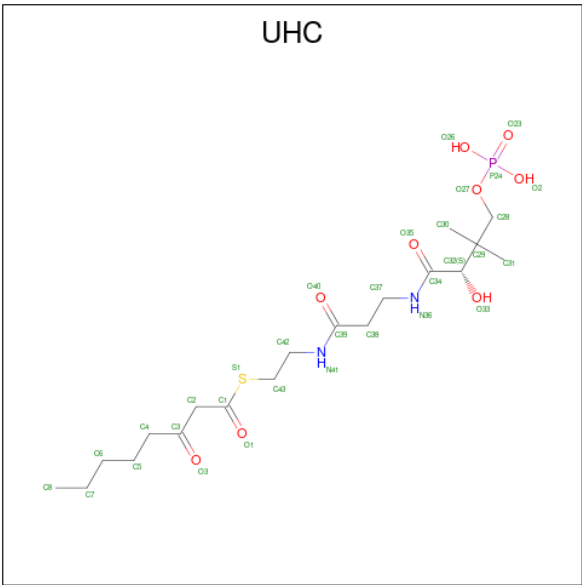
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP G2M827
B	0	SER	-	expression tag	UNP G2M827
C	0	SER	-	expression tag	UNP G2M827
D	0	SER	-	expression tag	UNP G2M827
E	0	SER	-	expression tag	UNP G2M827
F	0	SER	-	expression tag	UNP G2M827

- Molecule 2 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	73	Total	C	N	O	S	0	0	0
			566	359	85	121	1			
2	H	15	Total	C	N	O	S	0	0	0
			110	71	16	22	1			
2	I	9	Total	C	N	O	S	0	0	0
			68	45	9	13	1			

- # NAP

- Molecule 4 is {S}-[2-[3-[[2 {S}]-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] 3-oxidanylideneoctanethioate (CCD ID: UHC) (formula: C₁₉H₃₅N₂O₉PS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			29	17	2	8	1	1		

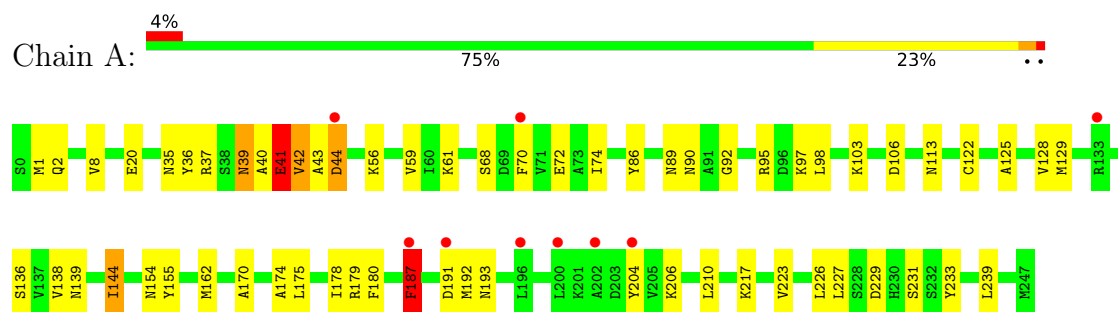
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	21	Total	O	0	0
			21	21		
5	C	7	Total	O	0	0
			7	7		
5	D	9	Total	O	0	0
			9	9		
5	E	10	Total	O	0	0
			10	10		
5	F	11	Total	O	0	0
			11	11		
5	G	3	Total	O	0	0
			3	3		

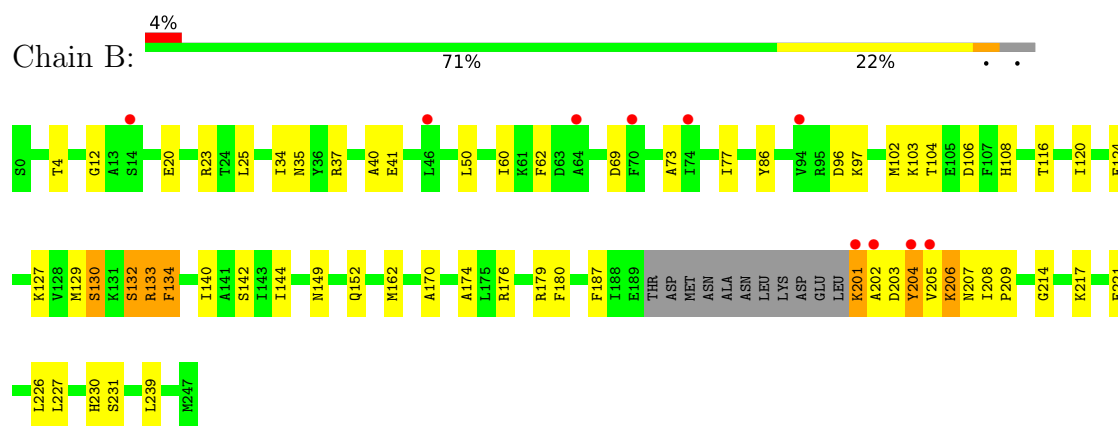
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

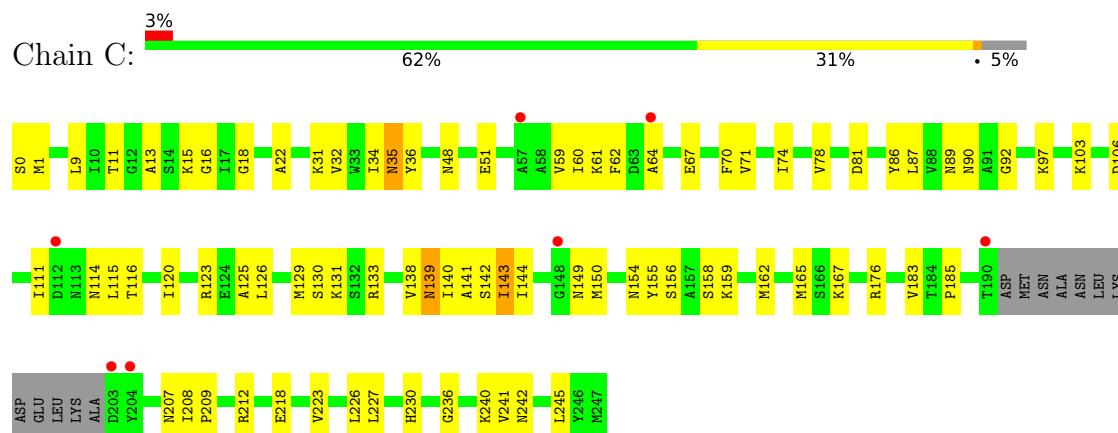
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



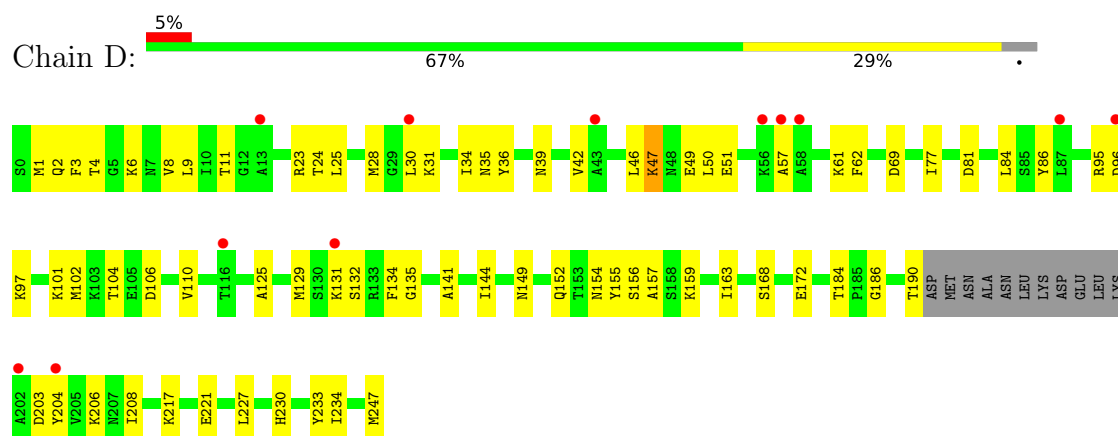
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



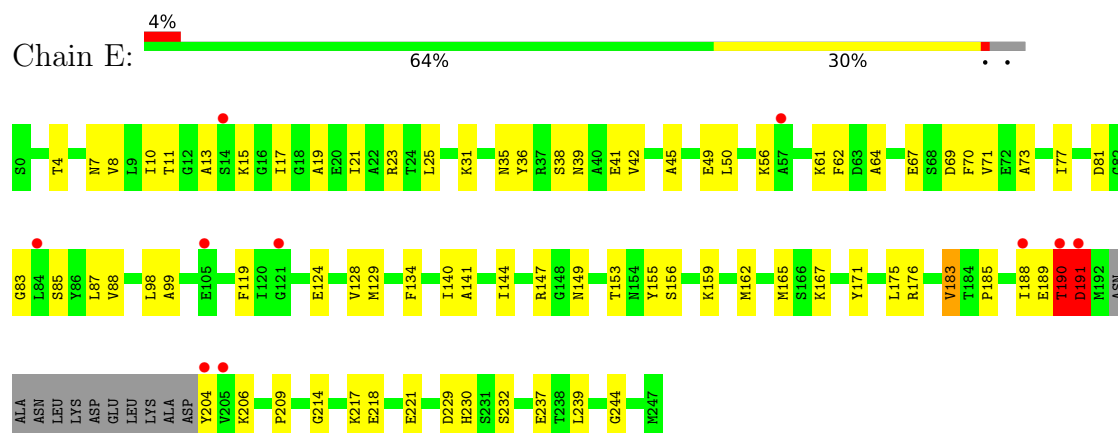
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



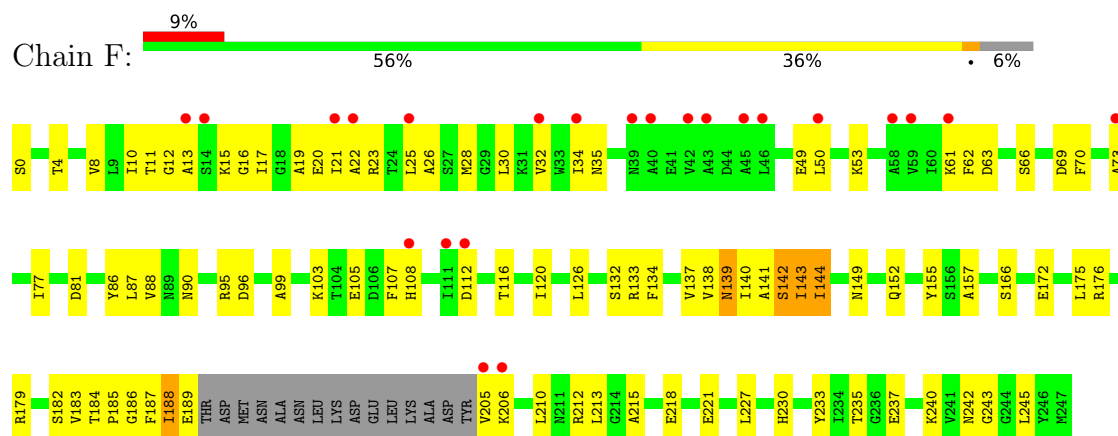
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



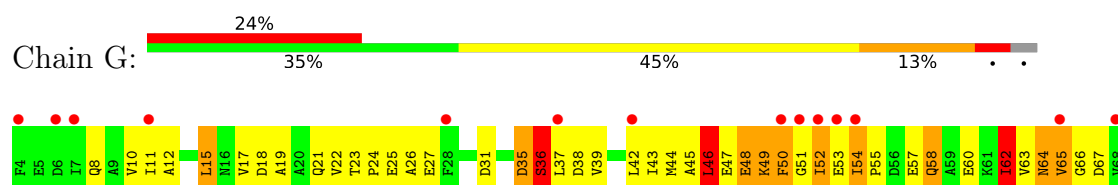
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] reductase

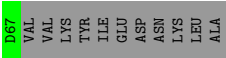
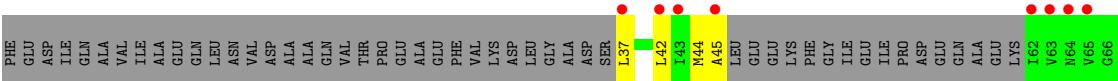


- Molecule 2: Acyl carrier protein

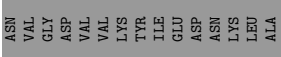
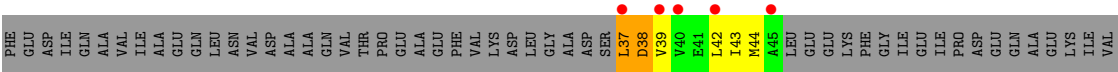




