



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 12:14 AM EDT

PDB ID : 3ND7
Title : Crystal structure of phosphopantetheine adenylyltransferase from *Enterococcus faecalis* in the ligand-unbound state and in complex with ATP and pantetheine
Authors : Yoon, H.J.; Lee, H.H.; Suh, S.W.
Deposited on : 2010-06-07
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

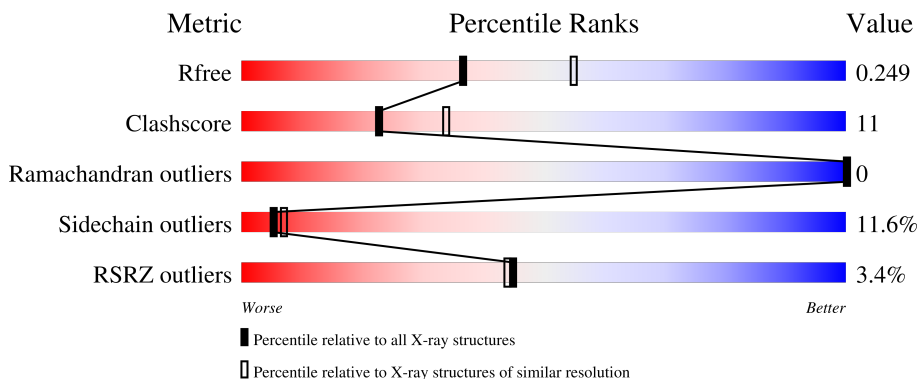
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	171	 63% 19% 6% 11%
1	B	171	 64% 19% 6% 11%
1	C	171	 61% 24% • 11%
1	D	171	 63% 22% • 11%

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Mol	Chain	Length	Quality of chain
1	E	171	 <p>%</p> <p>68% 18% 11%</p>
1	F	171	 <p>5%</p> <p>64% 18% 6% 11%</p>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 7706 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	152	1224	791	201	227	5	0	0	0
1	B	152	1224	791	201	227	5	0	0	0
1	C	152	1224	791	201	227	5	0	0	0
1	D	152	1224	791	201	227	5	0	0	0
1	E	152	1224	791	201	227	5	0	0	0
1	F	152	1224	791	201	227	5	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

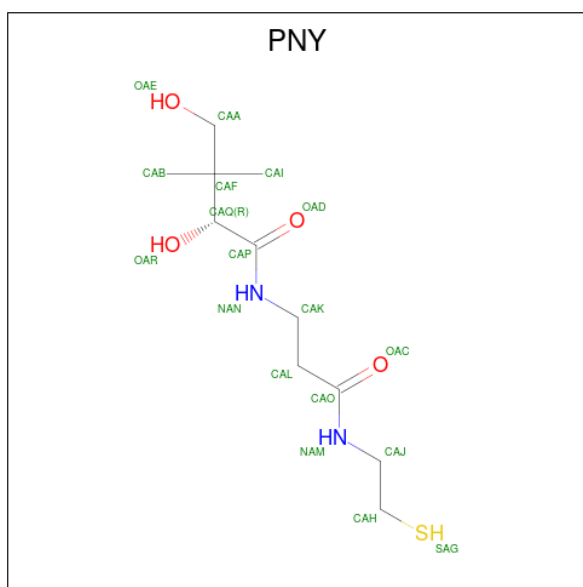
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	LEU	-	expression tag	UNP Q831P9
A	165	GLU	-	expression tag	UNP Q831P9
A	166	HIS	-	expression tag	UNP Q831P9
A	167	HIS	-	expression tag	UNP Q831P9
A	168	HIS	-	expression tag	UNP Q831P9
A	169	HIS	-	expression tag	UNP Q831P9
A	170	HIS	-	expression tag	UNP Q831P9
A	171	HIS	-	expression tag	UNP Q831P9
B	164	LEU	-	expression tag	UNP Q831P9
B	165	GLU	-	expression tag	UNP Q831P9
B	166	HIS	-	expression tag	UNP Q831P9
B	167	HIS	-	expression tag	UNP Q831P9
B	168	HIS	-	expression tag	UNP Q831P9
B	169	HIS	-	expression tag	UNP Q831P9
B	170	HIS	-	expression tag	UNP Q831P9
B	171	HIS	-	expression tag	UNP Q831P9
C	164	LEU	-	expression tag	UNP Q831P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	165	GLU	-	expression tag	UNP Q831P9
C	166	HIS	-	expression tag	UNP Q831P9
C	167	HIS	-	expression tag	UNP Q831P9
C	168	HIS	-	expression tag	UNP Q831P9
C	169	HIS	-	expression tag	UNP Q831P9
C	170	HIS	-	expression tag	UNP Q831P9
C	171	HIS	-	expression tag	UNP Q831P9
D	164	LEU	-	expression tag	UNP Q831P9
D	165	GLU	-	expression tag	UNP Q831P9
D	166	HIS	-	expression tag	UNP Q831P9
D	167	HIS	-	expression tag	UNP Q831P9
D	168	HIS	-	expression tag	UNP Q831P9
D	169	HIS	-	expression tag	UNP Q831P9
D	170	HIS	-	expression tag	UNP Q831P9
D	171	HIS	-	expression tag	UNP Q831P9
E	164	LEU	-	expression tag	UNP Q831P9
E	165	GLU	-	expression tag	UNP Q831P9
E	166	HIS	-	expression tag	UNP Q831P9
E	167	HIS	-	expression tag	UNP Q831P9
E	168	HIS	-	expression tag	UNP Q831P9
E	169	HIS	-	expression tag	UNP Q831P9
E	170	HIS	-	expression tag	UNP Q831P9
E	171	HIS	-	expression tag	UNP Q831P9
F	164	LEU	-	expression tag	UNP Q831P9
F	165	GLU	-	expression tag	UNP Q831P9
F	166	HIS	-	expression tag	UNP Q831P9
F	167	HIS	-	expression tag	UNP Q831P9
F	168	HIS	-	expression tag	UNP Q831P9
F	169	HIS	-	expression tag	UNP Q831P9
F	170	HIS	-	expression tag	UNP Q831P9
F	171	HIS	-	expression tag	UNP Q831P9

