



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:49 PM UTC

PDB ID : 6NKK / pdb_00006nkk
Title : Structure of PhqE Reductase/Diels-Alderase from *Penicillium fellutanum* in complex with NADP⁺ and premalbrancheamide
Authors : Newmister, S.A.; Dan, Q.; Smith, J.L.; Sherman, D.H.
Deposited on : 2019-01-07
Resolution : 2.30 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

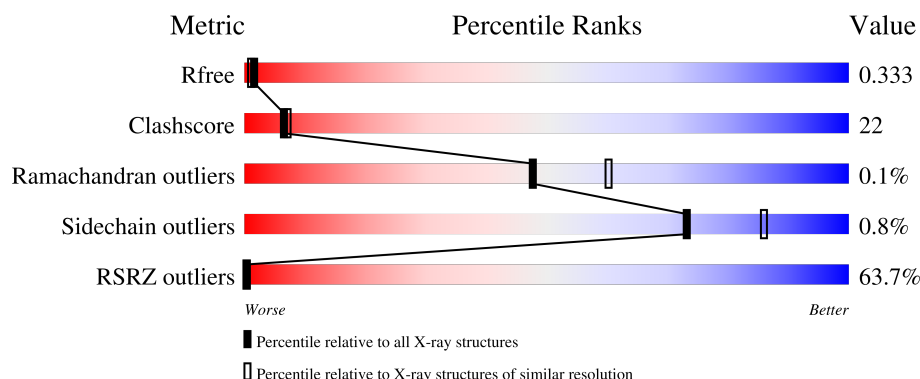
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	265	44% 72% 24% ..
1	B	265	40% 75% 20% ..
1	C	265	58% 67% 29% .
1	D	265	50% 65% 30% ..
1	E	265	84% 56% 39% ..

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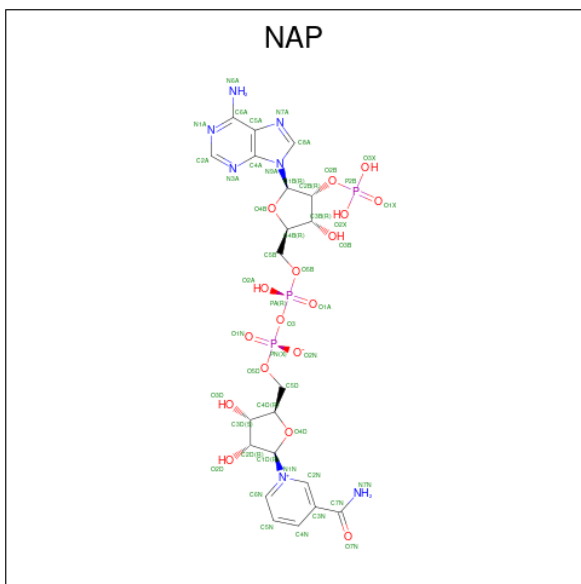
Mol	Chain	Length	Quality of chain
1	F	265	95% 49% 44% . .

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 Short chain dehydrogenase.

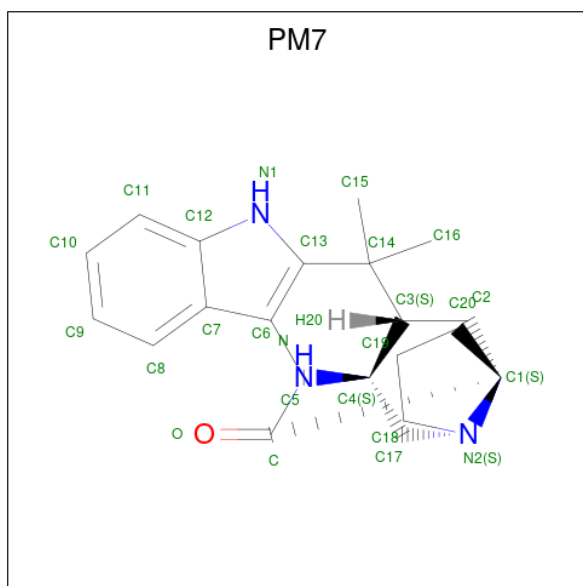
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	B	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	C	256	Total 1859	C 1163	N 320	O 364	S 12	0	0	0
1	D	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	E	256	Total 1859	C 1163	N 320	O 364	S 12	0	0	0
1	F	256	Total 1859	C 1163	N 320	O 364	S 12	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



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

- Molecule 3 is (5a*S*,12a*S*,13a*S*)-12,12-dimethyl-2,3,11,12,12a,13-hexahydro-1*H*,5*H*,6*H*-5a,13a-(epiminomethano)indolizino[7,6-*b*]carbazol-14-one (CCD ID: PM7) (formula: C₂₁H₂₅N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			25	21	3	1			
3	B	1	Total	C	N	O		0	0
			25	21	3	1			
3	C	1	Total	C	N	O		0	0
			25	21	3	1			
3	D	1	Total	C	N	O		0	0
			25	21	3	1			
3	E	1	Total	C	N	O		0	0
			25	21	3	1			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			25	21	3	1		

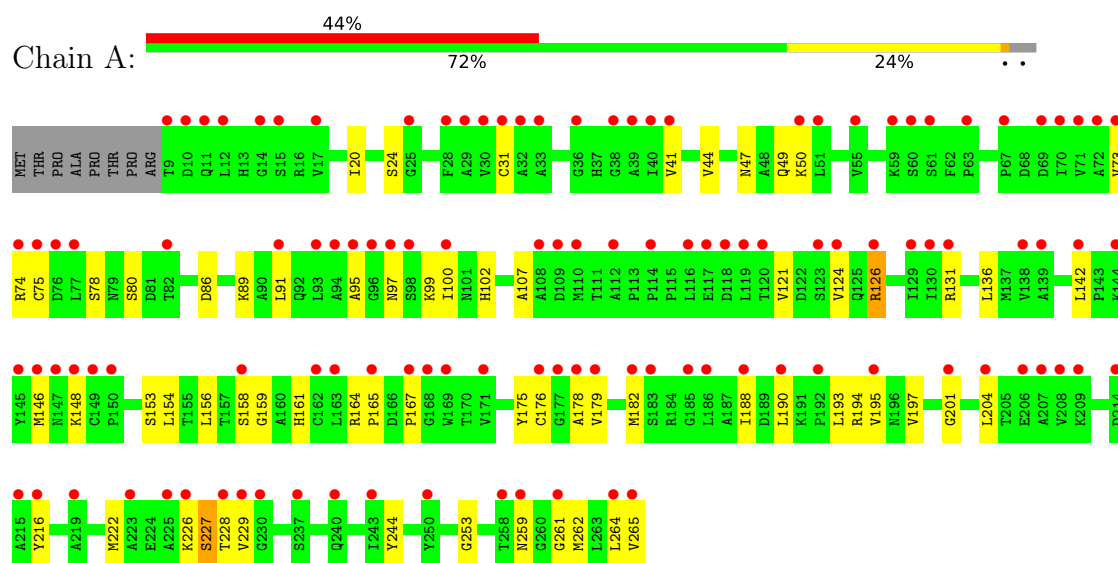
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	36	Total	O	0	0
			36	36		
4	C	22	Total	O	0	0
			22	22		
4	D	18	Total	O	0	0
			18	18		
4	E	1	Total	O	0	0
			1	1		

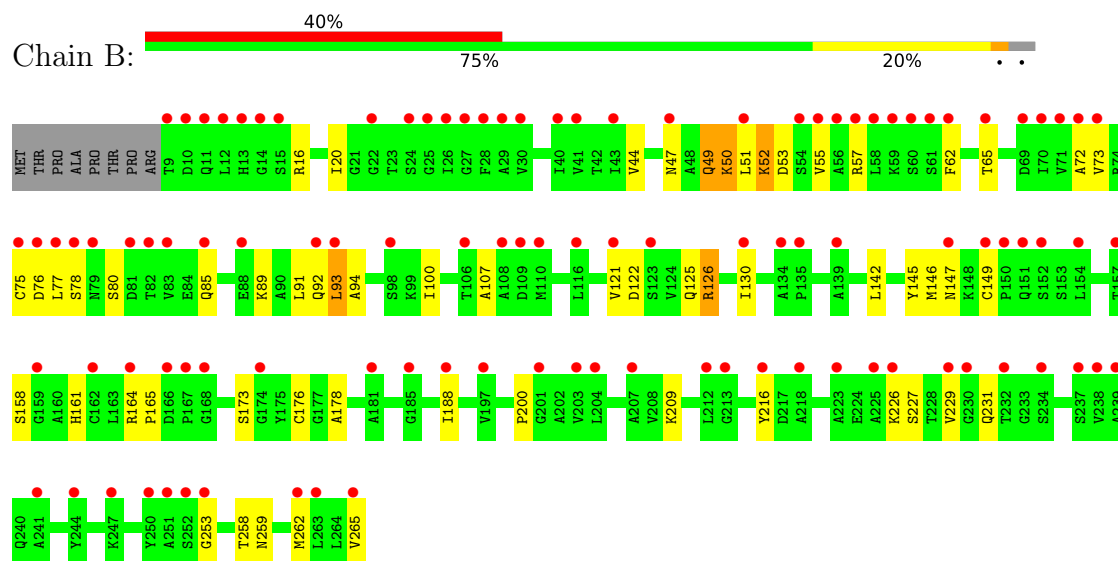
3 Residue-property plots [i](#)

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.

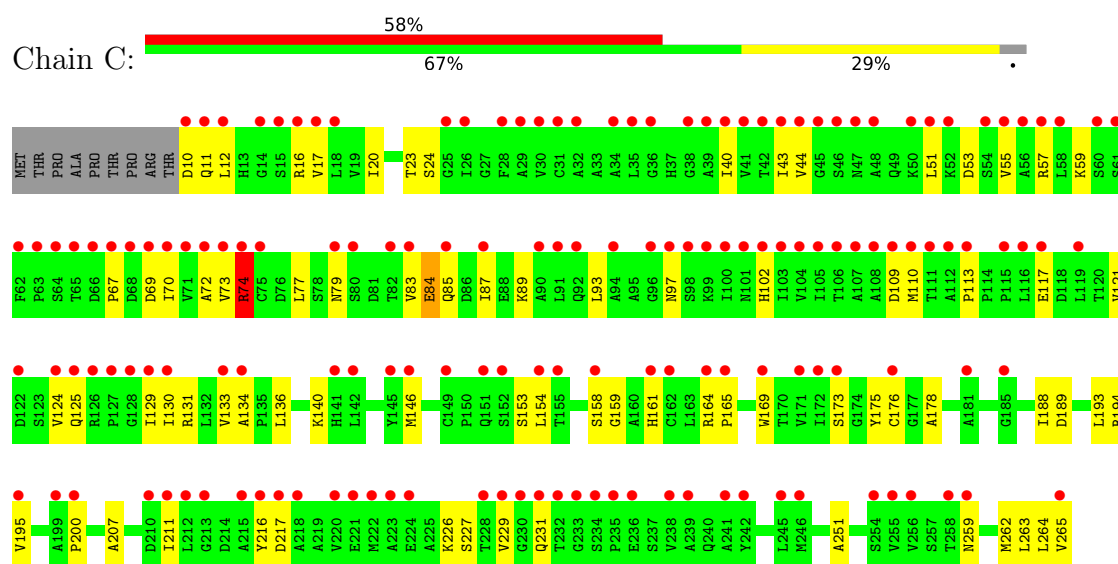
- Molecule 1: Short chain dehydrogenase



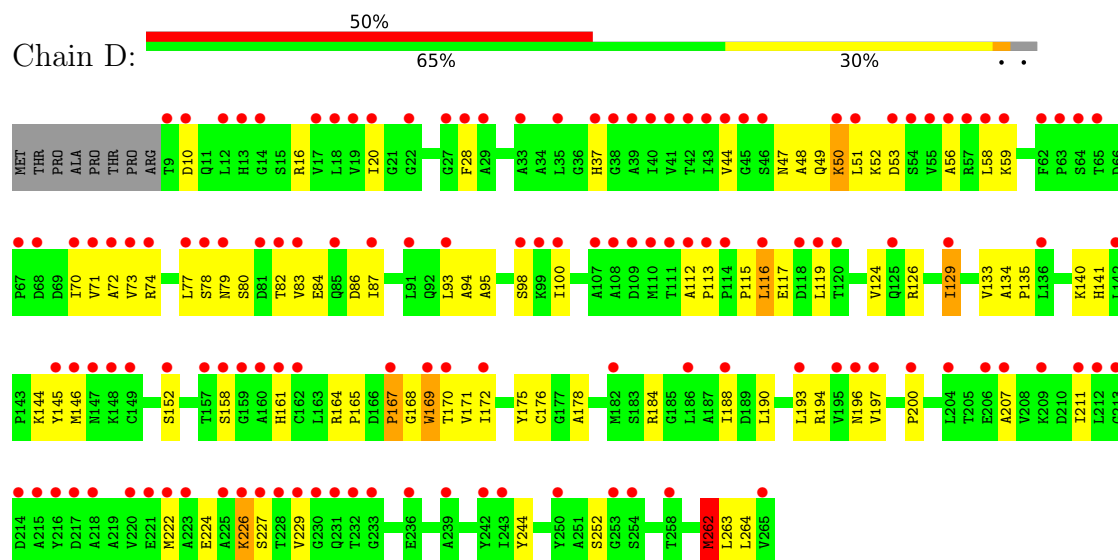
- Molecule 1: Short chain dehydrogenase



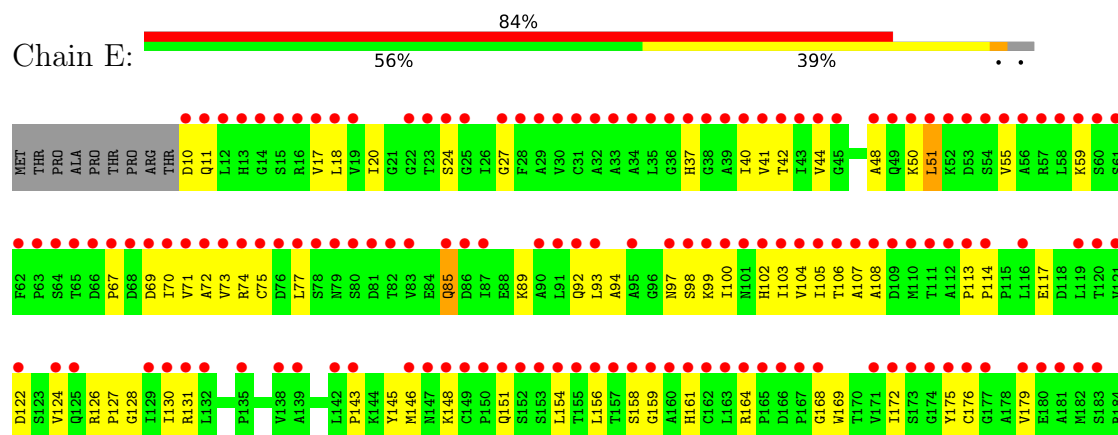
- Molecule 1: Short chain dehydrogenase

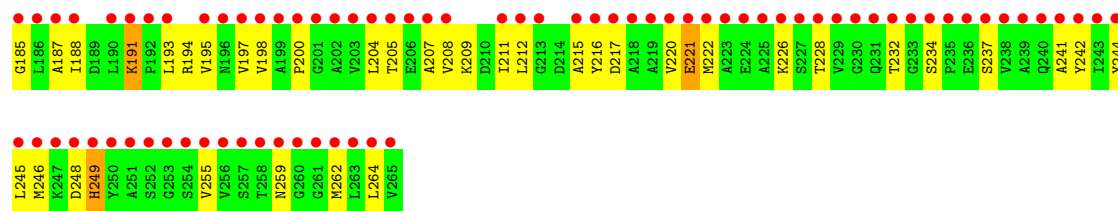


• Molecule 1: Short chain dehydrogenase

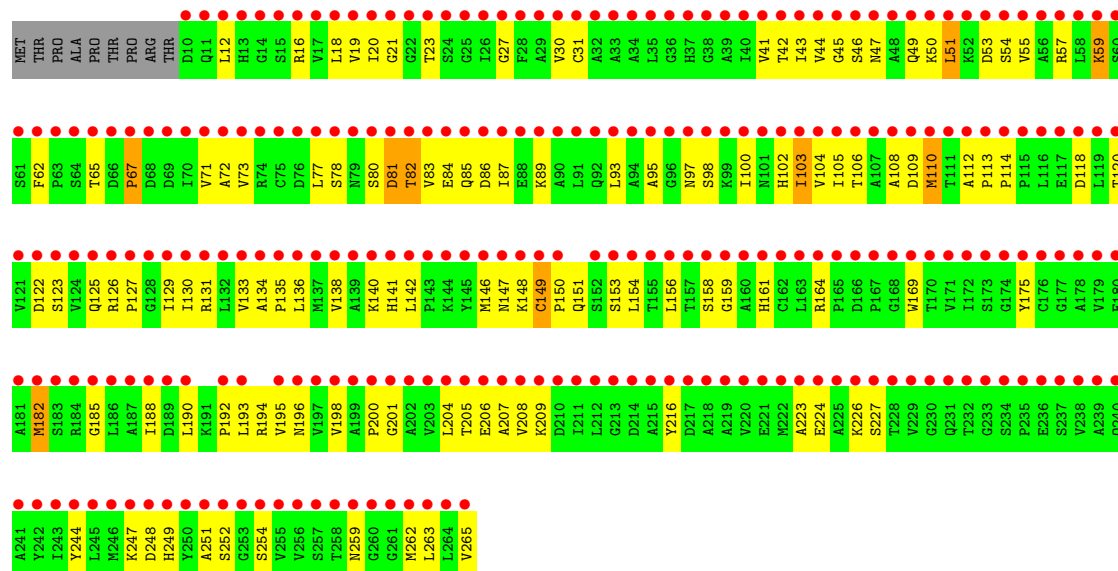


• Molecule 1: Short chain dehydrogenase





● Molecule 1: Short chain dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.59Å 117.25Å 64.81Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	46.38 – 2.30 46.38 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.38-2.30) 99.2 (46.38-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.293 , 0.336 0.294 , 0.333	Depositor DCC
R_{free} test set	3169 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11722	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, PM7

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	0.76	4/1895 (0.2%)	0.67	0/2580
1	B	0.60	4/1895 (0.2%)	0.70	6/2580 (0.2%)
1	C	0.44	2/1888 (0.1%)	0.65	0/2570
1	D	0.73	8/1895 (0.4%)	0.75	5/2580 (0.2%)
1	E	0.54	0/1888	1.00	11/2570 (0.4%)
1	F	0.70	1/1888 (0.1%)	1.25	19/2570 (0.7%)
All	All	0.64	19/11349 (0.2%)	0.86	41/15450 (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	D	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	149	CYS	C-N	8.35	1.43	1.34
1	D	169	TRP	C-O	-7.54	1.12	1.23
1	B	126	ARG	C-O	-7.12	1.17	1.24
1	D	167	PRO	C-O	-6.95	1.16	1.23
1	D	262	MET	C-O	-6.94	1.15	1.24
1	D	168	GLY	C-O	-6.91	1.14	1.23
1	D	263	LEU	C-O	-6.38	1.15	1.24
1	A	222	MET	C-O	-6.16	1.17	1.24
1	A	126	ARG	C-O	-6.07	1.18	1.24
1	A	91	LEU	C-O	-5.82	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	LYS	C-O	-5.42	1.17	1.24
1	D	74	ARG	C-O	-5.35	1.17	1.24
1	B	125	GLN	C-O	-5.29	1.17	1.24
1	D	262	MET	N-CA	-5.22	1.39	1.46
1	A	99	LYS	CA-C	-5.20	1.46	1.52
1	C	74	ARG	C-O	-5.18	1.17	1.24
1	C	84	GLU	C-O	-5.12	1.18	1.24
1	B	57	ARG	C-O	-5.09	1.18	1.24
1	D	169	TRP	N-CA	-5.08	1.40	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	MET	CB-CG-SD	-10.93	79.91	112.70
1	F	67	PRO	CA-C-N	-8.45	105.41	122.55
1	F	67	PRO	C-N-CA	-8.45	105.41	122.55
1	B	125	GLN	N-CA-C	8.33	120.44	111.36
1	F	110	MET	CB-CG-SD	8.08	136.93	112.70
1	F	110	MET	CA-CB-CG	7.74	129.59	114.10
1	E	85	GLN	CA-CB-CG	-7.56	98.98	114.10
1	E	92	GLN	CB-CA-C	-7.53	98.28	110.79
1	F	59	LYS	CB-CG-CD	-6.76	95.76	111.30
1	F	103	ILE	CA-CB-CG1	6.60	121.62	110.40
1	D	226	LYS	CB-CG-CD	-6.50	96.35	111.30
1	F	182	MET	N-CA-CB	6.33	119.53	110.16
1	B	89	LYS	CA-CB-CG	6.27	126.63	114.10
1	F	108	ALA	CA-C-N	-6.26	111.79	122.56
1	F	108	ALA	C-N-CA	-6.26	111.79	122.56
1	B	50	LYS	N-CA-C	-6.25	104.47	111.28
1	B	49	GLN	N-CA-C	6.12	117.75	111.14
1	F	110	MET	CA-C-N	-5.87	113.22	122.73
1	F	110	MET	C-N-CA	-5.87	113.22	122.73
1	F	81	ASP	CA-C-N	-5.75	116.26	126.45
1	F	81	ASP	C-N-CA	-5.75	116.26	126.45
1	F	87	ILE	CA-CB-CG1	5.75	120.18	110.40
1	E	248	ASP	CA-C-N	-5.59	111.12	122.31
1	E	248	ASP	C-N-CA	-5.59	111.12	122.31
1	F	149	CYS	O-C-N	-5.58	117.00	121.80
1	E	191	LYS	CB-CG-CD	5.57	124.12	111.30
1	B	89	LYS	CB-CA-C	-5.56	101.39	110.85
1	F	110	MET	CB-CA-C	-5.55	103.54	112.09
1	F	82	THR	N-CA-CB	-5.54	107.85	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	LEU	CA-CB-CG	5.54	135.69	116.30
1	B	89	LYS	N-CA-CB	5.46	118.23	110.16
1	E	191	LYS	CD-CE-NZ	5.40	129.19	111.90
1	E	168	GLY	N-CA-C	-5.37	97.73	113.30
1	E	117	GLU	CA-CB-CG	5.30	124.70	114.10
1	E	249	HIS	N-CA-CB	5.25	118.54	110.46
1	D	129	ILE	CA-CB-CG1	-5.13	101.69	110.40
1	D	48	ALA	N-CA-C	5.12	116.86	111.28
1	E	51	LEU	CA-CB-CG	5.08	134.09	116.30
1	F	46	SER	CA-CB-OG	5.07	121.25	111.10
1	D	169	TRP	N-CA-C	-5.02	104.80	111.87
1	E	221	GLU	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	PRO	Peptide
1	D	167	PRO	Peptide

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	1866	0	1899	50	0
1	B	1866	0	1899	45	0
1	C	1859	0	1892	75	0
1	D	1866	0	1899	72	0
1	E	1859	0	1892	115	0
1	F	1859	0	1892	167	1
2	A	48	0	23	3	0
2	B	48	0	25	2	0
2	C	48	0	23	2	0
2	D	48	0	23	2	0
2	E	48	0	25	5	0
2	F	48	0	22	12	0
3	A	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	0	0
3	C	25	0	0	0	0
3	D	25	0	0	0	0
3	E	25	0	0	0	0
3	F	25	0	0	2	0
4	A	32	0	0	1	0
4	B	36	0	0	2	0
4	C	22	0	0	1	0
4	D	18	0	0	0	0
4	E	1	0	0	0	0
All	All	11722	0	11514	503	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 22.