• Molecule 2: Acyl carrier protein



• Molecule 2: Acyl carrier protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	85.84Å 252.65Å 166.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.16 – 2.38 63.16 – 2.38	Depositor EDS
% Data completeness (in resolution range)	55.4 (63.16-2.38) 55.4 (63.16-2.38)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.37Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.206 , 0.225 0.206 , 0.225	Depositor DCC
R_{free} test set	2022 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å ²)	48.7	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11923	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: UHC, 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	0.72	6/1899 (0.3%)	0.81	3/2553 (0.1%)
1	B	0.85	13/1812 (0.7%)	0.85	8/2434 (0.3%)
1	C	0.75	7/1805 (0.4%)	0.71	0/2426
1	D	0.41	0/1810	0.69	3/2433 (0.1%)
1	E	0.53	1/1813 (0.1%)	0.83	7/2436 (0.3%)
1	F	1.04	15/1777 (0.8%)	0.94	5/2387 (0.2%)
2	G	1.53	11/571 (1.9%)	1.67	12/774 (1.6%)
2	H	0.34	0/108	0.93	0/145
2	I	0.69	0/67	1.58	4/90 (4.4%)
All	All	0.80	53/11662 (0.5%)	0.88	42/15678 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
2	G	0	2
All	All	0	4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	138	VAL	C-O	-15.65	1.08	1.24
1	F	183	VAL	C-O	-14.18	1.08	1.24
1	F	185	PRO	C-O	-13.88	1.08	1.23
1	C	138	VAL	C-O	-12.37	1.11	1.24
1	B	209	PRO	C-O	-10.30	1.11	1.24
1	A	42	VAL	C-O	-10.27	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	36	SER	CA-CB	-10.07	1.37	1.54
1	C	142	SER	C-O	-9.85	1.12	1.23
1	F	137	VAL	C-O	-9.41	1.14	1.24
1	B	129	MET	C-O	-9.36	1.11	1.24
1	A	44	ASP	C-O	-9.21	1.13	1.24
1	F	140	ILE	C-O	-8.95	1.13	1.23
1	F	139	ASN	C-O	-8.94	1.13	1.24
1	B	133	ARG	C-O	-8.42	1.12	1.23
1	F	182	SER	C-O	-8.36	1.13	1.23
2	G	62	ILE	C-O	-8.35	1.15	1.24
2	G	55	PRO	C-O	-8.32	1.14	1.23
1	B	206	LYS	C-O	-8.03	1.13	1.24
1	C	140	ILE	C-O	-7.97	1.14	1.23
1	F	187	PHE	C-O	-7.88	1.14	1.24
1	C	141	ALA	C-O	-7.76	1.14	1.24
1	A	40	ALA	C-O	-7.56	1.14	1.24
2	G	45	ALA	C-O	-7.47	1.14	1.24
1	B	205	VAL	C-O	-7.47	1.14	1.24
1	B	134	PHE	C-O	-7.21	1.14	1.23
1	F	143	ILE	C-O	-7.21	1.15	1.24
1	B	130	SER	CA-CB	-7.15	1.42	1.53
1	C	139	ASN	C-O	-7.12	1.15	1.24
1	F	142	SER	C-O	-7.05	1.15	1.23
1	B	132	SER	C-O	-6.82	1.14	1.24
2	G	51	GLY	C-O	-6.64	1.18	1.24
1	A	41	GLU	C-O	-6.57	1.15	1.24
1	B	130	SER	C-O	-6.37	1.16	1.24
2	G	19	ALA	C-O	-6.32	1.16	1.24
1	F	144	ILE	C-O	-6.29	1.16	1.24
1	F	141	ALA	C-O	-6.27	1.16	1.24
1	F	184	THR	C-O	-6.16	1.17	1.24
1	C	208	ILE	CA-C	-6.08	1.46	1.52
2	G	44	MET	C-O	-6.05	1.16	1.24
1	B	208	ILE	C-O	-6.03	1.16	1.24
1	A	39	ASN	C-O	-5.98	1.16	1.24
2	G	15	LEU	C-O	-5.66	1.17	1.23
1	A	43	ALA	C-O	-5.62	1.17	1.24
1	B	203	ASP	C-O	-5.59	1.16	1.24
2	G	48	GLU	C-O	-5.42	1.16	1.24
1	B	207	ASN	C-O	-5.41	1.17	1.24
2	G	47	GLU	C-O	-5.40	1.16	1.24
1	E	189	GLU	C-O	-5.28	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	TYR	C-O	-5.18	1.17	1.24
1	C	143	ILE	C-O	-5.04	1.17	1.24
2	G	60	GLU	C-O	-5.03	1.18	1.24
1	F	188	ILE	C-O	-5.02	1.18	1.24
1	F	103	LYS	CG-CD	5.01	1.67	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	CG-CD-NE	8.58	130.88	112.00
1	E	41	GLU	CA-CB-CG	8.48	131.06	114.10
2	G	51	GLY	N-CA-C	-8.19	98.20	110.97
2	G	50	PHE	CA-C-N	-8.02	113.76	120.98
2	G	50	PHE	C-N-CA	-8.02	113.76	120.98
1	F	187	PHE	CB-CA-C	7.75	122.75	110.19
1	F	175	LEU	CB-CG-CD2	-7.60	87.90	110.70
1	E	190	THR	N-CA-CB	-7.28	99.35	111.57
1	E	189	GLU	CB-CG-CD	6.96	124.43	112.60
1	B	203	ASP	N-CA-C	-5.96	106.17	113.50
2	I	38	ASP	CA-C-N	-5.87	113.16	120.56
2	I	38	ASP	C-N-CA	-5.87	113.16	120.56
2	G	49	LYS	CA-C-N	5.66	132.13	123.47
2	G	49	LYS	C-N-CA	5.66	132.13	123.47
1	E	183	VAL	CA-C-N	-5.49	116.05	123.46
1	E	183	VAL	C-N-CA	-5.49	116.05	123.46
1	B	204	TYR	CB-CA-C	-5.49	99.03	109.95
1	E	191	ASP	CA-C-O	-5.49	115.06	120.82
2	G	52	ILE	CA-C-N	5.46	131.96	121.54
2	G	52	ILE	C-N-CA	5.46	131.96	121.54
1	A	187	PHE	CB-CA-C	5.45	119.67	110.79
1	F	185	PRO	CB-CA-C	-5.44	103.97	111.21
1	F	184	THR	CA-CB-OG1	-5.41	101.48	109.60
2	G	58	GLN	N-CA-CB	-5.41	103.70	110.90
1	D	104	THR	CA-C-N	5.39	127.50	120.28
1	D	104	THR	C-N-CA	5.39	127.50	120.28
1	F	175	LEU	CB-CG-CD1	5.33	126.70	110.70
2	I	38	ASP	N-CA-C	-5.32	105.49	111.28
2	G	36	SER	CA-CB-OG	-5.31	100.49	111.10
1	A	56	LYS	CA-CB-CG	5.24	124.58	114.10
1	D	47	LYS	CG-CD-CE	5.23	123.32	111.30
2	G	58	GLN	N-CA-C	-5.20	107.61	114.31
1	E	190	THR	OG1-CB-CG2	5.19	119.67	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	53	GLU	O-C-N	5.17	129.47	122.59
1	B	34	ILE	CA-C-N	-5.16	114.14	122.81
1	B	34	ILE	C-N-CA	-5.16	114.14	122.81
1	B	202	ALA	CA-C-N	5.14	130.82	121.92
1	B	202	ALA	C-N-CA	5.14	130.82	121.92
2	I	38	ASP	CA-C-O	-5.14	115.11	120.55
2	G	58	GLN	CB-CG-CD	-5.09	103.94	112.60
1	B	203	ASP	CA-C-N	5.02	131.37	121.58
1	B	203	ASP	C-N-CA	5.02	131.37	121.58