- Molecule 2 is (2R)-2,4-dihydroxy-3,3-dimethyl-N-{3-oxo-3-[(2-sulfanylethyl)amino]propyl}butanamide (three-letter code: PNY) (formula: C₁₁H₂₂N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	18	11	2	4	1	0	0
2	B	1	18	11	2	4	1	0	0
2	C	1	18	11	2	4	1	0	0
2	D	1	18	11	2	4	1	0	0
2	E	1	18	11	2	4	1	0	0
2	F	1	18	11	2	4	1	0	0

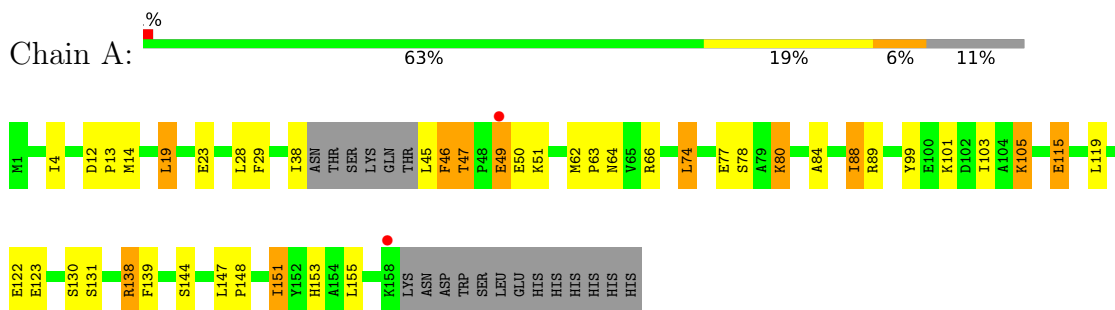
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	48	48	48	0	0
3	B	42	42	42	0	0
3	C	40	40	40	0	0
3	D	36	36	36	0	0
3	E	50	50	50	0	0
3	F	38	38	38	0	0

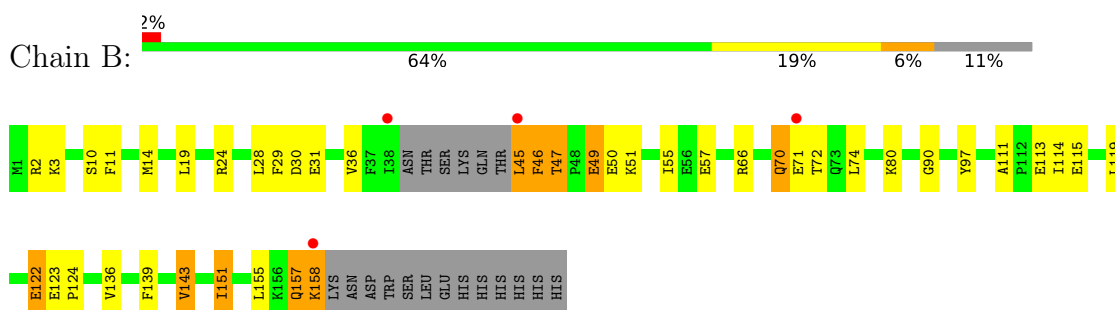
3 Residue-property plots [i](#)