All (503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASN:CB	1:F:50:LYS:HD2	1.72	1.18
2:F:801:NAP:O4B	2:F:801:NAP:C1B	1.63	1.17
1:F:59:LYS:HZ2	1:F:67:PRO:HB3	1.05	1.16
1:C:73:VAL:HG11	1:C:93:LEU:HD12	1.27	1.12
1:F:81:ASP:O	1:F:82:THR:HB	1.48	1.11
1:B:50:LYS:NZ	2:B:801:NAP:O1X	1.82	1.10
1:F:164:ARG:HD2	1:F:262:MET:HE2	1.29	1.07
1:F:47:ASN:ND2	1:F:50:LYS:HE3	1.70	1.06
1:F:47:ASN:HB3	1:F:50:LYS:HD2	1.11	1.06
1:C:16:ARG:HH12	1:C:40:ILE:HG12	1.21	1.04
1:B:73:VAL:HG11	1:B:93:LEU:HD23	1.39	1.03
1:F:59:LYS:NZ	1:F:67:PRO:HB3	1.72	1.03
1:F:45:GLY:HA3	1:F:51:LEU:HD12	1.41	1.02
1:F:47:ASN:HB3	1:F:50:LYS:CD	1.89	1.02
1:C:84:GLU:OE2	1:C:140:LYS:NZ	1.95	1.00
1:F:135:PRO:O	1:F:138:VAL:HG12	1.61	0.98
1:F:244:TYR:CE1	1:F:248:ASP:OD2	2.17	0.98
1:F:244:TYR:CZ	1:F:248:ASP:OD2	2.16	0.97
1:F:164:ARG:CD	1:F:262:MET:HE2	1.94	0.95
1:E:131:ARG:CZ	1:E:175:TYR:HB3	1.95	0.95
1:E:10:ASP:OD2	1:E:37:HIS:HD2	1.50	0.94
1:B:73:VAL:CG1	1:B:93:LEU:HD23	1.99	0.92
1:F:147:ASN:ND2	1:F:149:CYS:SG	2.43	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASN:CG	1:F:50:LYS:HG3	1.96	0.90
1:F:47:ASN:HD22	1:F:50:LYS:HE3	1.35	0.89
1:C:73:VAL:HG11	1:C:93:LEU:CD1	2.01	0.89
1:E:151:GLN:HA	1:E:249:HIS:HD2	1.39	0.87
1:F:45:GLY:CA	1:F:51:LEU:HD12	2.04	0.86
1:B:265:VAL:HG23	1:B:265:VAL:OXT	1.75	0.86
1:F:50:LYS:CD	2:F:801:NAP:O3X	2.24	0.86
1:F:23:THR:HG23	1:F:54:SER:OG	1.74	0.86
1:C:16:ARG:HH12	1:C:40:ILE:CG1	1.88	0.85
1:C:16:ARG:NH1	1:C:40:ILE:CG1	2.39	0.85
1:E:48:ALA:HB2	1:E:74:ARG:HD2	1.58	0.85
1:F:47:ASN:CB	1:F:50:LYS:CD	2.48	0.84
1:B:147:ASN:CG	1:B:149:CYS:HB3	2.02	0.84
1:F:45:GLY:N	1:F:51:LEU:HD11	1.93	0.83
1:E:122:ASP:O	1:E:126:ARG:HG2	1.78	0.83
1:C:55:VAL:HG21	1:C:72:ALA:HB2	1.61	0.83
1:C:16:ARG:NH1	1:C:40:ILE:HG12	1.93	0.82
1:F:77:LEU:HB2	1:F:130:ILE:HG12	1.61	0.81
1:E:131:ARG:HH22	1:E:176:CYS:CA	1.93	0.81
1:F:140:LYS:HB3	1:F:141:HIS:HD2	1.44	0.81
1:C:11:GLN:HG3	1:F:89:LYS:HG3	1.64	0.79
1:E:20:ILE:HA	1:E:44:VAL:HG22	1.65	0.79
1:E:131:ARG:NH1	1:E:175:TYR:HB2	1.98	0.78
1:C:17:VAL:HG12	1:C:102:HIS:HB2	1.63	0.78
1:F:49:GLN:OE1	1:F:53:ASP:OD1	2.02	0.78
1:A:102:HIS:HD2	1:A:153:SER:HB3	1.48	0.78
1:E:131:ARG:HH22	1:E:176:CYS:N	1.83	0.77
1:F:120:THR:HG21	1:F:122:ASP:OD2	1.85	0.77
1:F:164:ARG:CD	1:F:262:MET:CE	2.63	0.76
1:C:154:LEU:HB3	1:C:195:VAL:HG12	1.65	0.76
1:E:24:SER:OG	2:E:801:NAP:O1A	2.00	0.76
1:F:110:MET:HE1	3:F:802:PM7:O	1.87	0.75
1:B:16:ARG:NH1	1:B:94:ALA:O	2.20	0.75
1:E:151:GLN:HA	1:E:249:HIS:CD2	2.22	0.75
1:C:16:ARG:CZ	1:C:40:ILE:HG21	2.18	0.74
1:E:131:ARG:HH22	1:E:176:CYS:HA	1.52	0.74
1:F:21:GLY:H	1:F:44:VAL:HG22	1.50	0.74
1:D:113:PRO:HD3	1:D:169:TRP:CZ3	2.23	0.74
1:F:45:GLY:CA	1:F:51:LEU:CD1	2.66	0.73
1:D:51:LEU:HD21	1:D:72:ALA:HB1	1.70	0.73
1:F:45:GLY:HA3	1:F:51:LEU:CD1	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:LYS:O	1:E:50:LYS:HG2	1.88	0.73
1:E:55:VAL:HG13	1:E:70:ILE:HG22	1.70	0.73
1:F:50:LYS:HD2	2:F:801:NAP:O3X	1.87	0.72
1:C:97:ASN:HD21	1:F:97:ASN:HB2	1.53	0.72
1:E:131:ARG:CZ	1:E:175:TYR:CB	2.68	0.72
1:F:129:ILE:HG22	1:F:130:ILE:HG13	1.70	0.72
1:A:164:ARG:NH1	4:A:901:HOH:O	2.21	0.72
1:E:10:ASP:OD2	1:E:37:HIS:CD2	2.40	0.72
1:F:43:ILE:HD12	1:F:55:VAL:HG12	1.72	0.71
1:F:50:LYS:HD3	2:F:801:NAP:O3X	1.90	0.71
1:F:20:ILE:HA	1:F:44:VAL:HG22	1.71	0.71
1:F:62:PHE:O	1:F:65:THR:HG22	1.88	0.71
1:C:77:LEU:HA	1:C:83:VAL:HG12	1.70	0.71
1:E:20:ILE:HB	1:E:105:ILE:HA	1.73	0.71
1:E:50:LYS:HD2	2:E:801:NAP:O2X	1.91	0.71
1:E:131:ARG:NH1	1:E:175:TYR:CB	2.55	0.70
1:E:59:LYS:NZ	1:E:67:PRO:HB3	2.07	0.70
1:C:10:ASP:OD2	1:C:12:LEU:HB2	1.92	0.69
1:F:102:HIS:HD2	1:F:153:SER:HB3	1.57	0.69
1:F:95:ALA:HB2	1:F:100:ILE:HD12	1.75	0.69
1:F:110:MET:HG3	1:F:207:ALA:HB1	1.73	0.69
1:E:187:ALA:O	1:E:191:LYS:HB3	1.93	0.69
1:D:71:VAL:HG21	1:D:93:LEU:HD11	1.73	0.69
1:F:193:LEU:HD23	1:F:194:ARG:N	2.08	0.69
1:A:78:SER:O	1:A:126:ARG:NH2	2.26	0.69
1:D:28:PHE:CZ	1:D:58:LEU:HD11	2.28	0.68
1:B:161:HIS:NE2	1:B:176:CYS:SG	2.66	0.68
1:C:89:LYS:O	1:C:93:LEU:HG	1.94	0.67
1:F:20:ILE:HA	1:F:44:VAL:CG2	2.23	0.67
1:F:85:GLN:N	1:F:85:GLN:OE1	2.27	0.67
1:A:259:ASN:HB2	1:A:262:MET:HG2	1.77	0.67
1:F:131:ARG:NH2	2:F:801:NAP:O3D	2.28	0.67
1:B:147:ASN:ND2	1:B:149:CYS:HB3	2.10	0.66
1:F:95:ALA:HB2	1:F:100:ILE:CD1	2.26	0.66
1:A:161:HIS:NE2	1:A:176:CYS:SG	2.69	0.66
1:A:148:LYS:NZ	1:A:190:LEU:HA	2.10	0.65
1:C:178:ALA:HB2	1:D:178:ALA:HB2	1.78	0.65
1:E:126:ARG:HB2	1:E:127:PRO:HD3	1.77	0.65
1:E:122:ASP:OD2	1:E:126:ARG:NH1	2.29	0.65
1:F:194:ARG:HA	1:F:252:SER:OG	1.96	0.65
1:E:17:VAL:HB	1:E:41:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ASN:HB2	1:F:50:LYS:HD2	1.72	0.65
1:F:55:VAL:HG11	1:F:72:ALA:HB2	1.78	0.65
1:B:73:VAL:HG11	1:B:93:LEU:CD2	2.22	0.65
1:F:47:ASN:HB3	1:F:50:LYS:CG	2.27	0.65
1:E:154:LEU:HB3	1:E:195:VAL:HG12	1.77	0.65
1:C:125:GLN:CD	1:D:129:ILE:HD11	2.21	0.65
1:D:193:LEU:HD22	1:D:194:ARG:H	1.60	0.65
1:E:105:ILE:HD11	1:E:156:LEU:HD22	1.79	0.65
1:E:148:LYS:HA	1:E:193:LEU:HB2	1.79	0.64
1:E:20:ILE:N	1:E:104:VAL:O	2.29	0.64
1:F:259:ASN:HB2	1:F:262:MET:HG2	1.79	0.64
1:E:234:SER:HB2	1:E:237:SER:HB3	1.77	0.64
1:F:151:GLN:HA	1:F:249:HIS:ND1	2.12	0.64
1:C:110:MET:SD	1:C:211:ILE:HD11	2.38	0.64
1:F:44:VAL:HG12	1:F:73:VAL:CG2	2.28	0.64
1:F:140:LYS:HB3	1:F:141:HIS:CD2	2.30	0.64
1:F:47:ASN:CG	1:F:50:LYS:CG	2.71	0.63
1:C:23:THR:HG22	1:C:51:LEU:HD13	1.80	0.63
1:F:154:LEU:HD12	1:F:195:VAL:HG13	1.81	0.63
1:F:16:ARG:HD2	1:F:98:SER:HB2	1.80	0.63
1:F:204:LEU:HA	1:F:208:VAL:HG21	1.79	0.63
1:C:161:HIS:NE2	1:C:176:CYS:SG	2.70	0.63
1:D:158:SER:HB2	1:D:197:VAL:HG11	1.80	0.63
1:F:226:LYS:HD3	1:F:265:VAL:OXT	1.99	0.63
1:F:265:VAL:OXT	1:F:265:VAL:HG23	1.97	0.62
1:D:16:ARG:HE	1:D:98:SER:HB3	1.64	0.62
1:E:156:LEU:HB2	1:E:197:VAL:HG12	1.82	0.61
1:F:45:GLY:N	1:F:51:LEU:CD1	2.63	0.61
1:F:109:ASP:OD1	2:F:801:NAP:N7A	2.33	0.61
1:C:16:ARG:NH1	1:C:40:ILE:HG21	2.14	0.61
1:F:20:ILE:N	1:F:104:VAL:O	2.29	0.61
1:E:85:GLN:O	1:E:85:GLN:HG2	1.99	0.61
1:F:78:SER:C	1:F:129:ILE:HG21	2.26	0.61
1:F:20:ILE:O	1:F:106:THR:N	2.28	0.61
1:F:193:LEU:HD23	1:F:194:ARG:O	2.01	0.61
1:F:164:ARG:HD3	1:F:262:MET:CE	2.31	0.61
1:C:73:VAL:CG1	1:C:93:LEU:CD1	2.77	0.61
1:C:259:ASN:HB2	1:C:262:MET:HG2	1.82	0.61
1:D:161:HIS:NE2	1:D:176:CYS:SG	2.74	0.60
1:C:74:ARG:HG2	1:C:74:ARG:NH2	2.15	0.60
1:D:113:PRO:HD3	1:D:169:TRP:CH2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:ARG:NH2	1:E:175:TYR:C	2.58	0.60
1:F:205:THR:HG21	2:F:801:NAP:O1N	2.01	0.60
1:F:127:PRO:HB2	1:F:175:TYR:CE2	2.36	0.60
1:F:110:MET:CE	3:F:802:PM7:O	2.48	0.60
1:E:128:GLY:HA2	1:E:131:ARG:HB2	1.84	0.60
1:F:81:ASP:O	1:F:82:THR:CB	2.29	0.60
1:F:23:THR:HG23	1:F:54:SER:CB	2.32	0.59
1:F:226:LYS:CD	1:F:265:VAL:OXT	2.49	0.59
1:E:228:THR:HG21	1:E:264:LEU:HD12	1.84	0.59
1:E:242:TYR:O	1:E:246:MET:HG3	2.03	0.59
1:B:227:SER:OG	1:B:229:VAL:O	2.11	0.59
1:C:16:ARG:NH1	1:C:40:ILE:HD13	2.17	0.59
1:F:135:PRO:C	1:F:138:VAL:HG12	2.28	0.59
1:C:74:ARG:HG2	1:C:74:ARG:HH21	1.68	0.59
1:F:42:THR:HA	1:F:71:VAL:HG13	1.84	0.59
1:A:265:VAL:O	1:C:164:ARG:NH1	2.36	0.58
1:E:100:ILE:HB	1:E:146:MET:HG2	1.84	0.58
1:D:49:GLN:O	1:D:52:LYS:N	2.36	0.58
1:B:265:VAL:OXT	1:B:265:VAL:CG2	2.48	0.58
1:C:16:ARG:NH1	1:C:40:ILE:CB	2.67	0.58
1:F:31:CYS:HB3	1:F:41:VAL:HG21	1.84	0.58
1:E:131:ARG:NH2	1:E:176:CYS:N	2.51	0.58
1:F:259:ASN:ND2	1:F:263:LEU:HD12	2.18	0.58
1:E:17:VAL:O	1:E:41:VAL:HA	2.04	0.57
1:B:259:ASN:HB2	1:B:262:MET:HG2	1.86	0.57
1:E:75:CYS:HB3	1:E:77:LEU:HD21	1.85	0.57
1:F:196:ASN:OD1	1:F:254:SER:N	2.27	0.57
1:A:44:VAL:HG22	1:A:73:VAL:CG2	2.34	0.57
1:E:131:ARG:NH2	1:E:176:CYS:HA	2.18	0.57
1:F:196:ASN:OD1	1:F:254:SER:HB3	2.05	0.57
1:C:227:SER:OG	1:C:229:VAL:O	2.11	0.57
1:F:45:GLY:H	1:F:51:LEU:HD11	1.66	0.57
1:C:158:SER:O	1:C:200:PRO:HD2	2.05	0.57
1:A:121:VAL:HG11	1:B:80:SER:HB3	1.87	0.57
1:A:164:ARG:HH22	1:A:226:LYS:CE	2.18	0.57
1:C:16:ARG:NH1	1:C:40:ILE:CD1	2.67	0.57
1:D:158:SER:HB2	1:D:197:VAL:CG1	2.34	0.56
1:A:142:LEU:HD22	1:A:146:MET:HE2	1.88	0.56
1:C:43:ILE:HD12	1:C:55:VAL:HG22	1.86	0.56
1:B:76:ASP:OD1	1:B:78:SER:OG	2.21	0.56
1:C:24:SER:OG	2:C:801:NAP:O1A	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ILE:HB	1:D:146:MET:HG2	1.87	0.56
1:F:205:THR:OG1	1:F:206:GLU:N	2.36	0.56
1:E:108:ALA:O	2:E:801:NAP:H8A	2.06	0.56
1:A:164:ARG:HH22	1:A:226:LYS:HE3	1.71	0.56
1:F:130:ILE:O	1:F:135:PRO:HD3	2.05	0.56
1:A:24:SER:OG	2:A:801:NAP:O1A	2.20	0.56
1:E:154:LEU:O	1:E:195:VAL:HA	2.07	0.55
1:C:16:ARG:HH11	1:C:40:ILE:HD13	1.72	0.55
1:D:164:ARG:NH2	1:D:262:MET:O	2.37	0.55
1:F:19:VAL:HG11	1:F:31:CYS:SG	2.46	0.55
1:C:131:ARG:NH1	4:C:901:HOH:O	2.40	0.55
1:F:248:ASP:OD1	1:F:248:ASP:O	2.24	0.55
1:E:198:VAL:HG12	1:E:200:PRO:HD3	1.89	0.55
1:E:77:LEU:HB2	1:E:130:ILE:CD1	2.36	0.55
1:F:135:PRO:HA	1:F:138:VAL:HG12	1.86	0.55
1:F:51:LEU:CD2	1:F:72:ALA:HB1	2.37	0.55
1:A:164:ARG:NH2	1:A:226:LYS:HE2	2.21	0.55
1:A:49:GLN:HE22	1:E:215:ALA:HB3	1.72	0.54
1:A:154:LEU:HD22	1:A:195:VAL:HG13	1.89	0.54
1:F:120:THR:CG2	1:F:122:ASP:OD2	2.52	0.54
1:D:49:GLN:OE1	1:D:49:GLN:HA	2.07	0.54
1:E:59:LYS:HZ3	1:E:67:PRO:HB3	1.73	0.54
1:A:156:LEU:HB2	1:A:197:VAL:HG22	1.90	0.54
1:E:194:ARG:NH2	1:E:245:LEU:O	2.28	0.54
1:F:105:ILE:HG12	1:F:156:LEU:HD22	1.90	0.54
1:B:231:GLN:NE2	4:B:902:HOH:O	2.32	0.54
1:E:205:THR:O	1:E:208:VAL:HG12	2.07	0.54
1:F:164:ARG:HD2	1:F:262:MET:CE	2.17	0.54
1:F:142:LEU:HD11	1:F:190:LEU:HD22	1.89	0.53
1:C:154:LEU:O	1:C:195:VAL:HA	2.08	0.53
1:E:185:GLY:O	1:E:188:ILE:HG13	2.07	0.53
1:E:209:LYS:HG2	1:E:216:TYR:CD1	2.43	0.53
1:A:264:LEU:HB3	1:D:188:ILE:HD11	1.90	0.53
1:C:117:GLU:O	1:D:140:LYS:HE3	2.08	0.53
1:A:148:LYS:HZ2	1:A:190:LEU:HA	1.73	0.53
1:A:227:SER:OG	1:A:229:VAL:O	2.21	0.53
1:A:164:ARG:NH2	1:A:226:LYS:CE	2.72	0.53
1:C:77:LEU:HD23	1:C:134:ALA:HB1	1.91	0.53
1:E:10:ASP:OD1	1:E:11:GLN:N	2.38	0.53
1:E:151:GLN:CB	1:E:249:HIS:CD2	2.92	0.53
1:E:42:THR:HA	1:E:71:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:HIS:HA	1:F:164:ARG:O	2.09	0.52
1:C:77:LEU:HA	1:C:83:VAL:CG1	2.40	0.52
1:C:229:VAL:HG23	1:C:231:GLN:H	1.72	0.52
1:E:208:VAL:HG22	1:E:212:LEU:HD11	1.90	0.52
1:F:196:ASN:HD21	1:F:251:ALA:C	2.17	0.52
1:D:20:ILE:HA	1:D:44:VAL:HB	1.90	0.52
1:A:165:PRO:HG2	1:B:188:ILE:HD12	1.92	0.52
1:E:216:TYR:CZ	1:E:220:VAL:HG21	2.45	0.52
1:F:110:MET:HE1	2:F:801:NAP:H2D	1.92	0.52
1:D:196:ASN:HD21	1:D:252:SER:HA	1.74	0.52
1:F:201:GLY:O	2:F:801:NAP:H4N	2.11	0.51
1:A:102:HIS:CD2	1:A:153:SER:HB3	2.38	0.51
1:F:49:GLN:OE1	1:F:53:ASP:CG	2.53	0.51
1:C:169:TRP:O	1:C:173:SER:HB2	2.10	0.51
1:E:40:ILE:HG23	1:E:69:ASP:HA	1.92	0.51
1:A:74:ARG:HH12	1:E:114:PRO:HB3	1.76	0.51
1:E:127:PRO:O	1:E:131:ARG:HG3	2.11	0.51
1:A:146:MET:HE3	1:A:193:LEU:HD11	1.91	0.51
1:E:102:HIS:CD2	1:E:246:MET:HA	2.46	0.51
1:F:89:LYS:O	1:F:93:LEU:HD23	2.11	0.51
1:A:178:ALA:HB2	1:B:178:ALA:HB2	1.93	0.51
1:F:194:ARG:HA	1:F:252:SER:HG	1.74	0.51
1:B:91:LEU:HB3	1:B:145:TYR:CD2	2.46	0.51
1:E:105:ILE:HG13	1:E:156:LEU:HA	1.93	0.51
1:F:82:THR:HG23	1:F:86:ASP:OD2	2.10	0.51
1:E:98:SER:OG	1:E:99:LYS:N	2.44	0.51
1:F:223:ALA:O	1:F:227:SER:OG	2.24	0.51
1:A:95:ALA:HB2	1:A:100:ILE:HG13	1.92	0.51
1:F:47:ASN:OD1	1:F:50:LYS:HG3	2.08	0.51
1:B:62:PHE:O	1:B:65:THR:HG22	2.10	0.50
1:E:169:TRP:HB3	1:E:172:ILE:HG22	1.93	0.50
1:F:47:ASN:CB	1:F:50:LYS:CG	2.88	0.50
1:F:83:VAL:HG13	1:F:84:GLU:N	2.26	0.50
1:D:49:GLN:O	1:D:51:LEU:N	2.45	0.50
1:E:151:GLN:CA	1:E:249:HIS:HD2	2.18	0.50
1:E:24:SER:HG	2:E:801:NAP:PA	2.26	0.50
1:E:105:ILE:CG1	1:E:156:LEU:HA	2.41	0.50
1:E:105:ILE:CD1	1:E:156:LEU:HD22	2.41	0.50
1:E:151:GLN:HG2	1:E:249:HIS:CD2	2.46	0.50
1:F:27:GLY:O	1:F:30:VAL:HG22	2.12	0.50
1:A:47:ASN:HB3	1:A:50:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:CYS:HB3	1:B:77:LEU:HD21	1.94	0.50
1:E:204:LEU:HA	1:E:208:VAL:HG11	1.92	0.50
1:F:50:LYS:O	1:F:53:ASP:N	2.44	0.50
1:E:161:HIS:HA	1:E:164:ARG:O	2.12	0.50
1:E:209:LYS:HE3	1:E:216:TYR:CE2	2.47	0.50
1:A:44:VAL:HG22	1:A:73:VAL:HG23	1.93	0.49
1:A:148:LYS:HA	1:A:193:LEU:HD12	1.93	0.49
1:F:97:ASN:OD1	1:F:98:SER:N	2.45	0.49
1:E:102:HIS:CD2	1:E:246:MET:HB3	2.48	0.49
1:F:114:PRO:HB2	1:F:118:ASP:HB2	1.94	0.49
1:E:217:ASP:O	1:E:221:GLU:HG2	2.11	0.49
1:B:122:ASP:OD2	1:B:126:ARG:NE	2.42	0.49
1:C:216:TYR:HD2	1:C:217:ASP:OD1	1.94	0.49
1:A:188:ILE:HD12	1:B:165:PRO:HG2	1.94	0.49
1:F:130:ILE:HD11	2:F:801:NAP:N6A	2.28	0.49
1:F:78:SER:HA	1:F:129:ILE:HG21	1.94	0.49
1:F:125:GLN:HA	1:F:175:TYR:OH	2.12	0.49
1:D:87:ILE:HD11	1:D:141:HIS:HD2	1.78	0.49
1:B:100:ILE:HB	1:B:146:MET:HG2	1.95	0.49
1:C:20:ILE:HA	1:C:44:VAL:HB	1.94	0.49
1:C:74:ARG:HH21	1:C:74:ARG:CG	2.25	0.49
1:D:49:GLN:C	1:D:51:LEU:H	2.21	0.49
1:D:49:GLN:C	1:D:51:LEU:N	2.70	0.49
1:D:78:SER:OG	2:D:801:NAP:N6A	2.45	0.49
1:B:158:SER:O	1:B:200:PRO:HD2	2.13	0.49
1:C:59:LYS:NZ	1:C:67:PRO:O	2.45	0.49
1:D:193:LEU:HD22	1:D:194:ARG:N	2.28	0.49
1:F:103:ILE:HG13	1:F:154:LEU:HD23	1.95	0.49
1:F:131:ARG:NH2	2:F:801:NAP:O2D	2.46	0.49
1:D:59:LYS:HG2	1:D:70:ILE:HD12	1.94	0.48
1:F:47:ASN:HB3	1:F:50:LYS:HB2	1.93	0.48
1:E:204:LEU:HD13	1:E:216:TYR:OH	2.12	0.48
1:D:124:VAL:O	1:D:175:TYR:OH	2.24	0.48
1:E:55:VAL:HG13	1:E:70:ILE:CG2	2.39	0.48
1:E:51:LEU:HD13	1:E:72:ALA:HB1	1.94	0.48
1:E:107:ALA:HA	2:E:801:NAP:O4B	2.13	0.48
1:F:150:PRO:O	1:F:194:ARG:NE	2.37	0.48
1:B:147:ASN:ND2	1:B:149:CYS:CB	2.76	0.48
1:A:148:LYS:HZ1	1:A:190:LEU:HA	1.76	0.48
1:D:52:LYS:O	1:D:56:ALA:N	2.46	0.48
1:D:16:ARG:HD3	1:D:94:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:MET:O	1:D:226:LYS:HG2	2.13	0.48
1:D:115:PRO:HB2	1:D:117:GLU:OE1	2.13	0.47
1:E:124:VAL:O	1:E:127:PRO:HD2	2.14	0.47
1:F:47:ASN:CG	1:F:50:LYS:CD	2.87	0.47
1:E:151:GLN:CA	1:E:249:HIS:CD2	2.96	0.47
1:B:44:VAL:HG13	1:B:75:CYS:HB2	1.95	0.47
1:D:129:ILE:HD12	1:D:129:ILE:N	2.29	0.47
1:E:158:SER:O	1:E:200:PRO:HD2	2.14	0.47
1:F:21:GLY:N	1:F:44:VAL:HG22	2.26	0.47
1:B:77:LEU:HB2	1:B:130:ILE:HD12	1.96	0.47
1:E:113:PRO:HD3	1:E:169:TRP:CZ3	2.49	0.47
1:A:75:CYS:SG	1:A:86:ASP:HB3	2.54	0.47
1:D:10:ASP:OD2	1:D:37:HIS:ND1	2.40	0.47
1:A:124:VAL:O	1:A:175:TYR:OH	2.27	0.47
1:F:80:SER:O	1:F:83:VAL:HG12	2.15	0.47
1:F:89:LYS:O	1:F:93:LEU:CD2	2.62	0.47
1:A:158:SER:OG	1:A:159:GLY:N	2.47	0.47
1:C:265:VAL:HG22	1:C:265:VAL:OXT	2.13	0.47
1:E:18:LEU:HD12	1:E:42:THR:O	2.14	0.47
1:F:146:MET:CE	1:F:193:LEU:HD11	2.45	0.47
1:F:194:ARG:NE	1:F:249:HIS:HA	2.29	0.47
1:D:84:GLU:OE2	1:D:140:LYS:NZ	2.28	0.47
1:E:143:PRO:HG3	1:E:148:LYS:HD3	1.97	0.47
1:E:207:ALA:O	1:E:211:ILE:HD12	2.14	0.47
1:F:100:ILE:HB	1:F:146:MET:HG2	1.96	0.47
1:B:51:LEU:HD11	1:B:72:ALA:HB1	1.97	0.47
1:D:58:LEU:HD12	1:D:58:LEU:HA	1.70	0.47
1:C:124:VAL:O	1:C:175:TYR:OH	2.26	0.46
1:D:226:LYS:HA	1:D:226:LYS:HD3	1.72	0.46
1:F:95:ALA:N	1:F:100:ILE:HD11	2.31	0.46
1:F:127:PRO:HB2	1:F:175:TYR:CD2	2.50	0.46
1:F:133:VAL:HA	1:F:136:LEU:HB2	1.97	0.46
1:D:158:SER:O	1:D:200:PRO:HD2	2.15	0.46
1:F:158:SER:OG	1:F:159:GLY:N	2.48	0.46
1:C:165:PRO:HB3	1:C:173:SER:OG	2.15	0.46
1:E:44:VAL:HG12	1:E:73:VAL:CG1	2.45	0.46
1:C:40:ILE:HG13	1:C:69:ASP:HB3	1.97	0.46
1:F:185:GLY:HA2	1:F:188:ILE:HD12	1.97	0.46
1:C:102:HIS:HA	1:C:153:SER:O	2.16	0.46
1:E:97:ASN:OD1	1:E:98:SER:N	2.49	0.46
1:D:184:ARG:O	1:D:188:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ALA:O	1:D:211:ILE:HG13	2.15	0.45
1:E:228:THR:CG2	1:E:264:LEU:HD12	2.46	0.45
1:A:31:CYS:HB3	1:A:41:VAL:HG11	1.98	0.45
1:E:18:LEU:HD21	1:E:20:ILE:HD11	1.98	0.45
1:A:153:SER:HB2	1:A:194:ARG:NH2	2.31	0.45
1:E:11:GLN:NE2	1:E:249:HIS:HE1	2.15	0.45
1:D:79:ASN:O	1:D:83:VAL:HG13	2.16	0.45
1:E:77:LEU:HB2	1:E:130:ILE:HD13	1.98	0.45
1:E:164:ARG:NE	1:E:164:ARG:HA	2.31	0.45
1:B:107:ALA:HB1	1:B:130:ILE:HD11	1.99	0.45
1:E:222:MET:O	1:E:226:LYS:HB2	2.16	0.45
1:F:194:ARG:CZ	1:F:249:HIS:HA	2.47	0.45
1:A:131:ARG:HD3	1:A:175:TYR:HB3	1.99	0.45
1:B:20:ILE:HA	1:B:44:VAL:HB	1.98	0.45
1:B:44:VAL:HG22	1:B:73:VAL:CG2	2.46	0.45
1:C:85:GLN:N	1:C:85:GLN:OE1	2.49	0.45
1:B:73:VAL:HG12	1:B:93:LEU:HD23	1.93	0.45
1:F:23:THR:HG22	1:F:23:THR:O	2.16	0.45
1:C:159:GLY:HA3	2:C:801:NAP:H5N	1.98	0.45
1:E:99:LYS:HD3	1:E:145:TYR:C	2.42	0.45
1:E:158:SER:OG	1:E:159:GLY:N	2.50	0.45
1:E:18:LEU:HB3	1:E:103:ILE:HG22	1.99	0.45
1:F:59:LYS:NZ	1:F:67:PRO:CB	2.62	0.45
1:A:136:LEU:HG	1:A:182:MET:HE1	1.98	0.45
1:B:55:VAL:HG21	1:B:72:ALA:HB2	1.98	0.45
1:C:53:ASP:O	1:C:57:ARG:HB2	2.17	0.44
1:D:152:SER:CB	1:D:193:LEU:HD23	2.47	0.44
1:C:16:ARG:NH1	1:C:40:ILE:CG2	2.79	0.44
1:D:196:ASN:ND2	1:D:252:SER:HA	2.32	0.44
1:A:204:LEU:HD13	1:A:216:TYR:OH	2.18	0.44
1:A:228:THR:OG1	1:A:261:GLY:HA3	2.18	0.44
1:B:93:LEU:HD12	1:B:93:LEU:HA	1.75	0.44
1:C:146:MET:HE3	1:C:193:LEU:HD11	2.00	0.44
1:D:152:SER:HB2	1:D:193:LEU:HD23	2.00	0.44
1:E:197:VAL:HG23	1:E:255:VAL:HA	1.99	0.44
1:F:95:ALA:CB	1:F:100:ILE:HD12	2.46	0.44
1:D:95:ALA:HB2	1:D:100:ILE:HG13	1.99	0.44
1:F:120:THR:HB	1:F:123:SER:H	1.82	0.44
1:E:259:ASN:HB2	1:E:262:MET:HE3	2.00	0.44
1:F:224:GLU:O	1:F:227:SER:HB2	2.18	0.44
1:D:77:LEU:HA	1:D:83:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:HD21	1:C:87:ILE:HD11	2.00	0.43
1:F:196:ASN:CG	1:F:254:SER:HB3	2.42	0.43
1:C:188:ILE:HD12	1:D:165:PRO:HG2	2.00	0.43
1:C:207:ALA:O	1:C:211:ILE:HG13	2.18	0.43
1:E:148:LYS:CA	1:E:193:LEU:HB2	2.48	0.43
1:F:131:ARG:HH22	2:F:801:NAP:C3D	2.28	0.43
1:F:209:LYS:HG2	1:F:216:TYR:CE1	2.53	0.43
1:C:226:LYS:O	1:C:262:MET:HA	2.18	0.43
1:D:171:VAL:HG13	1:D:172:ILE:HG13	2.00	0.43
1:D:224:GLU:O	1:D:227:SER:OG	2.36	0.43
1:D:227:SER:OG	1:D:229:VAL:O	2.19	0.43
1:E:102:HIS:CD2	1:E:246:MET:CB	3.01	0.43
1:F:30:VAL:HG21	1:F:104:VAL:HG11	1.99	0.43
1:F:102:HIS:CD2	1:F:153:SER:HB3	2.46	0.43
1:F:134:ALA:HB3	1:F:135:PRO:HD3	2.00	0.43
1:C:55:VAL:HG13	1:C:70:ILE:HG22	1.99	0.43
1:D:80:SER:O	1:D:83:VAL:HG22	2.19	0.43
1:E:27:GLY:CA	1:E:106:THR:HG21	2.48	0.43
1:F:196:ASN:HD21	1:F:252:SER:HA	1.83	0.43
1:C:17:VAL:HA	1:C:102:HIS:O	2.19	0.43
1:D:28:PHE:CZ	1:D:58:LEU:CD1	3.00	0.43
1:E:94:ALA:HB3	1:E:100:ILE:HD11	2.00	0.43
1:B:52:LYS:HG2	1:B:53:ASP:N	2.34	0.43
1:B:209:LYS:HG2	1:B:216:TYR:CE1	2.54	0.43
1:D:28:PHE:HZ	1:D:58:LEU:HD11	1.81	0.43
1:F:57:ARG:HH11	1:F:57:ARG:HD2	1.49	0.43
1:F:135:PRO:CA	1:F:138:VAL:HG12	2.48	0.43
1:A:107:ALA:HA	2:A:801:NAP:O4B	2.19	0.43
1:D:44:VAL:HG22	1:D:73:VAL:HG13	1.99	0.43
1:F:47:ASN:HB3	1:F:50:LYS:CB	2.49	0.43
1:B:262:MET:HE3	1:B:262:MET:HB2	1.87	0.43
1:F:23:THR:HG21	1:F:50:LYS:C	2.44	0.43
1:D:116:LEU:HA	1:D:119:LEU:HB2	2.00	0.43
1:F:148:LYS:O	1:F:192:PRO:HD2	2.19	0.43
1:C:129:ILE:O	1:C:133:VAL:HB	2.19	0.42
1:E:104:VAL:HG13	1:E:242:TYR:CD1	2.54	0.42
1:F:20:ILE:HB	1:F:105:ILE:HA	2.00	0.42
1:F:47:ASN:ND2	1:F:50:LYS:CE	2.60	0.42
1:F:105:ILE:HG12	1:F:156:LEU:CD2	2.49	0.42
1:F:135:PRO:HA	1:F:138:VAL:CG1	2.49	0.42
1:B:142:LEU:HD13	1:B:146:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:ALA:HA	1:F:169:TRP:CH2	2.54	0.42
1:C:164:ARG:HH21	1:C:263:LEU:HA	1.84	0.42
1:E:164:ARG:HA	1:E:164:ARG:HE	1.84	0.42
1:C:121:VAL:HG11	1:D:80:SER:HB2	2.01	0.42
1:E:11:GLN:O	1:E:11:GLN:HG3	2.18	0.42
1:F:16:ARG:NE	1:F:95:ALA:O	2.53	0.42
1:C:189:ASP:OD2	1:D:170:THR:OG1	2.27	0.42
1:D:82:THR:CG2	1:D:86:ASP:OD2	2.68	0.42
1:E:244:TYR:CD2	1:E:245:LEU:HG	2.55	0.42
1:F:16:ARG:NH2	1:F:97:ASN:OD1	2.53	0.42
1:F:18:LEU:HD11	1:F:44:VAL:HG13	2.01	0.42
1:F:113:PRO:HD3	1:F:169:TRP:CZ3	2.55	0.42
1:F:196:ASN:ND2	1:F:252:SER:HA	2.35	0.42
1:A:20:ILE:HA	1:A:44:VAL:HB	2.01	0.42
1:D:129:ILE:HA	1:D:133:VAL:HB	2.01	0.42
1:F:158:SER:O	1:F:200:PRO:HD2	2.20	0.42
1:A:80:SER:HB2	1:B:121:VAL:HG11	2.01	0.42
1:A:201:GLY:O	2:A:801:NAP:H4N	2.20	0.42
1:C:109:ASP:OD1	1:C:130:ILE:HG21	2.20	0.42
1:C:136:LEU:HB3	1:D:119:LEU:CD2	2.50	0.42
1:D:82:THR:HG22	1:D:86:ASP:OD2	2.20	0.42
1:F:20:ILE:HA	1:F:44:VAL:HG21	2.00	0.42
1:E:17:VAL:HG11	1:E:246:MET:HE1	2.02	0.41
1:F:12:LEU:HD23	1:F:12:LEU:HA	1.77	0.41
1:E:131:ARG:HH21	1:E:179:VAL:CG2	2.32	0.41
1:F:147:ASN:OD1	1:F:147:ASN:N	2.48	0.41
1:D:144:LYS:HG3	1:D:145:TYR:CE2	2.55	0.41
1:E:59:LYS:HZ1	1:E:67:PRO:HB3	1.84	0.41
1:F:182:MET:HE2	1:F:182:MET:HB3	1.75	0.41
1:D:190:LEU:O	1:D:193:LEU:HB3	2.20	0.41
1:B:47:ASN:ND2	4:B:906:HOH:O	2.46	0.41
1:C:59:LYS:HE2	1:C:59:LYS:HB3	1.74	0.41
1:F:198:VAL:HG12	1:F:200:PRO:HD3	2.03	0.41
1:F:247:LYS:O	1:F:249:HIS:HD2	2.03	0.41
1:B:50:LYS:NZ	2:B:801:NAP:P2B	2.90	0.41
1:D:50:LYS:HD3	1:D:53:ASP:HB2	2.02	0.41
1:F:142:LEU:HD22	1:F:146:MET:HE2	2.02	0.41
1:B:161:HIS:O	1:B:173:SER:OG	2.36	0.41
1:C:79:ASN:O	1:C:83:VAL:HG13	2.21	0.41
1:C:194:ARG:HD2	1:C:251:ALA:O	2.21	0.41
1:D:112:ALA:HA	1:D:113:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ALA:HB3	1:D:135:PRO:HD3	2.01	0.41
1:E:204:LEU:HG	1:E:232:THR:OG1	2.21	0.41
1:A:175:TYR:O	1:A:179:VAL:HG23	2.20	0.41
1:A:253:GLY:HA3	1:D:264:LEU:HD11	2.03	0.41
1:D:126:ARG:HG3	1:D:126:ARG:HH11	1.85	0.41
1:E:131:ARG:HH21	1:E:179:VAL:HG23	1.86	0.41
1:F:27:GLY:CA	1:F:106:THR:HG21	2.51	0.41
1:A:244:TYR:HB2	1:D:244:TYR:HB2	2.04	0.40
1:C:113:PRO:HD3	1:C:169:TRP:CZ3	2.56	0.40
1:D:47:ASN:N	2:D:801:NAP:O3X	2.51	0.40
1:E:113:PRO:HD3	1:E:169:TRP:CE3	2.55	0.40
1:F:205:THR:O	1:F:208:VAL:HG22	2.21	0.40
1:A:78:SER:O	1:A:126:ARG:CZ	2.67	0.40
1:C:16:ARG:HH12	1:C:40:ILE:CD1	2.31	0.40
1:F:146:MET:HE3	1:F:193:LEU:HD11	2.03	0.40
1:C:125:GLN:OE1	1:D:129:ILE:HD11	2.19	0.40
1:E:20:ILE:HB	1:E:105:ILE:HG22	2.03	0.40
1:E:128:GLY:CA	1:E:131:ARG:HB2	2.51	0.40
1:E:241:ALA:O	1:E:245:LEU:HD12	2.22	0.40
1:F:16:ARG:HB2	1:F:100:ILE:HA	2.04	0.40
1:F:78:SER:CA	1:F:129:ILE:HG21	2.51	0.40
1:A:86:ASP:O	1:A:89:LYS:HG2	2.21	0.40
1:B:85:GLN:OE1	1:B:85:GLN:N	2.52	0.40
1:D:164:ARG:NH2	1:D:262:MET:HG3	2.36	0.40
1:E:89:LYS:O	1:E:93:LEU:HD12	2.22	0.40
1:E:197:VAL:CG2	1:E:255:VAL:HG22	2.51	0.40
1:B:164:ARG:NH1	1:B:226:LYS:HD3	2.37	0.40
1:B:253:GLY:HA3	1:C:264:LEU:HD11	2.04	0.40
1:F:126:ARG:HG3	1:F:126:ARG:HH11	1.86	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:F:125:GLN:OE1	1:F:125:GLN:OE1[2_556]	2.03	0.17