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	PHE	Sidechain
1	F	142	SER	Mainchain
2	G	46	LEU	Mainchain
2	G	64	ASN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1875	0	1894	46	0
1	B	1789	0	1811	40	1
1	C	1782	0	1800	73	0
1	D	1787	0	1805	59	0
1	E	1790	0	1808	61	0
1	F	1755	0	1780	78	0
2	G	566	0	553	33	1
2	H	110	0	115	4	0
2	I	68	0	74	19	0
3	A	48	0	24	7	0
3	B	48	0	24	5	0
3	C	48	0	24	5	0
3	D	48	0	24	3	0
3	E	48	0	23	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	48	0	24	1	0
4	A	29	0	0	3	0
5	A	23	0	0	2	0
5	B	21	0	0	2	0
5	C	7	0	0	0	0
5	D	9	0	0	3	0
5	E	10	0	0	1	0
5	F	11	0	0	1	0
5	G	3	0	0	0	0
All	All	11923	0	11783	379	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (379) 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)
4:A:302:UHC:P24	2:G:36:SER:OG	1.97	1.23
1:B:201:LYS:HD2	5:B:403:HOH:O	0.99	1.15
1:C:176:ARG:NH2	2:I:37:LEU:HD12	1.65	1.10
1:C:176:ARG:CZ	2:I:37:LEU:HD12	1.87	1.05
1:C:176:ARG:NH1	2:I:37:LEU:HD12	1.73	1.04
1:C:176:ARG:HH22	2:I:37:LEU:HD12	1.22	1.03
1:C:133:ARG:HG2	1:C:176:ARG:HD2	1.40	1.00
1:F:105:GLU:HA	1:F:108:HIS:HD2	1.28	0.97
2:I:38:ASP:O	2:I:42:LEU:HD13	1.64	0.96
1:F:15:LYS:HA	1:F:19:ALA:HB2	1.49	0.95
1:C:176:ARG:NH2	2:I:37:LEU:CD1	2.29	0.94
1:C:176:ARG:HH22	2:I:37:LEU:CD1	1.85	0.89
1:C:176:ARG:NH1	2:I:37:LEU:CD1	2.36	0.89
1:C:176:ARG:HH12	2:I:37:LEU:HD12	1.32	0.89
1:C:236:GLY:HA3	1:D:247:MET:HE2	1.56	0.87
1:E:7:ASN:ND2	1:E:83:GLY:O	2.10	0.84
1:C:176:ARG:CZ	2:I:37:LEU:CD1	2.54	0.84
1:E:176:ARG:HH12	2:H:37:LEU:HD21	1.42	0.83
1:F:105:GLU:HA	1:F:108:HIS:CD2	2.13	0.83
2:G:25:GLU:OE1	2:G:64:ASN:ND2	2.11	0.83
1:F:0:SER:HA	1:F:28:MET:HE2	1.61	0.83
1:A:179:ARG:NH1	1:A:231:SER:O	2.12	0.83
1:E:176:ARG:NH1	2:H:37:LEU:HD21	1.96	0.81
1:F:12:GLY:H	1:F:35:ASN:HD22	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:HH12	2:I:37:LEU:CD1	1.94	0.79
1:D:101:LYS:HA	2:H:44:MET:HE1	1.64	0.79
1:F:17:ILE:HD11	1:F:188:ILE:HG21	1.65	0.77
1:E:191:ASP:OD1	1:E:191:ASP:N	2.18	0.77
1:E:229:ASP:O	1:E:232:SER:OG	2.03	0.76
1:F:86:TYR:HB3	1:F:227:LEU:HD22	1.69	0.75
1:E:230:HIS:HB3	1:F:221:GLU:HB3	1.69	0.75
1:D:190:THR:HB	3:D:301:NAP:H72N	1.51	0.74
1:E:221:GLU:OE1	1:F:230:HIS:ND1	2.16	0.74
3:C:301:NAP:N7N	3:C:301:NAP:O1N	2.20	0.74
2:G:36:SER:O	2:G:37:LEU:C	2.32	0.73
1:E:218:GLU:OE1	1:F:233:TYR:HB2	1.90	0.72
1:B:37:ARG:HH12	3:B:301:NAP:P2B	2.13	0.72
1:A:36:TYR:HE1	1:A:61:LYS:HD2	1.55	0.72
1:C:67:GLU:OE2	1:C:123:ARG:NH2	2.20	0.70
1:E:45:ALA:O	1:E:49:GLU:HG2	1.90	0.70
1:A:128:VAL:O	5:A:401:HOH:O	2.10	0.69
2:G:62:ILE:HD13	2:G:67:ASP:HB2	1.75	0.69
1:F:144:ILE:HD12	1:F:149:ASN:HB2	1.75	0.68
1:E:39:ASN:N	1:E:39:ASN:OD1	2.26	0.68
1:A:68:SER:O	1:A:72:GLU:HG3	1.94	0.68
2:G:64:ASN:ND2	2:G:64:ASN:O	2.27	0.68
1:A:191:ASP:HB3	3:A:301:NAP:O1A	1.93	0.67
1:F:8:VAL:HG13	1:F:10:ILE:HD11	1.74	0.67
1:F:144:ILE:HG21	1:F:155:TYR:HD2	1.58	0.67
1:C:242:ASN:OD1	1:C:245:LEU:N	2.28	0.67
1:E:73:ALA:O	1:E:77:ILE:HD12	1.95	0.67
1:D:141:ALA:HB3	1:D:184:THR:HG22	1.78	0.66
2:G:48:GLU:HG3	2:G:48:GLU:O	1.95	0.66
1:B:62:PHE:HB2	1:B:69:ASP:HB3	1.77	0.66
1:B:144:ILE:HD12	1:B:149:ASN:HB2	1.78	0.64
1:E:36:TYR:CE2	1:E:61:LYS:HE3	2.32	0.64
2:G:66:GLY:O	2:G:69:VAL:HG22	1.98	0.64
1:F:12:GLY:H	1:F:35:ASN:ND2	1.95	0.64
1:B:217:LYS:O	1:B:221:GLU:HG3	1.97	0.64
2:G:12:ALA:HB1	2:G:17:VAL:O	1.97	0.64
1:F:15:LYS:CA	1:F:19:ALA:HB2	2.26	0.64
1:F:108:HIS:O	1:F:112:ASP:HB2	1.97	0.64
1:F:20:GLU:O	1:F:23:ARG:N	2.32	0.63
2:G:36:SER:C	2:G:38:ASP:N	2.52	0.63
2:I:39:VAL:O	2:I:43:ILE:HG12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASN:HD22	1:A:139:ASN:HD21	1.48	0.62
1:E:209:PRO:HG2	1:E:244:GLY:HA3	1.81	0.62
1:D:8:VAL:HG11	1:D:25:LEU:HD23	1.81	0.62
1:A:36:TYR:CE1	1:A:61:LYS:HD2	2.35	0.61
1:F:149:ASN:ND2	1:F:152:GLN:OE1	2.27	0.61
4:A:302:UHC:P24	2:G:36:SER:CB	2.87	0.61
1:B:73:ALA:O	1:B:77:ILE:HD12	2.01	0.61
1:E:124:GLU:O	1:E:128:VAL:HG12	2.01	0.61
2:G:36:SER:O	2:G:39:VAL:N	2.31	0.61
1:A:90:ASN:ND2	3:A:301:NAP:H4D	2.15	0.60
1:C:241:VAL:HG12	1:D:233:TYR:HD2	1.66	0.60
1:F:139:ASN:HD22	1:F:166:SER:HB2	1.66	0.60
1:F:112:ASP:O	1:F:116:THR:HB	2.02	0.60
1:D:204:TYR:O	1:D:208:ILE:HG13	2.01	0.60
1:D:46:LEU:O	1:D:49:GLU:HG2	2.01	0.60
1:D:203:ASP:HA	1:D:206:LYS:NZ	2.16	0.60
1:C:144:ILE:HG22	1:C:156:SER:HB3	1.83	0.59
1:A:206:LYS:NZ	5:A:402:HOH:O	2.28	0.59
1:D:155:TYR:CE1	1:D:159:LYS:HE2	2.37	0.59
1:A:89:ASN:HD22	1:A:139:ASN:ND2	2.00	0.59
1:F:95:ARG:NH1	5:F:401:HOH:O	2.29	0.59
1:C:212:ARG:NH2	1:C:218:GLU:OE2	2.31	0.59
1:A:97:LYS:NZ	1:A:106:ASP:OD2	2.26	0.59
2:G:10:VAL:HG11	2:G:46:LEU:HD11	1.84	0.58
2:G:49:LYS:O	2:G:49:LYS:HG2	2.03	0.58
1:E:23:ARG:HG3	1:E:50:LEU:HD21	1.84	0.58
1:F:63:ASP:HB3	1:F:66:SER:OG	2.04	0.58
1:E:64:ALA:HA	1:E:70:PHE:HD2	1.69	0.58
1:B:60:ILE:HD13	1:B:77:ILE:HD11	1.85	0.57
1:B:174:ALA:C	1:B:176:ARG:H	2.11	0.57
2:G:11:ILE:HD11	2:G:22:VAL:HG22	1.86	0.57
1:D:36:TYR:CZ	1:D:61:LYS:HB2	2.39	0.57
2:G:11:ILE:HG22	2:G:42:LEU:HD11	1.86	0.57
1:C:133:ARG:HG2	1:C:176:ARG:CD	2.25	0.57
1:C:64:ALA:HA	1:C:70:PHE:HD2	1.70	0.56
1:D:31:LYS:NZ	1:D:81:ASP:OD1	2.37	0.56
1:D:190:THR:HB	3:D:301:NAP:N7N	2.20	0.56
1:E:8:VAL:HG21	1:E:25:LEU:HD13	1.87	0.56
1:F:25:LEU:O	1:F:30:LEU:HB2	2.05	0.56
3:B:301:NAP:H52A	3:B:301:NAP:H52N	1.87	0.56
1:B:187:PHE:CE2	1:B:204:TYR:HD2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:ILE:HD12	1:E:149:ASN:HB2	1.88	0.56
1:D:131:LYS:HG3	1:D:132:SER:N	2.20	0.56
1:E:39:ASN:HD22	1:E:42:VAL:CG2	2.19	0.56
1:B:201:LYS:C	1:B:201:LYS:HD3	2.31	0.55
1:D:42:VAL:HG23	5:D:408:HOH:O	2.06	0.55
1:A:20:GLU:OE1	1:A:217:LYS:HE3	2.05	0.55
2:G:10:VAL:HG11	2:G:46:LEU:CD1	2.36	0.55
1:B:37:ARG:NH1	3:B:301:NAP:O1X	2.38	0.55
1:A:144:ILE:HD11	1:A:155:TYR:HD2	1.70	0.55
1:D:34:ILE:HD13	1:D:46:LEU:HD23	1.88	0.55
2:I:38:ASP:O	2:I:42:LEU:CD1	2.48	0.55
1:C:35:ASN:ND2	1:C:62:PHE:CZ	2.74	0.55
1:C:90:ASN:OD1	3:C:301:NAP:H4D	2.06	0.55
1:F:189:GLU:OE1	1:F:215:ALA:HA	2.06	0.55
1:F:16:GLY:O	1:F:19:ALA:HB3	2.06	0.55
1:C:15:LYS:NZ	3:C:301:NAP:H3B	2.22	0.55
1:F:20:GLU:OE1	1:F:21:ILE:N	2.39	0.55
1:C:35:ASN:OD1	1:C:35:ASN:C	2.50	0.55
1:C:0:SER:O	1:C:1:MET:HG3	2.07	0.54
1:C:86:TYR:HB3	1:C:227:LEU:HD22	1.89	0.54
1:E:237:GLU:OE1	1:F:240:LYS:HE3	2.05	0.54
1:F:20:GLU:CD	1:F:20:GLU:C	2.74	0.54
1:F:210:LEU:HD12	1:F:243:GLY:HA2	1.89	0.54
2:G:58:GLN:HG3	2:G:71:TYR:CD1	2.42	0.54
1:F:35:ASN:HD21	3:F:301:NAP:H2A	1.72	0.54
2:G:50:PHE:HD1	2:G:50:PHE:O	1.90	0.54
1:C:165:MET:HB2	1:F:157:ALA:HB2	1.89	0.54
1:F:143:ILE:CG2	1:F:186:GLY:HA2	2.37	0.54
1:B:96:ASP:O	1:B:97:LYS:HG3	2.08	0.54
2:G:8:GLN:HG3	2:G:22:VAL:HB	1.89	0.54
1:D:141:ALA:O	3:D:301:NAP:H6N	2.08	0.53
1:B:187:PHE:CE2	1:B:204:TYR:CD2	2.97	0.53
1:F:22:ALA:O	1:F:32:VAL:HG11	2.08	0.53
1:C:150:MET:HG3	1:F:172:GLU:HG2	1.91	0.53
1:D:217:LYS:O	1:D:221:GLU:HG3	2.09	0.53
2:G:54:ILE:O	2:G:54:ILE:HG13	2.06	0.53
1:F:73:ALA:O	1:F:77:ILE:HD12	2.09	0.52
1:A:192:MET:HE1	3:A:301:NAP:H2D	1.90	0.52
1:C:11:THR:O	1:C:90:ASN:HB3	2.10	0.52
1:C:144:ILE:HD12	1:C:149:ASN:HB2	1.90	0.52
1:D:110:VAL:HG21	1:D:154:ASN:ND2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:THR:HB	1:B:134:PHE:CZ	2.45	0.52
1:A:1:MET:HE2	1:B:230:HIS:CD2	2.44	0.52
1:B:142:SER:HB2	3:B:301:NAP:H5N	1.90	0.52
1:D:47:LYS:O	1:D:51:GLU:HG2	2.09	0.52
1:D:101:LYS:O	1:D:101:LYS:HG2	2.10	0.52
1:A:2:GLN:OE1	1:A:229:ASP:OD2	2.27	0.52
1:E:85:SER:C	1:E:129:MET:HE2	2.35	0.52
1:F:143:ILE:HG21	1:F:186:GLY:HA2	1.92	0.52
2:G:36:SER:O	2:G:38:ASP:N	2.42	0.52
1:F:23:ARG:HA	1:F:50:LEU:HD21	1.92	0.51
1:B:124:GLU:OE1	1:B:127:LYS:HD2	2.09	0.51
1:C:176:ARG:NH2	2:I:37:LEU:HD13	2.21	0.51
1:D:168:SER:O	1:D:172:GLU:HG3	2.10	0.51
1:F:20:GLU:HA	1:F:23:ARG:HE	1.74	0.51
1:C:176:ARG:NH1	2:I:37:LEU:HD11	2.21	0.51
1:B:103:LYS:O	1:B:106:ASP:N	2.43	0.51
1:F:21:ILE:O	1:F:25:LEU:HD23	2.10	0.51
1:A:35:ASN:OD1	1:A:36:TYR:N	2.44	0.51
3:A:301:NAP:H51N	3:A:301:NAP:H52A	1.91	0.51
1:C:116:THR:O	1:C:120:ILE:HG12	2.11	0.51
1:D:102:MET:HE1	1:D:154:ASN:CG	2.36	0.51
1:D:3:PHE:HE2	1:D:28:MET:HB3	1.76	0.51
1:E:4:THR:HB	1:E:134:PHE:CZ	2.46	0.51
1:A:187:PHE:HD2	1:A:204:TYR:CD2	2.29	0.51
1:B:201:LYS:CD	5:B:403:HOH:O	1.87	0.51
1:E:31:LYS:NZ	1:E:81:ASP:OD1	2.44	0.50
1:D:86:TYR:HB3	1:D:227:LEU:HD22	1.93	0.50
1:D:4:THR:HB	1:D:134:PHE:CZ	2.47	0.50
1:C:115:LEU:CD2	1:F:107:PHE:HZ	2.24	0.50
1:A:125:ALA:HB1	1:A:129:MET:CE	2.41	0.50
1:E:144:ILE:HG22	1:E:156:SER:HB3	1.93	0.50
1:E:39:ASN:ND2	1:E:42:VAL:HB	2.27	0.50
1:F:12:GLY:N	1:F:35:ASN:HD22	2.03	0.49
2:G:24:PRO:O	2:G:65:VAL:HG13	2.12	0.49
1:C:115:LEU:HD22	1:F:107:PHE:CZ	2.47	0.49
1:D:47:LYS:HG2	1:D:57:ALA:CB	2.41	0.49
1:F:116:THR:O	1:F:120:ILE:HG13	2.12	0.49
1:D:62:PHE:HB2	1:D:69:ASP:HB3	1.94	0.49
1:B:104:THR:HG22	1:B:108:HIS:CD2	2.47	0.49
1:B:201:LYS:C	1:B:201:LYS:CD	2.85	0.49
1:E:204:TYR:C	1:E:206:LYS:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:HG12	1:F:21:ILE:HG22	1.95	0.49
1:B:179:ARG:NH1	1:B:231:SER:O	2.46	0.49
1:E:141:ALA:O	3:E:301:NAP:H6N	2.13	0.49
1:A:187:PHE:CE1	1:A:193:ASN:CG	2.91	0.48
1:F:62:PHE:CE2	1:F:70:PHE:CD1	3.01	0.48
1:A:179:ARG:NH2	1:A:226:LEU:O	2.47	0.48
1:E:147:ARG:NH2	5:E:401:HOH:O	2.36	0.48
1:B:86:TYR:HB3	1:B:227:LEU:HD22	1.94	0.48
1:F:77:ILE:O	1:F:81:ASP:HB2	2.12	0.48
1:C:89:ASN:HB2	1:C:139:ASN:HD22	1.78	0.48
1:F:205:VAL:HG22	1:F:213:LEU:HD21	1.95	0.48
2:I:44:MET:HB3	2:I:44:MET:HE3	1.79	0.48
1:A:154:ASN:OD1	1:A:155:TYR:N	2.45	0.48
1:C:115:LEU:HD22	1:F:107:PHE:HZ	1.79	0.48
1:A:70:PHE:HE1	1:A:74:ILE:HD11	1.78	0.47
1:A:187:PHE:HB2	4:A:302:UHC:C6	2.44	0.47
1:E:35:ASN:OD1	1:E:36:TYR:N	2.47	0.47
1:F:212:ARG:NH2	1:F:218:GLU:OE2	2.33	0.47
2:G:50:PHE:O	2:G:50:PHE:CD1	2.67	0.47
1:A:39:ASN:OD1	1:A:39:ASN:N	2.42	0.47
1:D:144:ILE:HG22	1:D:156:SER:HB3	1.97	0.47
1:E:39:ASN:HD22	1:E:42:VAL:HG23	1.79	0.47
1:F:49:GLU:O	1:F:53:LYS:HG3	2.15	0.47
1:A:239:LEU:HD13	1:B:239:LEU:HD13	1.96	0.47
1:E:87:LEU:HD12	1:E:88:VAL:H	1.79	0.47
2:G:64:ASN:ND2	2:G:64:ASN:C	2.72	0.47
1:C:230:HIS:HA	1:D:221:GLU:OE1	2.14	0.47
1:E:62:PHE:HB2	1:E:69:ASP:HB3	1.96	0.47
1:E:62:PHE:HE2	1:E:70:PHE:CD2	2.32	0.47
1:F:212:ARG:HH22	1:F:218:GLU:CD	2.20	0.47
1:E:67:GLU:O	1:E:71:VAL:HG23	2.15	0.47
1:C:62:PHE:HE2	1:C:70:PHE:CD2	2.33	0.47
1:C:48:ASN:O	1:C:51:GLU:N	2.48	0.47
1:D:9:LEU:HD22	1:D:77:ILE:HD12	1.97	0.47
1:F:61:LYS:O	1:F:62:PHE:HB3	2.15	0.47
1:D:11:THR:HA	1:D:35:ASN:HB3	1.98	0.46
1:F:139:ASN:ND2	1:F:166:SER:HB2	2.28	0.46
2:G:35:ASP:OD1	2:G:36:SER:N	2.49	0.46
1:D:95:ARG:NH1	1:D:106:ASP:HA	2.30	0.46
1:A:89:ASN:HB2	1:A:139:ASN:HD22	1.81	0.46
3:B:301:NAP:H2N	3:B:301:NAP:O1N	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:SER:O	1:E:129:MET:HE2	2.15	0.46
1:A:95:ARG:NH1	1:A:106:ASP:OD1	2.49	0.46
1:B:174:ALA:C	1:B:176:ARG:N	2.74	0.46
1:C:92:GLY:HA2	1:C:114:ASN:OD1	2.16	0.46
1:D:97:LYS:HG2	1:D:101:LYS:HD3	1.98	0.46
1:A:122:CYS:O	1:A:125:ALA:HB3	2.16	0.45
1:F:144:ILE:HD12	1:F:149:ASN:CB	2.45	0.45
1:E:99:ALA:HB2	1:E:153:THR:HG21	1.98	0.45
1:C:18:GLY:HA3	1:C:90:ASN:ND2	2.30	0.45
1:D:47:LYS:HD2	1:D:47:LYS:C	2.40	0.45
1:E:190:THR:HG21	3:E:301:NAP:H72N	1.82	0.45
1:C:15:LYS:HZ3	3:C:301:NAP:H3B	1.82	0.45
1:C:207:ASN:O	1:C:209:PRO:HD3	2.17	0.45
1:E:217:LYS:O	1:E:221:GLU:HG3	2.16	0.45
1:B:23:ARG:HA	1:B:50:LEU:HD21	1.98	0.45
1:E:119:PHE:HB2	1:E:165:MET:SD	2.56	0.45
1:A:8:VAL:HA	1:A:86:TYR:O	2.16	0.45
1:E:31:LYS:HG3	1:E:56:LYS:HB3	1.98	0.45
1:E:204:TYR:C	1:E:206:LYS:N	2.75	0.45
1:F:87:LEU:HG	1:F:88:VAL:N	2.30	0.45
1:F:132:SER:O	1:F:133:ARG:HG2	2.17	0.45
1:C:74:ILE:O	1:C:78:VAL:HG23	2.17	0.45
2:G:27:GLU:O	2:G:31:ASP:HB2	2.17	0.45
1:F:25:LEU:HD12	1:F:30:LEU:HD12	1.99	0.45
1:A:175:LEU:O	1:A:175:LEU:HD23	2.17	0.45
1:D:129:MET:HB3	1:D:134:PHE:O	2.17	0.45
1:C:67:GLU:O	1:C:71:VAL:HG23	2.17	0.44
1:D:96:ASP:OD1	1:D:152:GLN:HG2	2.17	0.44
1:F:11:THR:O	1:F:90:ASN:HB3	2.17	0.44
1:C:240:LYS:HB3	1:C:242:ASN:HD22	1.82	0.44
1:A:92:GLY:HA3	3:A:301:NAP:H3D	1.99	0.44
1:C:176:ARG:NH2	2:I:38:ASP:OD1	2.50	0.44
1:F:4:THR:HB	1:F:134:PHE:CZ	2.52	0.44
1:C:36:TYR:CZ	1:C:61:LYS:HB2	2.52	0.44
2:G:49:LYS:HE2	2:G:49:LYS:HB2	1.79	0.44
1:A:113:ASN:HD22	3:A:301:NAP:H61A	1.64	0.44
1:F:206:LYS:HD2	1:F:206:LYS:N	2.32	0.44
1:E:155:TYR:CZ	1:E:159:LYS:HE3	2.53	0.44
1:F:144:ILE:HD13	1:F:144:ILE:HA	1.70	0.44
1:C:183:VAL:HG12	1:C:185:PRO:HD3	1.99	0.44
1:E:188:ILE:HG23	1:E:214:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:38:ASP:OD1	2:I:38:ASP:N	2.48	0.44
1:A:41:GLU:H	1:A:41:GLU:HG3	1.61	0.43
1:B:102:MET:HG2	1:B:106:ASP:HB2	2.00	0.43
1:D:102:MET:HE1	1:D:154:ASN:HB3	1.99	0.43
1:D:125:ALA:O	1:D:129:MET:HG3	2.18	0.43
1:E:87:LEU:HD12	1:E:88:VAL:N	2.32	0.43
1:C:230:HIS:ND1	1:D:1:MET:HE2	2.33	0.43
1:D:24:THR:O	1:D:28:MET:HG3	2.18	0.43
1:E:183:VAL:O	1:E:185:PRO:HD3	2.18	0.43
1:A:90:ASN:HD21	3:A:301:NAP:H4D	1.82	0.43
1:A:103:LYS:O	1:A:106:ASP:N	2.52	0.43
1:D:47:LYS:HG2	1:D:57:ALA:HB1	2.00	0.43
1:E:175:LEU:HD12	1:E:175:LEU:H	1.83	0.43
1:B:40:ALA:O	1:B:41:GLU:C	2.61	0.43
1:C:126:LEU:HD23	1:C:126:LEU:HA	1.69	0.43
1:A:170:ALA:O	1:A:174:ALA:HB2	2.18	0.43
1:B:116:THR:O	1:B:120:ILE:HD12	2.19	0.43
1:C:226:LEU:HA	1:C:226:LEU:HD23	1.71	0.43
1:D:157:ALA:HB2	1:E:165:MET:HB2	2.00	0.43
1:C:13:ALA:HB3	1:C:34:ILE:HG23	2.01	0.42
1:B:96:ASP:OD1	1:B:152:GLN:HG2	2.18	0.42
1:C:125:ALA:HB1	1:C:129:MET:SD	2.59	0.42
1:A:44:ASP:OD1	1:A:59:VAL:HG21	2.19	0.42
1:C:9:LEU:O	1:C:87:LEU:HD12	2.19	0.42
1:E:175:LEU:O	1:E:176:ARG:HG3	2.19	0.42
1:B:37:ARG:NH1	1:B:37:ARG:HB3	2.33	0.42
1:C:97:LYS:HE3	1:C:97:LYS:HB2	1.81	0.42
1:E:15:LYS:HA	1:E:19:ALA:HB2	2.00	0.42
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.75	0.42
1:F:96:ASP:OD1	1:F:152:GLN:HG2	2.19	0.42
1:F:176:ARG:HG3	1:F:176:ARG:O	2.18	0.42
2:G:17:VAL:HB	2:G:21:GLN:HG3	2.02	0.42
1:C:36:TYR:HE1	1:C:59:VAL:CG1	2.32	0.42
1:A:139:ASN:HB3	1:A:162:MET:SD	2.60	0.42
1:B:25:LEU:HD21	1:B:227:LEU:CD1	2.49	0.42
1:C:35:ASN:HA	1:C:60:ILE:O	2.19	0.42
1:E:38:SER:O	1:E:39:ASN:C	2.60	0.42
1:D:217:LYS:HG2	1:D:221:GLU:OE2	2.19	0.42
1:F:144:ILE:HG21	1:F:155:TYR:CD2	2.46	0.42
1:B:226:LEU:HD23	1:B:226:LEU:HA	1.87	0.42
1:C:22:ALA:O	1:C:32:VAL:HG11	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:HD13	1:C:158:SER:HB3	2.01	0.42
1:C:131:LYS:HA	1:C:131:LYS:HD3	1.75	0.42
1:C:154:ASN:OD1	1:C:155:TYR:N	2.53	0.42
1:C:167:LYS:HG2	1:D:247:MET:HB3	2.02	0.42
1:D:39:ASN:HB3	5:D:408:HOH:O	2.19	0.42
1:E:17:ILE:O	1:E:21:ILE:HG13	2.19	0.42
1:F:66:SER:OG	1:F:69:ASP:HB3	2.19	0.42
1:F:144:ILE:CD1	1:F:149:ASN:HB2	2.49	0.42
1:F:179:ARG:HB3	1:F:235:THR:HG22	2.01	0.42
1:A:98:LEU:HD23	1:A:98:LEU:HA	1.88	0.42
1:E:190:THR:HG21	3:E:301:NAP:N7N	2.34	0.42
2:G:23:THR:CG2	2:G:26:ALA:HB2	2.50	0.42
2:G:46:LEU:HA	2:G:46:LEU:HD12	1.69	0.42
2:G:72:ILE:HD13	2:G:72:ILE:HA	1.90	0.42
1:C:35:ASN:ND2	1:C:62:PHE:CE2	2.88	0.42
1:F:126:LEU:HD23	1:F:126:LEU:HA	1.90	0.42
1:A:187:PHE:HE1	1:A:193:ASN:CG	2.28	0.41
1:D:144:ILE:HD12	1:D:149:ASN:HB2	2.02	0.41
1:F:210:LEU:O	1:F:212:ARG:HG2	2.20	0.41
1:B:170:ALA:HB2	1:B:180:PHE:HB2	2.01	0.41
1:C:159:LYS:HD3	1:C:162:MET:HE2	2.01	0.41
1:E:232:SER:HB2	1:F:218:GLU:OE2	2.21	0.41
1:F:17:ILE:O	1:F:21:ILE:HD12	2.20	0.41
1:A:178:ILE:HG22	1:A:180:PHE:CE1	2.55	0.41
1:C:241:VAL:HG22	1:D:234:ILE:HD11	2.01	0.41
2:H:42:LEU:HA	2:H:45:ALA:HB3	2.03	0.41
1:B:20:GLU:HA	1:B:20:GLU:OE1	2.19	0.41
1:D:6:LYS:HA	1:D:30:LEU:HD22	2.03	0.41
1:C:240:LYS:HB3	1:C:242:ASN:ND2	2.36	0.41
1:F:23:ARG:HG2	1:F:50:LEU:HD21	2.02	0.41
1:D:84:LEU:HD12	1:D:84:LEU:HA	1.82	0.41
1:D:131:LYS:HG3	1:D:132:SER:H	1.85	0.41
1:E:62:PHE:HE2	1:E:70:PHE:CE2	2.38	0.41
1:E:167:LYS:O	1:E:171:TYR:HD1	2.03	0.41
1:B:140:ILE:O	1:B:162:MET:HE1	2.21	0.41
1:F:13:ALA:HB3	1:F:34:ILE:HG23	2.03	0.41
1:D:97:LYS:HE2	1:D:101:LYS:NZ	2.36	0.41
2:G:18:ASP:OD1	2:G:18:ASP:N	2.54	0.41
1:A:233:TYR:CE2	1:B:214:GLY:HA3	2.55	0.41
1:B:23:ARG:HE	1:B:23:ARG:HB2	1.52	0.41
1:C:126:LEU:HD12	1:F:99:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ARG:HA	1:D:50:LEU:HD11	2.03	0.41
1:D:203:ASP:OD1	5:D:401:HOH:O	2.22	0.41
1:E:11:THR:HA	1:E:35:ASN:HD22	1.86	0.41
1:F:17:ILE:CD1	1:F:188:ILE:HG21	2.44	0.41
1:F:242:ASN:OD1	1:F:245:LEU:N	2.53	0.41
2:G:49:LYS:O	2:G:49:LYS:CG	2.69	0.41
2:I:38:ASP:C	2:I:42:LEU:HD13	2.39	0.41
1:C:16:GLY:HA3	3:C:301:NAP:O2N	2.21	0.41
1:C:31:LYS:NZ	1:C:81:ASP:OD1	2.51	0.41
1:C:126:LEU:O	1:C:130:SER:OG	2.34	0.41
1:D:154:ASN:OD1	1:D:155:TYR:N	2.54	0.41
1:E:140:ILE:C	1:E:162:MET:HE1	2.46	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.65	0.40
1:B:37:ARG:HB3	1:B:37:ARG:HH11	1.86	0.40
1:C:183:VAL:HG21	1:C:223:VAL:HG22	2.02	0.40
1:D:2:GLN:HB3	1:D:230:HIS:CE1	2.56	0.40
1:E:10:ILE:HG22	1:E:13:ALA:HB2	2.02	0.40
1:A:138:VAL:HG11	1:A:223:VAL:HG22	2.03	0.40
1:B:12:GLY:N	1:B:35:ASN:OD1	2.45	0.40
1:E:239:LEU:HD12	1:F:237:GLU:HG2	2.04	0.40
1:E:190:THR:O	1:E:190:THR:CG2	2.66	0.40
1:A:136:SER:OG	1:A:227:LEU:HA	2.21	0.40
1:D:34:ILE:HD12	1:D:47:LYS:HB2	2.03	0.40
1:D:134:PHE:CD1	1:D:135:GLY:N	2.89	0.40
1:D:159:LYS:O	1:D:163:ILE:HG13	2.21	0.40
1:C:103:LYS:O	1:C:106:ASP:N	2.54	0.40
1:F:26:ALA:HA	1:F:30:LEU:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ARG:NH2	2:G:37:LEU:CD1[3_455]	1.64	0.56