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

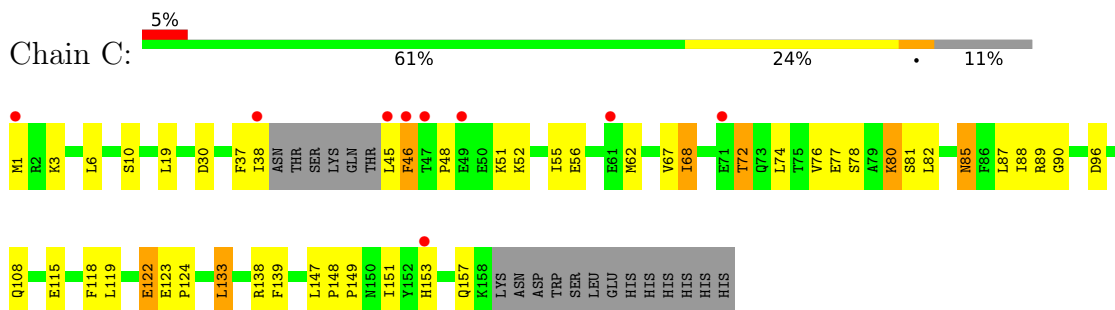
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

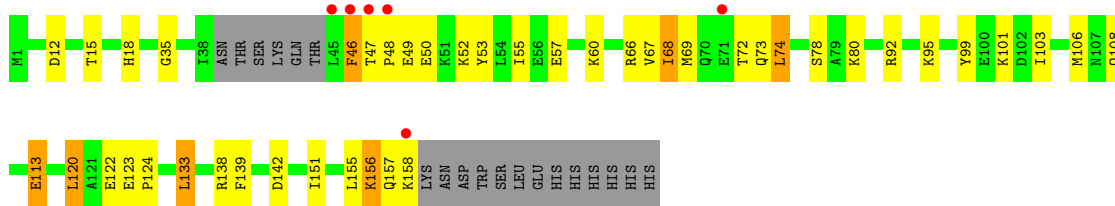


- Molecule 1: Phosphopantetheine adenylyltransferase

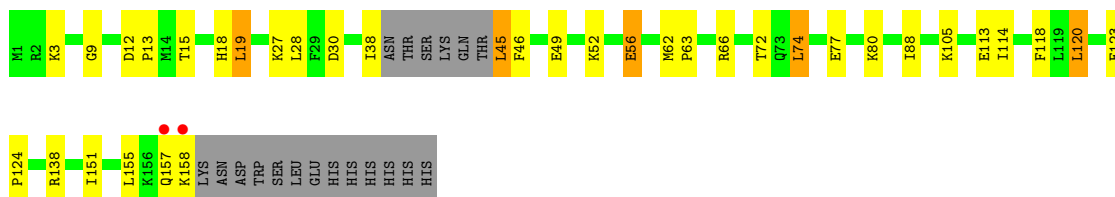


- Molecule 1: Phosphopantetheine adenylyltransferase

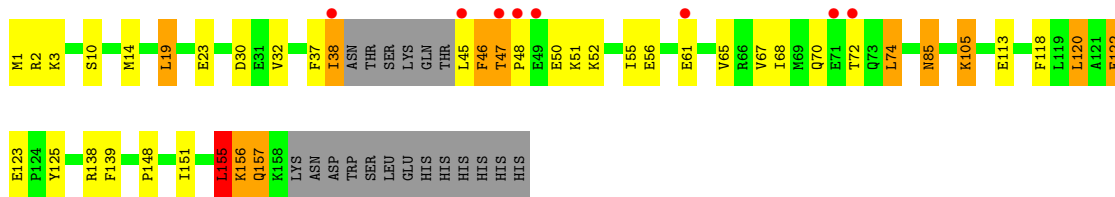




• Molecule 1: Phosphopantetheine adenylyltransferase



• Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.64Å 125.79Å 125.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.40 19.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.89-2.40) 99.5 (19.89-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 2.41Å)	Xtrriage
Refinement program	CNS, REFMAC 5.5.0102	Depositor
R, R_{free}	0.213 , 0.262 0.206 , 0.249	Depositor DCC
R_{free} test set	6884 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtrriage
Anisotropy	0.678	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.044 for -h,l,k	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7706	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: PNY