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	255/265 (96%)	250 (98%)	5 (2%)	0	100	100
1	B	255/265 (96%)	246 (96%)	9 (4%)	0	100	100
1	C	254/265 (96%)	248 (98%)	6 (2%)	0	100	100
1	D	255/265 (96%)	246 (96%)	8 (3%)	1 (0%)	30	38
1	E	254/265 (96%)	248 (98%)	6 (2%)	0	100	100
1	F	254/265 (96%)	242 (95%)	12 (5%)	0	100	100
All	All	1527/1590 (96%)	1480 (97%)	46 (3%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	50	LYS

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	204/211 (97%)	202 (99%)	2 (1%)	68	82
1	B	204/211 (97%)	199 (98%)	5 (2%)	42	60
1	C	203/211 (96%)	202 (100%)	1 (0%)	81	90
1	D	204/211 (97%)	203 (100%)	1 (0%)	81	90
1	E	203/211 (96%)	203 (100%)	0	100	100
1	F	203/211 (96%)	202 (100%)	1 (0%)	81	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1221/1266 (96%)	1211 (99%)	10 (1%)	73 86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	227	SER
1	B	49	GLN
1	B	52	LYS
1	B	92	GLN
1	B	93	LEU
1	B	258	THR
1	C	74	ARG
1	D	262	MET
1	F	51	LEU

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	49	GLN
1	A	102	HIS
1	B	13	HIS
1	B	49	GLN
1	B	79	ASN
1	E	11	GLN
1	E	37	HIS
1	E	101	ASN
1	E	249	HIS
1	F	79	ASN
1	F	102	HIS
1	F	151	GLN
1	F	240	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	A	801	-	50,52,52	3.77	18 (36%)	71,80,80	1.89	17 (23%)
2	NAP	B	801	-	50,52,52	2.65	25 (50%)	71,80,80	2.10	23 (32%)
2	NAP	F	801	-	50,52,52	3.92	17 (34%)	71,80,80	2.08	19 (26%)
2	NAP	D	801	-	50,52,52	3.80	17 (34%)	71,80,80	1.91	17 (23%)
3	PM7	A	802	-	26,30,30	5.33	11 (42%)	34,51,51	1.67	8 (23%)
3	PM7	C	802	-	26,30,30	5.35	11 (42%)	34,51,51	1.65	7 (20%)
3	PM7	E	802	-	26,30,30	5.34	12 (46%)	34,51,51	1.88	8 (23%)
3	PM7	F	802	-	26,30,30	5.40	12 (46%)	34,51,51	2.09	9 (26%)
2	NAP	E	801	-	50,52,52	1.96	14 (28%)	71,80,80	2.07	21 (29%)
3	PM7	D	802	-	26,30,30	5.36	11 (42%)	34,51,51	1.66	8 (23%)
3	PM7	B	802	-	26,30,30	5.35	11 (42%)	34,51,51	1.73	9 (26%)
2	NAP	C	801	-	50,52,52	3.80	18 (36%)	71,80,80	1.91	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
2	NAP	A	801	-	-	13/35/67/67	0/5/5/5
2	NAP	B	801	-	-	10/35/67/67	0/5/5/5
2	NAP	F	801	-	-	12/35/67/67	0/5/5/5
2	NAP	D	801	-	-	11/35/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	E	801	-	-	8/35/67/67	0/5/5/5
2	NAP	C	801	-	-	12/35/67/67	0/5/5/5

