



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:56 AM EDT

PDB ID : 6NKK
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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

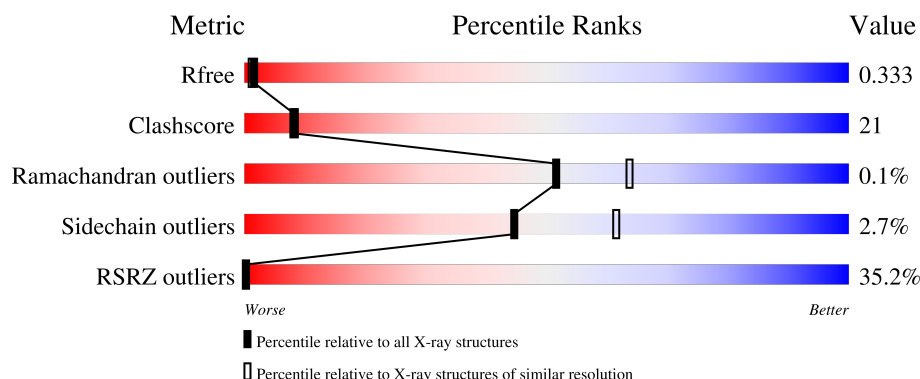
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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	<div> <div>14%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
1	B	265	<div> <div>12%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	C	265	<div> <div>20%</div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	D	265	<div> <div>24%</div> <div>66%</div> <div>28%</div> <div>..</div> </div>
1	E	265	<div> <div>54%</div> <div>55%</div> <div>39%</div> <div>..</div> </div>

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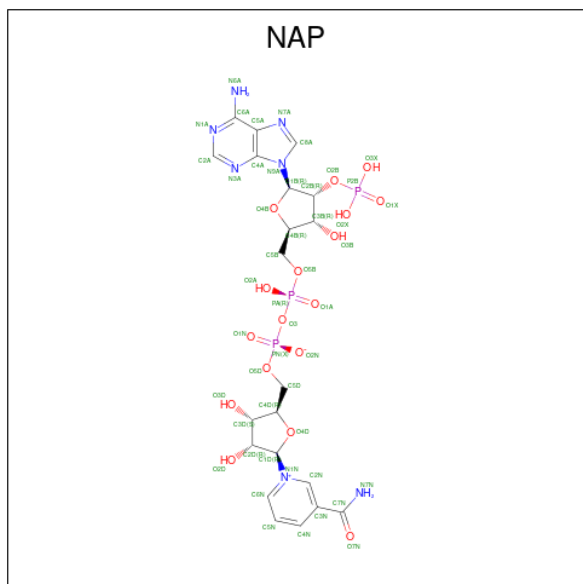
Mol	Chain	Length	Quality of chain
1	F	265	<div><div></div><div>81%</div><div>49%</div><div>43%</div><div>5%</div><div></div></div>

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.

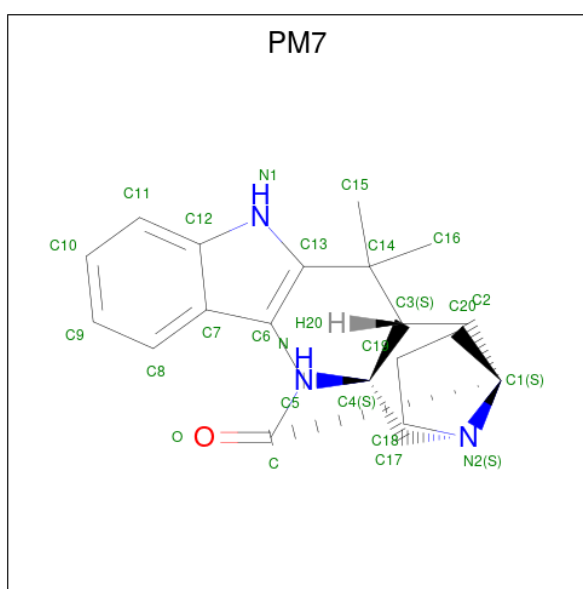
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	B	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	C	256	Total 1859	C 1163	N 320	O 364	S 12	0	0	0
1	D	257	Total 1866	C 1167	N 321	O 366	S 12	0	0	0
1	E	256	Total 1859	C 1163	N 320	O 364	S 12	0	0	0
1	F	256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

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: 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 (5aS,12aS,13aS)-12,12-dimethyl-2,3,11,12,12a,13-hexahydro-1H,5H,6H-5a,13a-(epiminomethano)indolizino[7,6-b]carbazol-14-one (three-letter code: PM7) (formula: $C_{21}H_{25}N_3O$) (labeled as "Ligand of Interest" by depositor).



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

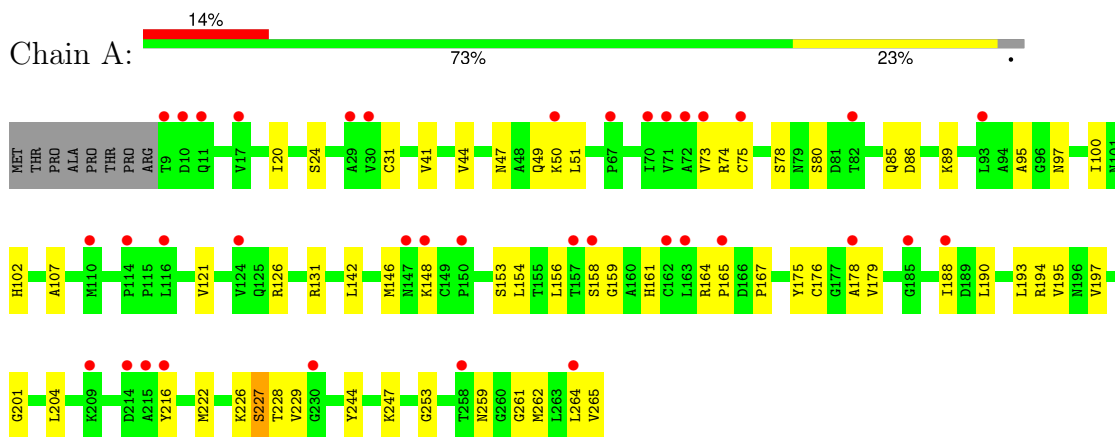
- Molecule 4 is water.

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		

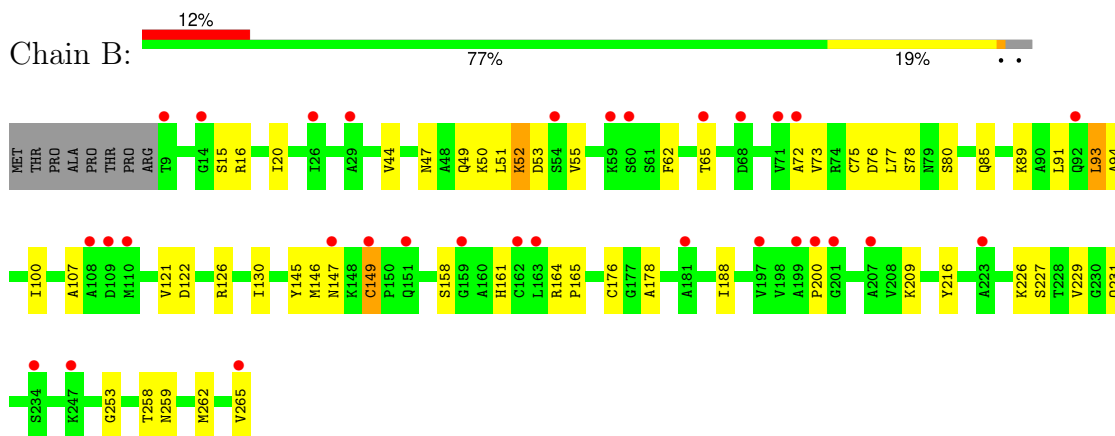
3 Residue-property plots [i](#)

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.

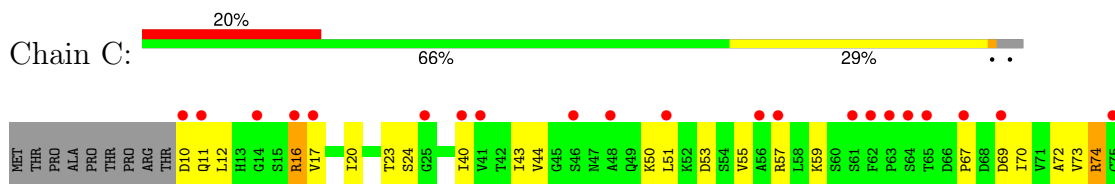
- Molecule 1: Short chain dehydrogenase

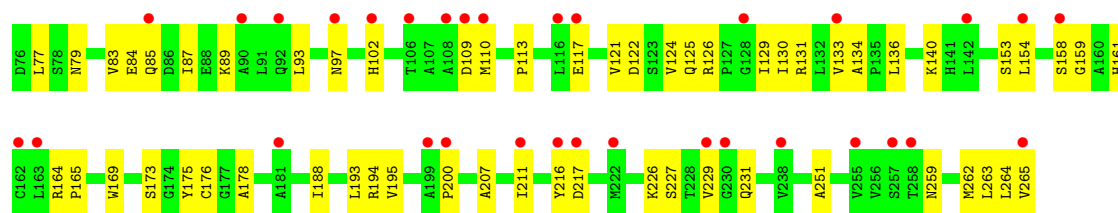


- Molecule 1: Short chain dehydrogenase

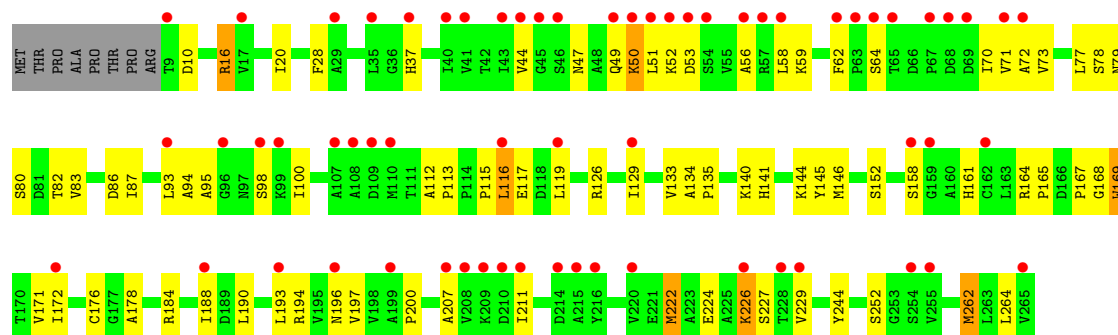


- Molecule 1: Short chain dehydrogenase

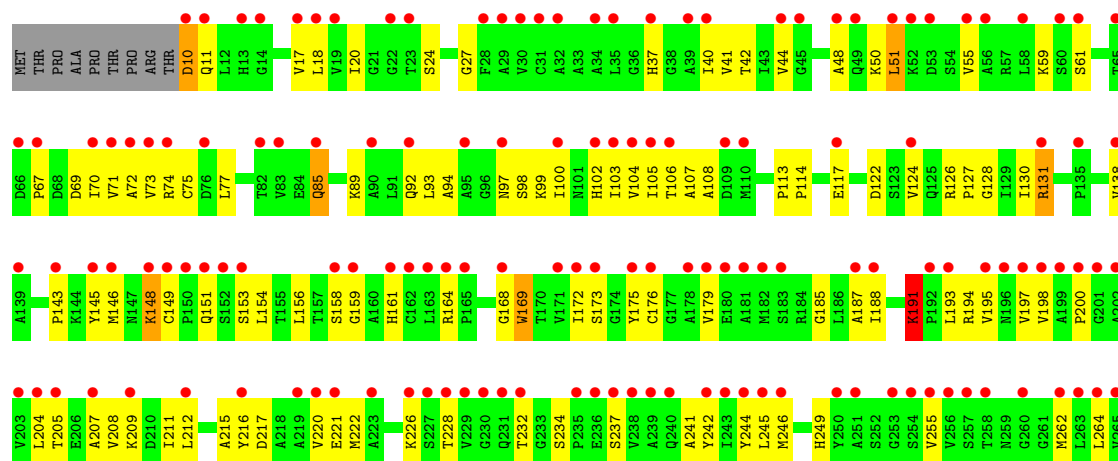




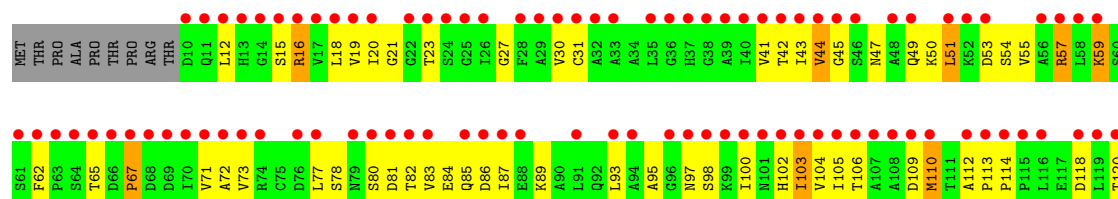
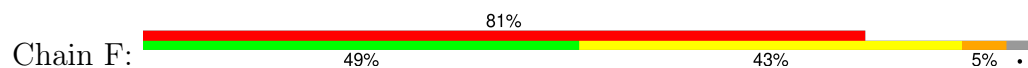
• Molecule 1: Short chain dehydrogenase

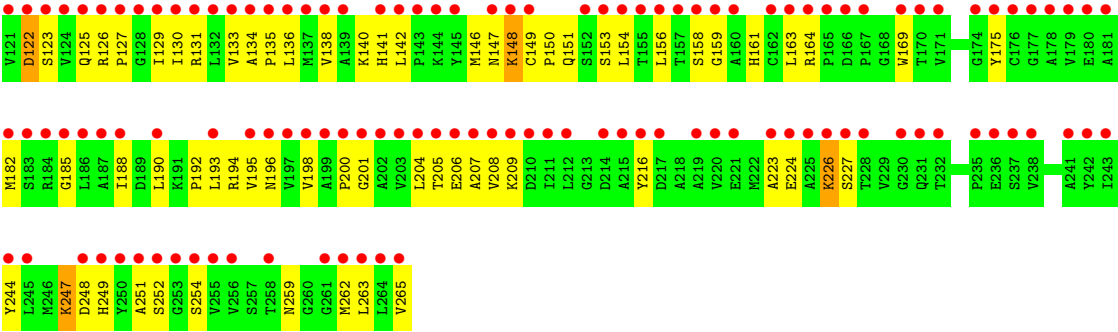


• Molecule 1: Short chain dehydrogenase



• 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) 99.3 (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	3153 reflections (4.80%)	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)	0.29 , 44.2	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	0.91	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 [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/1895	0.64	0/2580
1	B	0.44	0/1895	0.63	1/2580 (0.0%)
1	C	0.42	0/1888	0.63	0/2570
1	D	0.61	3/1895 (0.2%)	0.73	3/2580 (0.1%)
1	E	0.57	1/1888 (0.1%)	0.93	12/2570 (0.5%)
1	F	0.61	0/1888	1.09	11/2570 (0.4%)
All	All	0.55	4/11349 (0.0%)	0.80	27/15450 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	169	TRP	CB-CG	-6.87	1.37	1.50
1	D	168	GLY	C-O	-5.66	1.14	1.23
1	D	169	TRP	C-O	-5.49	1.12	1.23
1	D	169	TRP	CG-CD1	-5.16	1.29	1.36