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/248 (99%)	234 (95%)	12 (5%)	0	100	100
1	B	233/248 (94%)	220 (94%)	13 (6%)	0	100	100
1	C	232/248 (94%)	219 (94%)	13 (6%)	0	100	100
1	D	233/248 (94%)	214 (92%)	18 (8%)	1 (0%)	30	40
1	E	233/248 (94%)	211 (91%)	22 (9%)	0	100	100
1	F	229/248 (92%)	210 (92%)	19 (8%)	0	100	100
2	G	71/75 (95%)	59 (83%)	11 (16%)	1 (1%)	9	11
2	H	11/75 (15%)	10 (91%)	1 (9%)	0	100	100
2	I	7/75 (9%)	6 (86%)	1 (14%)	0	100	100
All	All	1495/1713 (87%)	1383 (92%)	110 (7%)	2 (0%)	48	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	35	ASP
1	D	186	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/197 (100%)	194 (98%)	3 (2%)	57	75
1	B	187/197 (95%)	182 (97%)	5 (3%)	39	59
1	C	187/197 (95%)	185 (99%)	2 (1%)	65	81
1	D	187/197 (95%)	187 (100%)	0	100	100
1	E	188/197 (95%)	186 (99%)	2 (1%)	65	81
1	F	184/197 (93%)	184 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	62/63 (98%)	52 (84%)	10 (16%)	2	3
2	H	13/63 (21%)	13 (100%)	0	100	100
2	I	8/63 (13%)	7 (88%)	1 (12%)	4	5
All	All	1213/1371 (88%)	1190 (98%)	23 (2%)	50	69

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	42	VAL
1	A	144	ILE
1	B	130	SER
1	B	132	SER
1	B	133	ARG
1	B	201	LYS
1	B	206	LYS
1	C	35	ASN
1	C	143	ILE
1	E	190	THR
1	E	191	ASP
2	G	15	LEU
2	G	36	SER
2	G	43	ILE
2	G	46	LEU
2	G	52	ILE
2	G	54	ILE
2	G	57	GLU
2	G	62	ILE
2	G	63	VAL
2	G	65	VAL
2	I	37	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	113	ASN
1	A	139	ASN
1	B	230	HIS
1	C	39	ASN