All (177) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O4D-C1D	16.49	1.62	1.40
2	D	801	NAP	O4D-C1D	16.30	1.62	1.40
2	C	801	NAP	O4D-C1D	16.28	1.62	1.40
2	A	801	NAP	O4D-C1D	16.15	1.62	1.40
3	E	802	PM7	C-N	15.09	1.52	1.34
3	D	802	PM7	C-N	15.06	1.52	1.34
3	C	802	PM7	C-N	15.01	1.52	1.34
3	F	802	PM7	C-N	14.92	1.52	1.34
3	B	802	PM7	C-N	14.90	1.52	1.34
3	A	802	PM7	C-N	14.77	1.52	1.34
3	F	802	PM7	C2-C1	-13.87	1.40	1.54
3	C	802	PM7	C2-C1	-13.63	1.41	1.54
3	A	802	PM7	C2-C1	-13.51	1.41	1.54
3	B	802	PM7	C2-C1	-13.43	1.41	1.54
3	E	802	PM7	C2-C1	-13.40	1.41	1.54
3	D	802	PM7	C2-C1	-13.39	1.41	1.54
3	A	802	PM7	C4-N	-10.15	1.35	1.47
3	F	802	PM7	C4-N	-10.14	1.35	1.47
2	F	801	NAP	C2B-C1B	-10.11	1.28	1.53
3	B	802	PM7	C4-N	-10.08	1.35	1.47
3	C	802	PM7	C4-N	-10.06	1.35	1.47
3	D	802	PM7	C4-N	-10.02	1.35	1.47
3	E	802	PM7	C4-N	-9.89	1.36	1.47
2	F	801	NAP	O4B-C1B	9.36	1.63	1.42
2	D	801	NAP	O4B-C1B	9.10	1.63	1.42
2	C	801	NAP	C2B-C1B	-9.01	1.30	1.53
2	A	801	NAP	C2B-C1B	-8.94	1.31	1.53
2	C	801	NAP	O4B-C1B	8.86	1.62	1.42
2	D	801	NAP	C2B-C1B	-8.83	1.31	1.53
2	A	801	NAP	O4B-C1B	8.68	1.62	1.42
3	F	802	PM7	C5-C6	7.70	1.60	1.50
3	D	802	PM7	C5-C6	7.66	1.60	1.50
3	B	802	PM7	C5-C6	7.58	1.60	1.50
3	E	802	PM7	C5-C6	7.56	1.60	1.50
3	A	802	PM7	C5-C6	7.44	1.60	1.50
3	C	802	PM7	C5-C6	7.32	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	NAP	C7N-N7N	6.91	1.45	1.33
2	C	801	NAP	C7N-N7N	6.90	1.45	1.33
2	F	801	NAP	C7N-N7N	6.90	1.45	1.33
2	A	801	NAP	C7N-N7N	6.88	1.45	1.33
3	B	802	PM7	C17-C4	6.75	1.61	1.53
3	A	802	PM7	C1-C	6.73	1.67	1.53
3	B	802	PM7	C1-C	6.71	1.67	1.53
3	D	802	PM7	C1-C	6.71	1.67	1.53
3	C	802	PM7	C1-C	6.67	1.67	1.53
3	D	802	PM7	C17-C4	6.65	1.61	1.53
3	E	802	PM7	C1-C	6.64	1.67	1.53
2	F	801	NAP	O4B-C4B	-6.54	1.30	1.45
2	B	801	NAP	C5A-N7A	-6.53	1.27	1.39
3	A	802	PM7	C17-C4	6.52	1.61	1.53
3	F	802	PM7	C1-C	6.50	1.67	1.53
2	E	801	NAP	PN-O3	-6.45	1.52	1.59
3	E	802	PM7	C17-C4	6.44	1.61	1.53
3	F	802	PM7	C17-C4	6.42	1.61	1.53
2	B	801	NAP	C8A-N9A	-6.34	1.26	1.37
2	A	801	NAP	O4D-C4D	-6.30	1.31	1.45
3	C	802	PM7	C17-C4	6.23	1.61	1.53
2	A	801	NAP	O4B-C4B	-6.23	1.31	1.45
2	D	801	NAP	O4B-C4B	-6.15	1.31	1.45
2	C	801	NAP	O4D-C4D	-6.13	1.31	1.45
2	F	801	NAP	O4D-C4D	-6.08	1.31	1.45
2	C	801	NAP	O4B-C4B	-6.08	1.31	1.45
2	D	801	NAP	O4D-C4D	-6.06	1.31	1.45
2	C	801	NAP	PA-O3	5.35	1.65	1.59
2	D	801	NAP	PA-O3	5.34	1.65	1.59
2	C	801	NAP	PN-O3	5.28	1.65	1.59
2	B	801	NAP	C4A-N9A	-5.18	1.26	1.37
2	F	801	NAP	PA-O3	5.15	1.65	1.59
2	F	801	NAP	PN-O3	5.14	1.65	1.59
3	E	802	PM7	C13-C6	5.13	1.45	1.37
2	D	801	NAP	PN-O3	5.11	1.65	1.59
3	B	802	PM7	C13-C6	5.10	1.44	1.37
3	A	802	PM7	C13-C6	5.09	1.44	1.37
3	F	802	PM7	C13-C6	5.08	1.44	1.37
3	D	802	PM7	C13-C6	5.08	1.44	1.37
3	C	802	PM7	C13-C6	5.03	1.44	1.37
2	A	801	NAP	PN-O3	4.99	1.64	1.59
2	A	801	NAP	PA-O3	4.93	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	C6A-N6A	4.65	1.46	1.34
2	D	801	NAP	C6A-N6A	4.53	1.45	1.34
3	C	802	PM7	C14-C3	-4.48	1.50	1.56
2	B	801	NAP	O4D-C1D	-4.48	1.35	1.40
3	F	802	PM7	C14-C3	-4.42	1.50	1.56
2	C	801	NAP	C6A-N6A	4.39	1.45	1.34
2	A	801	NAP	C6A-N6A	4.29	1.45	1.34
3	A	802	PM7	C14-C3	-4.26	1.51	1.56
3	D	802	PM7	C14-C3	-4.20	1.51	1.56
3	C	802	PM7	C7-C6	-4.19	1.36	1.44
3	B	802	PM7	C14-C3	-4.18	1.51	1.56
3	E	802	PM7	C14-C3	-4.15	1.51	1.56
3	E	802	PM7	C7-C6	-4.09	1.36	1.44
2	B	801	NAP	PA-O2A	-4.08	1.36	1.55
2	E	801	NAP	C4A-N9A	-4.06	1.29	1.37
2	F	801	NAP	O3B-C3B	-4.04	1.32	1.43
2	B	801	NAP	P2B-O3X	-4.02	1.39	1.54
3	F	802	PM7	C7-C6	-4.00	1.36	1.44
3	B	802	PM7	C7-C6	-3.98	1.36	1.44
3	A	802	PM7	C7-C6	-3.96	1.36	1.44
2	E	801	NAP	C5A-N7A	-3.92	1.31	1.39
3	D	802	PM7	C7-C6	-3.90	1.37	1.44
2	B	801	NAP	O4D-C4D	-3.78	1.36	1.45
2	B	801	NAP	P2B-O2X	-3.75	1.40	1.54
2	F	801	NAP	O2B-C2B	3.56	1.56	1.44
3	B	802	PM7	C19-C18	3.54	1.64	1.51
3	E	802	PM7	C19-C18	3.53	1.63	1.51
3	F	802	PM7	C19-C18	3.53	1.63	1.51
3	D	802	PM7	C19-C18	3.51	1.63	1.51
2	B	801	NAP	O7N-C7N	-3.49	1.17	1.24
2	E	801	NAP	O7N-C7N	-3.48	1.17	1.24
3	A	802	PM7	C19-C18	3.45	1.63	1.51
3	C	802	PM7	C19-C18	3.40	1.63	1.51
2	B	801	NAP	PA-O1A	-3.39	1.39	1.50
2	B	801	NAP	PN-O1N	-3.35	1.39	1.50
2	D	801	NAP	P2B-O2B	3.27	1.65	1.59
2	E	801	NAP	C8A-N9A	-3.21	1.32	1.37
3	F	802	PM7	O-C	-3.19	1.17	1.22
2	A	801	NAP	P2B-O2B	3.14	1.65	1.59
2	C	801	NAP	P2B-O2B	3.13	1.65	1.59
2	B	801	NAP	PA-O3	-3.04	1.56	1.59
2	A	801	NAP	C5A-C4A	-3.02	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O3D-C3D	-2.93	1.35	1.43
2	B	801	NAP	C7N-N7N	-2.93	1.27	1.33
2	C	801	NAP	C5A-C4A	-2.92	1.33	1.39
2	F	801	NAP	O2D-C2D	2.86	1.50	1.43
2	C	801	NAP	O2D-C2D	2.85	1.50	1.43
2	D	801	NAP	C5A-C4A	-2.83	1.34	1.39
2	A	801	NAP	O3D-C3D	-2.81	1.36	1.43
2	D	801	NAP	O7N-C7N	-2.81	1.18	1.24
2	C	801	NAP	O7N-C7N	-2.80	1.18	1.24
2	A	801	NAP	O2D-C2D	2.80	1.49	1.43
2	B	801	NAP	PN-O2N	-2.80	1.42	1.55
2	C	801	NAP	O3B-C3B	-2.80	1.36	1.43
2	F	801	NAP	C5A-C4A	-2.79	1.34	1.39
2	F	801	NAP	O7N-C7N	-2.78	1.19	1.24
2	D	801	NAP	O2D-C2D	2.77	1.49	1.43
2	E	801	NAP	PN-O2N	-2.77	1.42	1.55
2	B	801	NAP	C2N-N1N	-2.76	1.32	1.35
2	A	801	NAP	O7N-C7N	-2.75	1.19	1.24
2	D	801	NAP	O3B-C3B	-2.74	1.36	1.43
2	D	801	NAP	O3D-C3D	-2.73	1.36	1.43
2	A	801	NAP	O3B-C3B	-2.72	1.36	1.43
2	C	801	NAP	O3D-C3D	-2.71	1.36	1.43
2	E	801	NAP	O4D-C4D	-2.70	1.39	1.45
2	B	801	NAP	O4B-C4B	-2.62	1.39	1.45
2	B	801	NAP	PN-O3	-2.61	1.56	1.59
2	C	801	NAP	C5A-N7A	-2.61	1.34	1.39
2	A	801	NAP	C5A-N7A	-2.59	1.34	1.39
2	D	801	NAP	C5A-N7A	-2.55	1.34	1.39
2	B	801	NAP	C4A-N3A	-2.48	1.29	1.34
2	E	801	NAP	O4D-C1D	-2.48	1.37	1.40
2	B	801	NAP	P2B-O2B	-2.47	1.55	1.59
2	E	801	NAP	PA-O2A	-2.45	1.44	1.55
3	D	802	PM7	O-C	-2.42	1.18	1.22
3	E	802	PM7	O-C	-2.38	1.18	1.22
2	B	801	NAP	C6N-N1N	-2.38	1.29	1.35
3	A	802	PM7	O-C	-2.37	1.18	1.22
2	F	801	NAP	C4N-C3N	-2.35	1.35	1.39
2	E	801	NAP	C6N-N1N	-2.35	1.30	1.35
3	C	802	PM7	O-C	-2.34	1.18	1.22
2	B	801	NAP	C6A-N1A	-2.33	1.29	1.35
2	A	801	NAP	C4N-C3N	-2.31	1.35	1.39
2	D	801	NAP	C4N-C3N	-2.31	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	NAP	P2B-O2B	-2.30	1.55	1.59
2	B	801	NAP	C2D-C3D	-2.28	1.47	1.53
2	C	801	NAP	C4N-C3N	-2.28	1.36	1.39
2	B	801	NAP	PA-O5B	-2.23	1.50	1.59
2	F	801	NAP	C5A-N7A	-2.22	1.35	1.39
3	B	802	PM7	O-C	-2.21	1.19	1.22
2	A	801	NAP	C8A-N9A	-2.17	1.33	1.37
2	E	801	NAP	P2B-O3X	-2.12	1.46	1.54
3	F	802	PM7	C2-C3	-2.10	1.50	1.54
2	E	801	NAP	C5A-C6A	2.09	1.46	1.41
2	E	801	NAP	P2B-O2X	-2.07	1.47	1.54
2	C	801	NAP	C8A-N9A	-2.03	1.34	1.37
2	B	801	NAP	C6A-N6A	-2.02	1.29	1.34
2	B	801	NAP	PN-O5D	-2.01	1.51	1.59
3	E	802	PM7	C2-C3	-2.00	1.50	1.54

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	802	PM7	C-C1-N2	-6.76	97.59	106.55
2	F	801	NAP	C5A-C4A-N3A	-6.41	117.89	126.72
2	F	801	NAP	N6A-C6A-N1A	-6.21	104.55	118.38
2	C	801	NAP	N6A-C6A-N1A	-6.18	104.62	118.38
2	D	801	NAP	N6A-C6A-N1A	-6.11	104.76	118.38
2	A	801	NAP	N6A-C6A-N1A	-5.97	105.07	118.38
2	B	801	NAP	C5A-C4A-N3A	-5.82	118.70	126.72
2	C	801	NAP	N3A-C2A-N1A	-5.63	120.06	128.58
2	A	801	NAP	N3A-C2A-N1A	-5.60	120.11	128.58
2	D	801	NAP	N3A-C2A-N1A	-5.54	120.19	128.58
3	F	802	PM7	C2-C1-N2	5.34	114.57	107.82
3	E	802	PM7	C-C1-N2	-5.33	99.49	106.55
2	E	801	NAP	C5A-C4A-N3A	-5.32	119.39	126.72
2	D	801	NAP	C5A-C4A-N3A	-5.26	119.47	126.72
3	E	802	PM7	C2-C1-N2	5.21	114.41	107.82
2	E	801	NAP	O3-PA-O1A	5.18	126.28	110.70
2	A	801	NAP	C5A-C4A-N3A	-5.12	119.67	126.72
2	C	801	NAP	C5A-C4A-N3A	-5.04	119.78	126.72
2	F	801	NAP	N3A-C2A-N1A	-4.86	121.22	128.58
2	C	801	NAP	C5A-C6A-N6A	4.67	134.86	123.29
2	E	801	NAP	N3A-C2A-N1A	-4.67	121.51	128.58
2	F	801	NAP	C5A-C6A-N6A	4.67	134.84	123.29
2	D	801	NAP	C5A-C6A-N6A	4.65	134.79	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	NAP	C2A-N3A-C4A	4.63	123.15	111.83
3	F	802	PM7	C2-C3-C14	-4.60	109.73	114.17
3	B	802	PM7	C2-C1-N2	4.59	113.63	107.82
2	F	801	NAP	N3A-C4A-N9A	4.53	134.88	127.17
2	B	801	NAP	C4A-C5A-N7A	-4.53	105.40	110.58
3	B	802	PM7	C-C1-N2	-4.46	100.65	106.55
2	A	801	NAP	C5A-C6A-N6A	4.44	134.29	123.29
3	D	802	PM7	C2-C1-N2	4.43	113.42	107.82
2	B	801	NAP	N3A-C4A-N9A	4.33	134.52	127.17
3	A	802	PM7	C2-C1-N2	4.32	113.28	107.82
2	B	801	NAP	N3A-C2A-N1A	-4.28	122.11	128.58
2	B	801	NAP	O3-PN-O1N	-4.24	97.95	110.70
3	C	802	PM7	C2-C1-N2	4.22	113.15	107.82
3	D	802	PM7	C-C1-N2	-4.20	100.98	106.55
2	B	801	NAP	C2A-N3A-C4A	4.18	122.05	111.83
3	A	802	PM7	C-C1-N2	-4.08	101.15	106.55
2	D	801	NAP	N9A-C8A-N7A	-4.06	108.17	113.94
2	A	801	NAP	N9A-C8A-N7A	-4.04	108.21	113.94
2	C	801	NAP	N9A-C8A-N7A	-4.04	108.21	113.94
2	C	801	NAP	C4A-N9A-C1B	-3.93	117.44	126.63
2	E	801	NAP	C4A-C5A-N7A	-3.92	106.10	110.58
3	C	802	PM7	C2-C3-C14	-3.89	110.42	114.17
2	B	801	NAP	O2X-P2B-O2B	-3.78	91.12	105.85
3	E	802	PM7	C2-C3-C14	-3.78	110.52	114.17
2	E	801	NAP	N3A-C4A-N9A	3.76	133.56	127.17
2	D	801	NAP	C4A-N9A-C1B	-3.72	117.93	126.63
2	F	801	NAP	C2A-N3A-C4A	3.69	120.84	111.83
2	B	801	NAP	C6N-N1N-C1D	-3.66	112.55	119.73
2	E	801	NAP	O5D-PN-O1N	-3.60	94.68	108.94
2	A	801	NAP	C4A-N9A-C1B	-3.59	118.24	126.63
2	E	801	NAP	O3-PN-O1N	3.55	121.39	110.70
2	E	801	NAP	C4A-N9A-C8A	3.52	109.43	105.74
2	F	801	NAP	N9A-C8A-N7A	-3.51	108.95	113.94
2	B	801	NAP	O2X-P2B-O1X	3.51	124.52	110.83
3	A	802	PM7	C2-C3-C14	-3.51	110.78	114.17
2	C	801	NAP	C2A-N3A-C4A	3.49	120.35	111.83
2	A	801	NAP	C2A-N3A-C4A	3.49	120.35	111.83
2	D	801	NAP	C2A-N3A-C4A	3.48	120.33	111.83
2	C	801	NAP	C1B-N9A-C8A	3.47	134.79	127.09
3	B	802	PM7	C2-C3-C14	-3.41	110.87	114.17
3	D	802	PM7	C2-C3-C14	-3.40	110.89	114.17
2	E	801	NAP	C6A-C5A-N7A	3.35	138.54	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	801	NAP	N9A-C8A-N7A	-3.31	109.25	113.94
2	D	801	NAP	C1B-N9A-C8A	3.27	134.35	127.09
3	C	802	PM7	C-C1-N2	-3.26	102.23	106.55
2	B	801	NAP	C5A-N7A-C8A	3.23	108.53	103.45
2	A	801	NAP	C2B-C1B-N9A	-3.23	108.44	113.75
2	B	801	NAP	C4A-N9A-C8A	3.23	109.12	105.74
2	F	801	NAP	O2B-C2B-C3B	3.22	123.21	111.68
2	A	801	NAP	N3A-C4A-N9A	3.21	132.62	127.17
2	C	801	NAP	C4D-O4D-C1D	-3.20	106.99	109.92
2	E	801	NAP	O3D-C3D-C4D	-3.16	102.00	111.08
2	D	801	NAP	N3A-C4A-N9A	3.13	132.49	127.17
2	F	801	NAP	C3B-C2B-C1B	-3.08	96.91	102.81
2	E	801	NAP	O2B-P2B-O1X	-3.03	98.54	109.33
2	F	801	NAP	O3X-P2B-O2X	-3.01	96.50	107.80
2	A	801	NAP	C1B-N9A-C8A	3.01	133.78	127.09
2	F	801	NAP	O2B-P2B-O1X	3.00	120.03	109.33
2	B	801	NAP	O4B-C1B-N9A	3.00	113.85	108.09
2	E	801	NAP	C5A-N7A-C8A	3.00	108.16	103.45
2	D	801	NAP	C5A-N7A-C8A	2.98	108.14	103.45
2	C	801	NAP	N3A-C4A-N9A	2.97	132.22	127.17
2	F	801	NAP	C4A-N9A-C1B	-2.94	119.75	126.63
2	F	801	NAP	C6A-C5A-C4A	2.93	121.18	117.18
3	C	802	PM7	C15-C14-C13	-2.88	106.27	109.98
3	F	802	PM7	C19-C18-N2	2.87	108.05	103.94
2	C	801	NAP	C5A-N7A-C8A	2.86	107.95	103.45
2	F	801	NAP	C5A-N7A-C8A	2.79	107.84	103.45
2	B	801	NAP	C6A-C5A-N7A	2.79	137.47	132.09
2	A	801	NAP	C5A-N7A-C8A	2.79	107.83	103.45
2	B	801	NAP	C4D-O4D-C1D	-2.74	107.42	109.92
2	E	801	NAP	O2N-PN-O1N	2.70	125.00	112.44
3	F	802	PM7	C16-C14-C13	-2.69	106.51	109.98
2	B	801	NAP	C3B-C2B-C1B	-2.69	97.66	102.81
3	E	802	PM7	C15-C14-C13	-2.68	106.53	109.98
3	D	802	PM7	C16-C14-C13	-2.67	106.54	109.98
2	B	801	NAP	C2N-N1N-C1D	2.66	125.01	119.13
2	B	801	NAP	N9A-C8A-N7A	-2.66	110.17	113.94
2	F	801	NAP	C1B-N9A-C8A	2.65	132.98	127.09
2	B	801	NAP	O4B-C1B-C2B	-2.61	102.09	106.59
2	C	801	NAP	C2B-C1B-N9A	-2.61	109.46	113.75
3	B	802	PM7	C16-C14-C13	-2.58	106.65	109.98
3	C	802	PM7	C11-C12-C7	-2.54	119.73	122.19
2	F	801	NAP	C4D-O4D-C1D	-2.54	107.60	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	NAP	C5B-C4B-C3B	-2.53	106.11	115.21
2	E	801	NAP	O4B-C1B-C2B	-2.51	102.27	106.59
2	B	801	NAP	O2N-PN-O1N	2.50	124.09	112.44
2	D	801	NAP	C4D-O4D-C1D	-2.47	107.67	109.92
2	E	801	NAP	O4B-C4B-C5B	-2.46	101.46	109.33
3	A	802	PM7	C20-C1-C	-2.45	112.17	115.26
3	B	802	PM7	C15-C14-C13	-2.44	106.83	109.98
3	E	802	PM7	C16-C14-C13	-2.43	106.86	109.98
3	C	802	PM7	C20-C1-C	-2.41	112.21	115.26
3	A	802	PM7	C11-C12-C7	-2.41	119.86	122.19
3	B	802	PM7	C11-C12-C7	-2.41	119.86	122.19
2	B	801	NAP	O2A-PA-O3	-2.38	100.85	107.27
2	A	801	NAP	P2B-O2B-C2B	-2.38	117.09	123.43
3	D	802	PM7	C11-C12-C7	-2.37	119.89	122.19
3	E	802	PM7	C11-C12-C7	-2.36	119.91	122.19
2	E	801	NAP	O2X-P2B-O1X	2.35	119.98	110.83
3	B	802	PM7	C20-C1-C	-2.33	112.32	115.26
2	A	801	NAP	C4D-O4D-C1D	-2.33	107.79	109.92
3	E	802	PM7	C20-C1-C	-2.33	112.32	115.26
2	D	801	NAP	C4A-C5A-N7A	-2.33	107.92	110.58
2	B	801	NAP	O2A-PA-O1A	2.32	123.23	112.44
2	D	801	NAP	C6N-N1N-C2N	-2.31	119.91	121.88
3	A	802	PM7	C15-C14-C13	-2.29	107.03	109.98
3	E	802	PM7	C1-C2-C3	2.28	112.34	108.49
3	C	802	PM7	C6-C13-N1	-2.27	107.55	109.95
2	E	801	NAP	O4B-C1B-N9A	2.26	112.42	108.09
2	E	801	NAP	O3X-P2B-O1X	2.25	119.62	110.83
3	F	802	PM7	C15-C14-C13	-2.23	107.11	109.98
3	D	802	PM7	C15-C14-C13	-2.23	107.11	109.98
3	A	802	PM7	C6-C13-N1	-2.21	107.60	109.95
3	A	802	PM7	C16-C14-C13	-2.20	107.14	109.98
2	C	801	NAP	C4A-C5A-N7A	-2.18	108.09	110.58
2	A	801	NAP	C3N-C7N-N7N	2.17	120.42	117.74
3	D	802	PM7	C1-C2-C3	2.16	112.15	108.49
3	B	802	PM7	C1-C2-C3	2.16	112.15	108.49
2	D	801	NAP	C3N-C7N-N7N	2.14	120.38	117.74
2	A	801	NAP	C4A-N9A-C8A	2.13	107.97	105.74
2	E	801	NAP	C3N-C7N-N7N	2.12	120.36	117.74
3	F	802	PM7	C11-C12-C7	-2.12	120.14	122.19
2	F	801	NAP	C5B-C4B-C3B	-2.11	107.62	115.21
2	B	801	NAP	O4D-C4D-C5D	-2.09	102.63	109.33
2	C	801	NAP	P2B-O2B-C2B	-2.08	117.86	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NAP	O4B-C1B-N9A	2.07	112.06	108.09
2	F	801	NAP	O4B-C4B-C3B	-2.07	101.05	105.15
3	D	802	PM7	C6-C13-N1	-2.06	107.77	109.95
2	D	801	NAP	C6A-C5A-C4A	2.05	119.98	117.18
2	D	801	NAP	C5A-C4A-N9A	2.04	108.04	105.81
3	F	802	PM7	C1-C2-C3	2.04	111.95	108.49
2	F	801	NAP	C4B-O4B-C1B	-2.04	104.97	109.47
3	F	802	PM7	C20-C1-C	-2.03	112.69	115.26
2	C	801	NAP	C6N-N1N-C2N	-2.02	120.16	121.88
2	A	801	NAP	C5B-C4B-C3B	-2.02	107.95	115.21
3	B	802	PM7	C6-C13-N1	-2.02	107.81	109.95
2	A	801	NAP	C4A-C5A-N7A	-2.01	108.29	110.58
2	B	801	NAP	O7N-C7N-C3N	2.01	122.05	119.60
2	C	801	NAP	C5A-C4A-N9A	2.00	107.99	105.81