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	182	MET	CB-CG-SD	-10.83	79.91	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	110	MET	CA-CB-CG	9.58	129.59	113.30
1	D	116	LEU	CA-CB-CG	8.87	135.69	115.30
1	F	110	MET	CB-CG-SD	8.18	136.93	112.40
1	E	51	LEU	CA-CB-CG	8.17	134.09	115.30
1	E	191	LYS	CD-CE-NZ	7.61	129.19	111.70
1	F	122	ASP	CB-CG-OD1	6.81	124.43	118.30
1	E	131	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	E	10	ASP	CB-CG-OD2	6.77	124.39	118.30
1	E	85	GLN	CA-CB-CG	-6.55	98.98	113.40
1	F	67	PRO	C-N-CA	-6.52	105.41	121.70
1	F	87	ILE	CG1-CB-CG2	6.45	125.58	111.40
1	F	57	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	E	168	GLY	N-CA-C	-6.15	97.73	113.10
1	F	59	LYS	CB-CG-CD	-6.09	95.76	111.60
1	E	92	GLN	CB-CA-C	-6.06	98.28	110.40
1	B	89	LYS	CA-CB-CG	6.01	126.63	113.40
1	F	44	VAL	CG1-CB-CG2	6.01	120.51	110.90
1	D	226	LYS	CB-CG-CD	-5.87	96.35	111.60
1	D	16	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	F	122	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	F	103	ILE	CA-CB-CG1	5.59	121.62	111.00
1	E	10	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	E	153	SER	N-CA-CB	5.22	118.33	110.50
1	E	148	LYS	C-N-CA	5.14	134.55	121.70
1	E	117	GLU	CA-CB-CG	5.13	124.70	113.40
1	E	138	VAL	CG1-CB-CG2	5.12	119.09	110.90

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	47	0
1	B	1866	0	1899	42	0
1	C	1859	0	1892	73	0
1	D	1866	0	1899	69	0
1	E	1859	0	1892	114	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
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	3	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	492	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 21.

All (492) 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: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: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:F:59:LYS:HZ2	1:F:67:PRO:HB3	1.16	1.05
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:F:47:ASN:CG	1:F:50:LYS:HG3	1.96	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: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:B:147:ASN:CG	1:B:149:CYS:HB3	2.02	0.79
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:24:SER:OG	2:E:801:NAP:O1A	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:ARG:CD	1:F:262:MET:HE2	2.15	0.76
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:F:164:ARG:HD2	1:F:262:MET:CE	2.17	0.74
1:F:164:ARG:HD2	1:F:262:MET:HE2	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:265:VAL:HG23	1:F:265:VAL:OXT	1.97	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: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: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:D:16:ARG:HE	1:D:98:SER:HB3	1.64	0.62
1:C:227:SER:OG	1:C:229:VAL:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:GLN:O	1:E:85:GLN:HG2	1.99	0.61
1:F:20:ILE:O	1:F:106:THR:N	2.28	0.61
1:F:110:MET:HE1	2:F:801:NAP:H2D	1.82	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
1:F:110:MET:CE	3:F:802:PM7:O	2.48	0.60
1:F:205:THR:HG21	2:F:801:NAP:O1N	2.01	0.60
1:C:125:GLN:CD	1:D:129:ILE:HD11	2.21	0.60
1:F:127:PRO:HB2	1:F:175:TYR:CE2	2.36	0.60
1:C:161:HIS:NE2	1:C:176:CYS:SG	2.70	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:F:47:ASN:CG	1:F:50:LYS:CG	2.71	0.59
1:C:16:ARG:NH1	1:C:40:ILE:HD13	2.17	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:205:THR:OG1	1:F:206:GLU:N	2.36	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:A:227:SER:OG	1:A:229:VAL:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:D:100:ILE:HB	1:D:146:MET:HG2	1.87	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:131:ARG:NH2	1:E:175:TYR:C	2.58	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:F:78:SER:C	1:F:129:ILE:HG21	2.26	0.55
1:C:131:ARG:NH1	4:C:901:HOH:O	2.40	0.55
1:F:59:LYS:HZ3	1:F:67:PRO:HB3	1.66	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:142:LEU:HD22	1:A:146:MET:HE2	1.88	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: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:F:164:ARG:HD2	1:F:262:MET:HE1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:ARG:CD	1:F:262:MET:HE1	2.38	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: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:F:47:ASN:OD1	1:F:50:LYS:HG3	2.08	0.53
1:E:42:THR:HA	1:E:71:VAL:HG23	1.92	0.52
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: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: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: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: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:E:24:SER:HG	2:E:801:NAP:PA	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:F:194:ARG:HA	1:F:252:SER:HG	1.77	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: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:E:55:VAL:HG13	1:E:70:ILE:CG2	2.39	0.48
1:E:59:LYS:HZ3	1:E:67:PRO:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:MET:HE3	1:F:193:LEU:HD11	1.94	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:F:196:ASN:HD21	1:F:251:ALA:C	2.17	0.48
1:F:135:PRO:C	1:F:138:VAL:HG12	2.28	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
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: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: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:E:59:LYS:HZ1	1:E:67:PRO:HB3	1.78	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: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:F:49:GLN:OE1	1:F:53:ASP:CG	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:F:110:MET:HE2	3:F:802:PM7:O	2.16	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: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: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:D:49:GLN:C	1:D:51:LEU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLN:C	1:D:51:LEU:N	2.70	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: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
1:C:77:LEU:HD21	1:C:87:ILE:HD11	2.00	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:110:MET:HE1	3:F:802:PM7:O	2.18	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:F:47:ASN:CG	1:F:50:LYS:CD	2.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:C:125:GLN:OE1	1:D:129:ILE:HD11	2.19	0.41
1:D:50:LYS:HD3	1:D:53:ASP:HB2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ALA:HA	1:D:113:PRO:HD3	1.94	0.41
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: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:E:99:LYS:HD3	1:E:145:TYR:C	2.42	0.40
1:E:226:LYS:NZ	1:E:262:MET:O	2.48	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%)	34	42
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%)	51	64

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%)	198 (97%)	6 (3%)	42	58
1	B	204/211 (97%)	198 (97%)	6 (3%)	42	58
1	C	203/211 (96%)	197 (97%)	6 (3%)	41	57
1	D	204/211 (97%)	200 (98%)	4 (2%)	55	72
1	E	203/211 (96%)	199 (98%)	4 (2%)	55	72
1	F	203/211 (96%)	196 (97%)	7 (3%)	37	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1221/1266 (96%)	1188 (97%)	33 (3%)	44 61

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	85	GLN
1	A	97	ASN
1	A	222	MET
1	A	227	SER
1	A	247	LYS
1	B	15	SER
1	B	49	GLN
1	B	52	LYS
1	B	93	LEU
1	B	149	CYS
1	B	258	THR
1	C	16	ARG
1	C	50	LYS
1	C	74	ARG
1	C	122	ASP
1	C	126	ARG
1	C	193	LEU
1	D	62	PHE
1	D	64	SER
1	D	222	MET
1	D	262	MET
1	E	61	SER
1	E	149	CYS
1	E	173	SER
1	E	191	LYS
1	F	15	SER
1	F	16	ARG
1	F	51	LEU
1	F	148	LYS
1	F	163	LEU
1	F	226	LYS
1	F	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	B	49	GLN
1	B	79	ASN
1	E	11	GLN
1	E	37	HIS
1	E	249	HIS
1	F	79	ASN
1	F	102	HIS
1	F	141	HIS
1	F	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	801	-	46,52,52	2.39	22 (47%)	61,80,80	1.88	18 (29%)
2	NAP	C	801	-	46,52,52	4.20	16 (34%)	61,80,80	2.05	8 (13%)
3	PM7	C	802	-	26,30,30	5.37	12 (46%)	30,51,51	1.75	5 (16%)
3	PM7	E	802	-	26,30,30	5.36	13 (50%)	30,51,51	1.97	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PM7	D	802	-	26,30,30	5.37	12 (46%)	30,51,51	1.72	5 (16%)
3	PM7	A	802	-	26,30,30	5.35	12 (46%)	30,51,51	1.74	5 (16%)
2	NAP	E	801	-	46,52,52	1.81	12 (26%)	61,80,80	1.82	16 (26%)
2	NAP	D	801	-	46,52,52	4.24	15 (32%)	61,80,80	2.02	9 (14%)
3	PM7	F	802	-	26,30,30	5.42	13 (50%)	30,51,51	2.20	7 (23%)
2	NAP	F	801	-	46,52,52	4.32	15 (32%)	61,80,80	2.22	12 (19%)
2	NAP	A	801	-	46,52,52	4.16	16 (34%)	61,80,80	1.97	8 (13%)
3	PM7	B	802	-	26,30,30	5.36	12 (46%)	30,51,51	1.79	6 (20%)

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	B	801	-	-	10/31/67/67	0/5/5/5
2	NAP	C	801	-	-	11/31/67/67	0/5/5/5
2	NAP	E	801	-	-	8/31/67/67	0/5/5/5
2	NAP	D	801	-	-	11/31/67/67	0/5/5/5
2	NAP	F	801	-	-	12/31/67/67	0/5/5/5
2	NAP	A	801	-	-	13/31/67/67	0/5/5/5