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	1.08	2/1248 (0.2%)	0.95	1/1683 (0.1%)
1	B	1.13	4/1248 (0.3%)	1.00	2/1683 (0.1%)
1	C	1.04	1/1248 (0.1%)	1.01	4/1683 (0.2%)
1	D	1.07	1/1248 (0.1%)	1.01	5/1683 (0.3%)
1	E	1.07	0/1248	1.01	2/1683 (0.1%)
1	F	1.08	2/1248 (0.2%)	0.94	1/1683 (0.1%)
All	All	1.08	10/7488 (0.1%)	0.99	15/10098 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CG-CD	5.84	1.60	1.51
1	B	122	GLU	CB-CG	5.74	1.63	1.52
1	A	115	GLU	CG-CD	5.59	1.60	1.51
1	A	29	PHE	CE1-CZ	5.56	1.48	1.37
1	C	122	GLU	CG-CD	5.38	1.60	1.51
1	B	113	GLU	CG-CD	5.29	1.59	1.51
1	B	97	TYR	CD1-CE1	5.12	1.47	1.39
1	F	61	GLU	CB-CG	5.10	1.61	1.52
1	F	125	TYR	CD2-CE2	5.06	1.47	1.39
1	D	113	GLU	CG-CD	5.05	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	133	LEU	CB-CG-CD2	-6.47	99.99	111.00
1	D	95	LYS	CD-CE-NZ	-6.46	96.85	111.70
1	C	96	ASP	CB-CG-OD1	-6.31	112.62	118.30
1	D	101	LYS	CD-CE-NZ	-6.08	97.71	111.70
1	E	19	LEU	CA-CB-CG	5.84	128.74	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	B	45	LEU	CA-CB-CG	5.58	128.14	115.30
1	D	142	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	142	ASP	CB-CG-OD1	5.43	123.19	118.30
1	E	66	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	85	ASN	CB-CA-C	-5.29	99.81	110.40
1	F	155	LEU	CA-CB-CG	-5.28	103.17	115.30
1	C	30	ASP	CB-CG-OD1	-5.25	113.57	118.30
1	D	92	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	101	LYS	CD-CE-NZ	-5.08	100.02	111.70

There are no chirality outliers.

There are no planarity outliers.