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	139	ASN
1	D	2	GLN
1	D	35	ASN
1	F	35	ASN
1	F	108	HIS
2	G	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	F	301	-	50,52,52	1.33	6 (12%)	71,80,80	1.62	14 (19%)
3	NAP	A	301	-	50,52,52	1.34	4 (8%)	71,80,80	1.69	14 (19%)
3	NAP	E	301	-	50,52,52	1.36	5 (10%)	71,80,80	1.72	17 (23%)
3	NAP	C	301	-	50,52,52	1.34	5 (10%)	71,80,80	1.90	25 (35%)
4	UHC	A	302	-	22,28,31	0.96	2 (9%)	28,36,41	1.90	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	D	301	-	50,52,52	1.20	4 (8%)	71,80,80	1.52	12 (16%)
3	NAP	B	301	-	50,52,52	1.20	5 (10%)	71,80,80	1.79	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
3	NAP	F	301	-	-	14/35/67/67	0/5/5/5
3	NAP	A	301	-	-	8/35/67/67	0/5/5/5
3	NAP	E	301	-	-	7/35/67/67	0/5/5/5
3	NAP	C	301	-	-	10/35/67/67	0/5/5/5
4	UHC	A	302	-	-	20/34/36/39	-
3	NAP	D	301	-	-	12/35/67/67	0/5/5/5
3	NAP	B	301	-	-	11/35/67/67	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	NAP	PA-O3	4.99	1.64	1.59
3	A	301	NAP	PA-O3	4.66	1.64	1.59
3	C	301	NAP	PA-O3	4.47	1.64	1.59
3	D	301	NAP	PA-O3	4.19	1.64	1.59
3	E	301	NAP	PN-O3	4.07	1.63	1.59
3	F	301	NAP	PA-O3	3.94	1.63	1.59
3	C	301	NAP	C3N-C7N	3.93	1.56	1.50
3	F	301	NAP	C2N-N1N	3.90	1.39	1.35
3	F	301	NAP	C6N-N1N	-3.79	1.26	1.35
3	C	301	NAP	C2N-N1N	3.76	1.39	1.35
3	E	301	NAP	C6N-N1N	-3.74	1.26	1.35
3	A	301	NAP	C2N-N1N	3.68	1.39	1.35
3	C	301	NAP	PN-O3	3.53	1.63	1.59
3	A	301	NAP	C6N-N1N	-3.52	1.27	1.35
3	B	301	NAP	C6N-N1N	-3.51	1.27	1.35
3	B	301	NAP	PA-O3	3.47	1.63	1.59
3	A	301	NAP	PN-O3	3.41	1.63	1.59
3	D	301	NAP	C6N-N1N	-3.37	1.27	1.35
3	B	301	NAP	C2N-N1N	3.26	1.38	1.35
3	D	301	NAP	C2N-N1N	3.11	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	NAP	PN-O3	3.09	1.62	1.59
3	C	301	NAP	C6N-N1N	-3.08	1.28	1.35
3	E	301	NAP	C2N-N1N	2.93	1.38	1.35
3	F	301	NAP	C3N-C7N	2.79	1.54	1.50
3	D	301	NAP	PN-O3	2.79	1.62	1.59
3	B	301	NAP	PN-O3	2.41	1.62	1.59
3	E	301	NAP	O4D-C4D	-2.35	1.39	1.45
3	B	301	NAP	C3N-C7N	2.30	1.54	1.50
4	A	302	UHC	O3-C3	-2.15	1.18	1.21
4	A	302	UHC	O1-C1	-2.11	1.17	1.21
3	F	301	NAP	C2N-C3N	2.11	1.42	1.39

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	NAP	O2B-C2B-C3B	6.90	136.43	111.68
3	E	301	NAP	O2B-C2B-C3B	6.86	136.27	111.68
3	A	301	NAP	O2B-C2B-C3B	6.72	135.79	111.68
3	C	301	NAP	O2B-C2B-C3B	6.71	135.76	111.68
3	D	301	NAP	O2B-C2B-C3B	6.48	134.94	111.68
3	B	301	NAP	O2B-C2B-C3B	6.28	134.20	111.68
4	A	302	UHC	C30-C29-C32	5.61	118.34	108.77
3	A	301	NAP	C6N-N1N-C2N	-5.37	117.31	121.88
3	B	301	NAP	C6N-N1N-C2N	-4.80	117.80	121.88
3	C	301	NAP	O4B-C1B-N9A	4.49	116.72	108.09
3	B	301	NAP	O2X-P2B-O2B	-4.42	88.63	105.85
3	A	301	NAP	C5N-C4N-C3N	-4.10	116.33	120.36
3	B	301	NAP	C5N-C4N-C3N	-4.09	116.35	120.36
3	C	301	NAP	O2D-C2D-C3D	-3.90	99.30	111.82
4	A	302	UHC	O3-C3-C2	-3.86	115.24	121.20
3	E	301	NAP	O2D-C2D-C3D	-3.70	99.96	111.82
3	D	301	NAP	P2B-O2B-C2B	3.65	133.18	123.43
3	C	301	NAP	O7N-C7N-N7N	-3.57	117.46	122.62
3	C	301	NAP	P2B-O2B-C2B	3.54	132.89	123.43
3	E	301	NAP	C6N-N1N-C2N	-3.44	118.95	121.88
3	E	301	NAP	C4D-O4D-C1D	-3.43	106.78	109.92
3	E	301	NAP	O2X-P2B-O2B	-3.42	92.52	105.85
3	A	301	NAP	O2N-PN-O3	3.35	116.32	107.27
3	C	301	NAP	C2N-C3N-C4N	-3.33	114.38	118.26
3	F	301	NAP	O4B-C1B-N9A	3.30	114.43	108.09
3	D	301	NAP	O2X-P2B-O2B	-3.29	93.04	105.85
3	B	301	NAP	O3D-C3D-C4D	3.26	120.46	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	NAP	O3D-C3D-C4D	3.26	120.45	111.08
3	C	301	NAP	PA-O5B-C5B	-3.23	102.82	121.35
3	B	301	NAP	O4B-C1B-C2B	-3.20	101.08	106.59
3	A	301	NAP	O2X-P2B-O2B	-3.20	93.39	105.85
3	B	301	NAP	O2B-C2B-C1B	3.16	121.17	110.05
3	F	301	NAP	P2B-O2B-C2B	3.12	131.76	123.43
3	D	301	NAP	O2D-C2D-C3D	-3.06	102.01	111.82
3	F	301	NAP	O2D-C2D-C3D	-2.99	102.24	111.82
3	F	301	NAP	O2X-P2B-O2B	-2.96	94.30	105.85
3	E	301	NAP	C2D-C3D-C4D	2.96	108.33	102.61
3	A	301	NAP	C6N-C5N-C4N	-2.94	115.21	119.45
3	F	301	NAP	O2B-C2B-C1B	2.90	120.25	110.05
4	A	302	UHC	C30-C29-C28	-2.87	103.48	108.22
3	C	301	NAP	C3B-C2B-C1B	-2.86	97.34	102.81
3	B	301	NAP	O2D-C2D-C3D	-2.83	102.76	111.82
3	A	301	NAP	O2D-C2D-C3D	-2.78	102.90	111.82
3	E	301	NAP	O2N-PN-O3	2.76	114.73	107.27
3	B	301	NAP	O7N-C7N-C3N	2.75	122.96	119.60
3	D	301	NAP	O2A-PA-O1A	2.74	125.19	112.44
3	A	301	NAP	P2B-O2B-C2B	2.73	130.72	123.43
3	E	301	NAP	O5D-C5D-C4D	2.72	118.25	108.99
3	B	301	NAP	O3-PN-O1N	-2.71	102.56	110.70
3	C	301	NAP	O2B-C2B-C1B	2.69	119.51	110.05
3	C	301	NAP	O2X-P2B-O2B	-2.68	95.42	105.85
3	D	301	NAP	C6N-N1N-C2N	-2.66	119.61	121.88
4	A	302	UHC	C31-C29-C28	-2.64	103.87	108.22
3	F	301	NAP	O4B-C1B-C2B	-2.64	102.05	106.59
3	E	301	NAP	O3-PN-O1N	-2.62	102.82	110.70
3	C	301	NAP	C4B-O4B-C1B	-2.61	103.71	109.47
3	F	301	NAP	O3D-C3D-C4D	2.58	118.49	111.08
3	B	301	NAP	C2B-C3B-C4B	-2.57	96.48	101.99
3	C	301	NAP	O3D-C3D-C4D	2.55	118.41	111.08
3	A	301	NAP	O5D-C5D-C4D	2.55	117.67	108.99
3	B	301	NAP	C2B-C1B-N9A	2.52	117.89	113.75
3	E	301	NAP	O3D-C3D-C4D	2.49	118.23	111.08
4	A	302	UHC	C6-C5-C4	-2.48	102.21	112.69
3	E	301	NAP	O2B-C2B-C1B	2.46	118.69	110.05
3	A	301	NAP	O2B-C2B-C1B	2.43	118.61	110.05
3	B	301	NAP	O2N-PN-O3	2.43	113.85	107.27
3	D	301	NAP	PA-O5B-C5B	-2.41	107.52	121.35
3	E	301	NAP	O4B-C1B-C2B	-2.41	102.44	106.59
4	A	302	UHC	C43-S1-C1	-2.39	94.77	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	NAP	C5N-C6N-N1N	-2.35	117.18	120.38
3	B	301	NAP	O3X-P2B-O2X	2.34	116.57	107.80
4	A	302	UHC	C37-C38-C39	-2.34	108.50	112.39
3	B	301	NAP	O2A-PA-O1A	2.34	123.31	112.44
3	D	301	NAP	O4B-C4B-C3B	2.32	109.75	105.15
3	C	301	NAP	O2A-PA-O1A	2.31	123.19	112.44
3	C	301	NAP	O3X-P2B-O2X	2.31	116.45	107.80
3	C	301	NAP	C4A-N9A-C1B	-2.30	121.26	126.63
3	B	301	NAP	C2N-C3N-C4N	-2.21	115.69	118.26
3	F	301	NAP	C6N-C5N-C4N	-2.21	116.27	119.45
3	C	301	NAP	C2B-C1B-N9A	2.19	117.35	113.75
3	F	301	NAP	C6N-N1N-C2N	-2.18	120.02	121.88
3	C	301	NAP	C6N-N1N-C2N	-2.18	120.02	121.88
3	A	301	NAP	O3D-C3D-C4D	2.18	117.34	111.08
3	B	301	NAP	C3B-C2B-C1B	-2.16	98.67	102.81
3	D	301	NAP	C5N-C4N-C3N	-2.16	118.25	120.36
3	C	301	NAP	O3-PA-O1A	-2.16	104.22	110.70
3	F	301	NAP	C4D-O4D-C1D	-2.14	107.96	109.92
3	C	301	NAP	O7N-C7N-C3N	2.14	122.22	119.60
3	A	301	NAP	O2A-PA-O1A	2.13	122.35	112.44
3	C	301	NAP	O2N-PN-O3	2.11	112.98	107.27
3	C	301	NAP	O4B-C1B-C2B	2.11	110.22	106.59
3	C	301	NAP	O5D-C5D-C4D	2.10	116.16	108.99
3	E	301	NAP	O7N-C7N-C3N	2.10	122.17	119.60
3	C	301	NAP	C3N-C7N-N7N	2.10	120.32	117.74
3	F	301	NAP	O3-PA-O1A	-2.09	104.41	110.70
3	D	301	NAP	C5N-C6N-N1N	2.09	123.23	120.38
3	D	301	NAP	O2N-PN-O3	2.08	112.89	107.27
3	C	301	NAP	O3-PN-O1N	-2.08	104.46	110.70
3	E	301	NAP	O2A-PA-O1A	2.07	122.10	112.44
3	A	301	NAP	C4B-O4B-C1B	-2.05	104.94	109.47
3	E	301	NAP	O2N-PN-O5D	2.05	116.85	107.57
3	E	301	NAP	O3D-C3D-C2D	-2.04	105.28	111.82
3	E	301	NAP	C5N-C4N-C3N	-2.03	118.37	120.36
3	C	301	NAP	C1B-N9A-C8A	2.02	131.59	127.09
3	A	301	NAP	O3-PN-O1N	-2.02	104.63	110.70
3	F	301	NAP	O2A-PA-O1A	2.01	121.82	112.44

There are no chirality outliers.

All (82) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NAP	C3B-C2B-O2B-P2B
3	A	301	NAP	O4D-C1D-N1N-C2N
3	B	301	NAP	C3B-C2B-O2B-P2B
3	B	301	NAP	O4D-C4D-C5D-O5D
3	B	301	NAP	C3D-C4D-C5D-O5D
3	B	301	NAP	O4D-C1D-N1N-C2N
3	C	301	NAP	C5B-O5B-PA-O1A
3	C	301	NAP	C3B-C2B-O2B-P2B
3	C	301	NAP	C5D-O5D-PN-O1N
3	D	301	NAP	C5B-O5B-PA-O2A
3	D	301	NAP	C3B-C2B-O2B-P2B
3	D	301	NAP	C5D-O5D-PN-O1N
3	E	301	NAP	C3B-C2B-O2B-P2B
3	E	301	NAP	O4D-C4D-C5D-O5D
3	F	301	NAP	C3B-C2B-O2B-P2B
3	F	301	NAP	O4D-C4D-C5D-O5D
3	F	301	NAP	C3D-C4D-C5D-O5D
3	F	301	NAP	O4D-C1D-N1N-C2N
3	F	301	NAP	O4D-C1D-N1N-C6N
4	A	302	UHC	O1-C1-S1-C43
4	A	302	UHC	C2-C1-S1-C43
4	A	302	UHC	C28-C29-C32-O33
4	A	302	UHC	C28-C29-C32-C34
4	A	302	UHC	C30-C29-C32-O33
4	A	302	UHC	C30-C29-C32-C34
4	A	302	UHC	C31-C29-C32-O33
4	A	302	UHC	C31-C29-C32-C34
4	A	302	UHC	N41-C42-C43-S1
4	A	302	UHC	C38-C39-N41-C42
3	A	301	NAP	O4D-C4D-C5D-O5D
3	D	301	NAP	O4D-C4D-C5D-O5D
3	D	301	NAP	C3D-C4D-C5D-O5D
3	E	301	NAP	C3D-C4D-C5D-O5D
4	A	302	UHC	O3-C3-C4-C5
4	A	302	UHC	C2-C3-C4-C5
4	A	302	UHC	O40-C39-N41-C42
3	A	301	NAP	C3D-C4D-C5D-O5D
3	C	301	NAP	O4D-C4D-C5D-O5D
3	C	301	NAP	C1B-C2B-O2B-P2B
4	A	302	UHC	C3-C4-C5-C6
3	C	301	NAP	C3B-C4B-C5B-O5B
3	D	301	NAP	O4B-C4B-C5B-O5B
4	A	302	UHC	O33-C32-C34-O35