All (170) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAP	O4B-C1B	17.33	1.63	1.40
2	D	801	NAP	O4B-C1B	16.86	1.63	1.40
2	F	801	NAP	O4D-C1D	16.49	1.62	1.40
2	C	801	NAP	O4B-C1B	16.44	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
2	A	801	NAP	O4B-C1B	16.14	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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
3	F	802	PM7	C5-C6	8.34	1.60	1.51
3	D	802	PM7	C5-C6	8.29	1.60	1.51
3	B	802	PM7	C5-C6	8.20	1.60	1.51
3	E	802	PM7	C5-C6	8.18	1.60	1.51
3	A	802	PM7	C5-C6	8.05	1.60	1.51
3	C	802	PM7	C5-C6	7.91	1.60	1.51
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
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	F	801	NAP	PA-O3	5.15	1.65	1.59
2	F	801	NAP	PN-O3	5.14	1.65	1.59
2	D	801	NAP	PN-O3	5.11	1.65	1.59
2	A	801	NAP	PN-O3	4.99	1.64	1.59
2	A	801	NAP	PA-O3	4.93	1.64	1.59
3	A	802	PM7	C14-C13	4.55	1.60	1.52
3	C	802	PM7	C14-C13	4.54	1.60	1.52
2	B	801	NAP	O4D-C1D	-4.48	1.35	1.40
3	D	802	PM7	C14-C13	4.45	1.60	1.52
3	E	802	PM7	C14-C13	4.42	1.60	1.52
3	B	802	PM7	C14-C13	4.38	1.60	1.52
2	B	801	NAP	C4A-N3A	-4.34	1.29	1.35
3	F	802	PM7	C14-C13	4.21	1.60	1.52
2	B	801	NAP	PA-O2A	-4.08	1.36	1.55
3	C	802	PM7	C14-C3	-4.05	1.50	1.55
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	C14-C3	-3.99	1.50	1.55
3	A	802	PM7	C14-C3	-3.81	1.51	1.55
3	C	802	PM7	C6-C7	-3.79	1.36	1.41
2	B	801	NAP	O4D-C4D	-3.78	1.36	1.45
3	D	802	PM7	C14-C3	-3.75	1.51	1.55
2	B	801	NAP	P2B-O2X	-3.75	1.40	1.54
3	B	802	PM7	C14-C3	-3.72	1.51	1.55
3	E	802	PM7	C14-C3	-3.69	1.51	1.55
3	E	802	PM7	C6-C7	-3.66	1.36	1.41
2	F	801	NAP	O2B-C2B	3.56	1.56	1.44
3	F	802	PM7	C6-C7	-3.55	1.36	1.41
3	B	802	PM7	C19-C18	3.54	1.64	1.51
2	B	801	NAP	C5A-N7A	-3.53	1.27	1.39
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	B	802	PM7	C6-C7	-3.52	1.36	1.41
3	D	802	PM7	C19-C18	3.51	1.63	1.51
2	B	801	NAP	O7N-C7N	-3.49	1.17	1.24
3	A	802	PM7	C6-C7	-3.49	1.36	1.41
2	E	801	NAP	O7N-C7N	-3.48	1.17	1.24
3	A	802	PM7	C19-C18	3.45	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802	PM7	C6-C7	-3.43	1.37	1.41
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	F	801	NAP	C6A-N6A	3.35	1.46	1.34
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	D	801	NAP	C6A-N6A	3.26	1.45	1.34
3	F	802	PM7	O-C	-3.19	1.17	1.22
2	C	801	NAP	C6A-N6A	3.17	1.45	1.34
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	A	801	NAP	C6A-N6A	3.10	1.45	1.34
2	B	801	NAP	PA-O3	-3.04	1.56	1.59
3	E	802	PM7	C6-C13	2.94	1.45	1.39
2	F	801	NAP	O3D-C3D	-2.93	1.35	1.43
2	B	801	NAP	C7N-N7N	-2.93	1.27	1.33
3	B	802	PM7	C6-C13	2.91	1.44	1.39
3	A	802	PM7	C6-C13	2.90	1.44	1.39
3	F	802	PM7	C6-C13	2.89	1.44	1.39
3	D	802	PM7	C6-C13	2.89	1.44	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
3	C	802	PM7	C6-C13	2.85	1.44	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	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	F	801	NAP	C2A-N3A	2.58	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
2	A	801	NAP	C2A-N3A	2.42	1.35	1.32
2	D	801	NAP	C2A-N3A	2.42	1.35	1.32
3	D	802	PM7	O-C	-2.42	1.18	1.22
2	E	801	NAP	C4A-N3A	-2.41	1.32	1.35
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	C	801	NAP	C2A-N3A	2.32	1.35	1.32
2	A	801	NAP	C4N-C3N	-2.31	1.35	1.39
2	D	801	NAP	C4N-C3N	-2.31	1.35	1.39
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	A	801	NAP	C1B-N9A	-2.22	1.44	1.49
2	E	801	NAP	C5A-N7A	-2.21	1.31	1.39
3	B	802	PM7	O-C	-2.21	1.19	1.22
2	B	801	NAP	C1B-N9A	-2.16	1.44	1.49
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	C	801	NAP	C1B-N9A	-2.08	1.44	1.49
2	E	801	NAP	P2B-O2X	-2.07	1.47	1.54
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 (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NAP	C5A-C6A-N6A	9.55	134.86	120.31
2	F	801	NAP	C5A-C6A-N6A	9.54	134.84	120.31
2	D	801	NAP	C5A-C6A-N6A	9.51	134.79	120.31
2	A	801	NAP	C5A-C6A-N6A	9.17	134.29	120.31
3	F	802	PM7	C-C1-N2	-6.76	97.59	106.55
2	F	801	NAP	N6A-C6A-N1A	-6.45	104.55	118.33
2	C	801	NAP	N6A-C6A-N1A	-6.42	104.62	118.33
2	D	801	NAP	N6A-C6A-N1A	-6.35	104.76	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	NAP	N3A-C2A-N1A	-6.35	120.06	128.67
2	A	801	NAP	N3A-C2A-N1A	-6.31	120.11	128.67
2	D	801	NAP	N3A-C2A-N1A	-6.25	120.19	128.67
2	A	801	NAP	N6A-C6A-N1A	-6.21	105.07	118.33
2	F	801	NAP	N3A-C2A-N1A	-5.49	121.22	128.67
2	F	801	NAP	C4B-O4B-C1B	-5.42	104.97	109.92
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	N3A-C2A-N1A	-5.28	121.51	128.67
2	C	801	NAP	C1B-N9A-C4A	-5.23	117.44	126.64
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	D	801	NAP	C1B-N9A-C4A	-4.96	117.93	126.64
2	B	801	NAP	N3A-C2A-N1A	-4.83	122.11	128.67
2	A	801	NAP	C1B-N9A-C4A	-4.78	118.24	126.64
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
3	B	802	PM7	C-C1-N2	-4.46	100.65	106.55
3	D	802	PM7	C2-C1-N2	4.43	113.42	107.82
3	A	802	PM7	C2-C1-N2	4.32	113.28	107.82
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
3	C	802	PM7	C13-C14-C3	4.19	118.45	109.63
3	D	802	PM7	C13-C14-C3	4.12	118.32	109.63
3	E	802	PM7	C13-C14-C3	4.11	118.29	109.63
3	A	802	PM7	C-C1-N2	-4.08	101.15	106.55
3	B	802	PM7	C13-C14-C3	4.07	118.22	109.63
3	A	802	PM7	C13-C14-C3	4.07	118.21	109.63
2	F	801	NAP	C1B-N9A-C4A	-3.92	119.75	126.64
3	F	802	PM7	C13-C14-C3	3.92	117.90	109.63
3	C	802	PM7	C2-C3-C14	-3.89	110.42	114.17
2	B	801	NAP	O4B-C1B-N9A	3.85	113.85	108.75
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	B	801	NAP	C4A-C5A-N7A	-3.72	105.40	109.34
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	E	801	NAP	O3-PN-O1N	3.55	121.39	110.70
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
3	B	802	PM7	C2-C3-C14	-3.41	110.87	114.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	802	PM7	C2-C3-C14	-3.40	110.89	114.17
3	C	802	PM7	C-C1-N2	-3.26	102.23	106.55
2	F	801	NAP	O2B-C2B-C3B	3.22	123.21	111.68
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	F	801	NAP	C3B-C2B-C1B	-3.08	96.91	102.81
2	E	801	NAP	C4A-C5A-N7A	-3.06	106.10	109.34
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	F	801	NAP	O2B-P2B-O1X	3.00	120.03	109.33
3	F	802	PM7	C19-C18-N2	2.87	108.05	103.94
2	E	801	NAP	O4B-C1B-N9A	2.77	112.42	108.75
2	B	801	NAP	C4B-O4B-C1B	2.75	112.44	109.92
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
2	B	801	NAP	C3B-C2B-C1B	-2.69	97.66	102.81
2	B	801	NAP	C2N-N1N-C1D	2.66	125.01	119.13
2	B	801	NAP	O4B-C1B-C2B	-2.65	102.09	106.61
2	E	801	NAP	O4B-C1B-C2B	-2.54	102.27	106.61
2	F	801	NAP	C4D-O4D-C1D	-2.54	107.60	109.92
2	E	801	NAP	C1B-N9A-C4A	-2.54	122.19	126.64
2	D	801	NAP	C5B-C4B-C3B	-2.53	106.11	115.21
2	B	801	NAP	O2N-PN-O1N	2.50	124.09	112.44
2	C	801	NAP	O4B-C1B-N9A	2.50	112.06	108.75
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	C	802	PM7	C20-C1-C	-2.41	112.21	115.26
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
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	B	801	NAP	C5A-C6A-N6A	2.33	123.86	120.31
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	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	E	802	PM7	C1-C2-C3	2.28	112.34	108.49
2	E	801	NAP	O3X-P2B-O1X	2.25	119.62	110.83
2	D	801	NAP	C4B-O4B-C1B	-2.23	107.89	109.92
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	E	801	NAP	C3N-C7N-N7N	2.12	120.36	117.74
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
2	F	801	NAP	O4B-C4B-C3B	-2.07	101.05	105.15
3	F	802	PM7	C1-C2-C3	2.04	111.95	108.49
3	F	802	PM7	C20-C1-C	-2.03	112.69	115.26
2	E	801	NAP	C4B-O4B-C1B	-2.02	108.08	109.92
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
2	B	801	NAP	O7N-C7N-C3N	2.01	122.05	119.60

There are no chirality outliers.

All (65) 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
2	D	801	NAP	C5D-O5D-PN-O3

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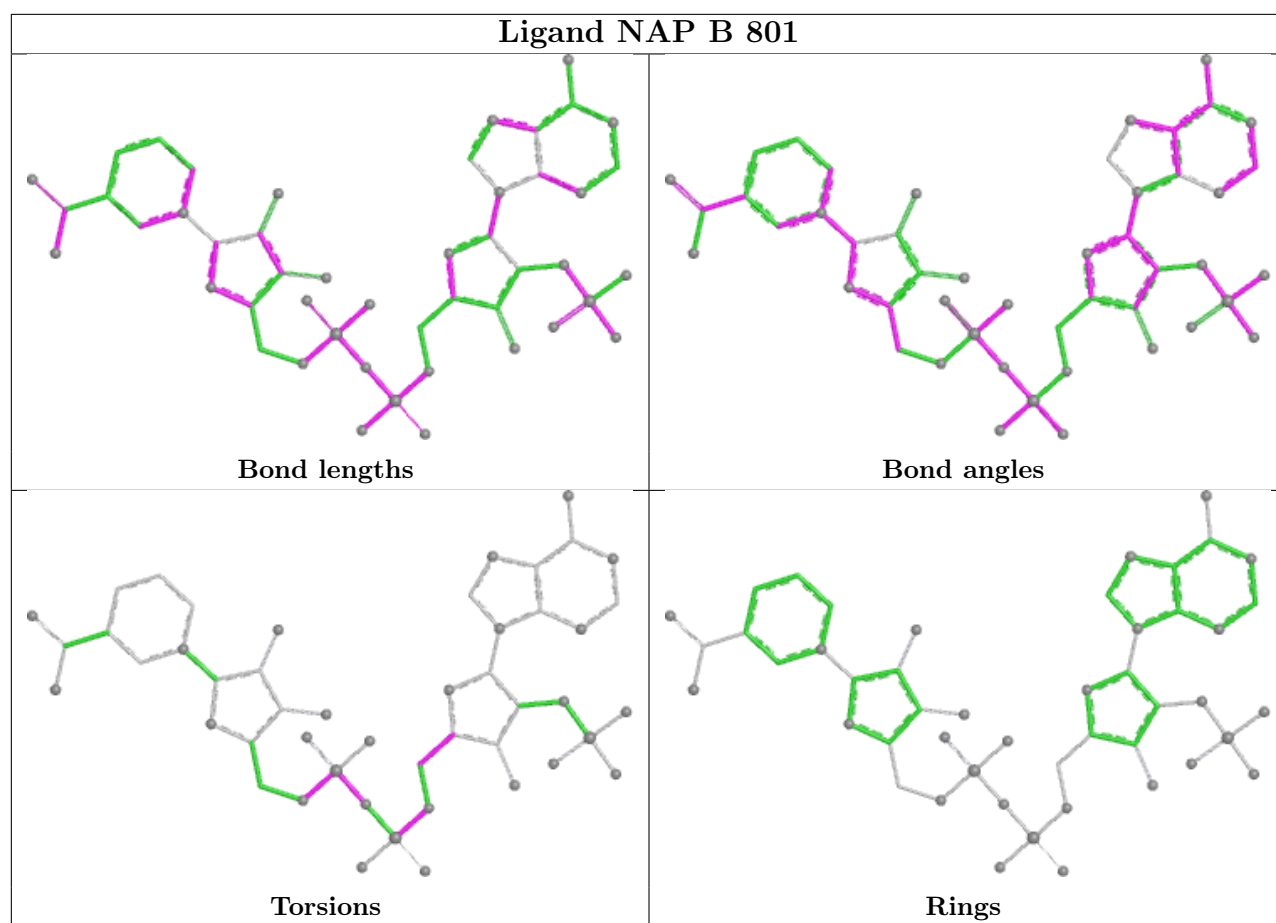
Mol	Chain	Res	Type	Atoms
2	D	801	NAP	C5D-O5D-PN-O1N
2	D	801	NAP	C5D-O5D-PN-O2N
2	E	801	NAP	C5D-O5D-PN-O3
2	F	801	NAP	C5B-O5B-PA-O1A
2	F	801	NAP	C5B-O5B-PA-O2A
2	F	801	NAP	C5B-O5B-PA-O3
2	F	801	NAP	C5D-O5D-PN-O3
2	F	801	NAP	C5D-O5D-PN-O1N
2	F	801	NAP	C5D-O5D-PN-O2N
2	F	801	NAP	C3B-C2B-O2B-P2B
2	B	801	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

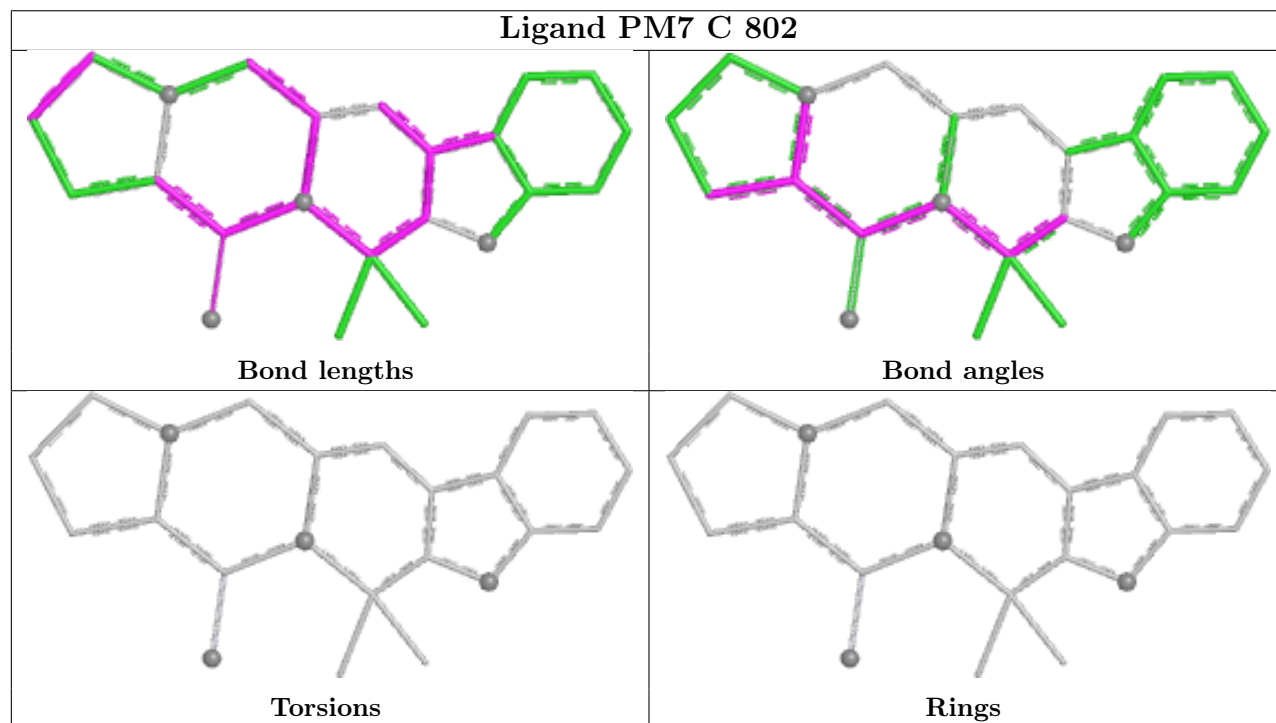
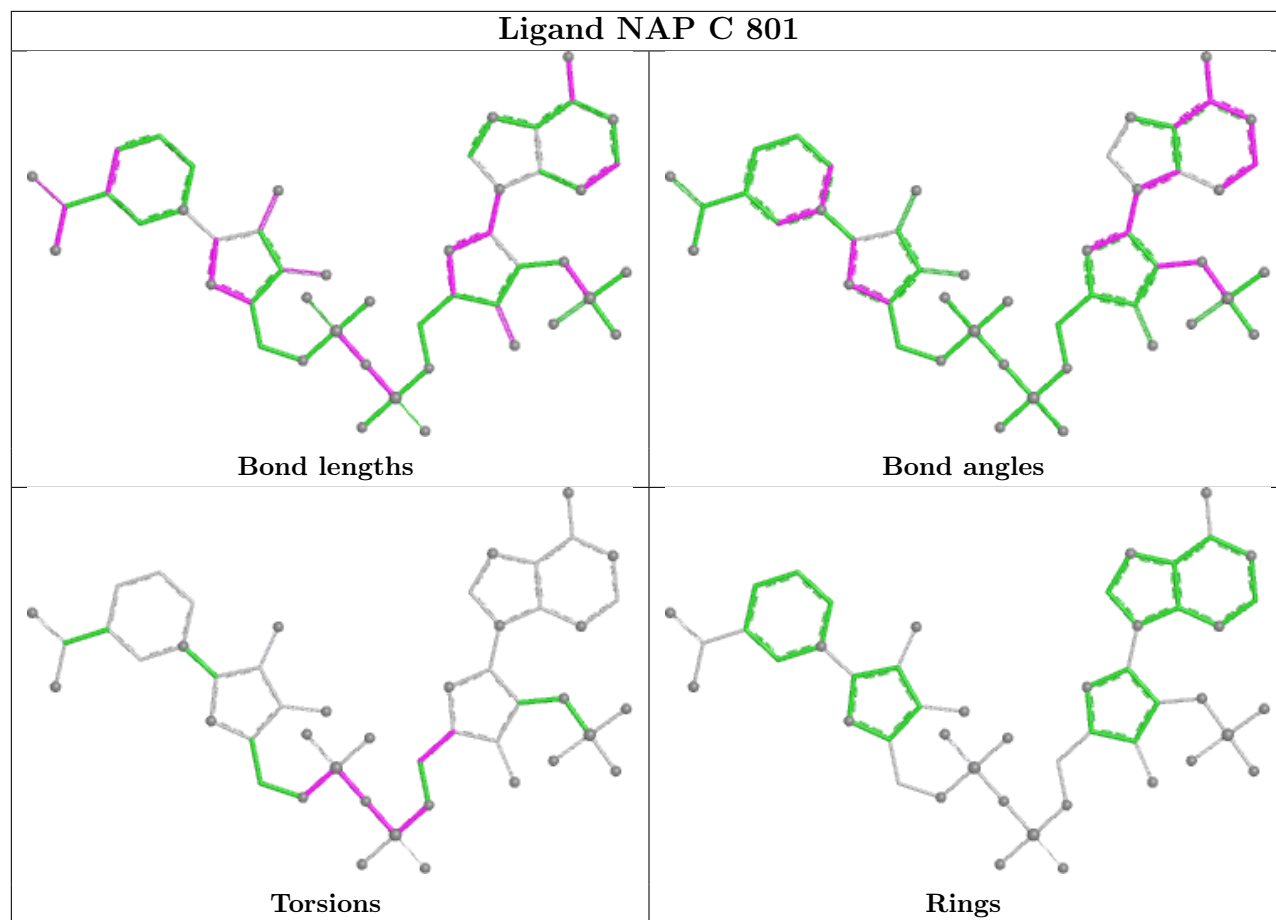
There are no ring outliers.