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	1224	0	1246	32	0
1	B	1224	0	1246	42	0
1	C	1224	0	1246	24	0
1	D	1224	0	1246	30	0
1	E	1224	0	1246	31	0
1	F	1224	0	1245	36	0
2	A	18	0	22	3	0
2	B	18	0	22	2	0
2	C	18	0	22	2	0
2	D	18	0	22	1	0
2	E	18	0	22	1	0
2	F	18	0	22	0	0
3	A	48	0	0	4	0
3	B	42	0	0	3	0
3	C	40	0	0	3	0
3	D	36	0	0	2	0
3	E	50	0	0	0	0
3	F	38	0	0	2	0
All	All	7706	0	7607	173	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (173) 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:B:47:THR:CG2	1:B:50:GLU:OE1	1.77	1.31
1:B:49:GLU:OE2	1:B:49:GLU:HA	1.42	1.12
1:B:47:THR:HG23	1:B:50:GLU:OE1	1.49	1.12
1:D:151:ILE:O	1:D:155:LEU:HD23	1.60	1.01
1:B:47:THR:HG22	1:B:50:GLU:OE1	1.61	0.97
1:B:47:THR:HG23	1:B:50:GLU:CG	1.95	0.96
1:A:105:LYS:HE3	1:B:123:GLU:HG2	1.44	0.96
2:C:503:PNY:HAI	2:C:503:PNY:OAD	1.68	0.93
1:B:47:THR:HG23	1:B:50:GLU:CD	1.91	0.91
2:A:501:PNY:HNAN	2:A:501:PNY:HAB	1.33	0.89
1:C:118:PHE:HE2	1:D:120:LEU:HD22	1.38	0.87
1:B:115:GLU:HG2	3:B:201:HOH:O	1.75	0.87
1:B:157:GLN:O	1:B:158:LYS:HG3	1.77	0.84
1:B:47:THR:CG2	1:B:50:GLU:CD	2.47	0.82
1:B:115:GLU:OE1	3:B:201:HOH:O	1.96	0.81
1:C:118:PHE:CE2	1:D:120:LEU:HD22	2.17	0.79
1:A:115:GLU:OE1	3:A:187:HOH:O	2.00	0.78
1:A:105:LYS:HE3	1:B:123:GLU:CG	2.14	0.78
2:A:501:PNY:HAB	2:A:501:PNY:NAN	1.99	0.77
1:F:156:LYS:HB2	1:F:157:GLN:OE1	1.85	0.76
1:B:49:GLU:OE2	1:B:49:GLU:CA	2.30	0.76
1:C:115:GLU:OE2	3:C:242:HOH:O	2.06	0.74
1:C:85:ASN:ND2	3:C:205:HOH:O	2.19	0.74
1:E:45:LEU:HD13	1:E:46:PHE:HD2	1.53	0.74
1:E:120:LEU:HD22	1:F:118:PHE:CE2	2.23	0.73
1:D:156:LYS:C	1:D:157:GLN:OE1	2.29	0.70
1:E:120:LEU:HD22	1:F:118:PHE:HE2	1.55	0.70
1:A:105:LYS:CE	1:B:123:GLU:HG2	2.18	0.70
1:B:47:THR:O	1:B:50:GLU:N	2.23	0.70
1:E:80:LYS:HE3	1:E:113:GLU:OE1	1.93	0.68
1:C:81:SER:O	3:C:193:HOH:O	2.11	0.68
1:B:47:THR:CG2	1:B:50:GLU:CG	2.70	0.68
1:E:123:GLU:CG	1:F:105:LYS:HE3	2.24	0.67
1:A:12:ASP:OD2	1:A:45:LEU:HD22	1.95	0.67
1:D:157:GLN:HB2	3:D:216:HOH:O	1.93	0.66
1:A:64:ASN:OD1	3:A:221:HOH:O	2.15	0.65
1:B:72:THR:HG22	1:F:139:PHE:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:PHE:CD2	1:B:46:PHE:N	2.64	0.65
1:F:157:GLN:OE1	1:F:157:GLN:N	2.29	0.65
1:C:118:PHE:CE2	1:D:120:LEU:CD2	2.80	0.65
1:E:80:LYS:HG3	1:E:114:ILE:HD11	1.79	0.64
1:D:157:GLN:OE1	1:D:157:GLN:N	2.31	0.64
1:E:118:PHE:CE2	1:F:120:LEU:HD22	2.33	0.64
1:A:12:ASP:OD1	1:A:46:PHE:HE2	1.80	0.63
1:A:88:ILE:HD11	1:A:119:LEU:HG	1.79	0.63
1:D:80:LYS:HE3	1:D:113:GLU:OE1	1.97	0.63
1:A:138:ARG:HG2	1:A:138:ARG:O	1.99	0.62
2:C:503:PNY:OAD	2:C:503:PNY:CAI	2.43	0.62
1:F:14:MET:HE1	1:F:148:PRO:HG2	1.82	0.62
1:F:52:LYS:O	1:F:56:GLU:HG2	1.99	0.62
1:B:47:THR:HG23	1:B:50:GLU:CB	2.29	0.61
1:B:70:GLN:NE2	1:B:70:GLN:HA	2.15	0.61
1:A:77:GLU:HA	1:A:80:LYS:HD2	1.81	0.61
1:E:123:GLU:HG3	1:F:105:LYS:HE3	1.83	0.60
1:B:70:GLN:HA	1:B:70:GLN:HE21	1.67	0.60
1:C:51:LYS:O	1:C:55:ILE:HD12	2.02	0.60
1:A:115:GLU:HG2	3:A:187:HOH:O	2.00	0.59
1:B:47:THR:CG2	1:B:50:GLU:HG3	2.33	0.59
1:A:12:ASP:OD1	1:A:46:PHE:CE2	2.55	0.59
1:B:28:LEU:HD23	1:B:29:PHE:CE2	2.38	0.59
1:C:90:GLY:HA2	1:C:119:LEU:O	2.04	0.58
1:B:47:THR:HG23	1:B:50:GLU:HB2	1.86	0.58
1:C:76:VAL:O	1:C:80:LYS:HD3	2.04	0.58
1:A:28:LEU:HD12	1:A:28:LEU:O	2.04	0.57
1:D:47:THR:HB	1:D:48:PRO:HD2	1.86	0.57
1:B:47:THR:HG23	1:B:50:GLU:HG3	1.83	0.57
1:A:144:SER:OG	3:A:184:HOH:O	2.18	0.56
1:B:115:GLU:CG	3:B:201:HOH:O	2.44	0.56
1:D:99:TYR:CZ	1:D:103:ILE:HD11	2.41	0.56
1:A:139:PHE:HB2	1:E:74:LEU:HD13	1.88	0.55
1:E:74:LEU:HB2	1:E:77:GLU:HG2	1.88	0.55
1:C:138:ARG:O	1:C:138:ARG:HG2	2.05	0.55
1:E:105:LYS:HE3	1:F:123:GLU:CD	2.27	0.54
1:D:15:THR:O	1:D:18:HIS:HB2	2.06	0.54
1:B:157:GLN:O	1:B:158:LYS:HE2	2.09	0.53
1:F:113:GLU:OE2	1:F:113:GLU:N	2.32	0.53
1:D:139:PHE:CB	1:F:74:LEU:HD13	2.39	0.53
1:F:148:PRO:HG2	1:F:151:ILE:HD13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:LYS:HB2	1:E:30:ASP:H	1.75	0.52
1:A:139:PHE:CB	1:E:74:LEU:HD13	2.40	0.51
1:B:111:ALA:HB1	1:B:114:ILE:HD12	1.91	0.51
1:F:3:LYS:HB2	1:F:30:ASP:H	1.76	0.50
1:F:46:PHE:HE2	3:F:203:HOH:O	1.94	0.50
1:C:88:ILE:O	1:C:89:ARG:HD2	2.12	0.50
1:A:151:ILE:O	1:A:155:LEU:HB2	2.12	0.50
1:C:46:PHE:CD2	1:C:46:PHE:N	2.80	0.50
1:D:55:ILE:HG22	1:D:67:VAL:HG21	1.93	0.50
1:C:89:ARG:HB2	1:C:118:PHE:CE1	2.47	0.50