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	NAP	C5B-O5B-PA-O1A
2	A	801	NAP	C5B-O5B-PA-O2A
2	A	801	NAP	C5B-O5B-PA-O3
2	A	801	NAP	PN-O3-PA-O5B
2	A	801	NAP	C5D-O5D-PN-O3
2	A	801	NAP	C5D-O5D-PN-O1N
2	A	801	NAP	C5D-O5D-PN-O2N
2	A	801	NAP	O4D-C1D-N1N-C2N
2	B	801	NAP	C5B-O5B-PA-O1A
2	B	801	NAP	C5B-O5B-PA-O2A
2	B	801	NAP	C5B-O5B-PA-O3
2	B	801	NAP	C5D-O5D-PN-O3
2	B	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	C5D-O5D-PN-O2N
2	C	801	NAP	C5B-O5B-PA-O1A
2	C	801	NAP	C5B-O5B-PA-O2A
2	C	801	NAP	C5B-O5B-PA-O3
2	C	801	NAP	C5D-O5D-PN-O3
2	C	801	NAP	C5D-O5D-PN-O1N
2	C	801	NAP	C5D-O5D-PN-O2N
2	D	801	NAP	C5B-O5B-PA-O1A
2	D	801	NAP	C5B-O5B-PA-O2A
2	D	801	NAP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	D	801	NAP	C5D-O5D-PN-O3
2	D	801	NAP	C5D-O5D-PN-O1N
2	D	801	NAP	C5D-O5D-PN-O2N
2	E	801	NAP	C5D-O5D-PN-O3
2	F	801	NAP	C5B-O5B-PA-O1A
2	F	801	NAP	C5B-O5B-PA-O2A
2	F	801	NAP	C5B-O5B-PA-O3
2	F	801	NAP	C5D-O5D-PN-O3
2	F	801	NAP	C5D-O5D-PN-O1N
2	F	801	NAP	C5D-O5D-PN-O2N
2	F	801	NAP	C3B-C2B-O2B-P2B
2	B	801	NAP	C3B-C4B-C5B-O5B
2	A	801	NAP	C3B-C4B-C5B-O5B
2	B	801	NAP	O4B-C4B-C5B-O5B
2	C	801	NAP	C3B-C4B-C5B-O5B
2	D	801	NAP	C3B-C4B-C5B-O5B
2	E	801	NAP	C3D-C4D-C5D-O5D
2	F	801	NAP	C3B-C4B-C5B-O5B
2	A	801	NAP	O4B-C4B-C5B-O5B
2	C	801	NAP	O4B-C4B-C5B-O5B
2	E	801	NAP	O4D-C4D-C5D-O5D
2	D	801	NAP	O4B-C4B-C5B-O5B
2	F	801	NAP	O4B-C4B-C5B-O5B
2	C	801	NAP	PN-O3-PA-O5B
2	D	801	NAP	PN-O3-PA-O5B
2	F	801	NAP	PN-O3-PA-O5B
2	A	801	NAP	PA-O3-PN-O1N
2	B	801	NAP	PA-O3-PN-O1N
2	D	801	NAP	PA-O3-PN-O1N
2	F	801	NAP	PA-O3-PN-O1N
2	E	801	NAP	C5B-O5B-PA-O1A
2	E	801	NAP	C5B-O5B-PA-O2A
2	E	801	NAP	C5D-O5D-PN-O1N
2	B	801	NAP	PA-O3-PN-O2N
2	C	801	NAP	PA-O3-PN-O1N
2	A	801	NAP	O4D-C1D-N1N-C6N
2	A	801	NAP	PA-O3-PN-O2N
2	C	801	NAP	PA-O3-PN-O2N
2	D	801	NAP	PA-O3-PN-O2N
2	E	801	NAP	PA-O3-PN-O2N
2	F	801	NAP	PA-O3-PN-O2N
2	E	801	NAP	C2B-O2B-P2B-O1X

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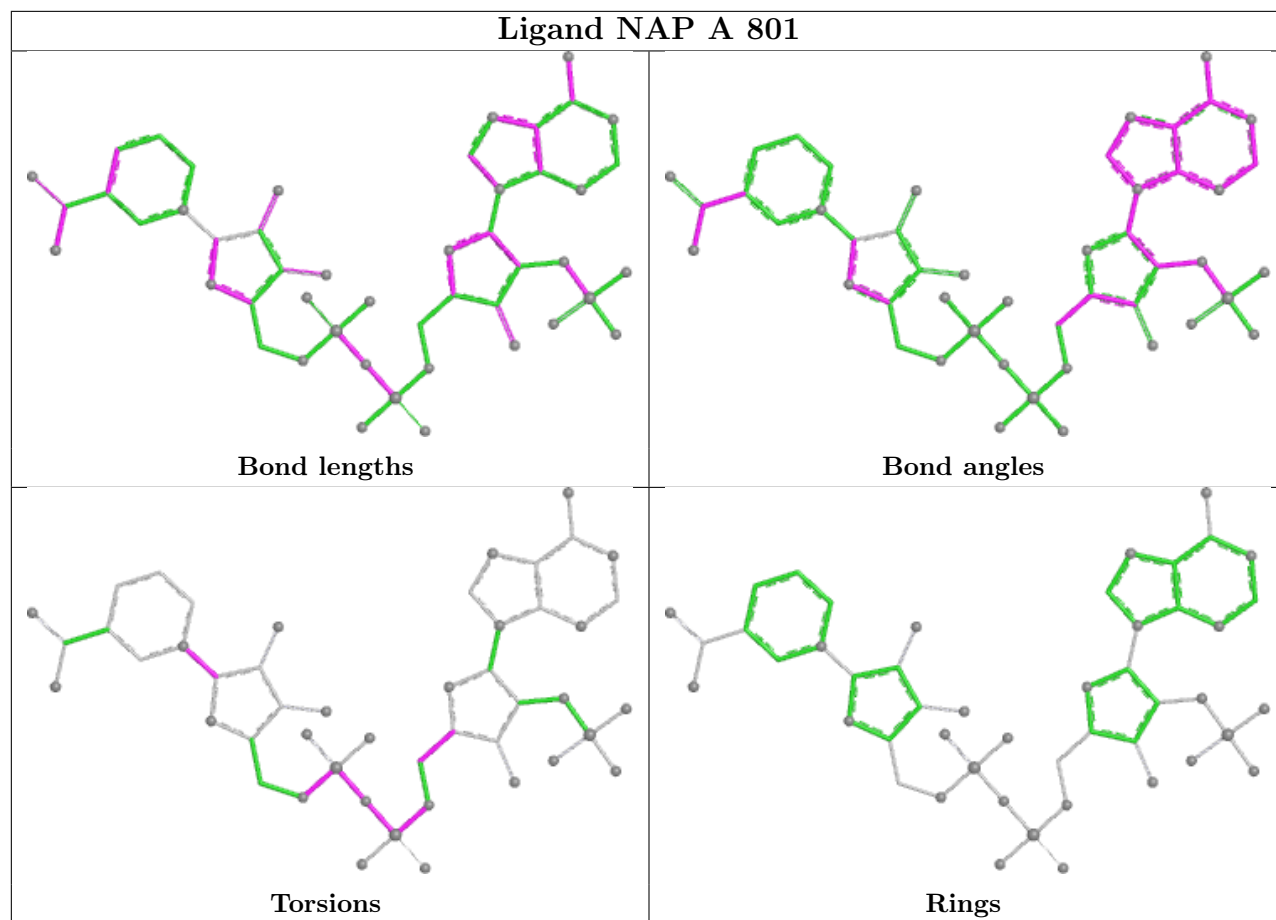
Mol	Chain	Res	Type	Atoms
2	C	801	NAP	C2B-C1B-N9A-C8A

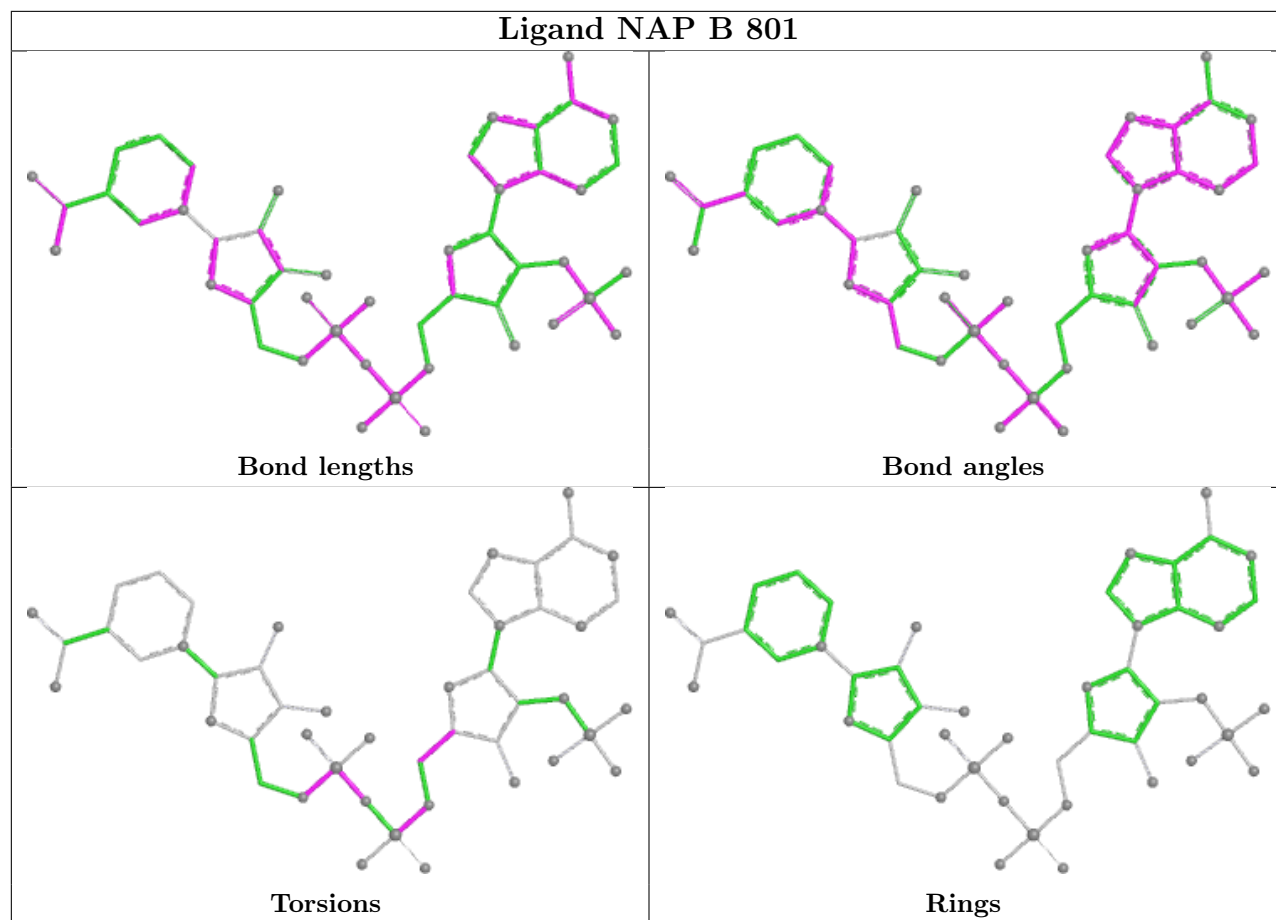
There are no ring outliers.

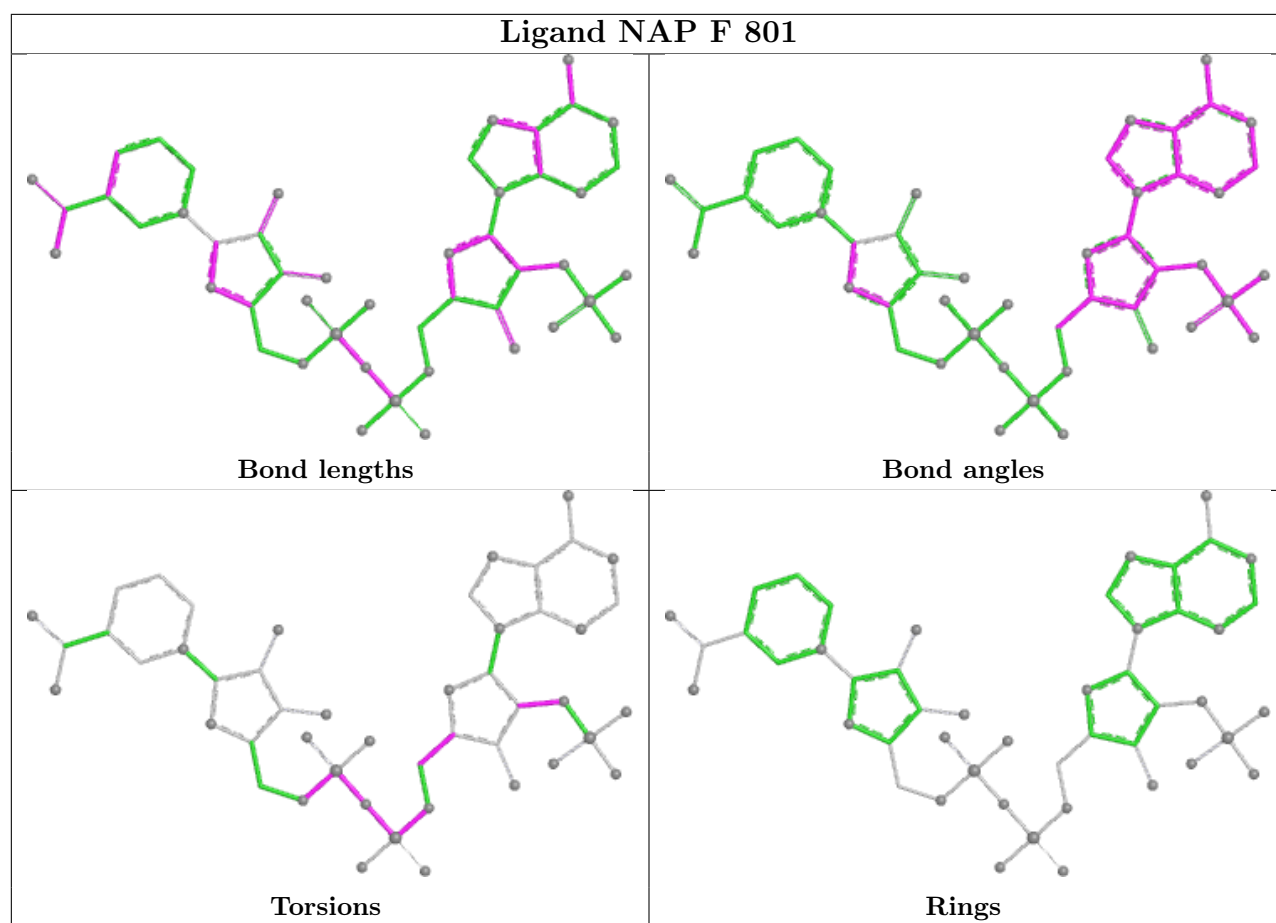
7 monomers are involved in 28 short contacts:

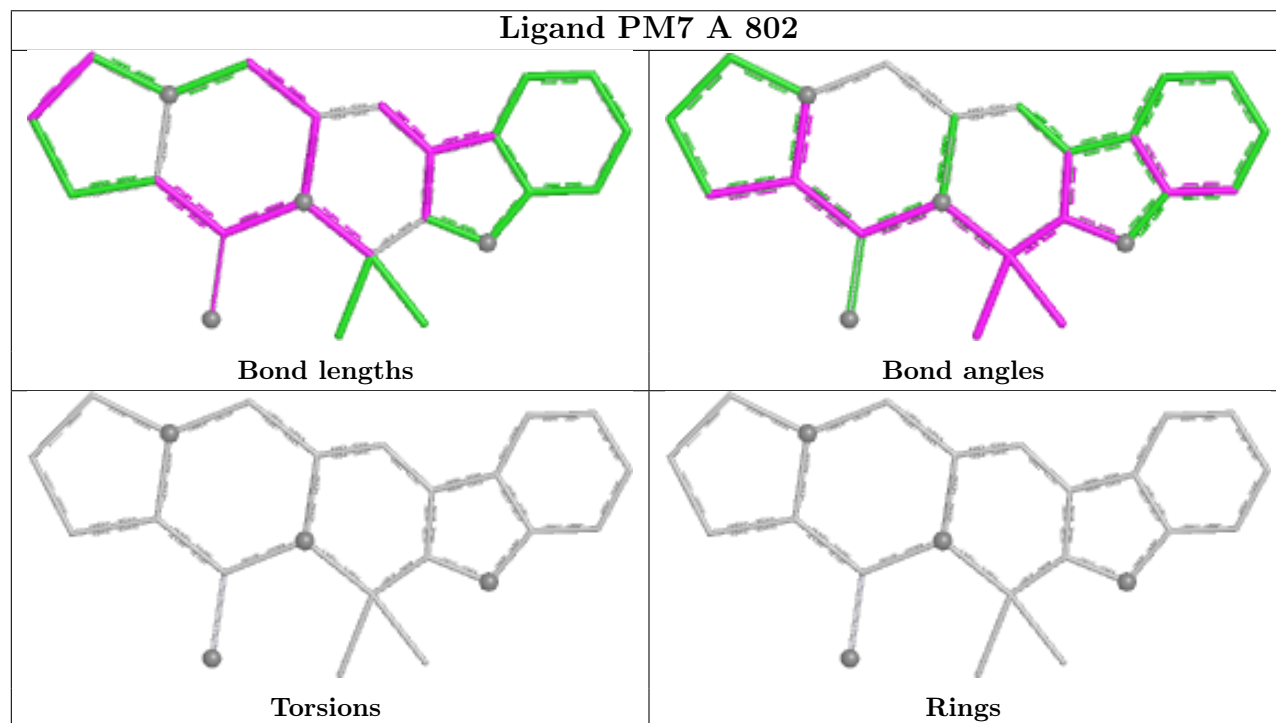
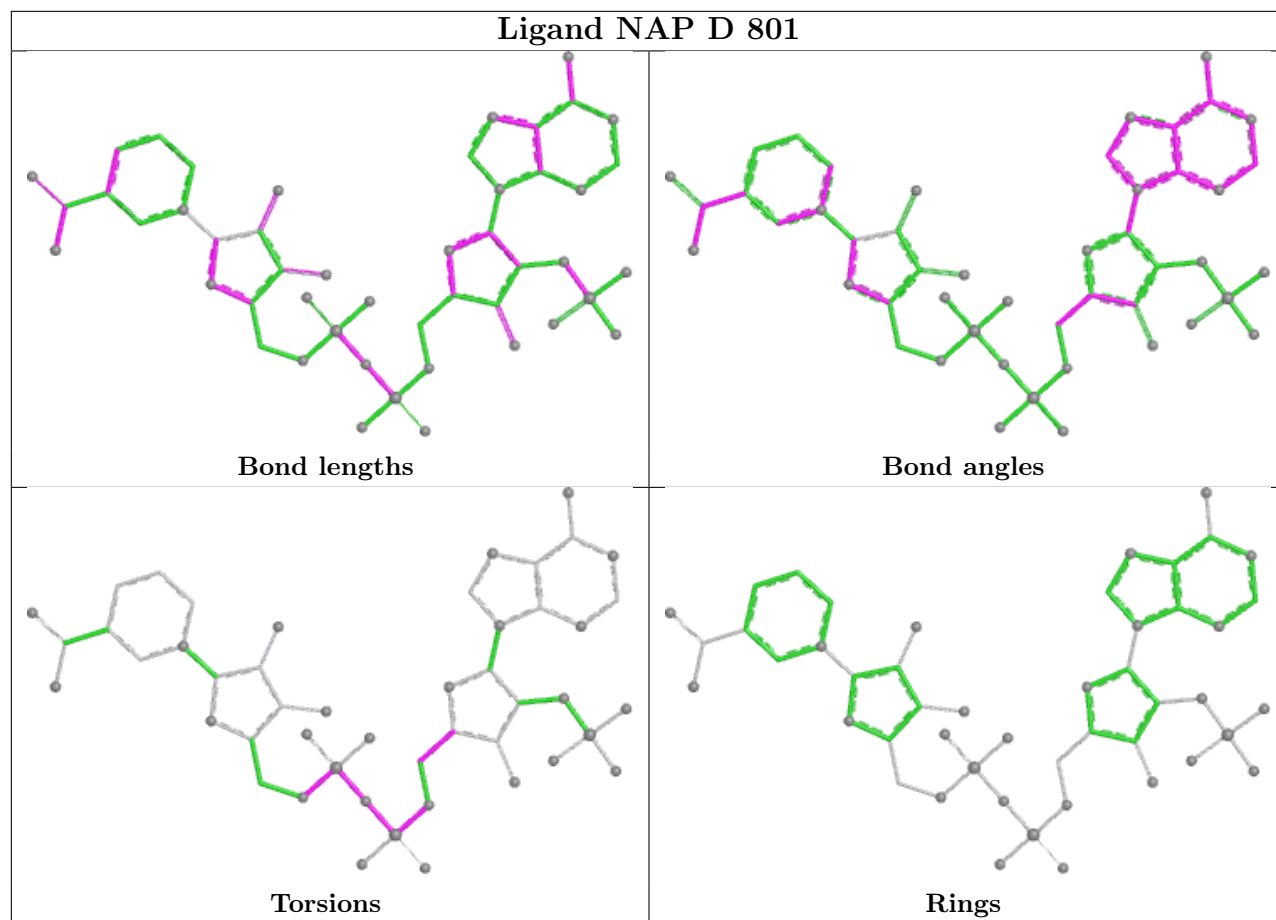
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	NAP	3	0
2	B	801	NAP	2	0
2	F	801	NAP	12	0
2	D	801	NAP	2	0
3	F	802	PM7	2	0
2	E	801	NAP	5	0
2	C	801	NAP	2	0