7 monomers are involved in 29 short contacts:

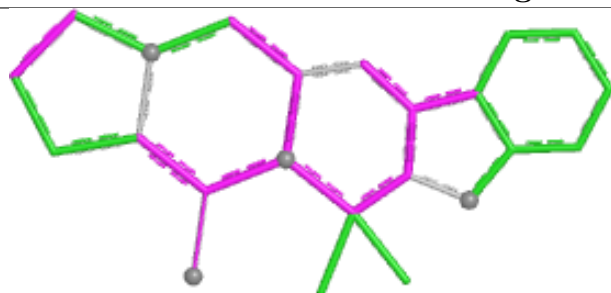
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	NAP	2	0
2	C	801	NAP	2	0
2	E	801	NAP	5	0
2	D	801	NAP	2	0
3	F	802	PM7	3	0
2	F	801	NAP	12	0
2	A	801	NAP	3	0

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.

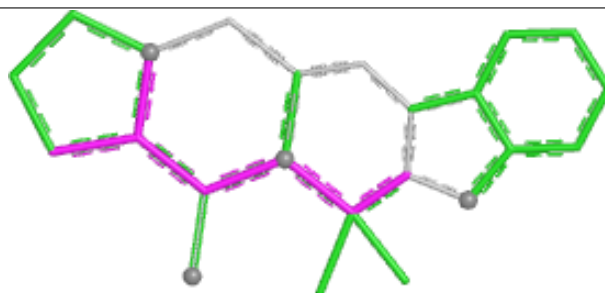




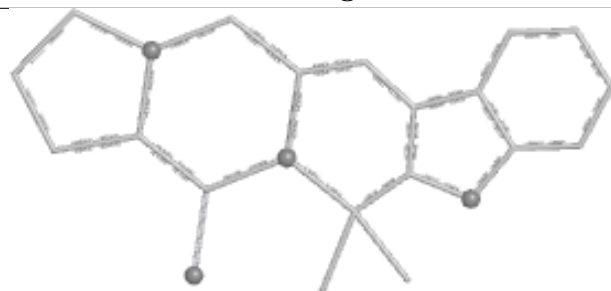
Ligand PM7 E 802



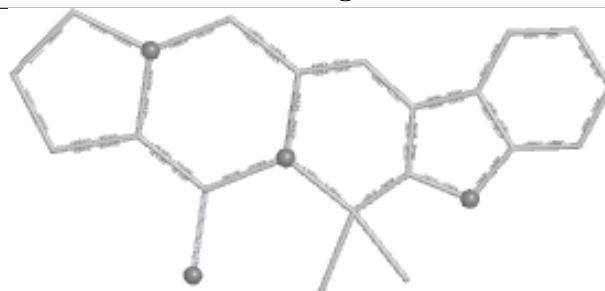
Bond lengths



Bond angles

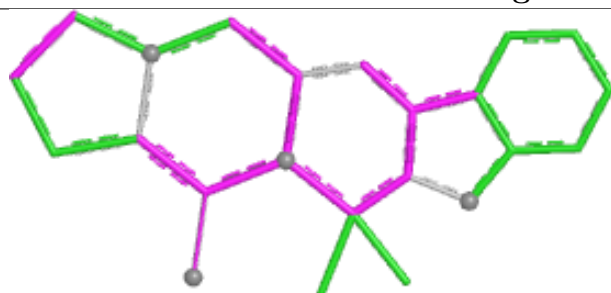


Torsions

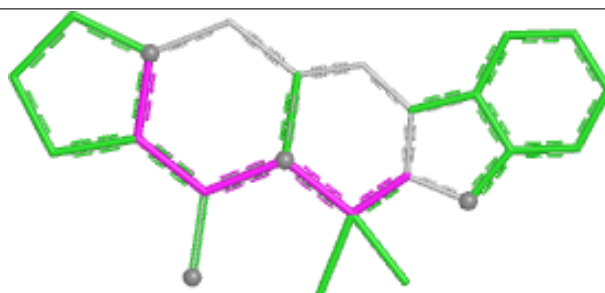


Rings

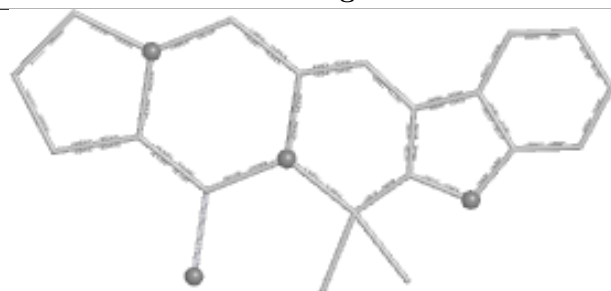
Ligand PM7 D 802



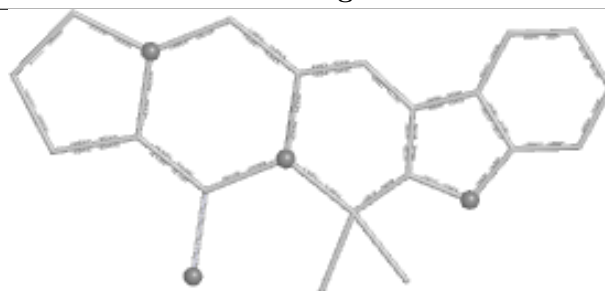
Bond lengths



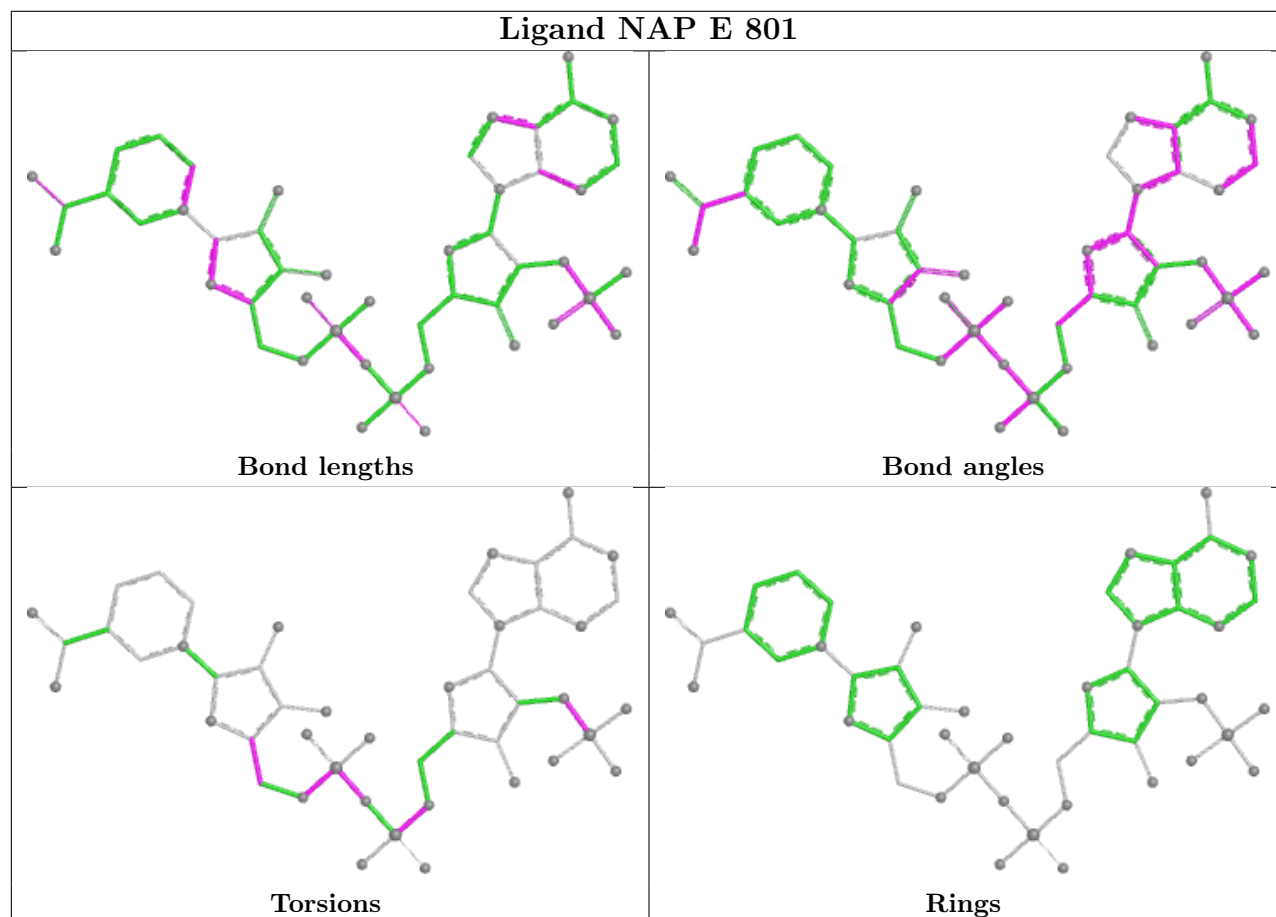
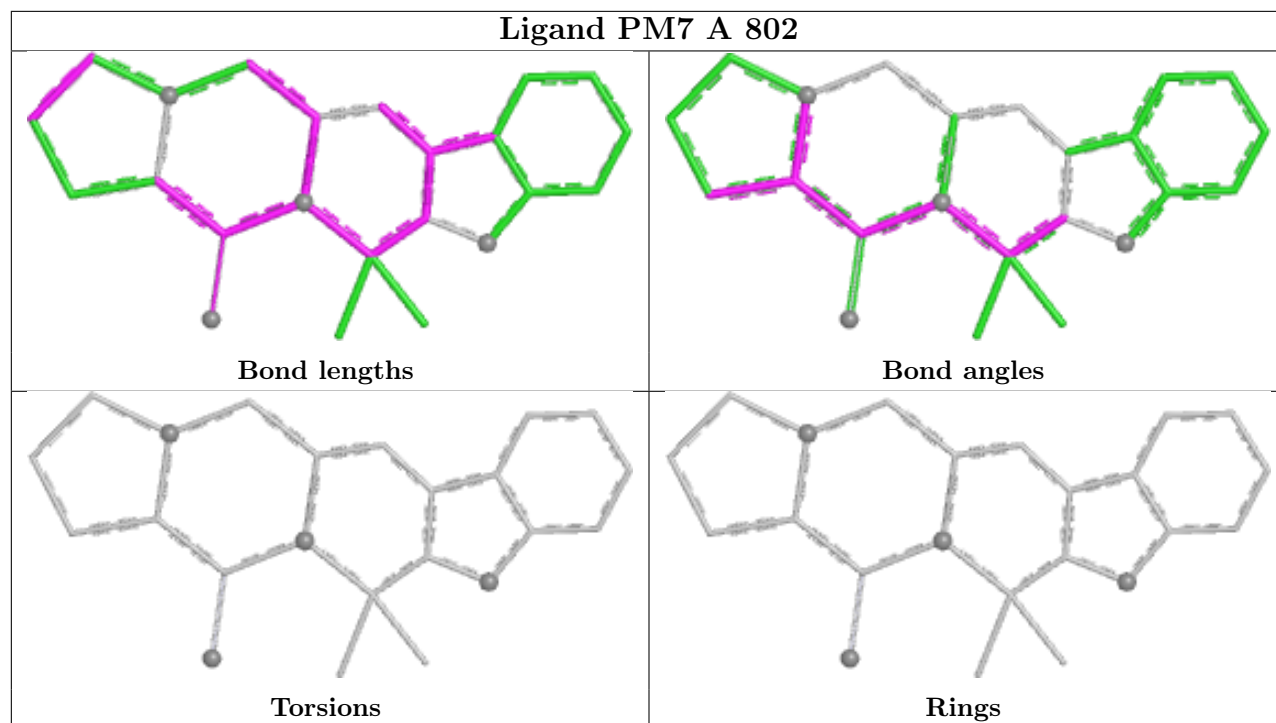
Bond angles