1:B:3:LYS:N	1:B:30:ASP:OD2	2.35	0.50
1:A:88:ILE:O	1:A:89:ARG:HD2	2.12	0.49
1:D:156:LYS:O	1:D:157:GLN:OE1	2.30	0.49
1:B:72:THR:HG22	1:F:139:PHE:CZ	2.47	0.49
1:D:52:LYS:HB2	1:D:69:MET:SD	2.52	0.49
1:B:123:GLU:N	1:B:124:PRO:HD2	2.28	0.49
1:E:105:LYS:HE3	1:F:123:GLU:CG	2.43	0.48
1:E:52:LYS:O	1:E:56:GLU:HB2	2.14	0.48
1:E:123:GLU:HG2	1:F:105:LYS:HE3	1.94	0.48
1:E:123:GLU:HG2	1:F:105:LYS:CE	2.44	0.48
1:B:10:SER:O	1:B:11:PHE:C	2.51	0.48
1:E:9:GLY:HA2	2:E:505:PNY:HABA	1.95	0.48
1:E:118:PHE:HE2	1:F:120:LEU:HD22	1.79	0.48
1:D:35:GLY:HA2	1:D:68:ILE:HG22	1.96	0.47
1:D:139:PHE:HB3	1:F:74:LEU:HD13	1.96	0.47
1:E:27:LYS:HB3	1:F:1:MET:HG3	1.95	0.47
1:B:157:GLN:O	1:B:158:LYS:CG	2.58	0.47
1:F:32:VAL:HB	1:F:65:VAL:HG22	1.97	0.47
1:D:99:TYR:CZ	1:D:103:ILE:CD1	2.97	0.47
1:C:6:LEU:HB3	1:C:87:LEU:HD23	1.97	0.47
1:D:57:GLU:HG2	1:D:60:LYS:NZ	2.30	0.46
1:F:38:ILE:HG21	1:F:48:PRO:HG3	1.98	0.46
2:A:501:PNY:NAN	2:A:501:PNY:CAB	2.73	0.46
1:C:68:ILE:HD13	1:C:82:LEU:HD22	1.98	0.46
1:C:108:GLN:HE21	1:C:108:GLN:HB3	1.61	0.46
1:E:120:LEU:CD2	1:F:118:PHE:CE2	2.98	0.45
1:B:151:ILE:O	1:B:155:LEU:HB2	2.16	0.45
1:F:55:ILE:HG22	1:F:67:VAL:HG21	1.99	0.45
1:A:74:LEU:HD13	1:C:139:PHE:HB2	1.97	0.45
1:C:56:GLU:HG3	1:C:67:VAL:CG2	2.47	0.45
1:F:122:GLU:OE2	3:F:204:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ASP:HB2	1:A:51:LYS:NZ	2.31	0.45
1:A:23:GLU:HG2	1:A:62:MET:SD	2.57	0.45
1:A:47:THR:OG1	1:A:50:GLU:OE1	2.30	0.45
1:A:12:ASP:HA	1:A:13:PRO:HA	1.29	0.44
1:A:47:THR:HB	1:A:49:GLU:HG2	1.99	0.44
1:F:37:PHE:HA	1:F:70:GLN:O	2.18	0.44
1:A:139:PHE:CE1	1:E:72:THR:HG22	2.53	0.44
1:B:90:GLY:HA2	1:B:119:LEU:O	2.19	0.43
1:E:123:GLU:N	1:E:124:PRO:HD2	2.34	0.43
1:E:74:LEU:CB	1:E:77:GLU:HG2	2.47	0.43
1:F:155:LEU:HA	1:F:155:LEU:HD12	1.17	0.43
1:B:24:ARG:NH2	1:B:119:LEU:HB3	2.34	0.43
1:B:139:PHE:CD1	1:D:73:GLN:HA	2.53	0.43
1:C:153:HIS:O	1:C:157:GLN:HG2	2.18	0.43
1:E:45:LEU:HD12	1:E:46:PHE:H	1.83	0.43
1:D:133:LEU:HD12	1:D:133:LEU:HA	1.82	0.43
1:A:99:TYR:CZ	1:A:103:ILE:HD11	2.53	0.43
1:B:136:VAL:HG11	1:B:143:VAL:HG13	2.00	0.43
1:D:50:GLU:O	1:D:53:TYR:N	2.52	0.43
1:D:106:MET:HB3	2:D:504:PNY:SAG	2.59	0.43
1:C:52:LYS:NZ	1:C:56:GLU:OE2	2.50	0.42
1:E:123:GLU:HG2	1:F:105:LYS:NZ	2.34	0.42
1:F:14:MET:CE	1:F:148:PRO:HG2	2.49	0.42
1:A:14:MET:CE	1:A:19:LEU:HG	2.49	0.42
1:A:153:HIS:C	1:A:155:LEU:N	2.73	0.42
1:D:108:GLN:HG3	3:D:196:HOH:O	2.18	0.42
1:F:19:LEU:O	1:F:23:GLU:HG3	2.19	0.42
1:B:36:VAL:HG21	1:B:55:ILE:CD1	2.50	0.42
1:F:47:THR:O	1:F:50:GLU:N	2.53	0.42
1:C:148:PRO:HA	1:C:149:PRO:HD3	1.93	0.42
1:A:62:MET:HA	1:A:63:PRO:HD2	1.88	0.42
2:B:502:PNY:OAD	2:B:502:PNY:HAB	2.19	0.42
1:D:99:TYR:CE1	1:D:103:ILE:HD11	2.55	0.42
1:D:156:LYS:HB3	1:D:156:LYS:HE2	1.73	0.42
1:C:37:PHE:HB3	1:C:72:THR:HG23	2.02	0.41
1:D:57:GLU:HG2	1:D:60:LYS:HZ1	1.86	0.41
1:E:15:THR:O	1:E:18:HIS:HB2	2.19	0.41
1:C:89:ARG:HB2	1:C:118:PHE:CD1	2.56	0.41
1:A:147:LEU:HA	1:A:148:PRO:HD3	1.94	0.41
1:A:4:ILE:HG22	1:A:84:ALA:HA	2.01	0.41
1:F:47:THR:HA	1:F:48:PRO:HD2	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLU:OE2	1:C:123:GLU:CD	2.59	0.41
1:F:2:ARG:O	1:F:85:ASN:ND2	2.54	0.41
1:A:13:PRO:HG2	1:A:147:LEU:HD21	2.02	0.41
1:B:80:LYS:HG3	1:B:114:ILE:HD11	2.02	0.41
2:B:502:PNY:OAD	2:B:502:PNY:HAI	2.21	0.41
1:B:31:GLU:OE1	1:B:66:ARG:NH1	2.52	0.41
1:E:28:LEU:HD12	1:E:28:LEU:O	2.21	0.40
1:D:123:GLU:N	1:D:124:PRO:CD	2.84	0.40
1:D:74:LEU:HD12	1:D:74:LEU:HA	1.85	0.40
1:E:12:ASP:HA	1:E:13:PRO:HA	1.84	0.40
1:D:12:ASP:OD1	1:D:46:PHE:CZ	2.74	0.40
1:E:151:ILE:O	1:E:155:LEU:HD23	2.22	0.40
1:E:62:MET:HA	1:E:63:PRO:HD2	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	148/171 (86%)	140 (95%)	8 (5%)	0	100	100
1	B	148/171 (86%)	146 (99%)	2 (1%)	0	100	100
1	C	148/171 (86%)	142 (96%)	6 (4%)	0	100	100
1	D	148/171 (86%)	142 (96%)	6 (4%)	0	100	100
1	E	148/171 (86%)	141 (95%)	7 (5%)	0	100	100
1	F	148/171 (86%)	146 (99%)	2 (1%)	0	100	100
All	All	888/1026 (86%)	857 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/154 (88%)	118 (87%)	17 (13%)	4	5
1	B	135/154 (88%)	120 (89%)	15 (11%)	6	8
1	C	135/154 (88%)	115 (85%)	20 (15%)	3	3
1	D	135/154 (88%)	122 (90%)	13 (10%)	8	12
1	E	135/154 (88%)	124 (92%)	11 (8%)	11	18
1	F	135/154 (88%)	117 (87%)	18 (13%)	4	4
All	All	810/924 (88%)	716 (88%)	94 (12%)	5	7