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

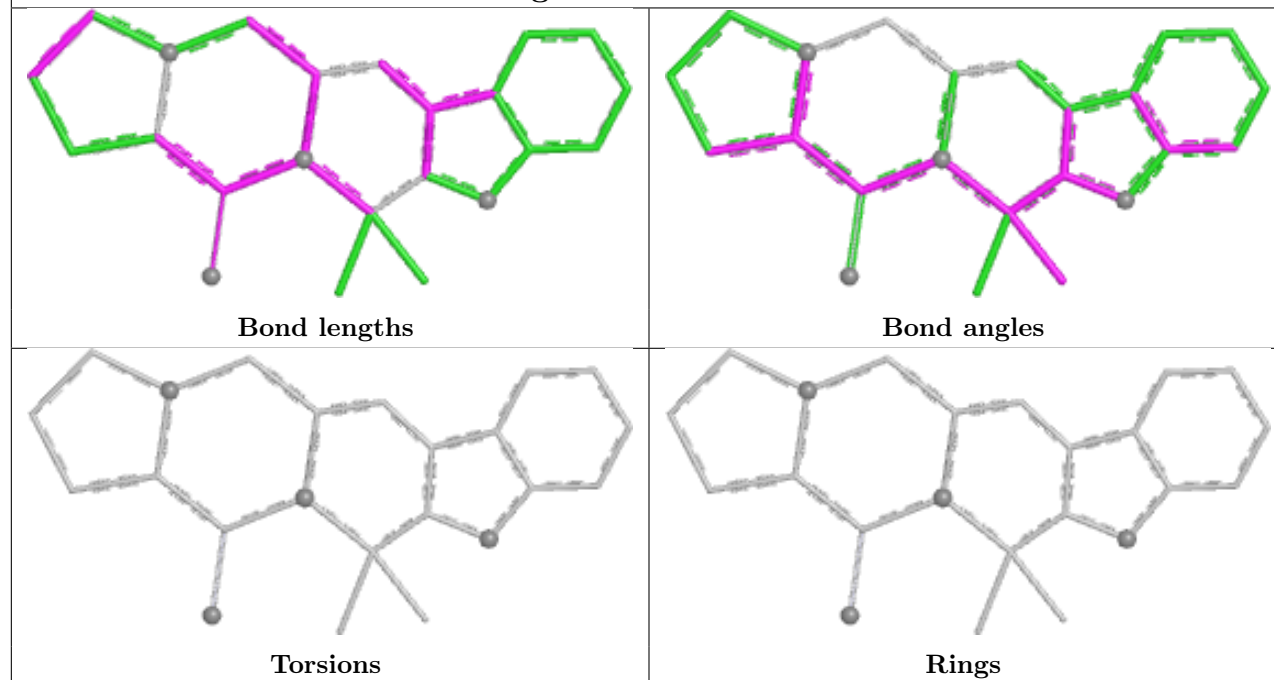




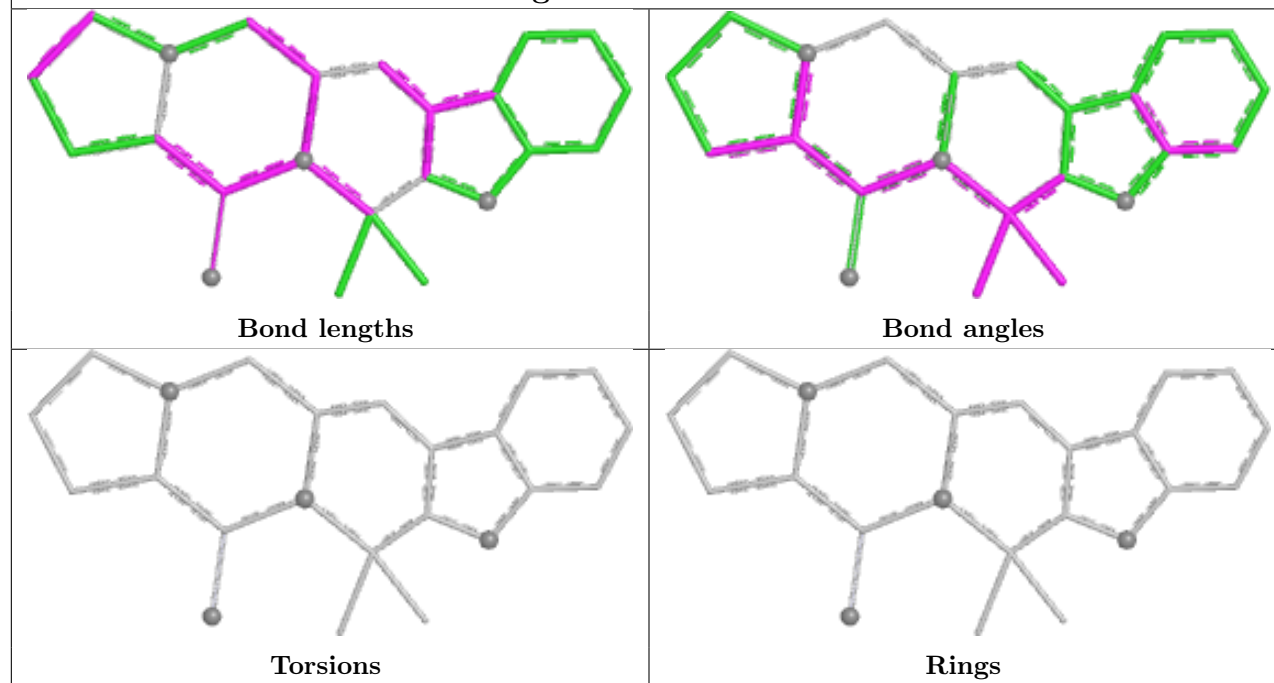




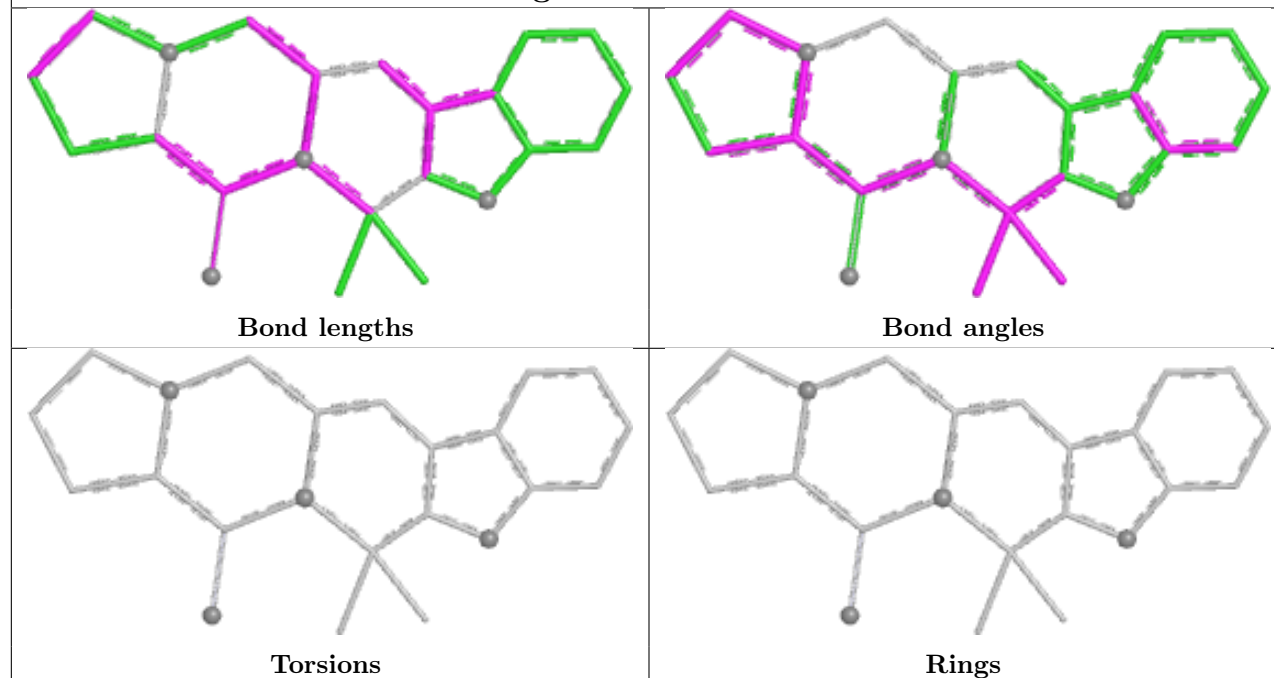
Ligand PM7 C 802



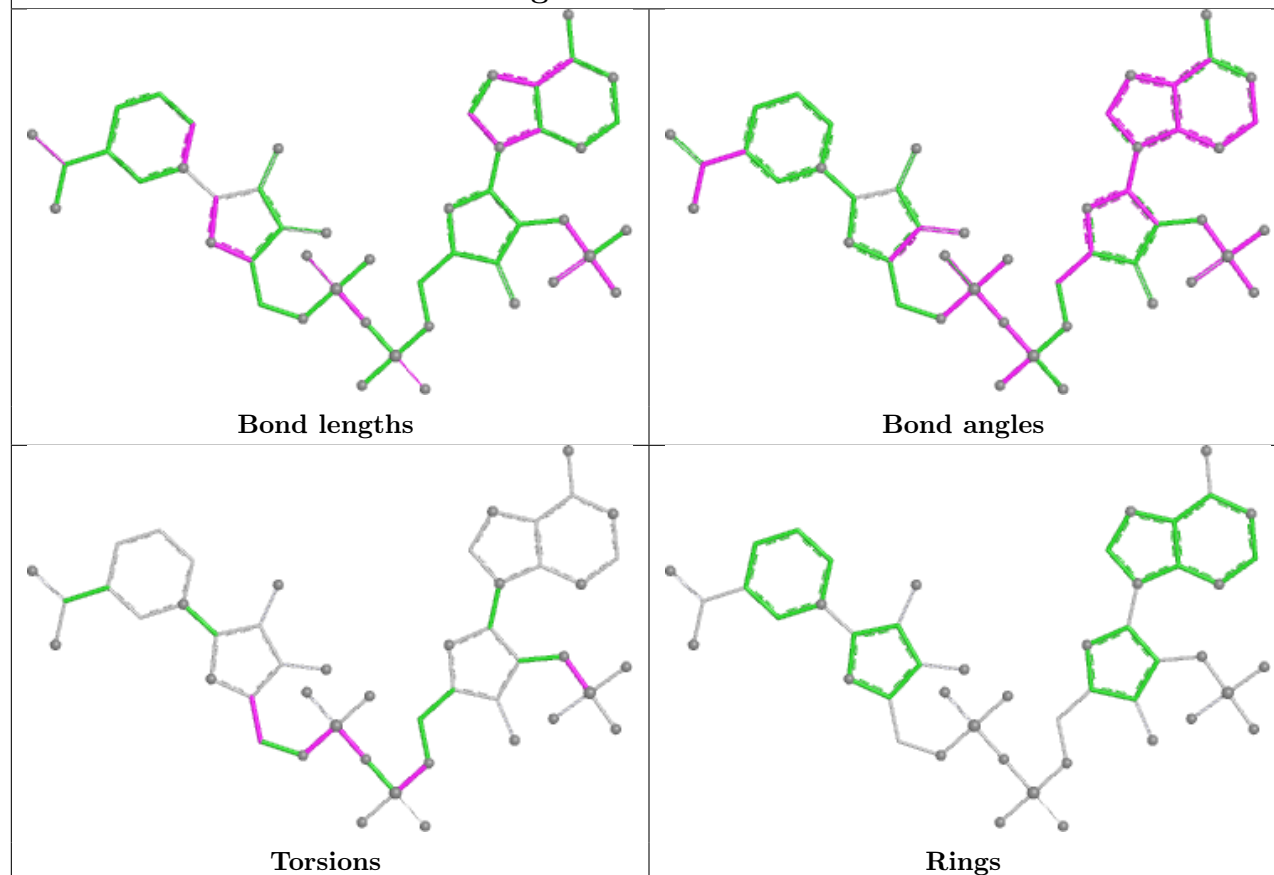
Ligand PM7 E 802



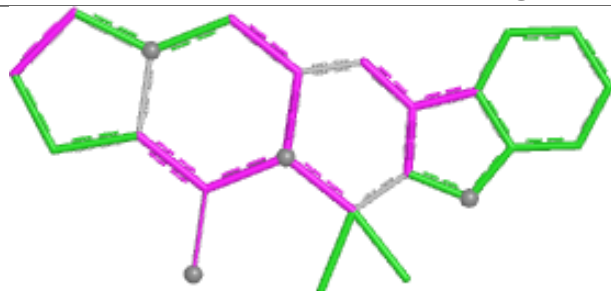
Ligand PM7 F 802



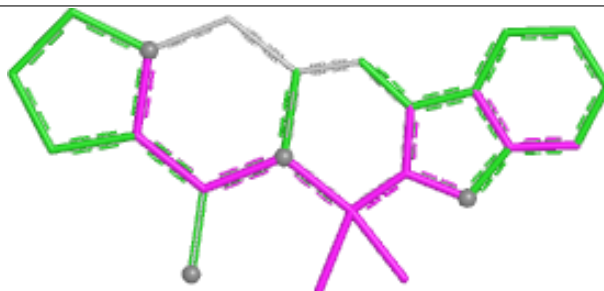
Ligand NAP E 801



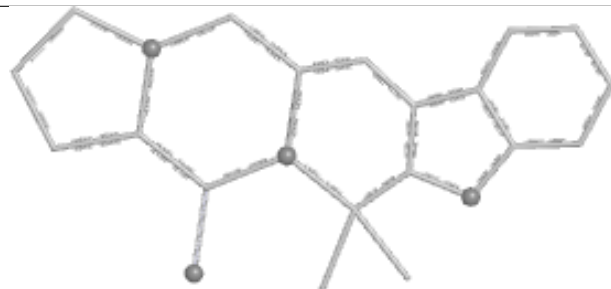
Ligand PM7 D 802



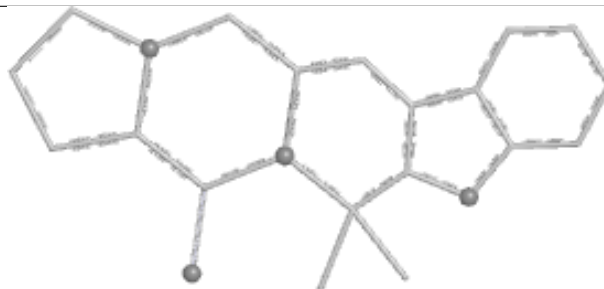
Bond lengths



Bond angles

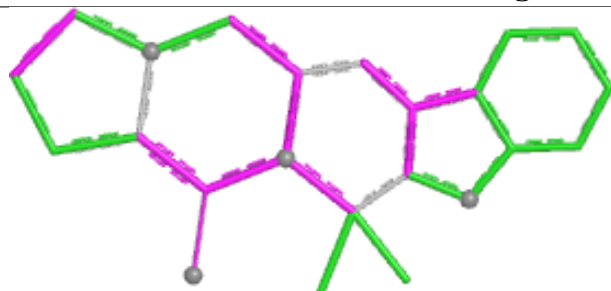


Torsions

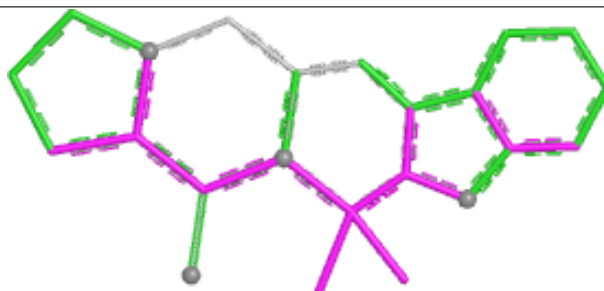


Rings

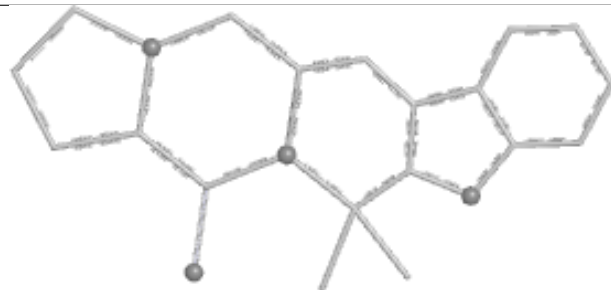
Ligand PM7 B 802



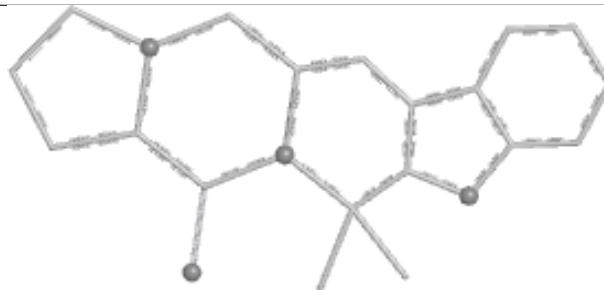
Bond lengths



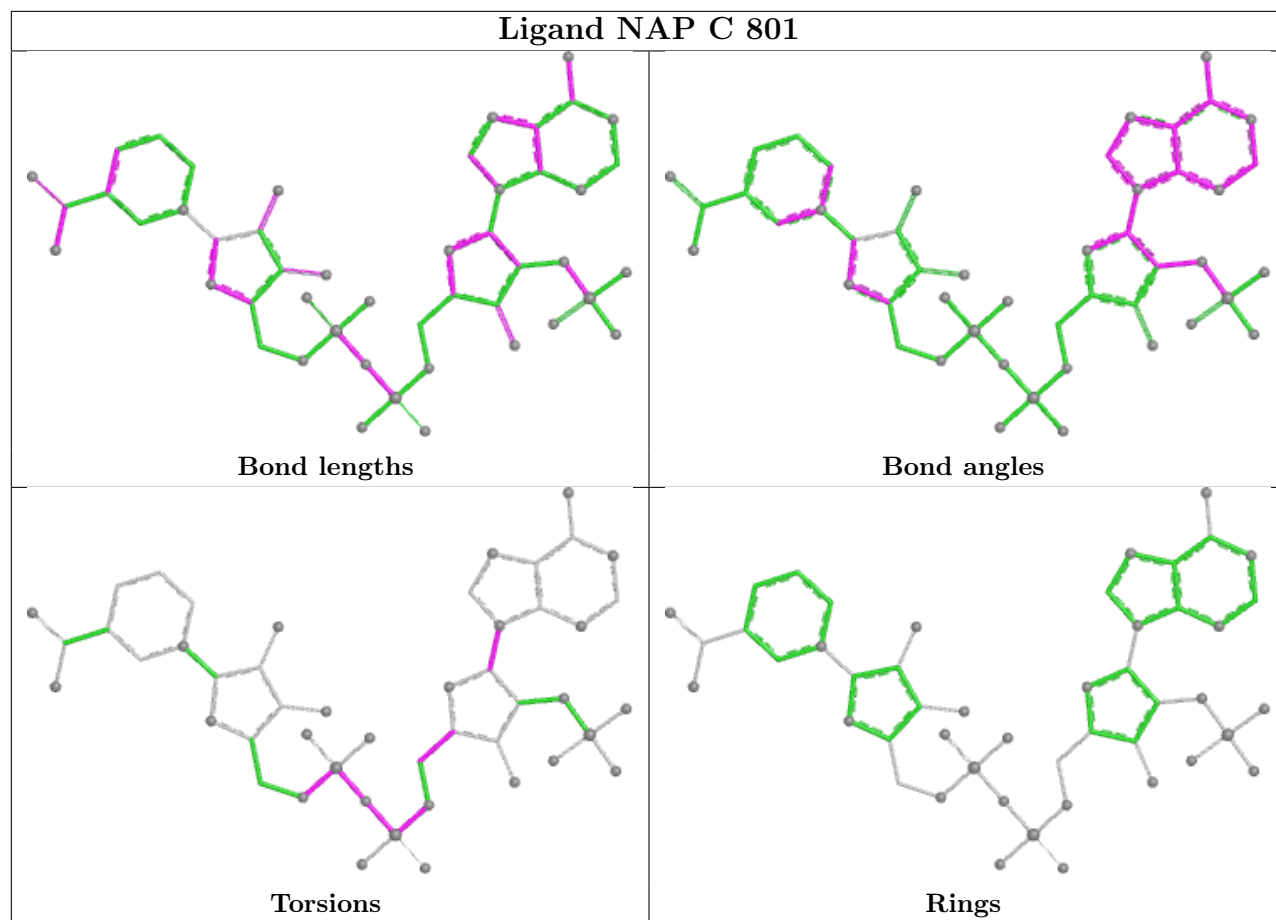
Bond angles



Torsions



Rings



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	257/265 (96%)	1.95	116 (45%) 0 0	32, 54, 78, 119	0
1	B	257/265 (96%)	1.92	105 (40%) 0 0	31, 50, 79, 114	0
1	C	256/265 (96%)	2.40	153 (59%) 0 0	32, 63, 105, 123	0
1	D	257/265 (96%)	2.18	132 (51%) 0 0	36, 63, 105, 141	0
1	E	256/265 (96%)	3.35	222 (86%) 0 0	55, 88, 123, 154	0
1	F	256/265 (96%)	4.28	253 (98%) 0 0	82, 117, 150, 176	0
All	All	1539/1590 (96%)	2.68	981 (63%) 0 0	31, 67, 130, 176	0

All (981) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	104	VAL	10.3
1	F	134	ALA	9.3
1	F	255	VAL	8.9
1	F	254	SER	8.4
1	F	121	VAL	8.4
1	B	14	GLY	8.3
1	C	17	VAL	8.1
1	F	130	ILE	8.0
1	F	17	VAL	7.9
1	F	12	LEU	7.4
1	F	77	LEU	7.4
1	F	19	VAL	7.4
1	F	135	PRO	7.4
1	F	133	VAL	7.3
1	E	197	VAL	7.0
1	F	244	TYR	7.0
1	F	155	THR	6.9
1	D	72	ALA	6.9
1	A	230	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	F	248	ASP	6.8
1	F	197	VAL	6.8
1	F	136	LEU	6.8
1	C	109	ASP	6.7
1	E	18	LEU	6.6
1	F	106	THR	6.6
1	F	157	THR	6.6
1	F	179	VAL	6.5
1	F	215	ALA	6.4
1	F	110	MET	6.4
1	E	198	VAL	6.4
1	E	223	ALA	6.4
1	E	240	GLN	6.3
1	C	110	MET	6.3
1	F	138	VAL	6.1
1	E	168	GLY	6.1
1	F	167	PRO	6.1
1	F	256	VAL	6.1
1	F	33	ALA	6.0
1	E	264	LEU	6.0
1	F	108	ALA	5.9
1	F	181	ALA	5.9
1	E	242	TYR	5.9
1	E	265	VAL	5.9
1	F	198	VAL	5.9
1	F	29	ALA	5.9
1	F	129	ILE	5.9
1	E	19	VAL	5.9
1	C	265	VAL	5.8
1	F	44	VAL	5.8
1	C	230	GLY	5.8
1	F	96	GLY	5.8
1	F	30	VAL	5.7
1	F	187	ALA	5.7
1	F	196	ASN	5.7
1	E	230	GLY	5.7
1	F	250	TYR	5.7
1	E	254	SER	5.7
1	F	43	ILE	5.6
1	F	91	LEU	5.6
1	C	229	VAL	5.6
1	E	228	THR	5.6