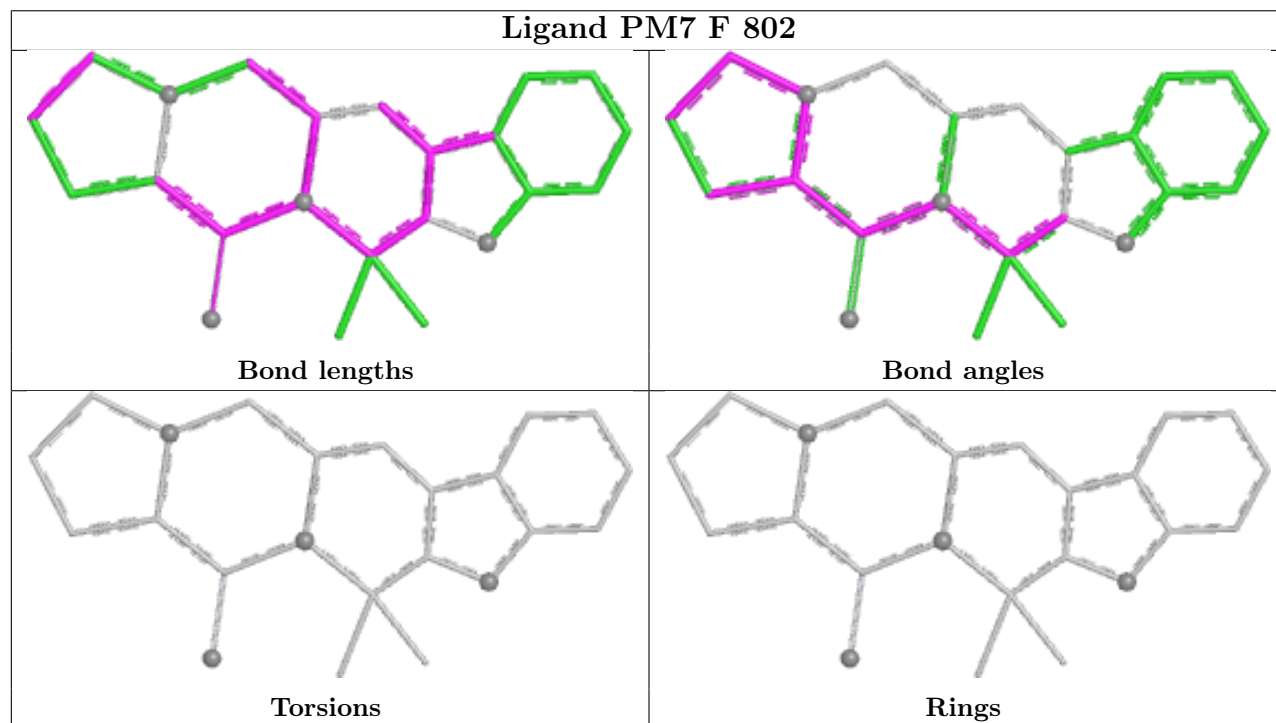
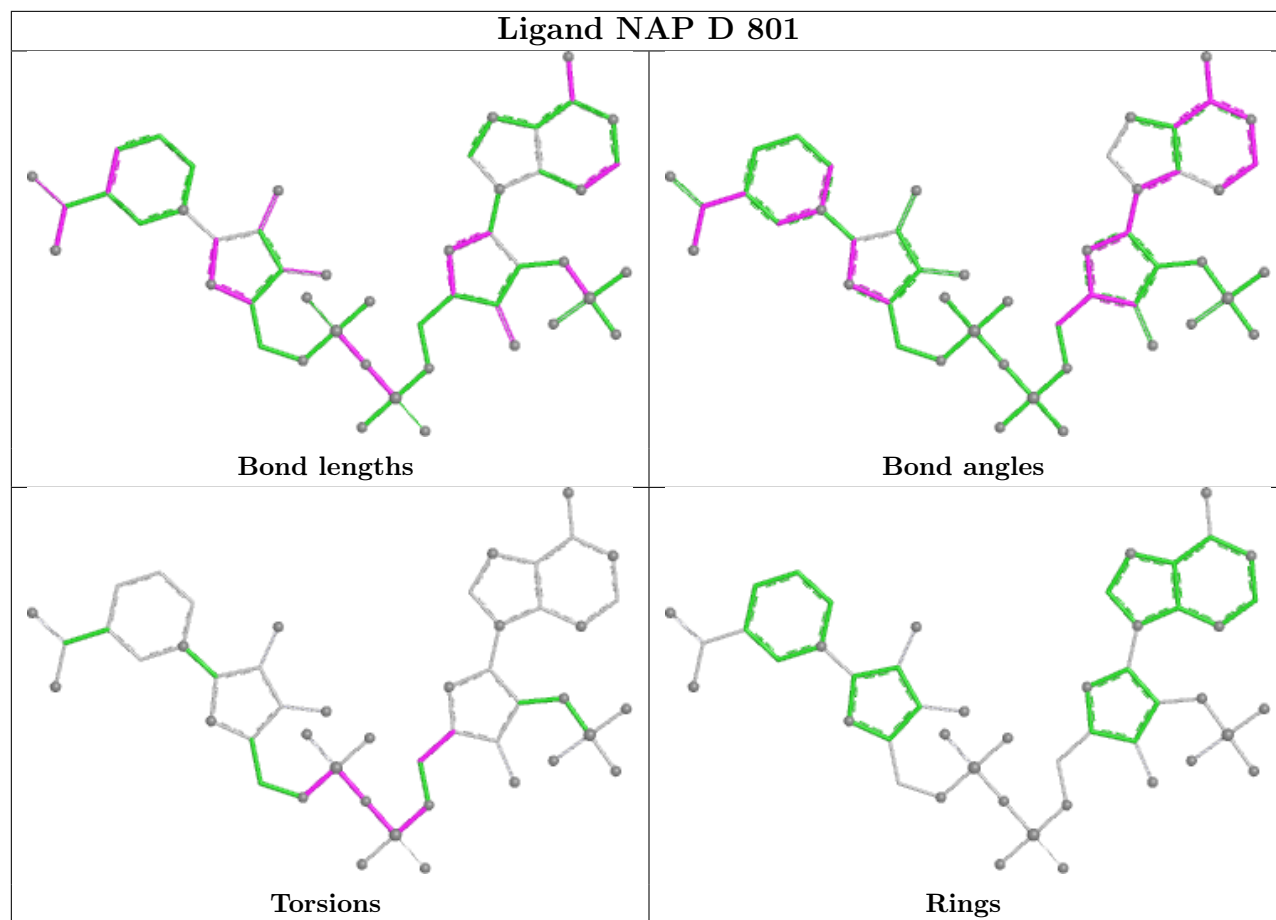


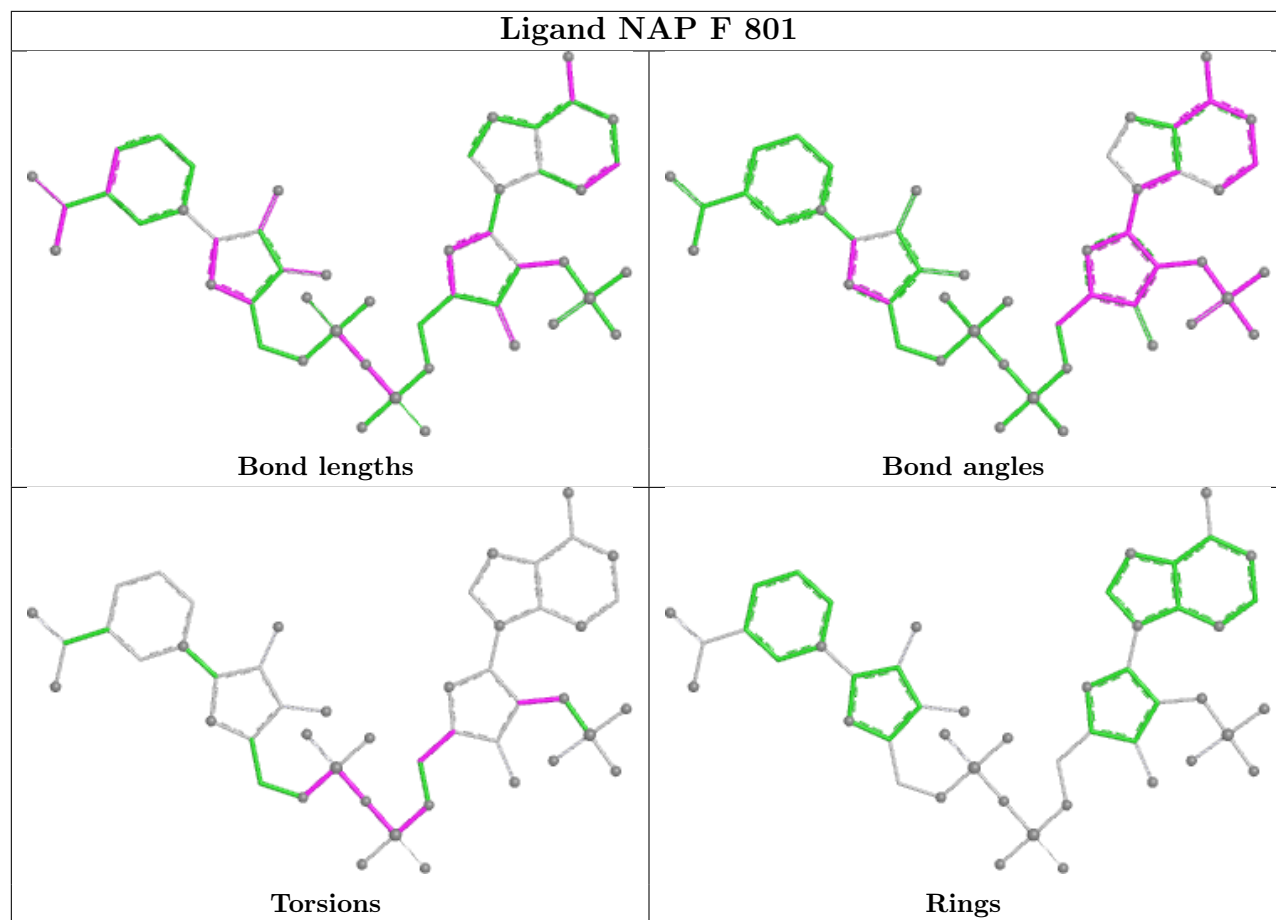
Torsions

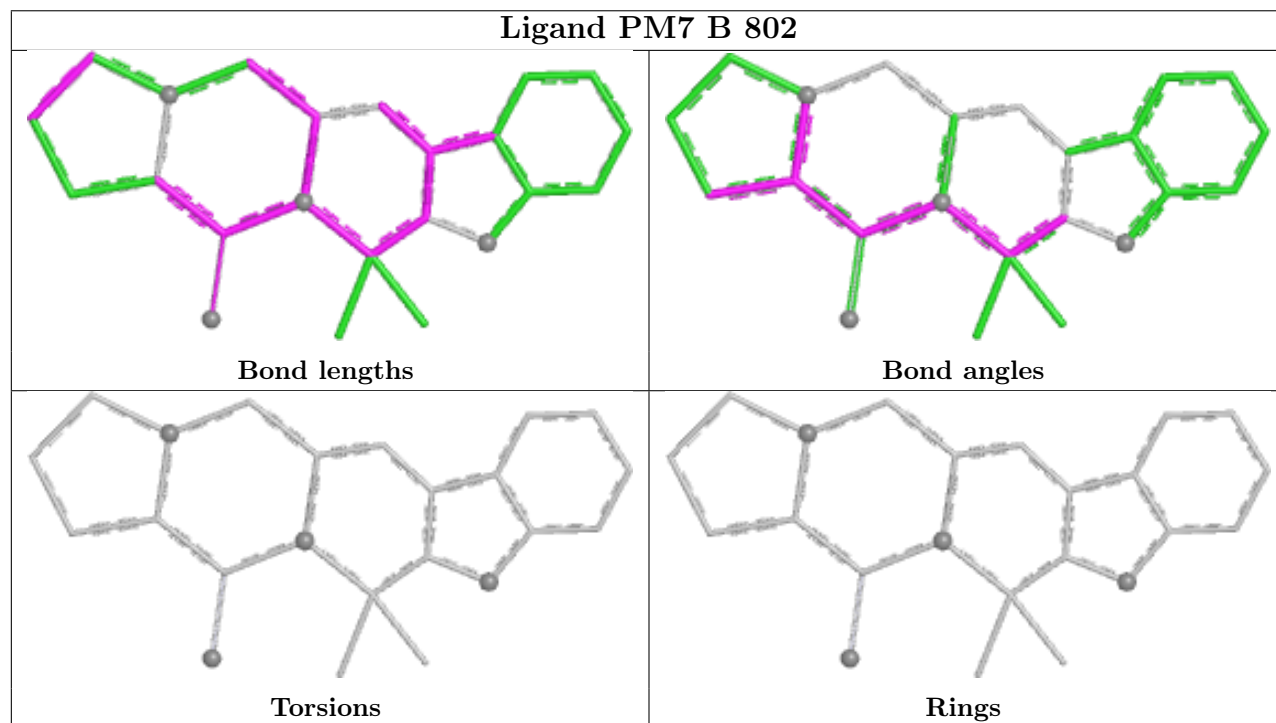
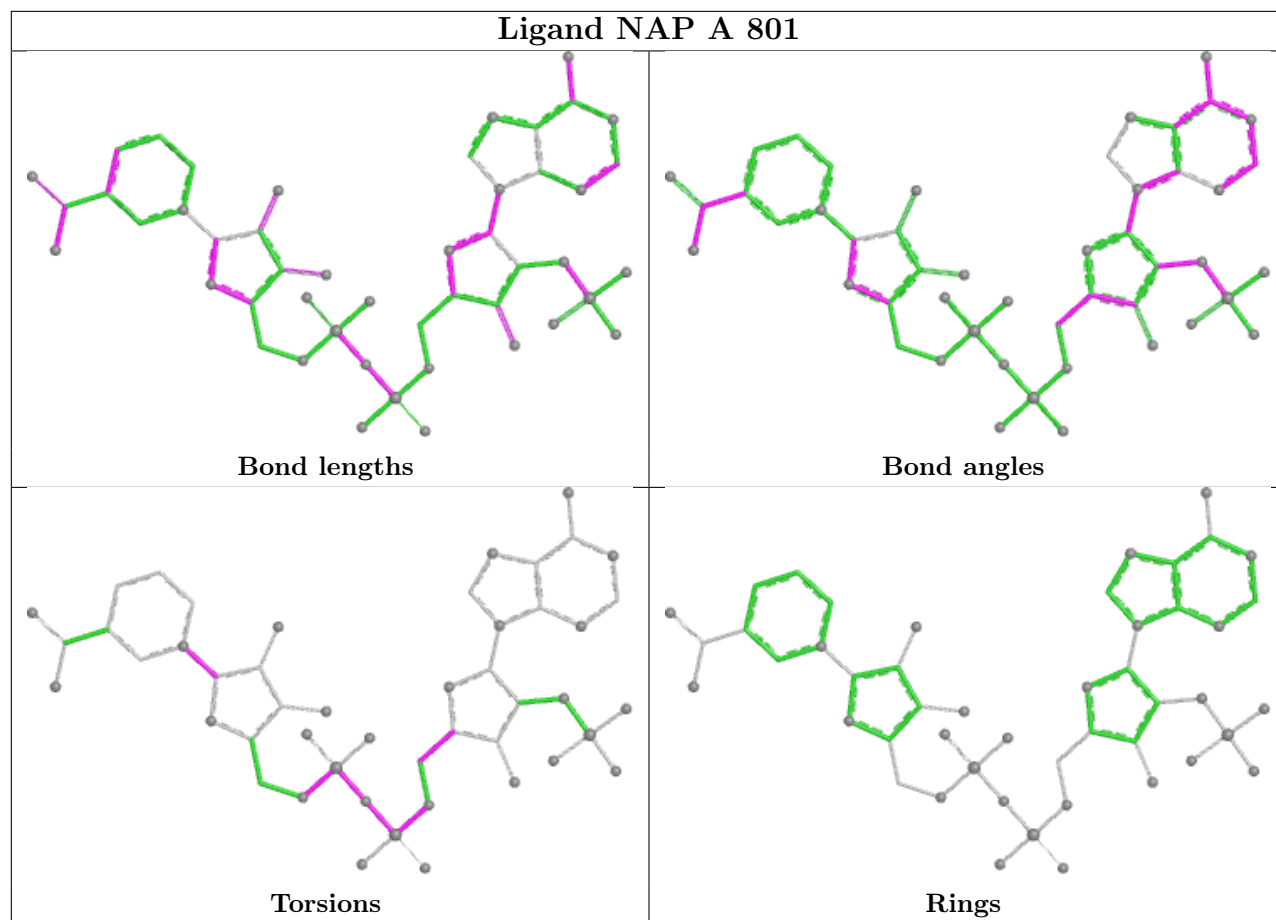