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	38	ILE
1	A	46	PHE
1	A	47	THR
1	A	49	GLU
1	A	66	ARG
1	A	74	LEU
1	A	78	SER
1	A	80	LYS
1	A	88	ILE
1	A	105	LYS
1	A	122	GLU
1	A	123	GLU
1	A	130	SER
1	A	131	SER
1	A	138	ARG
1	A	151	ILE
1	B	14	MET
1	B	19	LEU
1	B	45	LEU
1	B	46	PHE
1	B	47	THR

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Mol	Chain	Res	Type
1	B	49	GLU
1	B	51	LYS
1	B	70	GLN
1	B	71	GLU
1	B	74	LEU
1	B	122	GLU
1	B	143	VAL
1	B	151	ILE
1	B	157	GLN
1	B	158	LYS
1	C	1	MET
1	C	3	LYS
1	C	10	SER
1	C	19	LEU
1	C	38	ILE
1	C	45	LEU
1	C	46	PHE
1	C	48	PRO
1	C	62	MET
1	C	68	ILE
1	C	72	THR
1	C	74	LEU
1	C	77	GLU
1	C	78	SER
1	C	80	LYS
1	C	122	GLU
1	C	124	PRO
1	C	133	LEU
1	C	147	LEU
1	C	151	ILE
1	D	46	PHE
1	D	49	GLU
1	D	66	ARG
1	D	68	ILE
1	D	72	THR
1	D	74	LEU
1	D	78	SER
1	D	120	LEU
1	D	122	GLU
1	D	133	LEU
1	D	138	ARG
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	158	LYS
1	E	19	LEU
1	E	38	ILE
1	E	45	LEU
1	E	49	GLU
1	E	56	GLU
1	E	74	LEU
1	E	88	ILE
1	E	120	LEU
1	E	138	ARG
1	E	157	GLN
1	E	158	LYS
1	F	10	SER
1	F	19	LEU
1	F	38	ILE
1	F	45	LEU
1	F	46	PHE
1	F	47	THR
1	F	51	LYS
1	F	68	ILE
1	F	72	THR
1	F	74	LEU
1	F	85	ASN
1	F	105	LYS
1	F	120	LEU
1	F	122	GLU
1	F	138	ARG
1	F	155	LEU
1	F	156	LYS
1	F	157	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	108	GLN
1	C	108	GLN
1	F	85	ASN
1	F	108	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](#)