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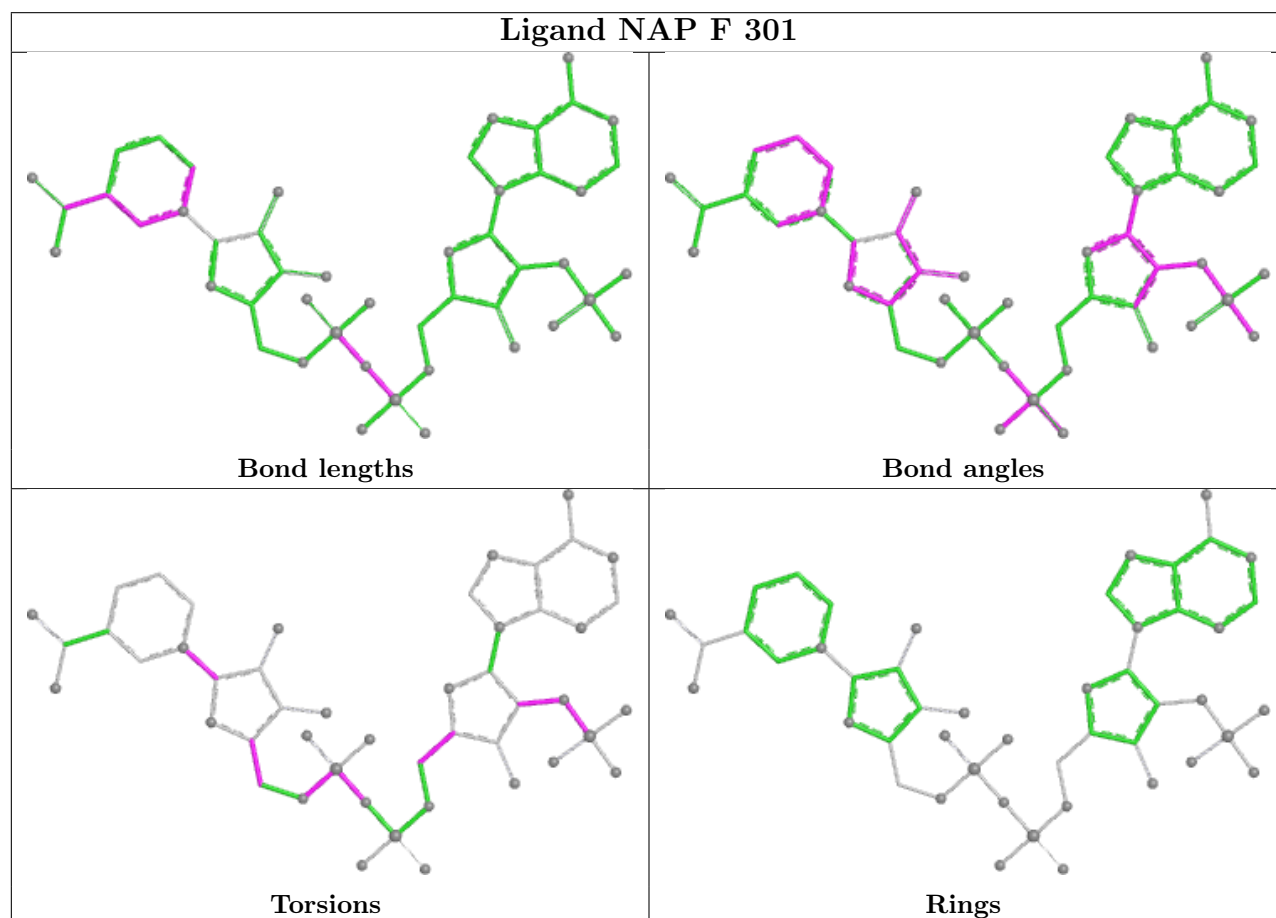
Mol	Chain	Res	Type	Atoms
3	C	301	NAP	C3D-C4D-C5D-O5D
3	D	301	NAP	C3B-C4B-C5B-O5B
3	C	301	NAP	O4B-C4B-C5B-O5B
4	A	302	UHC	N36-C37-C38-C39
4	A	302	UHC	C1-C2-C3-O3
3	B	301	NAP	PA-O3-PN-O2N
4	A	302	UHC	C42-C43-S1-C1
3	A	301	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C5D-O5D-PN-O3
3	B	301	NAP	C5D-O5D-PN-O1N
3	B	301	NAP	C5D-O5D-PN-O2N
3	C	301	NAP	C5D-O5D-PN-O3
3	D	301	NAP	C5B-O5B-PA-O3
3	D	301	NAP	C5D-O5D-PN-O3
3	D	301	NAP	C5D-O5D-PN-O2N
3	F	301	NAP	C5D-O5D-PN-O3
3	F	301	NAP	C5D-O5D-PN-O1N
3	F	301	NAP	C5D-O5D-PN-O2N
3	E	301	NAP	C4N-C3N-C7N-O7N
3	E	301	NAP	C4D-C5D-O5D-PN
4	A	302	UHC	O1-C1-C2-C3
3	E	301	NAP	C4N-C3N-C7N-N7N
3	A	301	NAP	PA-O3-PN-O1N
3	D	301	NAP	PA-O3-PN-O1N
3	F	301	NAP	PA-O3-PN-O2N
3	A	301	NAP	C2D-C1D-N1N-C2N
3	B	301	NAP	C2D-C1D-N1N-C2N
3	F	301	NAP	C2D-C1D-N1N-C6N
3	D	301	NAP	C1B-C2B-O2B-P2B
3	A	301	NAP	O4D-C1D-N1N-C6N
3	C	301	NAP	O4D-C1D-N1N-C2N
3	F	301	NAP	C2B-O2B-P2B-O1X
3	F	301	NAP	O4B-C4B-C5B-O5B
3	B	301	NAP	PA-O3-PN-O1N
3	F	301	NAP	PA-O3-PN-O1N
3	F	301	NAP	C2B-O2B-P2B-O2X
3	B	301	NAP	O4B-C4B-C5B-O5B
3	E	301	NAP	C2B-O2B-P2B-O1X
4	A	302	UHC	O33-C32-C34-N36

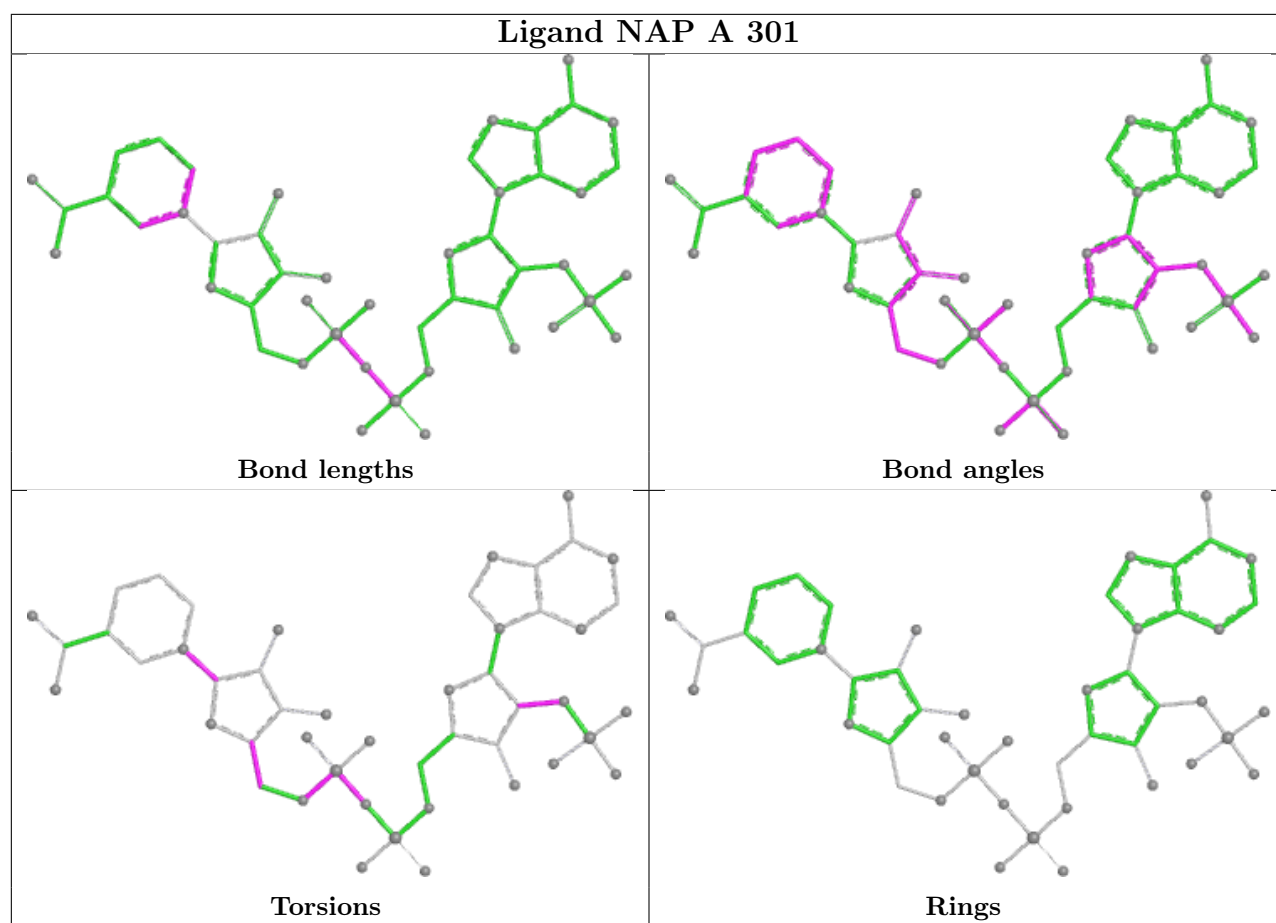
There are no ring outliers.

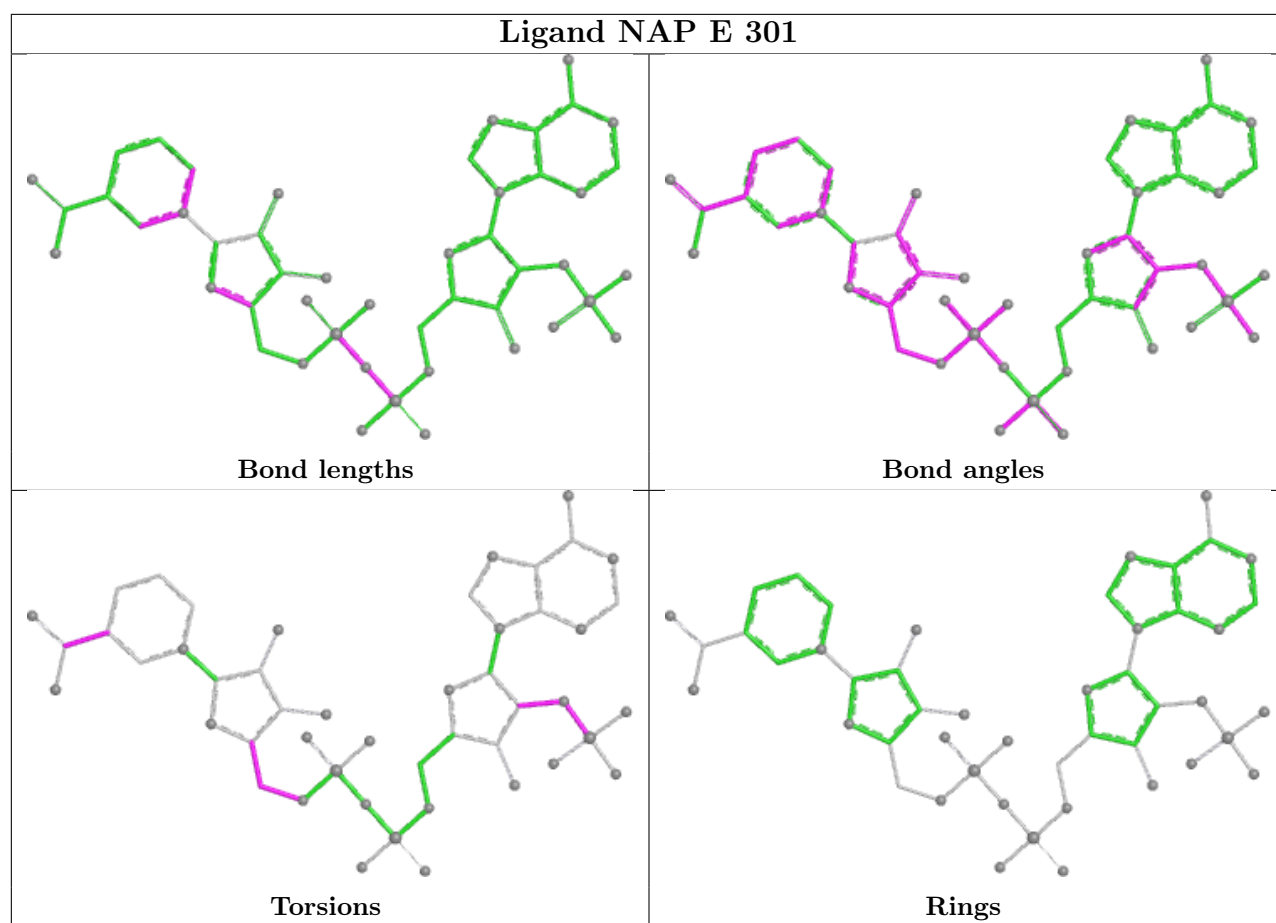
7 monomers are involved in 27 short contacts:

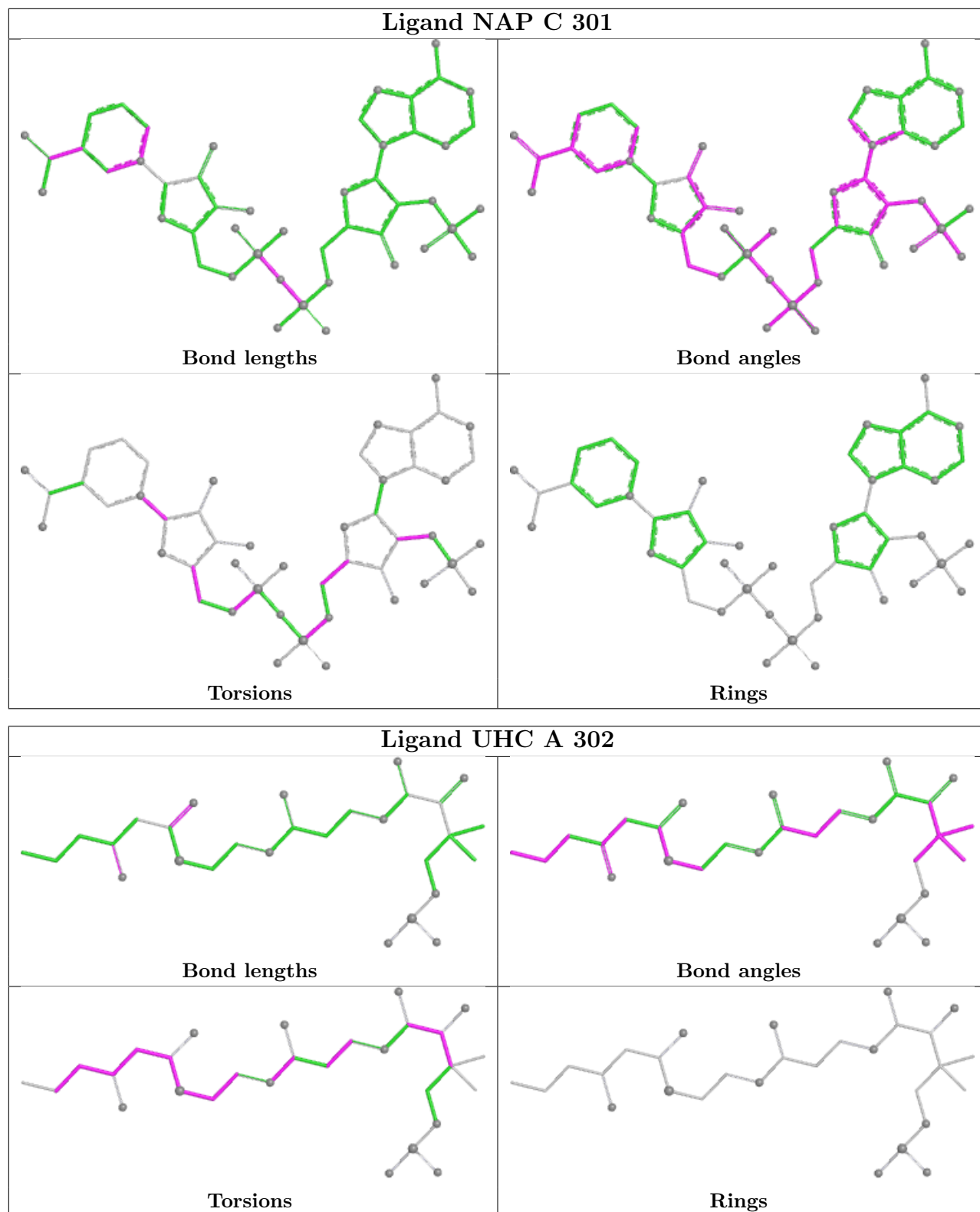
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	NAP	1	0
3	A	301	NAP	7	0
3	E	301	NAP	3	0
3	C	301	NAP	5	0
4	A	302	UHC	3	0
3	D	301	NAP	3	0
3	B	301	NAP	5	0

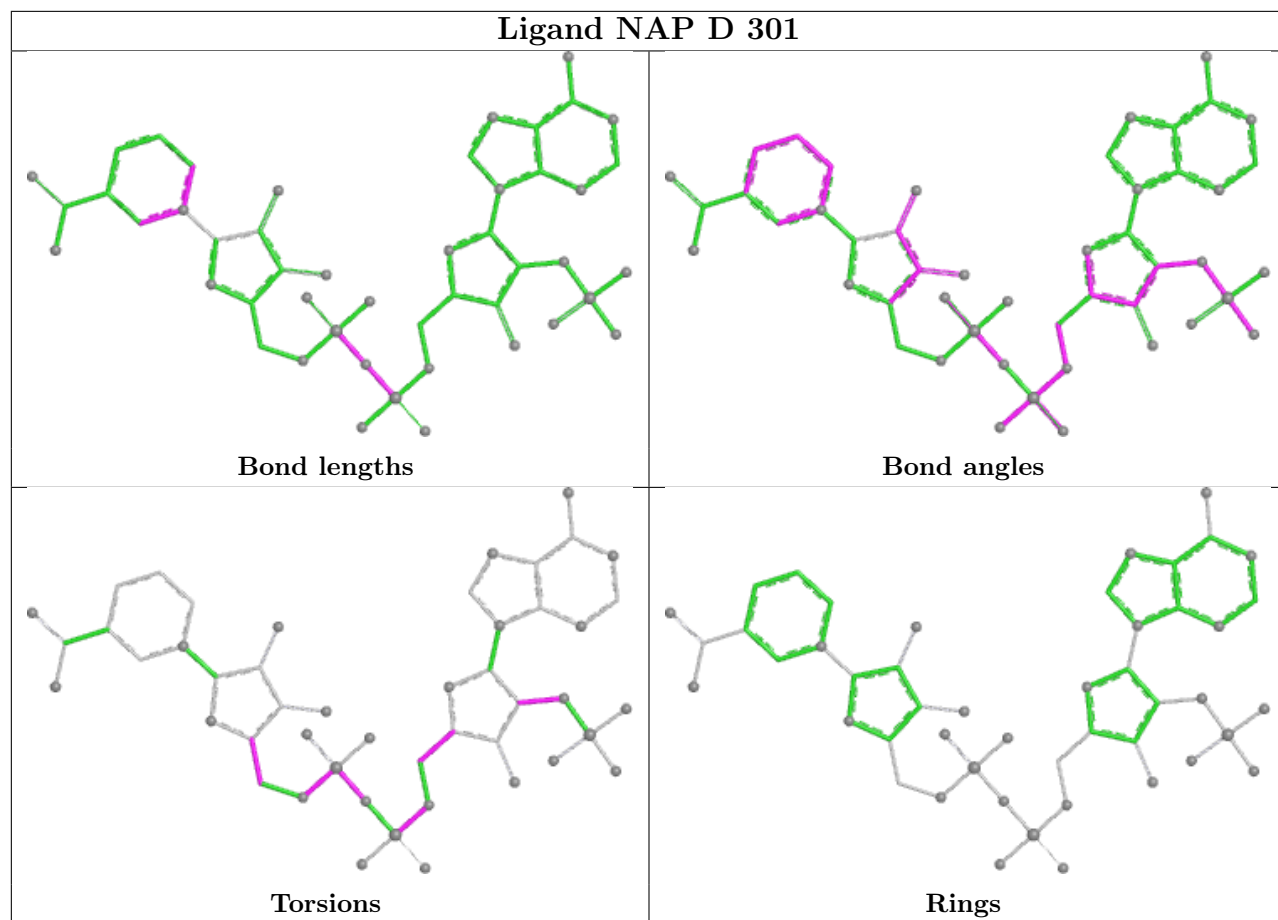
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

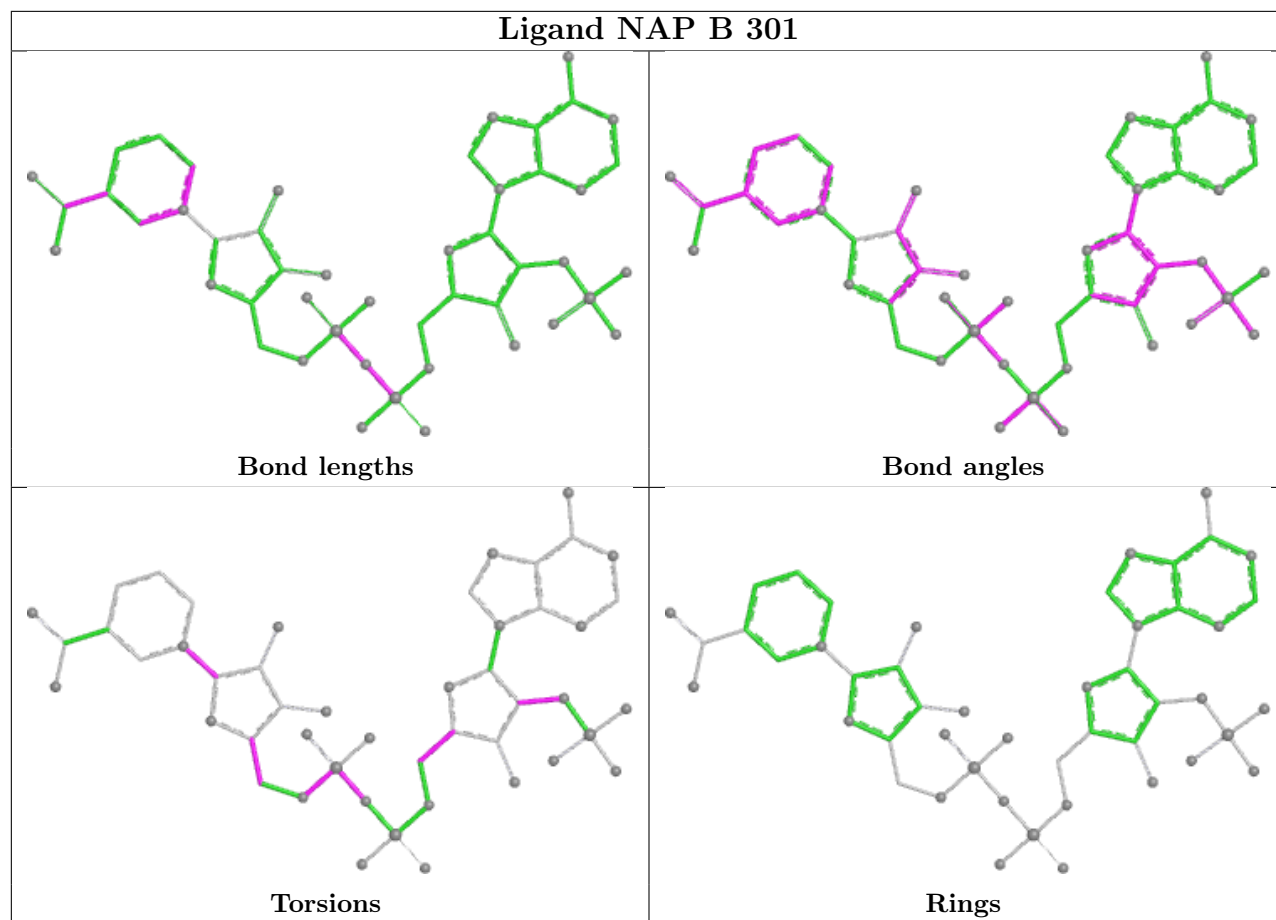












5.7 Other polymers [i](#)

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	248/248 (100%)	0.37	9 (3%) 46 46	20, 35, 74, 103	0
1	B	237/248 (95%)	0.41	10 (4%) 40 40	21, 38, 59, 79	0
1	C	236/248 (95%)	0.44	7 (2%) 52 52	24, 42, 62, 76	0
1	D	237/248 (95%)	0.73	12 (5%) 33 33	30, 50, 68, 92	0
1	E	237/248 (95%)	0.66	10 (4%) 40 40	31, 48, 69, 91	0
1	F	233/248 (93%)	0.86	23 (9%) 13 11	33, 52, 78, 97	0
2	G	73/75 (97%)	1.45	18 (24%) 2 1	53, 76, 91, 102	0
2	H	15/75 (20%)	2.16	8 (53%) 0 0	78, 89, 100, 107	0
2	I	9/75 (12%)	2.26	5 (55%) 0 0	74, 79, 86, 86	0
All	All	1525/1713 (89%)	0.65	102 (6%) 24 22	20, 45, 78, 107	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	ALA	6.4
1	F	112	ASP	6.2
1	D	202	ALA	5.1
2	G	28	PHE	4.5
2	G	52	ILE	4.5
1	F	58	ALA	4.5
2	H	63	VAL	4.3
1	F	22	ALA	4.2
2	I	45	ALA	4.1
1	E	191	ASP	4.1
1	D	13	ALA	4.1
2	G	37	LEU	4.1
1	D	204	TYR	4.1
2	H	65	VAL	4.0
1	D	96	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	G	51	GLY	3.8
1	A	204	TYR	3.7
1	C	112	ASP	3.7
1	D	30	LEU	3.6
1	A	187	PHE	3.6
1	E	204	TYR	3.5
1	E	190	THR	3.5
2	G	54	ILE	3.5
1	D	56	LYS	3.4
2	G	7	ILE	3.4
2	I	37	LEU	3.2
2	I	39	VAL	3.2
1	E	205	VAL	3.1
1	F	46	LEU	3.0
1	F	13	ALA	2.9
2	G	6	ASP	2.9
1	F	50	LEU	2.9
2	H	45	ALA	2.9
1	D	87	LEU	2.8
1	F	14	SER	2.8
1	D	43	ALA	2.7
1	E	57	ALA	2.7
1	F	25	LEU	2.7
2	I	42	LEU	2.7
1	B	202	ALA	2.7
1	F	45	ALA	2.7
1	F	42	VAL	2.7
2	H	62	ILE	2.7
2	G	4	PHE	2.6
2	G	50	PHE	2.6
2	G	74	ASP	2.6
1	F	111	ILE	2.6
1	F	108	HIS	2.6
2	G	72	ILE	2.6
1	D	58	ALA	2.5
2	G	53	GLU	2.5
1	C	190	THR	2.5
1	B	70	PHE	2.5
1	B	205	VAL	2.5
1	A	196	LEU	2.5
1	A	202	ALA	2.5
2	G	11	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	37	LEU	2.4
1	E	105	GLU	2.4
2	G	65	VAL	2.4
2	H	42	LEU	2.4
1	C	204	TYR	2.4
1	A	70	PHE	2.4
2	G	73	GLU	2.4
1	A	191	ASP	2.3
1	F	43	ALA	2.3
1	F	34	ILE	2.3
1	C	203	ASP	2.3
1	D	116	THR	2.3
2	G	69	VAL	2.3
2	H	64	ASN	2.3
1	B	204	TYR	2.3
1	E	121	GLY	2.3
1	F	73	ALA	2.3
2	H	43	ILE	2.3
1	B	94	VAL	2.3
1	F	40	ALA	2.3
1	E	84	LEU	2.2
2	G	68	VAL	2.3
1	A	200	LEU	2.2
1	C	57	ALA	2.2
1	C	64	ALA	2.2
1	F	61	LYS	2.2
1	A	44	ASP	2.2
1	C	148	GLY	2.2
1	B	46	LEU	2.2
1	F	21	ILE	2.2
1	B	201	LYS	2.2
1	B	14	SER	2.1
1	F	59	VAL	2.1
1	F	205	VAL	2.1
1	E	14	SER	2.1
1	E	188	ILE	2.1
1	F	39	ASN	2.1
1	A	133	ARG	2.1
1	D	131	LYS	2.0
2	G	42	LEU	2.0
1	F	32	VAL	2.0
2	I	40	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	206	LYS	2.0
1	B	64	ALA	2.0
1	B	74	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