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Mol	Chain	Res	Type	RSRZ
1	F	171	VAL	5.6
1	F	119	LEU	5.6
1	E	70	ILE	5.6
1	F	263	LEU	5.5
1	E	207	ALA	5.5
1	E	32	ALA	5.5
1	F	199	ALA	5.5
1	F	45	GLY	5.5
1	F	176	CYS	5.5
1	F	212	LEU	5.5
1	E	105	ILE	5.5
1	E	227	SER	5.4
1	C	65	THR	5.4
1	E	163	LEU	5.4
1	E	229	VAL	5.4
1	D	62	PHE	5.4
1	E	153	SER	5.3
1	E	58	LEU	5.3
1	E	243	ILE	5.3
1	F	145	TYR	5.3
1	F	202	ALA	5.3
1	F	93	LEU	5.3
1	E	172	ILE	5.2
1	F	225	ALA	5.2
1	E	212	LEU	5.2
1	E	263	LEU	5.2
1	E	237	SER	5.2
1	E	187	ALA	5.2
1	E	239	ALA	5.2
1	E	55	VAL	5.2
1	F	265	VAL	5.2
1	F	40	ILE	5.2
1	F	41	VAL	5.2
1	B	71	VAL	5.1
1	D	46	SER	5.1
1	E	61	SER	5.1
1	E	39	ALA	5.1
1	E	221	GLU	5.1
1	F	160	ALA	5.1
1	D	17	VAL	5.1
1	D	172	ILE	5.1
1	C	108	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	F	158	SER	5.1
1	F	105	ILE	5.0
1	F	80	SER	5.0
1	F	169	TRP	5.0
1	F	216	TYR	5.0
1	F	178	ALA	5.0
1	E	257	SER	5.0
1	C	14	GLY	5.0
1	E	235	PRO	5.0
1	F	20	ILE	5.0
1	F	100	ILE	5.0
1	E	82	THR	5.0
1	B	147	ASN	5.0
1	F	94	ALA	5.0
1	F	183	SER	4.9
1	F	124	VAL	4.9
1	F	168	GLY	4.9
1	F	175	TYR	4.9
1	F	62	PHE	4.9
1	F	186	LEU	4.9
1	E	13	HIS	4.9
1	F	32	ALA	4.9
1	F	153	SER	4.9
1	F	253	GLY	4.9
1	F	70	ILE	4.9
1	F	120	THR	4.9
1	F	18	LEU	4.9
1	B	70	ILE	4.9
1	F	182	MET	4.8
1	C	25	GLY	4.8
1	B	265	VAL	4.8
1	F	238	VAL	4.8
1	F	103	ILE	4.8
1	E	41	VAL	4.8
1	F	137	MET	4.8
1	A	148	LYS	4.8
1	F	34	ALA	4.8
1	F	63	PRO	4.8
1	F	165	PRO	4.8
1	E	104	VAL	4.8
1	F	28	PHE	4.7
1	F	22	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	40	ILE	4.7
1	F	86	ASP	4.7
1	F	109	ASP	4.7
1	E	22	GLY	4.7
1	F	207	ALA	4.7
1	F	132	LEU	4.7
1	E	201	GLY	4.7
1	F	139	ALA	4.7
1	C	69	ASP	4.7
1	F	162	CYS	4.7
1	D	116	LEU	4.7
1	F	174	GLY	4.7
1	E	29	ALA	4.7
1	C	15	SER	4.6
1	E	106	THR	4.6
1	D	58	LEU	4.6
1	E	188	ILE	4.6
1	E	238	VAL	4.6
1	C	211	ILE	4.6
1	E	103	ILE	4.6
1	F	188	ILE	4.6
1	F	185	GLY	4.6
1	F	39	ALA	4.6
1	E	71	VAL	4.6
1	B	72	ALA	4.5
1	F	112	ALA	4.5
1	D	9	THR	4.5
1	E	218	ALA	4.5
1	F	241	ALA	4.5
1	D	73	VAL	4.5
1	F	195	VAL	4.5
1	F	201	GLY	4.5
1	E	108	ALA	4.5
1	E	202	ALA	4.5
1	F	90	ALA	4.5
1	F	180	GLU	4.5
1	E	10	ASP	4.5
1	E	109	ASP	4.5
1	F	10	ASP	4.5
1	F	116	LEU	4.5
1	F	245	LEU	4.5
1	F	208	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	110	MET	4.5
1	F	264	LEU	4.4
1	F	131	ARG	4.4
1	E	226	LYS	4.4
1	E	34	ALA	4.4
1	E	131	ARG	4.4
1	E	255	VAL	4.4
1	E	236	GLU	4.3
1	E	93	LEU	4.3
1	F	58	LEU	4.3
1	F	156	LEU	4.3
1	F	163	LEU	4.3
1	F	243	ILE	4.3
1	F	257	SER	4.3
1	E	56	ALA	4.3
1	F	200	PRO	4.3
1	E	232	THR	4.3
1	A	147	ASN	4.3
1	F	166	ASP	4.3
1	F	235	PRO	4.3
1	E	65	THR	4.3
1	F	205	THR	4.3
1	E	14	GLY	4.3
1	F	236	GLU	4.3
1	F	218	ALA	4.3
1	B	109	ASP	4.2
1	C	10	ASP	4.2
1	C	241	ALA	4.2
1	D	14	GLY	4.2
1	E	167	PRO	4.2
1	C	128	GLY	4.2
1	C	233	GLY	4.2
1	E	211	ILE	4.2
1	D	265	VAL	4.2
1	C	75	CYS	4.2
1	F	64	SER	4.2
1	F	203	VAL	4.2
1	C	216	TYR	4.2
1	E	199	ALA	4.2
1	E	225	ALA	4.2
1	F	115	PRO	4.2
1	F	190	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	232	THR	4.2
1	E	149	CYS	4.1
1	D	229	VAL	4.1
1	E	158	SER	4.1
1	F	15	SER	4.1
1	E	139	ALA	4.1
1	F	221	GLU	4.1
1	F	204	LEU	4.1
1	A	82	THR	4.1
1	D	87	ILE	4.1
1	D	214	ASP	4.1
1	F	223	ALA	4.1
1	F	65	THR	4.1
1	F	82	THR	4.1
1	D	45	GLY	4.1
1	E	173	SER	4.1
1	D	41	VAL	4.1
1	E	256	VAL	4.1
1	D	67	PRO	4.1
1	E	165	PRO	4.1
1	E	258	THR	4.1
1	F	141	HIS	4.1
1	F	74	ARG	4.1
1	E	138	VAL	4.1
1	F	251	ALA	4.0
1	B	247	LYS	4.0
1	F	51	LEU	4.0
1	E	196	ASN	4.0
1	D	254	SER	4.0
1	E	146	MET	4.0
1	F	222	MET	4.0
1	F	262	MET	4.0
1	F	26	ILE	4.0
1	A	150	PRO	4.0
1	A	9	THR	4.0
1	D	40	ILE	4.0
1	D	100	ILE	4.0
1	F	71	VAL	3.9
1	E	260	GLY	3.9
1	E	52	LYS	3.9
1	F	184	ARG	3.9
1	F	83	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	94	ALA	3.9
1	F	14	GLY	3.9
1	F	228	THR	3.9
1	F	59	LYS	3.9
1	F	147	ASN	3.9
1	D	129	ILE	3.9
1	E	244	TYR	3.9
1	C	116	LEU	3.9
1	D	51	LEU	3.9
1	C	62	PHE	3.9
1	D	108	ALA	3.9
1	F	237	SER	3.8
1	A	70	ILE	3.8
1	F	87	ILE	3.8
1	A	77	LEU	3.8
1	F	36	GLY	3.8
1	A	29	ALA	3.8
1	F	23	THR	3.8
1	F	48	ALA	3.8
1	F	79	ASN	3.8
1	B	149	CYS	3.8
1	B	15	SER	3.8
1	E	200	PRO	3.8
1	F	73	VAL	3.8
1	C	12	LEU	3.8
1	C	51	LEU	3.8
1	C	142	LEU	3.8
1	F	261	GLY	3.8
1	F	13	HIS	3.8
1	B	9	THR	3.8
1	A	67	PRO	3.8
1	E	152	SER	3.8
1	E	246	MET	3.8
1	C	215	ALA	3.8
1	D	239	ALA	3.8
1	F	81	ASP	3.8
1	E	262	MET	3.8
1	E	60	SER	3.8
1	E	192	PRO	3.8
1	F	143	PRO	3.8
1	F	107	ALA	3.7
1	D	63	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	102	HIS	3.7
1	D	196	ASN	3.7
1	F	217	ASP	3.7
1	D	215	ALA	3.7
1	E	241	ALA	3.7
1	C	212	LEU	3.7
1	F	193	LEU	3.7
1	E	23	THR	3.7
1	F	170	THR	3.7
1	C	173	SER	3.7
1	F	249	HIS	3.7
1	F	149	CYS	3.7
1	C	11	GLN	3.7
1	E	77	LEU	3.7
1	F	142	LEU	3.7
1	D	145	TYR	3.7
1	F	85	GLN	3.6
1	A	93	LEU	3.6
1	A	264	LEU	3.6
1	E	31	CYS	3.6
1	A	165	PRO	3.6
1	C	158	SER	3.6
1	F	46	SER	3.6
1	E	28	PHE	3.6
1	F	211	ILE	3.6
1	A	190	LEU	3.6
1	B	29	ALA	3.6
1	A	209	LYS	3.6
1	C	113	PRO	3.6
1	E	251	ALA	3.6
1	D	50	LYS	3.6
1	E	250	TYR	3.6
1	F	227	SER	3.6
1	B	151	GLN	3.6
1	D	70	ILE	3.6
1	F	172	ILE	3.6
1	A	149	CYS	3.6
1	E	111	THR	3.6
1	B	13	HIS	3.6
1	F	113	PRO	3.6
1	D	158	SER	3.6
1	D	236	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	54	SER	3.6
1	E	51	LEU	3.6
1	F	69	ASP	3.6
1	F	99	LYS	3.6
1	F	101	ASN	3.6
1	C	56	ALA	3.6
1	F	49	GLN	3.5
1	C	16	ARG	3.5
1	E	253	GLY	3.5
1	F	159	GLY	3.5
1	B	77	LEU	3.5
1	C	238	VAL	3.5
1	B	201	GLY	3.5
1	E	45	GLY	3.5
1	E	261	GLY	3.5
1	F	25	GLY	3.5
1	A	51	LEU	3.5
1	E	116	LEU	3.5
1	F	102	HIS	3.5
1	C	127	PRO	3.5
1	E	73	VAL	3.5
1	F	220	VAL	3.5
1	D	226	LYS	3.5
1	A	259	ASN	3.5
1	C	97	ASN	3.5
1	F	229	VAL	3.5
1	C	107	ALA	3.5
1	E	160	ALA	3.5
1	C	52	LYS	3.5
1	D	64	SER	3.5
1	E	175	TYR	3.5
1	F	154	LEU	3.5
1	E	74	ARG	3.5
1	C	71	VAL	3.4
1	E	208	VAL	3.4
1	F	219	ALA	3.4
1	F	123	SER	3.4
1	F	37	HIS	3.4
1	E	224	GLU	3.4
1	E	245	LEU	3.4
1	E	124	VAL	3.4
1	F	72	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	233	GLY	3.4
1	E	195	VAL	3.4
1	E	219	ALA	3.4
1	F	60	SER	3.4
1	A	176	CYS	3.4
1	B	185	GLY	3.4
1	D	79	ASN	3.4
1	E	81	ASP	3.4
1	F	54	SER	3.4
1	F	61	SER	3.4
1	F	144	LYS	3.4
1	F	213	GLY	3.4
1	E	79	ASN	3.4
1	F	97	ASN	3.4
1	C	70	ILE	3.3
1	E	100	ILE	3.3
1	E	67	PRO	3.3
1	F	114	PRO	3.3
1	A	216	TYR	3.3
1	B	65	THR	3.3
1	F	242	TYR	3.3
1	E	147	ASN	3.3
1	E	87	ILE	3.3
1	F	78	SER	3.3
1	A	72	ALA	3.3
1	C	223	ALA	3.3
1	E	49	GLN	3.3
1	E	38	GLY	3.3
1	F	68	ASP	3.3
1	D	77	LEU	3.3
1	D	193	LEU	3.3
1	E	176	CYS	3.3
1	C	40	ILE	3.3
1	E	143	PRO	3.3
1	B	62	PHE	3.3
1	C	106	THR	3.3
1	E	107	ALA	3.3
1	E	119	LEU	3.3
1	F	75	CYS	3.3
1	F	127	PRO	3.3
1	A	158	SER	3.3
1	B	250	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	60	SER	3.3
1	B	168	GLY	3.2
1	F	177	GLY	3.2
1	E	91	LEU	3.2
1	D	209	LYS	3.2
1	E	102	HIS	3.2
1	E	64	SER	3.2
1	E	80	SER	3.2
1	F	234	SER	3.2
1	C	39	ALA	3.2
1	D	207	ALA	3.2
1	E	30	VAL	3.2
1	E	112	ALA	3.2
1	A	116	LEU	3.2
1	D	162	CYS	3.2
1	F	31	CYS	3.2
1	F	252	SER	3.2
1	C	239	ALA	3.2
1	A	185	GLY	3.2
1	B	159	GLY	3.2
1	F	76	ASP	3.2
1	F	148	LYS	3.2
1	F	259	ASN	3.2
1	D	119	LEU	3.2
1	D	228	THR	3.2
1	C	222	MET	3.2
1	F	164	ARG	3.2
1	B	27	GLY	3.2
1	F	206	GLU	3.2
1	C	101	ASN	3.2
1	E	69	ASP	3.2
1	E	76	ASP	3.2
1	E	179	VAL	3.2
1	F	55	VAL	3.2
1	A	163	LEU	3.2
1	F	42	THR	3.2
1	B	164	ARG	3.1
1	E	222	MET	3.2
1	F	98	SER	3.1
1	F	152	SER	3.1
1	C	213	GLY	3.1
1	C	218	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	177	GLY	3.1
1	D	55	VAL	3.1
1	E	17	VAL	3.1
1	C	242	TYR	3.1
1	B	58	LEU	3.1
1	C	67	PRO	3.1
1	E	85	GLN	3.1
1	B	162	CYS	3.1
1	E	75	CYS	3.1
1	C	152	SER	3.1
1	E	249	HIS	3.1
1	E	27	GLY	3.1
1	E	213	GLY	3.1
1	C	35	LEU	3.1
1	E	35	LEU	3.1
1	F	35	LEU	3.1
1	F	192	PRO	3.1
1	D	110	MET	3.1
1	D	82	THR	3.1
1	A	75	CYS	3.1
1	A	214	ASP	3.1
1	B	69	ASP	3.1
1	B	230	GLY	3.1
1	C	96	GLY	3.1
1	D	53	ASP	3.1
1	D	147	ASN	3.1
1	F	122	ASP	3.1
1	F	56	ALA	3.1
1	E	220	VAL	3.1
1	D	35	LEU	3.1
1	E	135	PRO	3.1
1	E	150	PRO	3.1
1	F	209	LYS	3.1
1	A	110	MET	3.1
1	C	258	THR	3.1
1	E	37	HIS	3.1
1	B	166	ASP	3.1
1	C	92	GLN	3.1
1	F	27	GLY	3.1
1	A	17	VAL	3.1
1	D	71	VAL	3.1
1	F	226	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	190	LEU	3.1
1	E	204	LEU	3.1
1	C	103	ILE	3.0
1	E	155	THR	3.0
1	C	61	SER	3.0
1	F	11	GLN	3.0
1	C	79	ASN	3.0
1	D	38	GLY	3.0
1	C	32	ALA	3.0
1	F	239	ALA	3.0
1	A	30	VAL	3.0
1	C	195	VAL	3.0
1	A	206	GLU	3.0
1	C	117	GLU	3.0
1	A	243	ILE	3.0
1	E	151	GLN	3.0
1	F	89	LYS	3.0
1	F	53	ASP	3.0
1	F	128	GLY	3.0
1	B	139	ALA	3.0
1	D	225	ALA	3.0
1	D	188	ILE	3.0
1	E	161	HIS	3.0
1	D	42	THR	3.0
1	D	170	THR	3.0
1	F	231	GLN	3.0
1	E	148	LYS	3.0
1	F	126	ARG	3.0
1	B	24	SER	3.0
1	B	60	SER	3.0
1	B	61	SER	3.0
1	D	109	ASP	3.0
1	E	36	GLY	3.0
1	C	72	ALA	3.0
1	D	57	ARG	3.0
1	F	92	GLN	3.0
1	D	65	THR	3.0
1	E	97	ASN	3.0
1	F	38	GLY	3.0
1	F	214	ASP	3.0
1	A	32	ALA	2.9
1	A	108	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	157	THR	2.9
1	D	227	SER	2.9
1	F	24	SER	2.9
1	D	182	MET	2.9
1	F	118	ASP	2.9
1	C	28	PHE	2.9
1	C	94	ALA	2.9
1	D	29	ALA	2.9
1	D	220	VAL	2.9
1	D	149	CYS	2.9
1	F	57	ARG	2.9
1	C	26	ILE	2.9
1	C	43	ILE	2.9
1	D	120	THR	2.9
1	B	150	PRO	2.9
1	D	59	LYS	2.9
1	C	34	ALA	2.9
1	D	12	LEU	2.9
1	E	231	GLN	2.9
1	A	73	VAL	2.9
1	E	44	VAL	2.9
1	B	234	SER	2.9
1	A	96	GLY	2.9
1	E	247	LYS	2.9
1	A	12	LEU	2.9
1	E	48	ALA	2.9
1	A	229	VAL	2.9
1	E	83	VAL	2.9
1	C	129	ILE	2.9
1	D	211	ILE	2.9
1	E	130	ILE	2.9
1	A	168	GLY	2.8
1	B	78	SER	2.8
1	C	98	SER	2.8
1	E	24	SER	2.8
1	F	140	LYS	2.8
1	C	85	GLN	2.8
1	C	91	LEU	2.8
1	E	62	PHE	2.8
1	A	208	VAL	2.8
1	C	133	VAL	2.8
1	C	130	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	78	SER	2.8
1	D	98	SER	2.8
1	E	164	ARG	2.8
1	D	112	ALA	2.8
1	E	203	VAL	2.8
1	F	111	THR	2.8
1	A	97	ASN	2.8
1	C	122	ASP	2.8
1	B	152	SER	2.8
1	E	252	SER	2.8
1	F	240	GLN	2.8
1	F	88	GLU	2.8
1	A	265	VAL	2.8
1	B	83	VAL	2.8
1	C	44	VAL	2.8
1	C	104	VAL	2.8
1	C	217	ASP	2.8
1	E	217	ASP	2.8
1	A	11	GLN	2.8
1	D	125	GLN	2.8
1	A	223	ALA	2.8
1	B	110	MET	2.8
1	B	251	ALA	2.8
1	A	130	ILE	2.7
1	C	111	THR	2.7
1	E	11	GLN	2.7
1	C	45	GLY	2.7
1	C	80	SER	2.7
1	D	142	LEU	2.7
1	B	216	TYR	2.7
1	B	76	ASP	2.7
1	C	82	THR	2.7
1	D	243	ILE	2.7
1	D	213	GLY	2.7
1	F	67	PRO	2.7
1	B	108	ALA	2.7
1	C	41	VAL	2.7
1	D	44	VAL	2.7
1	E	92	GLN	2.7
1	A	63	PRO	2.7
1	E	98	SER	2.7
1	C	126	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	92	GLN	2.7
1	E	216	TYR	2.7
1	A	124	VAL	2.7
1	A	138	VAL	2.7
1	B	10	ASP	2.7
1	C	255	VAL	2.7
1	C	155	THR	2.7
1	E	68	ASP	2.7
1	C	64	SER	2.7
1	D	152	SER	2.7
1	A	112	ALA	2.6
1	B	223	ALA	2.6
1	A	118	ASP	2.6
1	B	88	GLU	2.6
1	B	197	VAL	2.6
1	C	68	ASP	2.6
1	C	73	VAL	2.6
1	D	118	ASP	2.6
1	C	42	THR	2.6
1	E	205	THR	2.6
1	A	114	PRO	2.6
1	B	26	ILE	2.6
1	E	174	GLY	2.6
1	A	31	CYS	2.6
1	B	12	LEU	2.6
1	B	218	ALA	2.6
1	C	90	ALA	2.6
1	F	95	ALA	2.6
1	A	117	GLU	2.6
1	F	16	ARG	2.6
1	E	42	THR	2.6
1	E	180	GLU	2.6
1	F	117	GLU	2.6
1	A	95	ALA	2.6
1	C	112	ALA	2.6
1	D	68	ASP	2.6
1	A	25	GLY	2.6
1	A	177	GLY	2.6
1	A	258	THR	2.6
1	D	222	MET	2.6
1	D	113	PRO	2.6
1	D	233	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	226	LYS	2.6
1	C	58	LEU	2.6
1	D	186	LEU	2.6
1	D	221	GLU	2.6
1	C	164	ARG	2.6
1	D	33	ALA	2.6
1	E	215	ALA	2.6
1	E	259	ASN	2.6
1	F	47	ASN	2.6
1	C	146	MET	2.6
1	B	106	THR	2.6
1	C	63	PRO	2.6
1	D	230	GLY	2.6
1	C	124	VAL	2.6
1	C	87	ILE	2.6
1	D	250	TYR	2.6
1	E	156	LEU	2.5
1	C	74	ARG	2.5
1	C	29	ALA	2.5
1	C	31	CYS	2.5
1	C	181	ALA	2.5
1	A	10	ASP	2.5
1	B	79	ASN	2.5
1	C	200	PRO	2.5
1	E	114	PRO	2.5
1	E	78	SER	2.5
1	D	231	GLN	2.5
1	F	125	GLN	2.5
1	C	221	GLU	2.5
1	A	142	LEU	2.5
1	C	18	LEU	2.5
1	C	154	LEU	2.5
1	E	12	LEU	2.5
1	D	56	ALA	2.5
1	A	38	GLY	2.5
1	A	201	GLY	2.5
1	C	36	GLY	2.5
1	E	159	GLY	2.5
1	F	161	HIS	2.5
1	A	71	VAL	2.5
1	A	179	VAL	2.5
1	B	73	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	46	SER	2.5
1	E	171	VAL	2.5
1	A	40	ILE	2.5
1	C	259	ASN	2.5
1	D	148	LYS	2.5
1	E	181	ALA	2.5
1	E	248	ASP	2.5
1	A	162	CYS	2.5
1	E	113	PRO	2.5
1	F	260	GLY	2.5
1	B	11	GLN	2.5
1	A	237	SER	2.5
1	B	41	VAL	2.5
1	C	234	SER	2.5
1	C	57	ARG	2.5
1	C	256	VAL	2.5
1	D	83	VAL	2.5
1	D	195	VAL	2.5
1	B	244	TYR	2.5
1	E	66	ASP	2.5
1	A	207	ALA	2.5
1	E	72	ALA	2.5
1	D	253	GLY	2.5
1	F	230	GLY	2.5
1	F	84	GLU	2.4
1	F	224	GLU	2.4
1	A	98	SER	2.4
1	A	123	SER	2.4
1	B	28	PHE	2.4
1	C	83	VAL	2.4
1	D	19	VAL	2.4
1	D	99	LYS	2.4
1	F	52	LYS	2.4
1	B	56	ALA	2.4
1	B	253	GLY	2.4
1	B	82	THR	2.4
1	D	111	THR	2.4
1	E	121	VAL	2.4
1	B	59	LYS	2.4
1	E	59	LYS	2.4
1	A	204	LEU	2.4
1	B	154	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	57	ARG	2.4
1	B	25	GLY	2.4
1	A	188	ILE	2.4
1	B	40	ILE	2.4
1	E	125	GLN	2.4
1	B	81	ASP	2.4
1	D	10	ASP	2.4
1	E	63	PRO	2.4
1	A	14	GLY	2.4
1	A	33	ALA	2.4
1	A	36	GLY	2.4
1	B	174	GLY	2.4
1	D	22	GLY	2.4
1	D	223	ALA	2.4
1	A	144	LYS	2.4
1	F	247	LYS	2.4
1	C	54	SER	2.4
1	E	183	SER	2.4
1	A	146	MET	2.4
1	D	28	PHE	2.4
1	E	154	LEU	2.4
1	D	37	HIS	2.4
1	A	145	TYR	2.3
1	A	167	PRO	2.3
1	C	48	ALA	2.3
1	E	90	ALA	2.3
1	D	232	THR	2.3
1	B	262	MET	2.3
1	D	146	MET	2.3
1	B	188	ILE	2.3
1	B	238	VAL	2.3
1	A	126	ARG	2.3
1	C	149	CYS	2.3
1	E	142	LEU	2.3
1	E	193	LEU	2.3
1	C	47	ASN	2.3
1	C	66	ASP	2.3
1	C	99	LYS	2.3
1	C	115	PRO	2.3
1	C	235	PRO	2.3
1	A	39	ALA	2.3
1	B	134	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	123	SER	2.3
1	E	16	ARG	2.3
1	A	55	VAL	2.3
1	B	116	LEU	2.3
1	B	212	LEU	2.3
1	E	50	LYS	2.3
1	D	54	SER	2.3
1	A	195	VAL	2.3
1	E	122	ASP	2.3
1	C	185	GLY	2.3
1	F	21	GLY	2.3
1	B	241	ALA	2.3
1	A	120	THR	2.3
1	B	98	SER	2.3
1	D	13	HIS	2.3
1	A	240	GLN	2.3
1	F	50	LYS	2.3
1	A	28	PHE	2.2
1	C	119	LEU	2.2
1	A	76	ASP	2.2
1	F	210	ASP	2.2
1	B	167	PRO	2.2
1	F	146	MET	2.2
1	A	215	ALA	2.2
1	B	181	ALA	2.2
1	C	145	TYR	2.2
1	C	161	HIS	2.2
1	D	39	ALA	2.2
1	B	237	SER	2.2
1	C	254	SER	2.2
1	E	15	SER	2.2
1	E	234	SER	2.2
1	A	129	ILE	2.2
1	B	203	VAL	2.2
1	B	204	LEU	2.2
1	D	136	LEU	2.2
1	D	212	LEU	2.2
1	B	47	ASN	2.2
1	E	101	ASN	2.2
1	F	66	ASP	2.2
1	F	189	ASP	2.2
1	F	150	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	25	GLY	2.2
1	C	224	GLU	2.2
1	A	219	ALA	2.2
1	B	225	ALA	2.2
1	D	160	ALA	2.2
1	A	61	SER	2.2
1	C	100	ILE	2.2
1	E	129	ILE	2.2
1	A	91	LEU	2.2
1	A	119	LEU	2.2
1	C	30	VAL	2.2
1	C	55	VAL	2.2
1	C	171	VAL	2.2
1	A	74	ARG	2.2
1	A	182	MET	2.2
1	E	182	MET	2.2
1	B	22	GLY	2.2
1	C	236	GLU	2.2
1	A	50	LYS	2.2
1	C	231	GLN	2.2
1	D	161	HIS	2.2
1	A	178	ALA	2.2
1	B	207	ALA	2.2
1	D	107	ALA	2.2
1	B	43	ILE	2.2
1	E	132	LEU	2.2
1	E	86	ASP	2.2
1	C	50	LYS	2.2
1	B	85	GLN	2.2
1	B	213	GLY	2.2
1	D	27	GLY	2.2
1	B	157	THR	2.2
1	D	157	THR	2.2
1	A	250	TYR	2.1
1	E	43	ILE	2.1
1	B	30	VAL	2.1
1	C	220	VAL	2.1
1	D	81	ASP	2.1
1	D	197	VAL	2.1
1	A	192	PRO	2.1
1	D	114	PRO	2.1
1	D	200	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	125	GLN	2.1
1	C	141	HIS	2.1
1	C	38	GLY	2.1
1	D	159	GLY	2.1
1	B	75	CYS	2.1
1	A	60	SER	2.1
1	A	183	SER	2.1
1	B	54	SER	2.1
1	C	134	ALA	2.1
1	E	33	ALA	2.1
1	F	173	SER	2.1
1	F	258	THR	2.1
1	D	242	TYR	2.1
1	B	93	LEU	2.1
1	C	245	LEU	2.1
1	D	43	ILE	2.1
1	D	206	GLU	2.1
1	A	41	VAL	2.1
1	A	169	TRP	2.1
1	B	121	VAL	2.1
1	E	233	GLY	2.1
1	A	15	SER	2.1
1	C	228	THR	2.1
1	E	120	THR	2.1
1	D	218	ALA	2.1
1	C	246	MET	2.1
1	D	93	LEU	2.1
1	D	216	TYR	2.1
1	B	229	VAL	2.1
1	D	167	PRO	2.1
1	C	176	CYS	2.1
1	D	258	THR	2.1
1	E	162	CYS	2.1
1	F	246	MET	2.1
1	A	69	ASP	2.1
1	C	210	ASP	2.1
1	D	85	GLN	2.1
1	E	186	LEU	2.1
1	D	217	ASP	2.1
1	E	166	ASP	2.1
1	B	55	VAL	2.1
1	A	261	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	169	TRP	2.1
1	E	57	ARG	2.1
1	A	59	LYS	2.0
1	B	226	LYS	2.0
1	A	228	THR	2.0
1	B	232	THR	2.0
1	C	232	THR	2.0
1	A	139	ALA	2.0
1	A	225	ALA	2.0
1	B	239	ALA	2.0
1	C	162	CYS	2.0
1	C	151	GLN	2.0
1	A	186	LEU	2.0
1	B	263	LEU	2.0
1	D	18	LEU	2.0
1	D	91	LEU	2.0
1	A	100	ILE	2.0
1	B	130	ILE	2.0
1	C	105	ILE	2.0
1	C	172	ILE	2.0
1	B	135	PRO	2.0
1	C	165	PRO	2.0
1	A	171	VAL	2.0
1	D	74	ARG	2.0
1	E	185	GLY	2.0
1	E	99	LYS	2.0
1	D	169	TRP	2.0
1	B	252	SER	2.0
1	E	206	GLU	2.0
1	C	199	ALA	2.0
1	E	95	ALA	2.0
1	A	109	ASP	2.0
1	B	51	LEU	2.0
1	D	204	LEU	2.0
1	E	53	ASP	2.0
1	A	131	ARG	2.0
1	D	20	ILE	2.0
1	E	191	LYS	2.0