Rings









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%)	1.18	37 (14%) 2 3	32, 54, 78, 119	0
1	B	257/265 (96%)	1.14	31 (12%) 4 6	31, 50, 79, 114	0
1	C	256/265 (96%)	1.40	53 (20%) 1 1	32, 63, 105, 123	0
1	D	257/265 (96%)	1.47	63 (24%) 0 0	36, 63, 105, 141	0
1	E	256/265 (96%)	2.62	143 (55%) 0 0	55, 88, 123, 154	0
1	F	256/265 (96%)	4.23	214 (83%) 0 0	82, 117, 150, 176	0
All	All	1539/1590 (96%)	2.01	541 (35%) 0 0	31, 67, 130, 176	0

All (541) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	130	ILE	23.7
1	F	255	VAL	14.0
1	F	19	VAL	13.8
1	E	240	GLN	12.4
1	F	119	LEU	10.7
1	F	187	ALA	10.1
1	F	29	ALA	10.0
1	F	104	VAL	9.8
1	E	14	GLY	9.7
1	F	17	VAL	9.6
1	F	196	ASN	9.4
1	E	221	GLU	9.0
1	F	220	VAL	9.0
1	F	45	GLY	9.0
1	F	135	PRO	8.9
1	F	216	TYR	8.9
1	F	169	TRP	8.9
1	F	134	ALA	8.7
1	F	63	PRO	8.7

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Mol	Chain	Res	Type	RSRZ
1	F	62	PHE	8.6
1	F	106	THR	8.2
1	F	201	GLY	8.2
1	F	197	VAL	8.1
1	F	10	ASP	8.0
1	F	110	MET	7.9
1	F	176	CYS	7.7
1	F	121	VAL	7.7
1	F	182	MET	7.6
1	E	18	LEU	7.6
1	D	64	SER	7.5
1	F	219	ALA	7.5
1	E	56	ALA	7.5
1	E	32	ALA	7.4
1	F	223	ALA	7.3
1	F	158	SER	7.3
1	F	36	GLY	7.1
1	F	99	LYS	7.1
1	E	230	GLY	7.1
1	E	55	VAL	7.1
1	F	68	ASP	7.0
1	E	242	TYR	6.9
1	F	118	ASP	6.9
1	F	127	PRO	6.9
1	F	136	LEU	6.9
1	E	11	GLN	6.8
1	F	221	GLU	6.8
1	D	9	THR	6.7
1	F	186	LEU	6.7
1	C	17	VAL	6.7
1	F	175	TYR	6.6
1	F	198	VAL	6.6
1	F	236	GLU	6.6
1	F	23	THR	6.6
1	F	211	ILE	6.5
1	F	56	ALA	6.5
1	F	40	ILE	6.4
1	E	254	SER	6.3
1	F	179	VAL	6.3
1	E	19	VAL	6.3
1	F	65	THR	6.3
1	F	205	THR	6.2

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Mol	Chain	Res	Type	RSRZ
1	F	248	ASP	6.2
1	F	96	GLY	6.2
1	F	49	GLN	6.2
1	E	207	ALA	6.1
1	F	53	ASP	6.1
1	D	62	PHE	6.1
1	D	50	LYS	6.1
1	E	60	SER	6.0
1	E	40	ILE	5.9
1	F	77	LEU	5.9
1	E	82	THR	5.9
1	F	94	ALA	5.9
1	F	181	ALA	5.9
1	D	41	VAL	5.8
1	F	254	SER	5.8
1	E	223	ALA	5.8
1	F	103	ILE	5.8
1	E	255	VAL	5.8
1	F	82	THR	5.7
1	F	157	THR	5.7
1	F	72	ALA	5.7
1	F	108	ALA	5.7
1	F	133	VAL	5.7
1	F	109	ASP	5.7
1	F	28	PHE	5.6
1	F	120	THR	5.6
1	E	34	ALA	5.5
1	F	244	TYR	5.5
1	C	110	MET	5.4
1	F	207	ALA	5.4
1	F	256	VAL	5.4
1	F	33	ALA	5.4
1	E	243	ILE	5.3
1	D	67	PRO	5.3
1	F	215	ALA	5.3
1	E	263	LEU	5.3
1	F	70	ILE	5.2
1	E	168	GLY	5.2
1	D	116	LEU	5.2
1	F	100	ILE	5.2
1	F	204	LEU	5.2
1	F	131	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	163	LEU	5.2
1	B	9	THR	5.1
1	F	143	PRO	5.1
1	E	23	THR	5.1
1	E	264	LEU	5.1
1	F	93	LEU	5.1
1	D	63	PRO	5.1
1	F	22	GLY	5.1
1	F	138	VAL	5.0
1	E	13	HIS	5.0
1	F	105	ILE	5.0
1	F	137	MET	5.0
1	F	178	ALA	5.0
1	F	37	HIS	4.9
1	F	190	LEU	4.9
1	F	148	LYS	4.9
1	E	197	VAL	4.9
1	C	67	PRO	4.9
1	F	237	SER	4.9
1	F	44	VAL	4.9
1	E	29	ALA	4.9
1	F	122	ASP	4.9
1	F	145	TYR	4.9
1	E	257	SER	4.8
1	F	52	LYS	4.8
1	B	14	GLY	4.8
1	D	17	VAL	4.8
1	E	265	VAL	4.8
1	D	68	ASP	4.7
1	E	198	VAL	4.7
1	F	171	VAL	4.7
1	F	39	ALA	4.7
1	E	232	THR	4.7
1	F	162	CYS	4.7
1	F	12	LEU	4.7
1	F	147	ASN	4.6
1	E	49	GLN	4.6
1	F	20	ILE	4.6
1	A	148	LYS	4.6
1	F	153	SER	4.6
1	F	183	SER	4.6
1	E	237	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	64	SER	4.5
1	D	72	ALA	4.5
1	F	263	LEU	4.5
1	E	187	ALA	4.4
1	E	220	VAL	4.4
1	F	174	GLY	4.4
1	E	92	GLN	4.4
1	F	98	SER	4.3
1	D	45	GLY	4.3
1	E	153	SER	4.3
1	F	165	PRO	4.3
1	F	141	HIS	4.3
1	A	209	LYS	4.3
1	F	243	ILE	4.3
1	C	10	ASP	4.3
1	F	206	GLU	4.2
1	B	71	VAL	4.2
1	E	67	PRO	4.2
1	E	22	GLY	4.2
1	F	41	VAL	4.2
1	E	262	MET	4.2
1	E	235	PRO	4.2
1	A	11	GLN	4.2
1	F	97	ASN	4.2
1	F	113	PRO	4.1
1	F	74	ARG	4.1
1	F	193	LEU	4.1
1	C	265	VAL	4.1
1	F	180	GLU	4.1
1	F	18	LEU	4.1
1	F	123	SER	4.1
1	E	227	SER	4.1
1	F	81	ASP	4.0
1	E	139	ALA	4.0
1	C	230	GLY	4.0
1	C	216	TYR	4.0
1	B	147	ASN	4.0
1	F	184	ARG	4.0
1	F	250	TYR	4.0
1	C	229	VAL	4.0
1	F	13	HIS	4.0
1	A	82	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	69	ASP	3.9
1	F	209	LYS	3.9
1	E	246	MET	3.9
1	E	138	VAL	3.9
1	F	30	VAL	3.9
1	F	265	VAL	3.9
1	B	265	VAL	3.9
1	E	238	VAL	3.9
1	E	102	HIS	3.9
1	E	152	SER	3.8
1	A	230	GLY	3.8
1	F	159	GLY	3.8
1	F	167	PRO	3.8
1	E	44	VAL	3.8
1	F	195	VAL	3.8
1	A	163	LEU	3.8
1	F	166	ASP	3.8
1	E	181	ALA	3.8
1	F	203	VAL	3.8
1	F	156	LEU	3.7
1	F	126	ARG	3.7
1	F	142	LEU	3.7
1	E	31	CYS	3.7
1	E	256	VAL	3.7
1	A	264	LEU	3.7
1	D	51	LEU	3.7
1	C	16	ARG	3.7
1	D	56	ALA	3.6
1	E	175	TYR	3.6
1	F	208	VAL	3.6
1	F	210	ASP	3.6
1	F	227	SER	3.6
1	E	70	ILE	3.6
1	F	163	LEU	3.6
1	A	29	ALA	3.6
1	A	215	ALA	3.6
1	E	104	VAL	3.6
1	E	196	ASN	3.5
1	F	185	GLY	3.5
1	F	225	ALA	3.5
1	F	232	THR	3.5
1	F	80	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	177	GLY	3.5
1	F	51	LEU	3.5
1	F	155	THR	3.5
1	E	10	ASP	3.5
1	E	212	LEU	3.5
1	F	200	PRO	3.5
1	E	229	VAL	3.5
1	E	236	GLU	3.5
1	F	217	ASP	3.5
1	B	65	THR	3.4
1	E	95	ALA	3.4
1	E	226	LYS	3.4
1	D	162	CYS	3.4
1	F	114	PRO	3.4
1	F	253	GLY	3.4
1	D	172	ILE	3.4
1	E	51	LEU	3.4
1	F	212	LEU	3.4
1	D	129	ILE	3.4
1	E	97	ASN	3.4
1	E	173	SER	3.4
1	F	43	ILE	3.4
1	A	147	ASN	3.4
1	A	216	TYR	3.4
1	D	119	LEU	3.4
1	E	61	SER	3.3
1	F	46	SER	3.3
1	E	52	LYS	3.3
1	E	48	ALA	3.3
1	C	65	THR	3.3
1	A	214	ASP	3.3
1	F	48	ALA	3.3
1	F	86	ASP	3.3
1	C	142	LEU	3.3
1	F	264	LEU	3.3
1	D	46	SER	3.3
1	F	61	SER	3.3
1	E	65	THR	3.3
1	F	35	LEU	3.3
1	F	242	TYR	3.3
1	E	28	PHE	3.3
1	F	164	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	42	THR	3.3
1	F	112	ALA	3.2
1	A	178	ALA	3.2
1	F	91	LEU	3.2
1	F	129	ILE	3.2
1	C	238	VAL	3.2
1	F	102	HIS	3.2
1	D	57	ARG	3.2
1	E	109	ASP	3.2
1	F	66	ASP	3.2
1	F	149	CYS	3.2
1	F	115	PRO	3.2
1	F	71	VAL	3.2
1	C	109	ASP	3.2
1	E	219	ALA	3.1
1	A	110	MET	3.1
1	F	226	LYS	3.1
1	F	199	ALA	3.1
1	E	146	MET	3.1
1	F	154	LEU	3.1
1	E	117	GLU	3.1
1	F	235	PRO	3.1
1	D	193	LEU	3.1
1	F	14	GLY	3.1
1	B	109	ASP	3.1
1	F	228	THR	3.1
1	C	211	ILE	3.1
1	E	172	ILE	3.1
1	D	65	THR	3.0
1	A	67	PRO	3.0
1	D	211	ILE	3.0
1	B	199	ALA	3.0
1	F	85	GLN	3.0
1	F	262	MET	3.0
1	F	107	ALA	3.0
1	E	195	VAL	3.0
1	E	250	TYR	3.0
1	F	132	LEU	3.0
1	E	158	SER	3.0
1	D	229	VAL	3.0
1	E	253	GLY	2.9
1	D	35	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	193	LEU	2.9
1	E	216	TYR	2.9
1	D	71	VAL	2.9
1	E	228	THR	2.9
1	D	210	ASP	2.9
1	C	199	ALA	2.9
1	D	199	ALA	2.9
1	D	54	SER	2.9
1	F	241	ALA	2.9
1	F	15	SER	2.9
1	F	83	VAL	2.9
1	F	25	GLY	2.9
1	E	103	ILE	2.9
1	F	24	SER	2.8
1	F	76	ASP	2.8
1	D	158	SER	2.8
1	E	201	GLY	2.8
1	E	199	ALA	2.8
1	E	239	ALA	2.8
1	F	202	ALA	2.8
1	A	158	SER	2.8
1	A	10	ASP	2.8
1	E	71	VAL	2.8
1	E	200	PRO	2.8
1	F	38	GLY	2.8
1	A	165	PRO	2.8
1	E	72	ALA	2.8
1	F	67	PRO	2.8
1	B	68	ASP	2.8
1	B	201	GLY	2.8
1	F	214	ASP	2.7
1	C	64	SER	2.7
1	F	125	GLN	2.7
1	E	148	LYS	2.7
1	F	69	ASP	2.7
1	E	171	VAL	2.7
1	C	51	LEU	2.7
1	E	182	MET	2.7
1	F	57	ARG	2.7
1	C	25	GLY	2.7
1	C	48	ALA	2.7
1	D	99	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	116	LEU	2.7
1	E	105	ILE	2.7
1	C	158	SER	2.7
1	D	220	VAL	2.7
1	C	69	ASP	2.7
1	F	251	ALA	2.7
1	A	116	LEU	2.7
1	E	149	CYS	2.7
1	E	183	SER	2.6
1	E	209	LYS	2.6
1	F	160	ALA	2.6
1	E	204	LEU	2.6
1	E	165	PRO	2.6
1	B	72	ALA	2.6
1	C	181	ALA	2.6
1	F	188	ILE	2.6
1	B	159	GLY	2.6
1	E	188	ILE	2.6
1	E	251	ALA	2.6
1	B	163	LEU	2.6
1	E	179	VAL	2.6
1	E	164	ARG	2.6
1	F	224	GLU	2.6
1	B	207	ALA	2.6
1	F	31	CYS	2.6
1	A	258	THR	2.6
1	C	106	THR	2.6
1	E	106	THR	2.6
1	C	97	ASN	2.6
1	E	35	LEU	2.6
1	A	30	VAL	2.6
1	A	73	VAL	2.6
1	C	255	VAL	2.6
1	F	32	ALA	2.6
1	D	214	ASP	2.6
1	C	75	CYS	2.6
1	D	209	LYS	2.6
1	E	74	ARG	2.6
1	E	135	PRO	2.6
1	E	110	MET	2.6
1	E	231	GLN	2.6
1	D	29	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	150	PRO	2.5
1	F	231	GLN	2.5
1	C	108	ALA	2.5
1	C	40	ILE	2.5
1	F	58	LEU	2.5
1	F	245	LEU	2.5
1	C	162	CYS	2.5
1	D	188	ILE	2.5
1	F	11	GLN	2.5
1	C	102	HIS	2.5
1	E	17	VAL	2.5
1	A	150	PRO	2.5
1	E	45	GLY	2.5
1	F	116	LEU	2.5
1	C	92	GLN	2.5
1	D	207	ALA	2.5
1	E	192	PRO	2.5
1	D	110	MET	2.5
1	C	46	SER	2.5
1	C	217	ASP	2.5
1	D	216	TYR	2.5
1	F	258	THR	2.5
1	B	26	ILE	2.5
1	F	230	GLY	2.5
1	E	85	GLN	2.5
1	D	58	LEU	2.5
1	B	110	MET	2.4
1	F	252	SER	2.4
1	B	108	ALA	2.4
1	B	223	ALA	2.4
1	C	41	VAL	2.4
1	D	96	GLY	2.4
1	F	101	ASN	2.4
1	A	188	ILE	2.4
1	B	197	VAL	2.4
1	D	159	GLY	2.4
1	F	249	HIS	2.4
1	E	151	GLN	2.4
1	D	226	LYS	2.4
1	E	39	ALA	2.4
1	A	162	CYS	2.4
1	E	30	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	73	VAL	2.4
1	E	176	CYS	2.4
1	E	53	ASP	2.4
1	F	16	ARG	2.4
1	E	260	GLY	2.4
1	C	56	ALA	2.3
1	A	9	THR	2.3
1	B	60	SER	2.3
1	E	66	ASP	2.3
1	E	161	HIS	2.3
1	D	196	ASN	2.3
1	C	62	PHE	2.3
1	A	185	GLY	2.3
1	D	49	GLN	2.3
1	C	63	PRO	2.3
1	E	178	ALA	2.3
1	D	53	ASP	2.3
1	D	265	VAL	2.3
1	E	37	HIS	2.3
1	A	75	CYS	2.3
1	E	76	ASP	2.3
1	F	88	GLU	2.3
1	F	139	ALA	2.3
1	F	152	SER	2.3
1	C	128	GLY	2.3
1	D	52	LYS	2.3
1	F	87	ILE	2.3
1	F	261	GLY	2.3
1	E	131	ARG	2.3
1	B	200	PRO	2.3
1	A	72	ALA	2.3
1	C	61	SER	2.3
1	D	98	SER	2.3
1	C	163	LEU	2.2
1	D	228	THR	2.2
1	E	58	LEU	2.2
1	F	79	ASN	2.2
1	A	114	PRO	2.2
1	B	54	SER	2.2
1	D	40	ILE	2.2
1	F	26	ILE	2.2
1	D	93	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	244	TYR	2.2
1	C	117	GLU	2.2
1	C	200	PRO	2.2
1	F	238	VAL	2.2
1	E	162	CYS	2.2
1	D	108	ALA	2.2
1	E	258	THR	2.2
1	D	37	HIS	2.2
1	E	203	VAL	2.2
1	C	90	ALA	2.2
1	D	215	ALA	2.2
1	B	234	SER	2.2
1	E	145	TYR	2.2
1	E	180	GLU	2.2
1	D	255	VAL	2.2
1	A	17	VAL	2.1
1	D	208	VAL	2.1
1	F	73	VAL	2.1
1	F	124	VAL	2.1
1	C	258	THR	2.1
1	A	70	ILE	2.1
1	C	85	GLN	2.1
1	C	14	GLY	2.1
1	E	83	VAL	2.1
1	D	109	ASP	2.1
1	B	92	GLN	2.1
1	C	11	GLN	2.1
1	D	43	ILE	2.1
1	E	143	PRO	2.1
1	D	254	SER	2.1
1	A	93	LEU	2.1
1	C	222	MET	2.1
1	A	157	THR	2.1
1	A	71	VAL	2.1
1	B	29	ALA	2.1
1	B	181	ALA	2.1
1	C	154	LEU	2.1
1	B	151	GLN	2.1
1	E	202	ALA	2.1
1	C	133	VAL	2.1
1	B	247	LYS	2.1
1	F	128	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	245	LEU	2.1
1	F	170	THR	2.1
1	B	162	CYS	2.1
1	E	100	ILE	2.0
1	E	205	THR	2.0
1	E	90	ALA	2.0
1	B	59	LYS	2.0
1	E	159	GLY	2.0
1	A	124	VAL	2.0
1	D	44	VAL	2.0
1	E	124	VAL	2.0
1	B	149	CYS	2.0
1	A	50	LYS	2.0
1	C	57	ARG	2.0
1	C	257	SER	2.0
1	D	107	ALA	2.0
1	F	59	LYS	2.0
1	F	144	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PM7	F	802	25/25	0.54	0.37	72,94,107,112	0
2	NAP	F	801	48/48	0.76	0.27	77,100,116,121	0
3	PM7	E	802	25/25	0.81	0.39	80,90,106,107	0
2	NAP	C	801	48/48	0.84	0.21	42,58,83,85	0
3	PM7	A	802	25/25	0.84	0.22	51,60,68,74	0