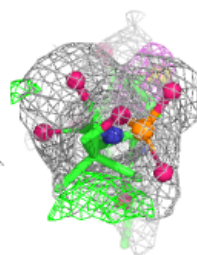
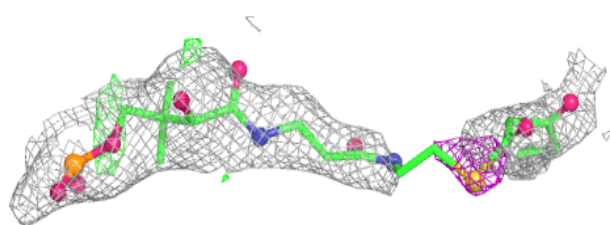
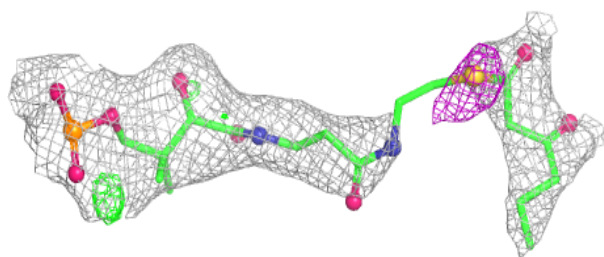
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	UHC	A	302	29/32	0.77	0.17	45,59,91,102	0
3	NAP	C	301	48/48	0.80	0.11	42,63,82,98	0
3	NAP	F	301	48/48	0.85	0.11	50,65,87,102	0
3	NAP	D	301	48/48	0.87	0.10	46,58,79,83	0
3	NAP	B	301	48/48	0.89	0.09	34,53,73,83	0
3	NAP	E	301	48/48	0.93	0.08	38,49,62,71	0
3	NAP	A	301	48/48	0.95	0.07	29,37,48,53	0

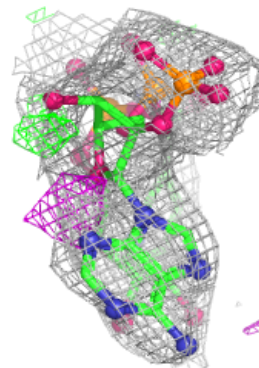
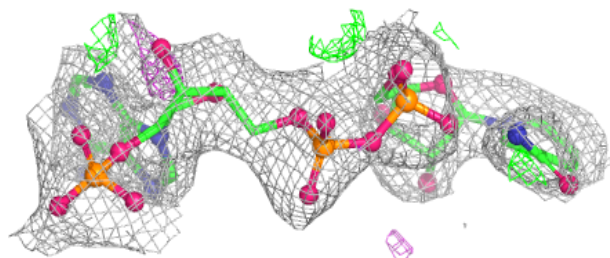
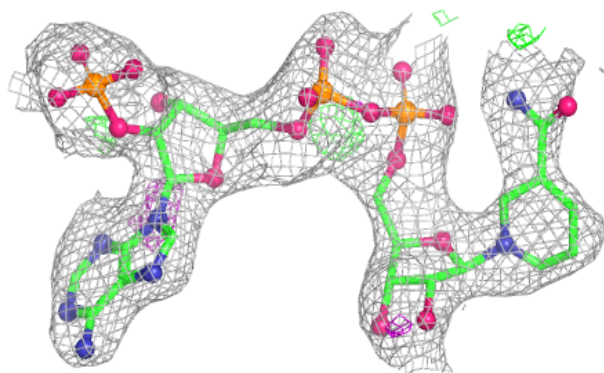
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UHC A 302:

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

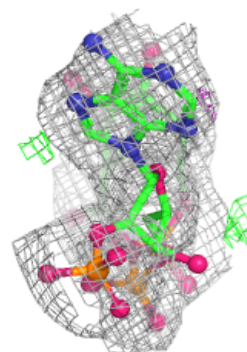
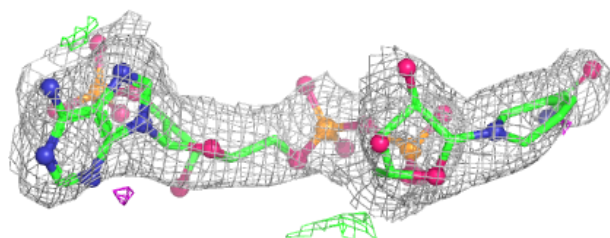
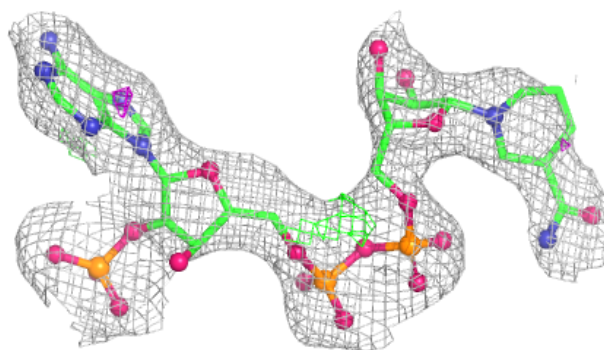
**Electron density around NAP C 301:**

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

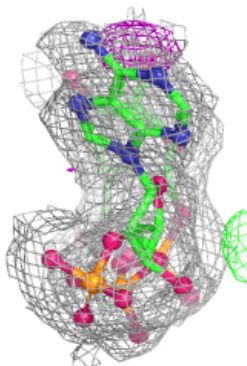
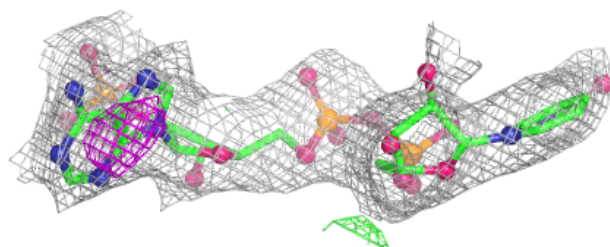
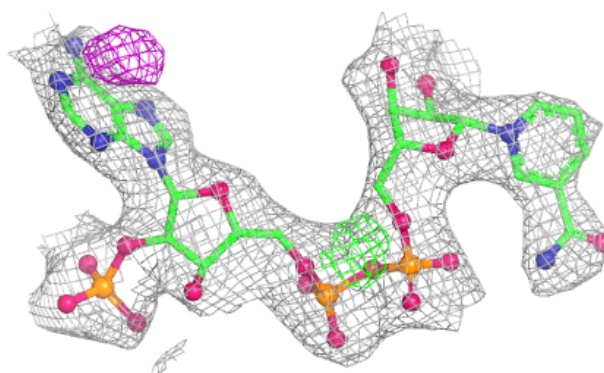


Electron density around NAP F 301:

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

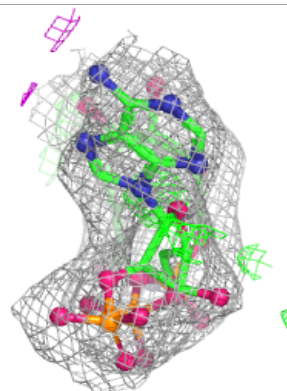
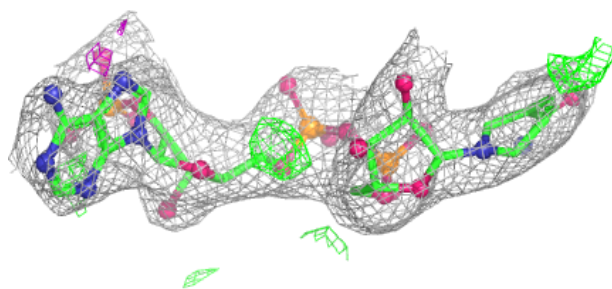
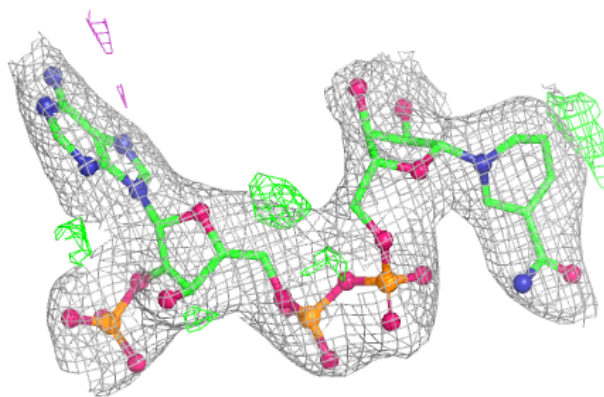
**Electron density around NAP D 301:**

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

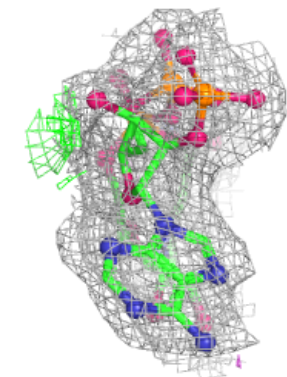
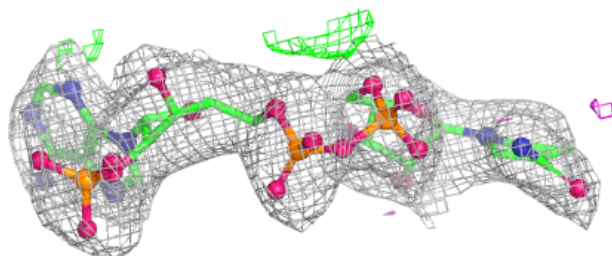
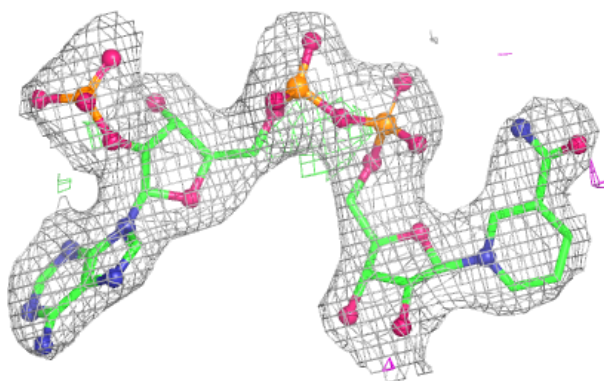


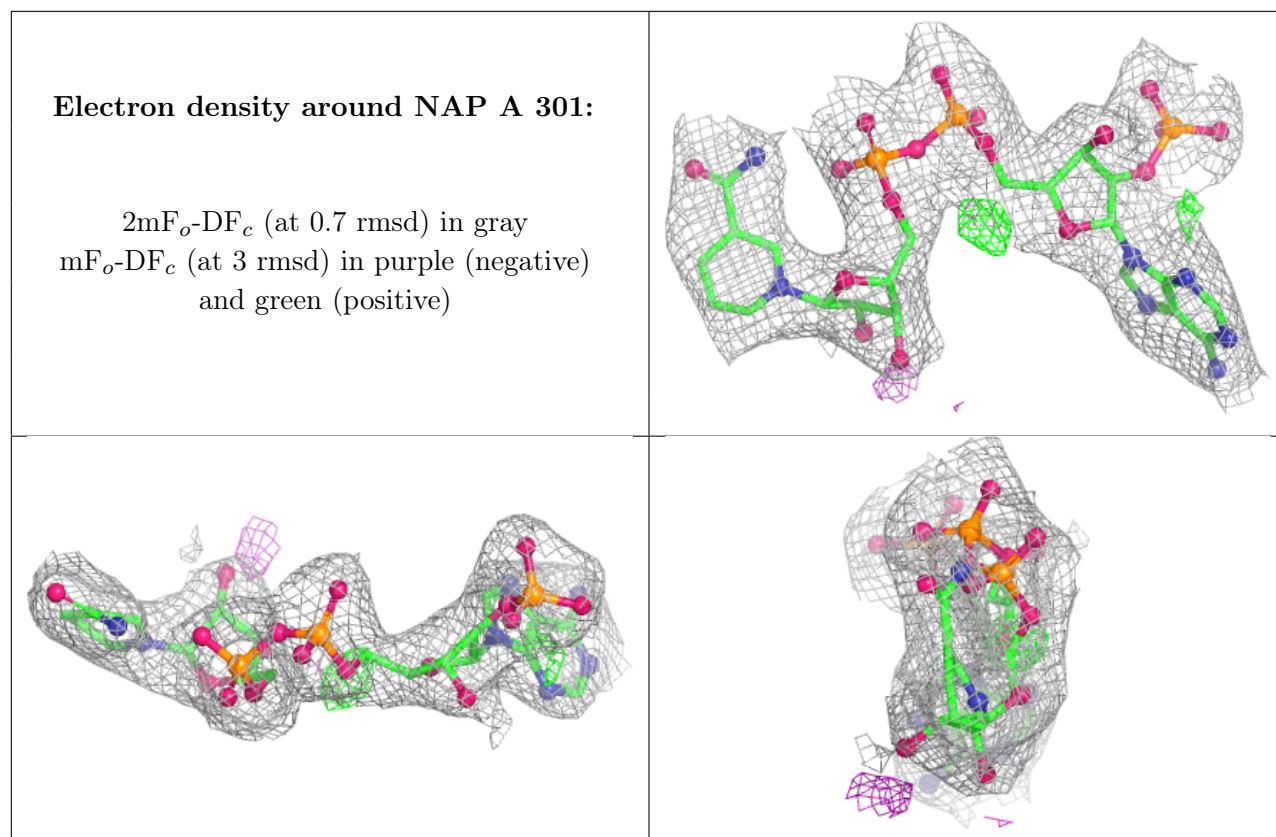
Electron density around NAP B 301:

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

**Electron density around NAP E 301:**

$2mF_o-DF_c$ (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.