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

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](#)

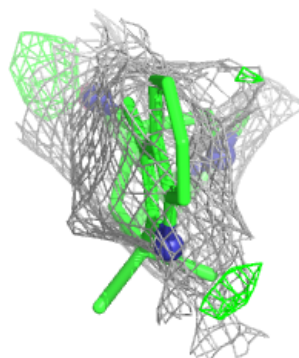
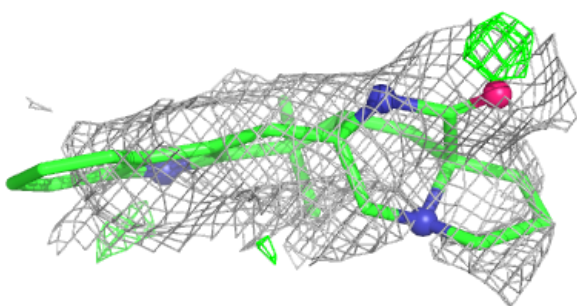
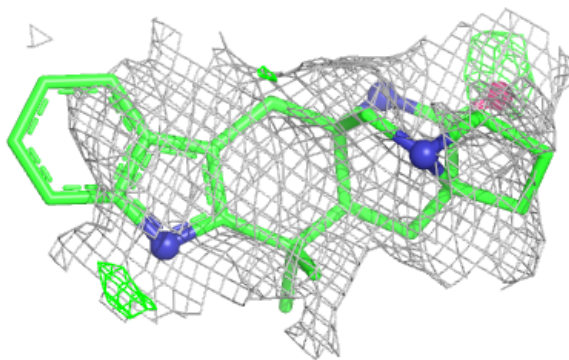
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PM7	F	802	25/25	0.58	0.24	72,94,107,112	0
2	NAP	F	801	48/48	0.75	0.18	77,100,116,121	0
3	PM7	E	802	25/25	0.81	0.22	80,90,106,107	0
2	NAP	C	801	48/48	0.84	0.16	42,58,83,85	0
2	NAP	E	801	48/48	0.85	0.15	63,78,89,97	0
3	PM7	B	802	25/25	0.86	0.16	33,47,51,60	0
3	PM7	D	802	25/25	0.86	0.15	59,63,69,70	0
2	NAP	A	801	48/48	0.86	0.14	35,51,62,69	0
3	PM7	A	802	25/25	0.86	0.16	51,60,68,74	0
3	PM7	C	802	25/25	0.88	0.15	51,61,72,74	0
2	NAP	D	801	48/48	0.88	0.13	42,63,76,77	0
2	NAP	B	801	48/48	0.92	0.11	33,44,60,65	0

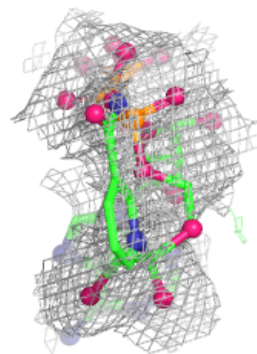
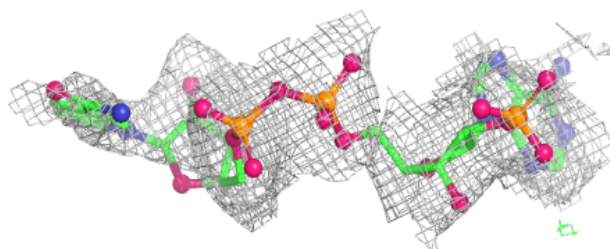
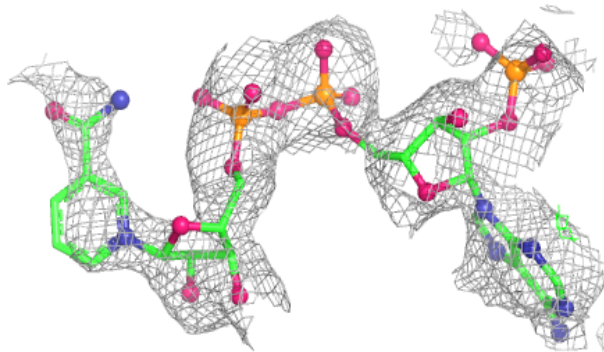
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PM7 F 802:

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

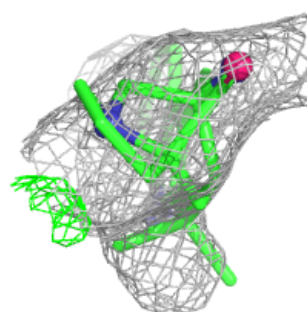
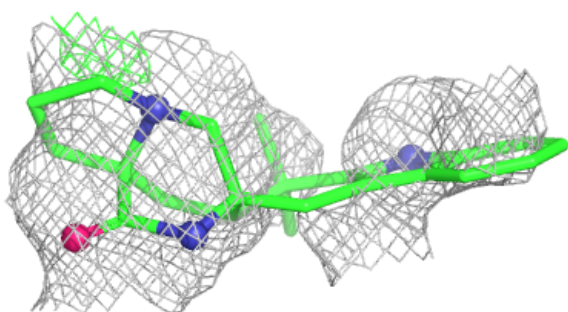
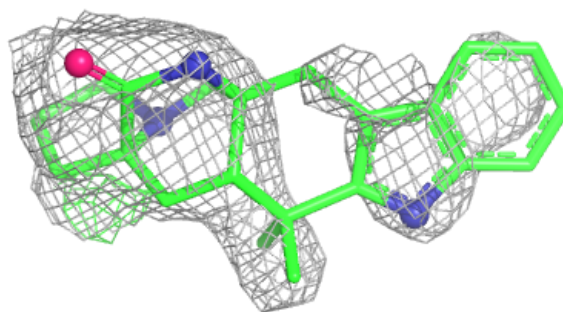
**Electron density around NAP F 801:**

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

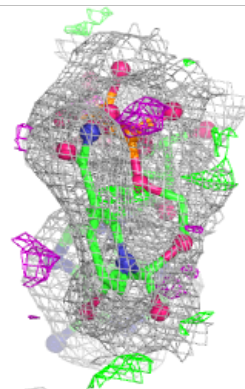
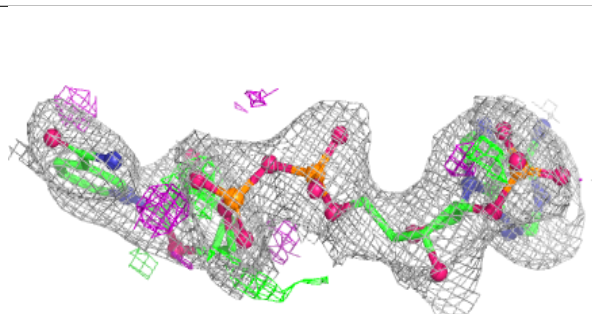
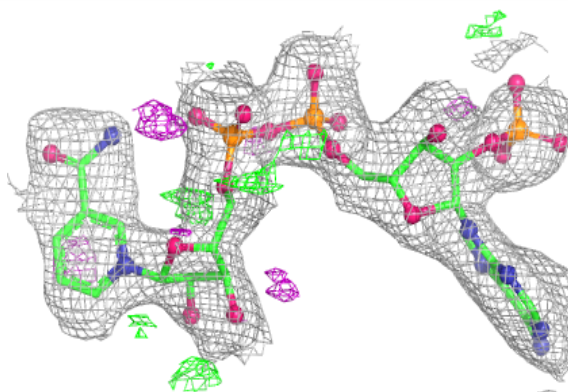


Electron density around PM7 E 802:

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

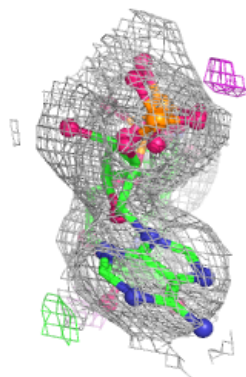
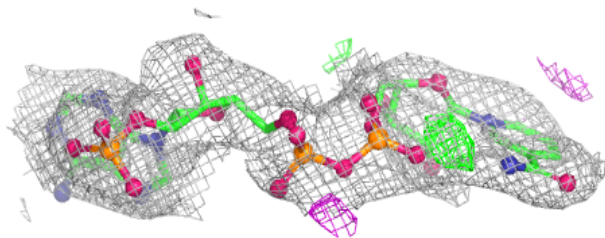
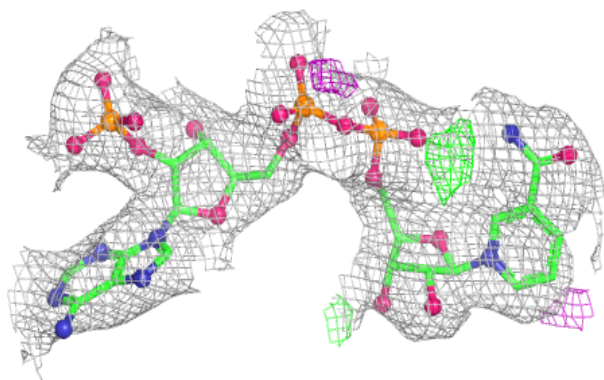
**Electron density around NAP C 801:**

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

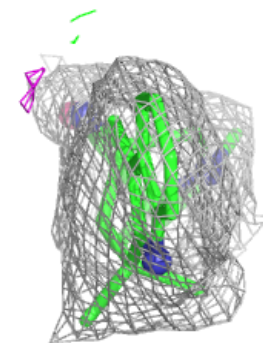
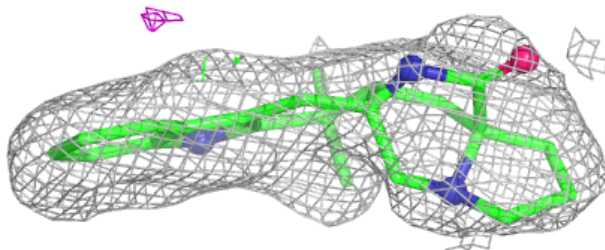
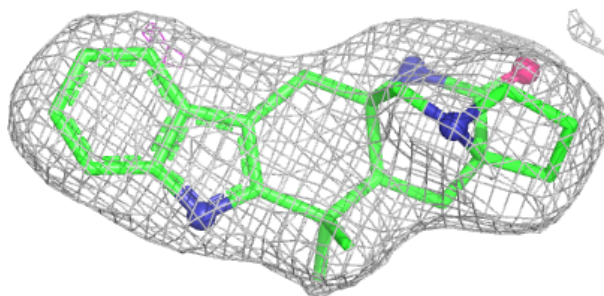


Electron density around NAP E 801:

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

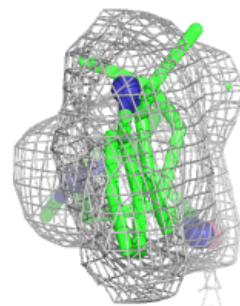
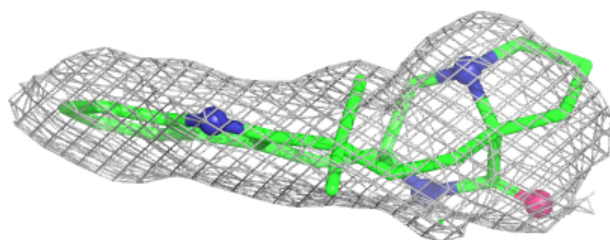
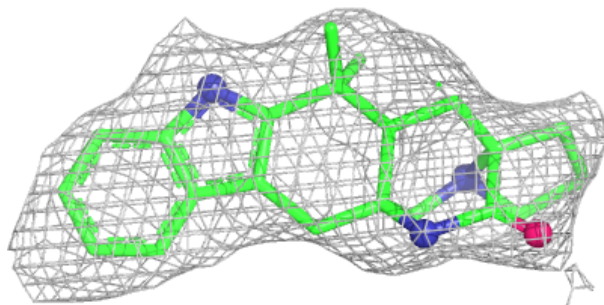
**Electron density around PM7 B 802:**

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

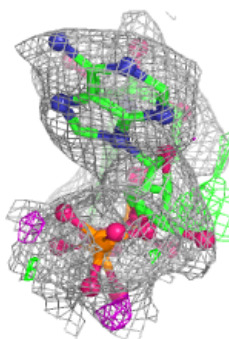
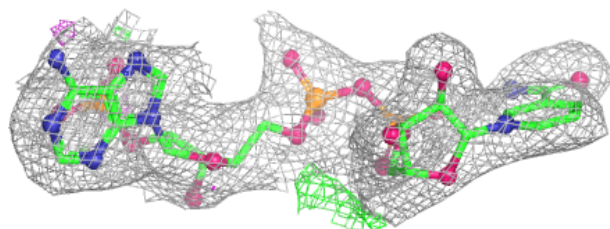
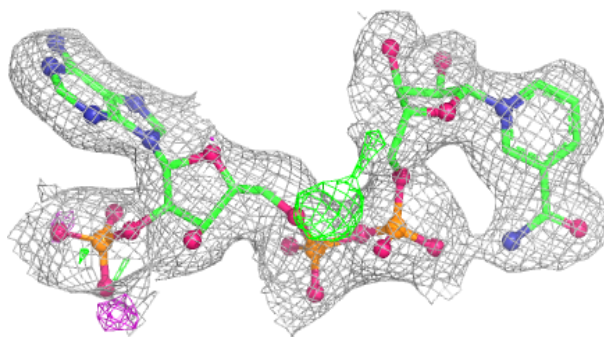


Electron density around PM7 D 802:

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

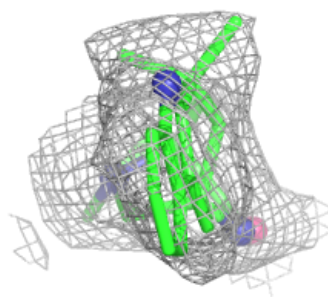
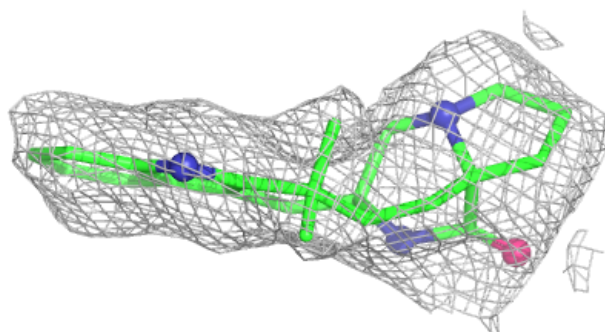
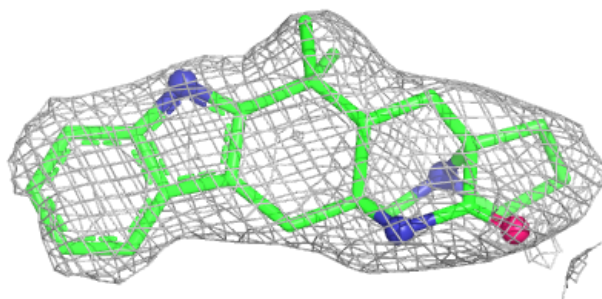
**Electron density around NAP A 801:**

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

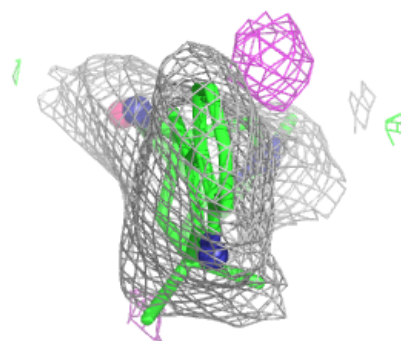
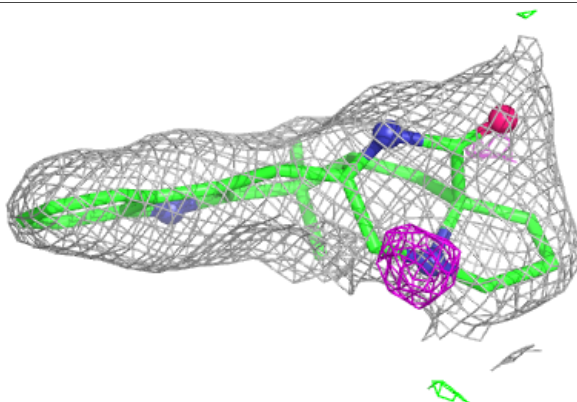
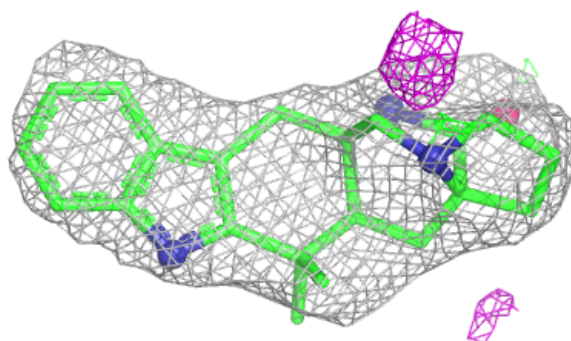


Electron density around PM7 A 802:

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

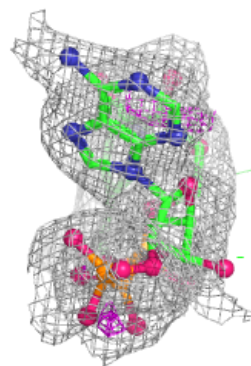
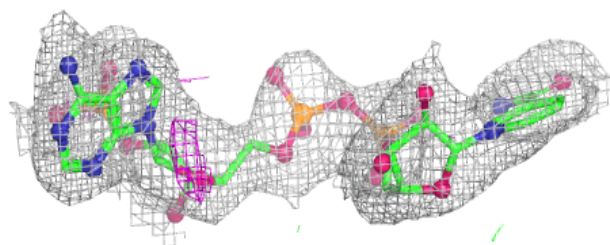
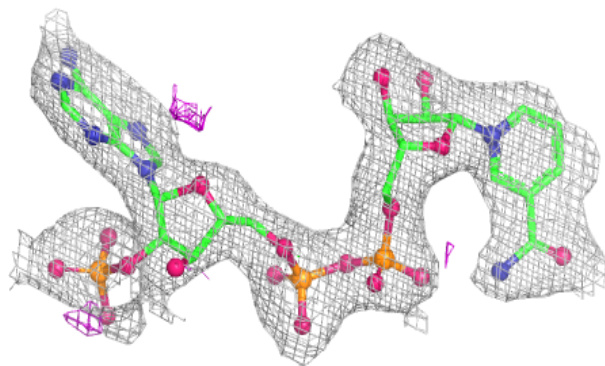
**Electron density around PM7 C 802:**

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

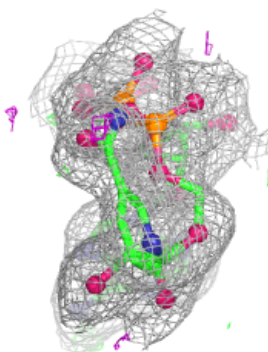
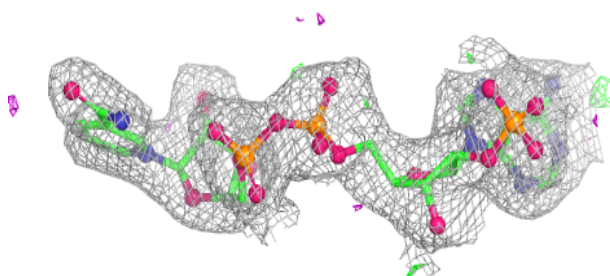
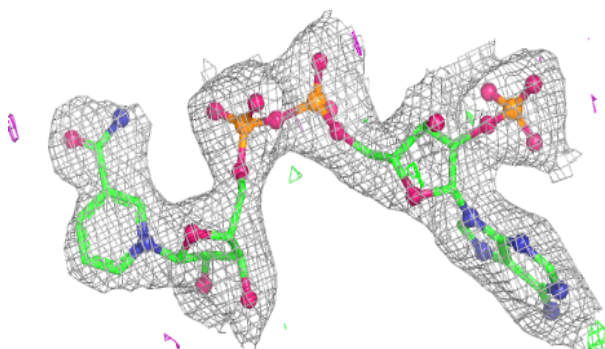


Electron density around NAP D 801:

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

**Electron density around NAP B 801:**

$2mF_o-DF_c$ (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.