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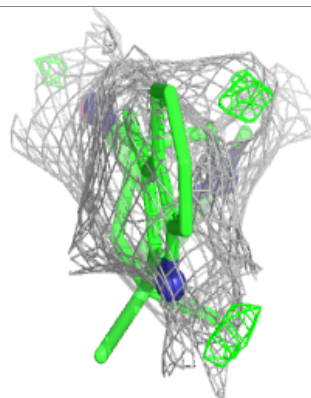
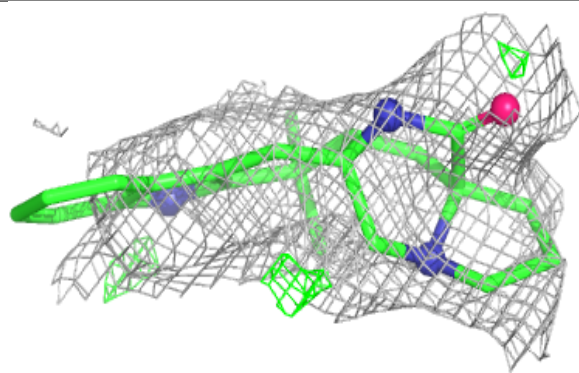
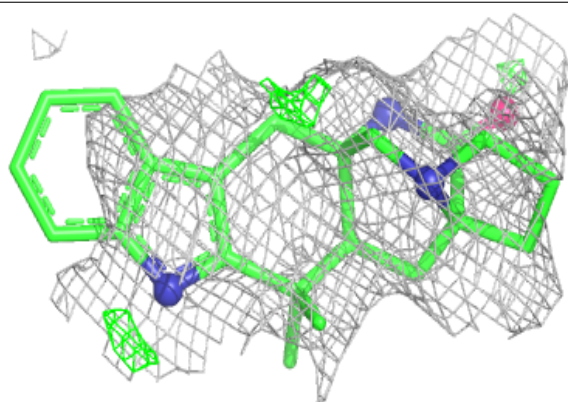
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PM7	D	802	25/25	0.85	0.24	59,63,69,70	0
2	NAP	E	801	48/48	0.86	0.17	63,78,89,97	0
3	PM7	B	802	25/25	0.86	0.19	33,47,51,60	0
3	PM7	C	802	25/25	0.86	0.20	51,61,72,74	0
2	NAP	A	801	48/48	0.87	0.18	35,51,62,69	0
2	NAP	D	801	48/48	0.88	0.17	42,63,76,77	0
2	NAP	B	801	48/48	0.93	0.15	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.

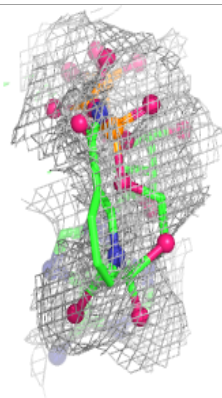
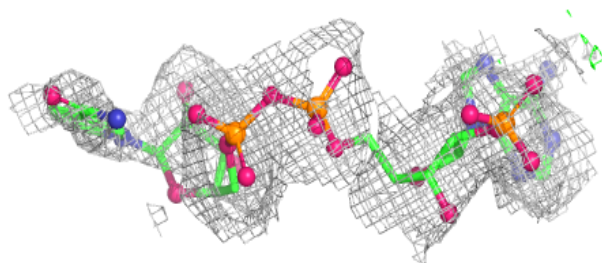
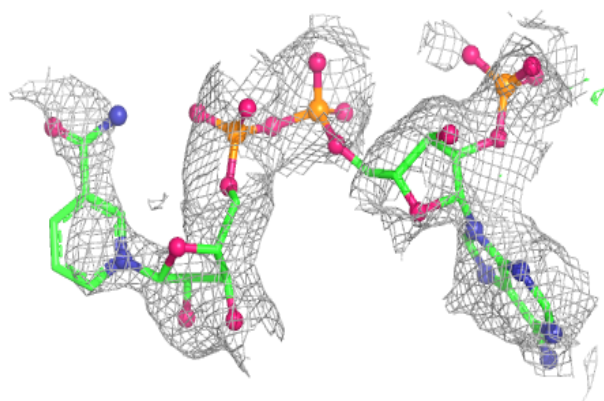
Electron density around PM7 F 802:

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

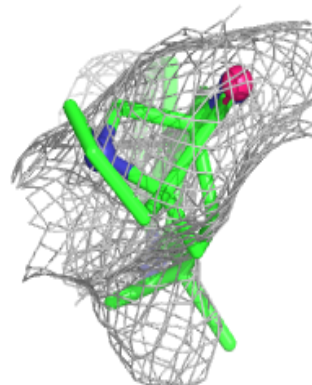
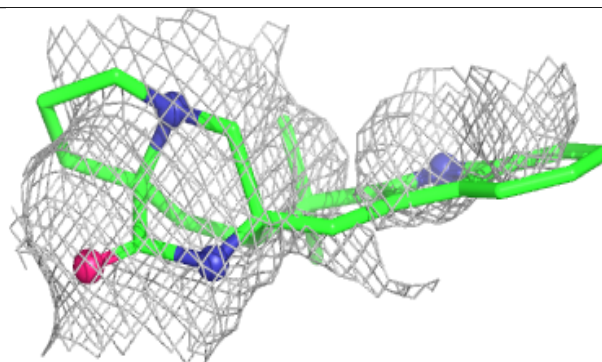
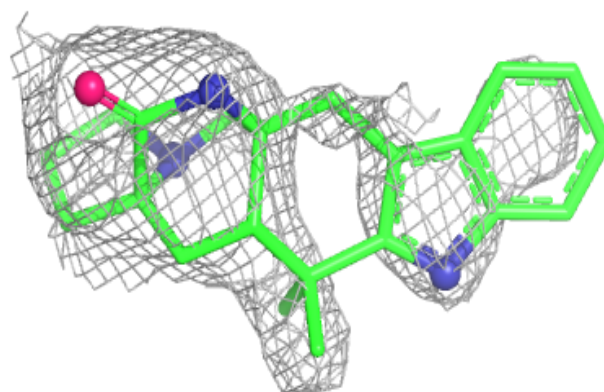


Electron density around NAP F 801:

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

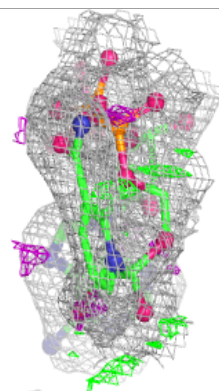
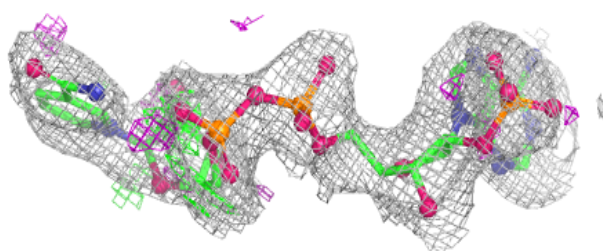
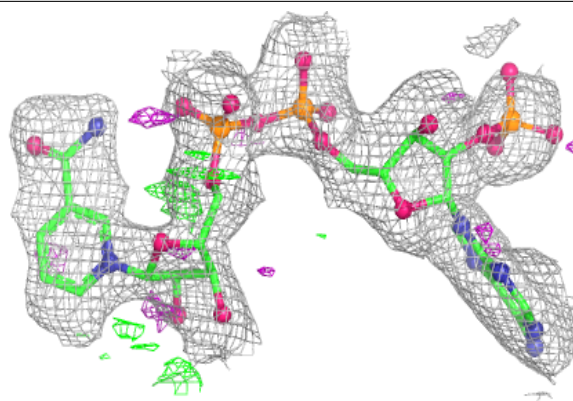
**Electron density around PM7 E 802:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

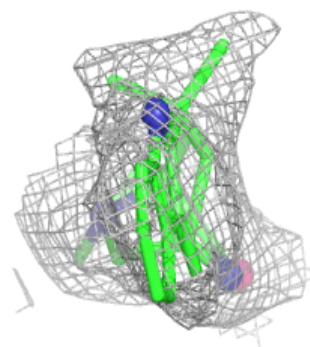
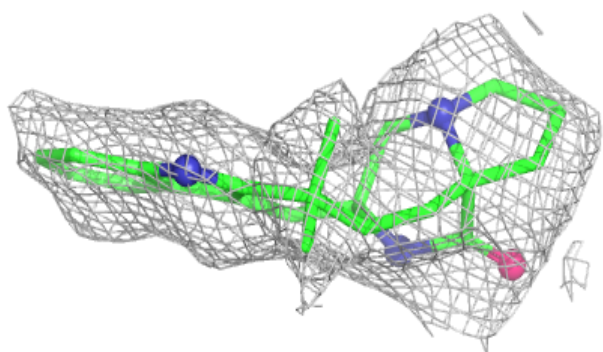
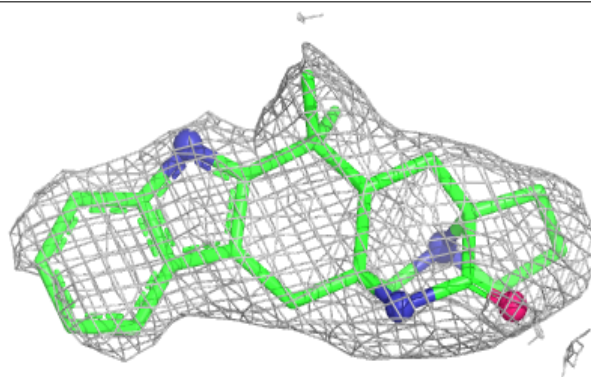


Electron density around NAP C 801:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

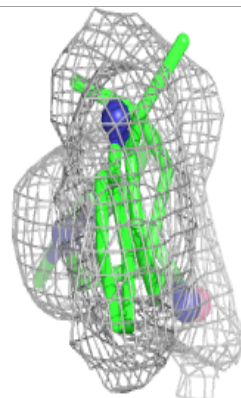
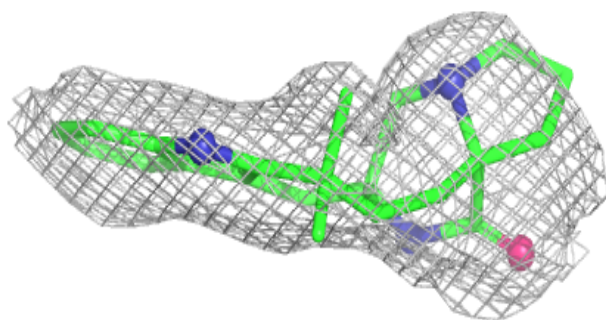
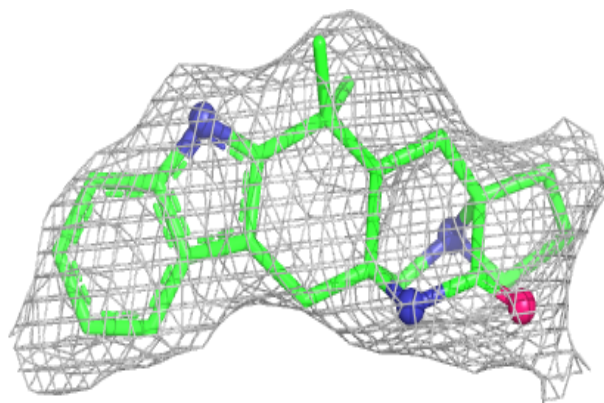
**Electron density around PM7 A 802:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

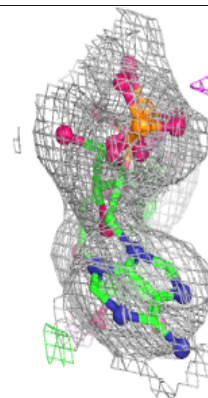
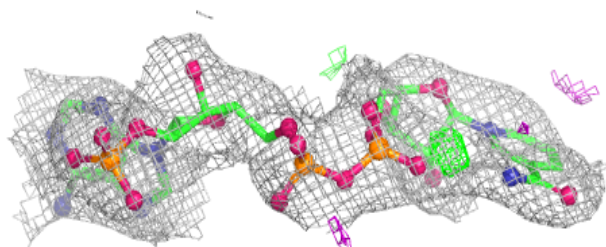
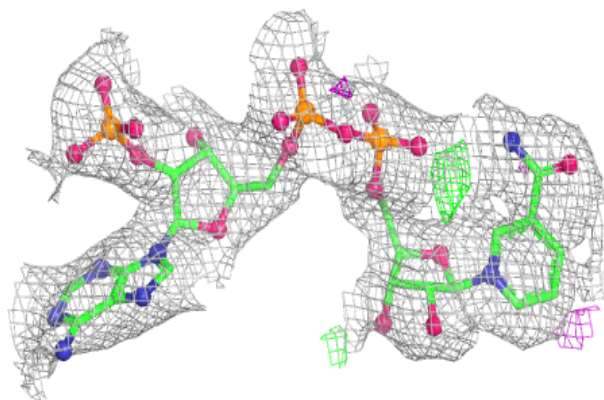


Electron density around PM7 D 802:

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

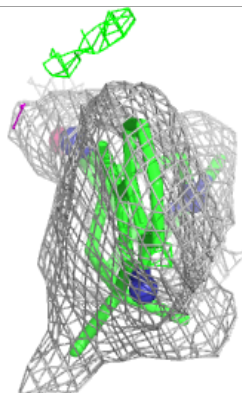
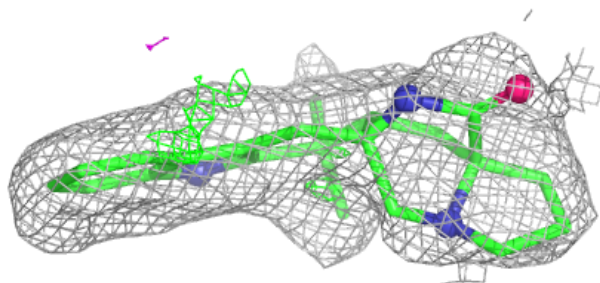
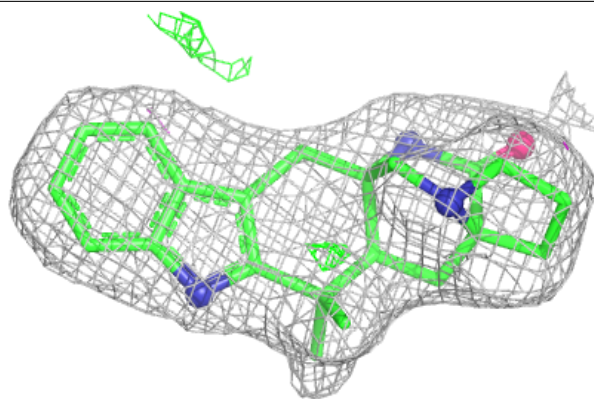
**Electron density around NAP E 801:**

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

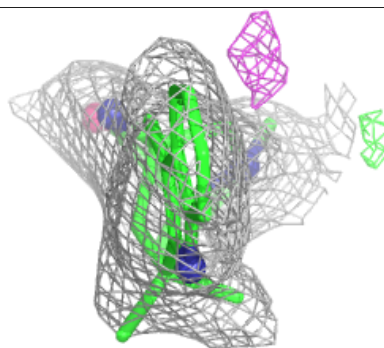
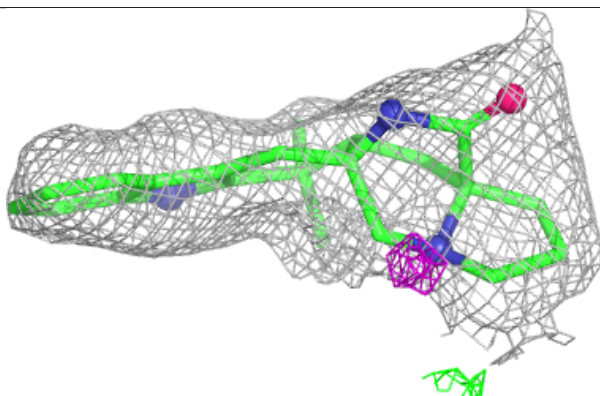
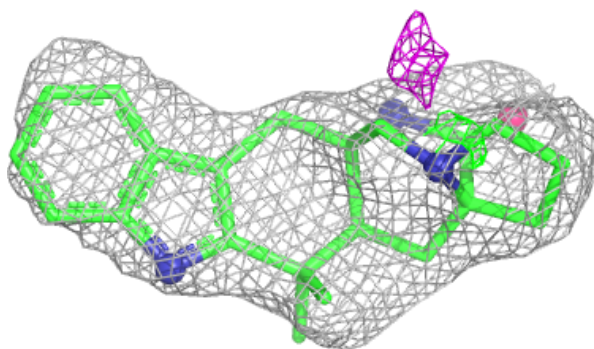


Electron density around PM7 B 802:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

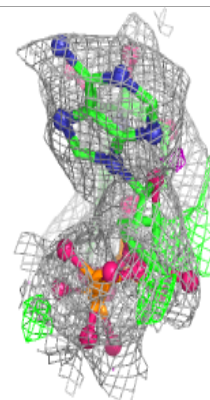
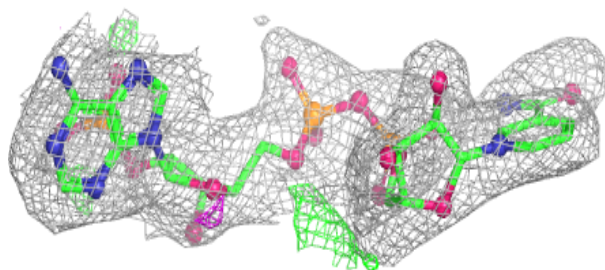
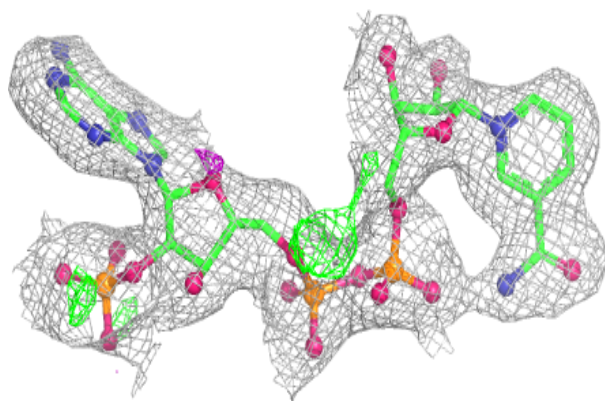
**Electron density around PM7 C 802:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

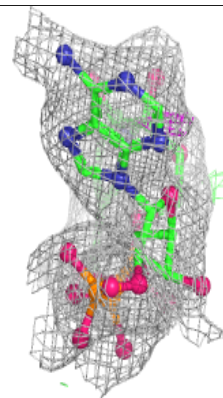
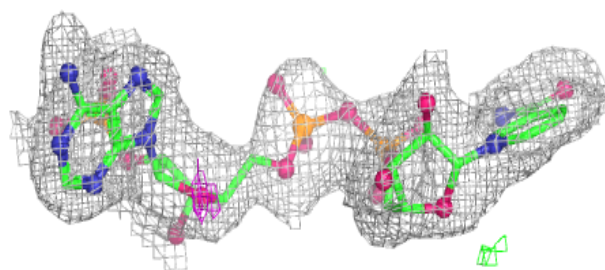
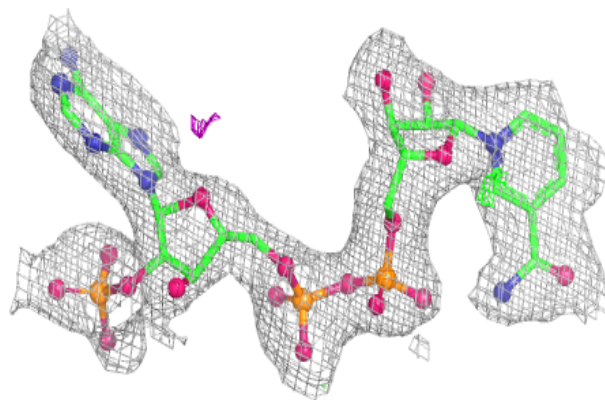


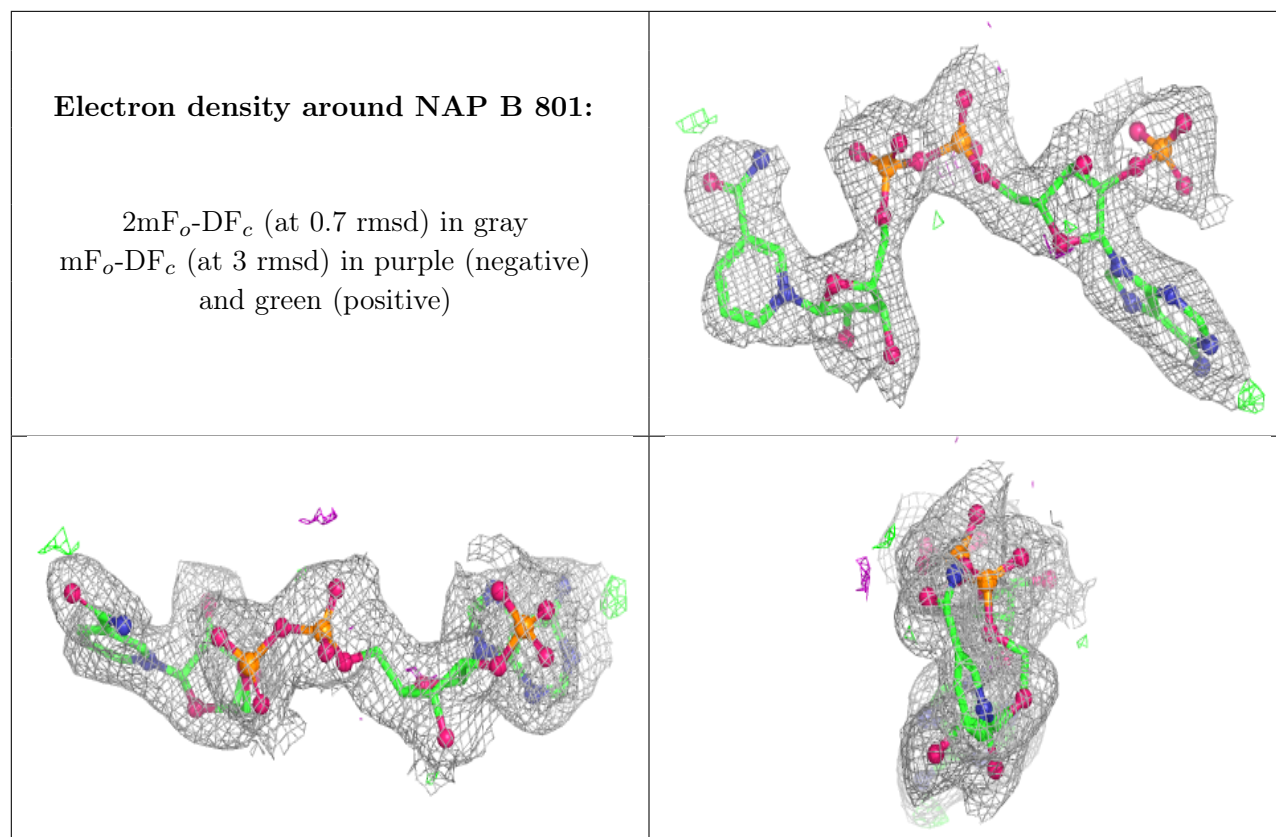
Electron density around NAP A 801:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.