6 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	PNY	F	506	-	14,17,17	1.01	1 (7%)	19,22,22	1.41	4 (21%)
2	PNY	C	503	-	14,17,17	0.71	0	19,22,22	1.60	4 (21%)
2	PNY	E	505	-	14,17,17	1.14	2 (14%)	19,22,22	1.58	4 (21%)
2	PNY	A	501	-	14,17,17	2.98	2 (14%)	19,22,22	1.29	1 (5%)
2	PNY	B	502	-	14,17,17	1.04	1 (7%)	19,22,22	1.70	3 (15%)
2	PNY	D	504	-	14,17,17	1.59	3 (21%)	19,22,22	1.14	2 (10%)

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	PNY	F	506	-	-	1/23/23/23	-
2	PNY	C	503	-	-	5/23/23/23	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PNY	E	505	-	-	8/23/23/23	-
2	PNY	A	501	-	-	9/23/23/23	-
2	PNY	B	502	-	-	4/23/23/23	-
2	PNY	D	504	-	-	3/23/23/23	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PNY	CAA-CAF	9.94	1.59	1.53
2	A	501	PNY	CAL-CAO	3.80	1.58	1.51
2	D	504	PNY	CAA-CAF	3.51	1.55	1.53
2	D	504	PNY	CAL-CAO	2.98	1.57	1.51
2	D	504	PNY	OAR-CAQ	2.60	1.47	1.42
2	E	505	PNY	CAA-CAF	2.47	1.55	1.53
2	E	505	PNY	CAL-CAO	2.47	1.56	1.51
2	F	506	PNY	CAL-CAO	2.38	1.55	1.51
2	B	502	PNY	CAA-CAF	2.14	1.55	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	PNY	CAL-CAO-NAM	-4.03	109.64	116.42
2	B	502	PNY	CAB-CAF-CAA	3.80	115.87	108.90
2	C	503	PNY	OAE-CAA-CAF	-3.80	106.16	112.96
2	E	505	PNY	CAL-CAO-NAM	-3.44	110.63	116.42
2	A	501	PNY	CAK-CAL-CAO	3.23	117.74	112.36
2	F	506	PNY	CAB-CAF-CAQ	2.85	113.75	108.82
2	D	504	PNY	CAJ-NAM-CAO	-2.80	117.65	122.84
2	F	506	PNY	CAK-CAL-CAO	2.75	116.93	112.36
2	E	505	PNY	CAI-CAF-CAQ	2.72	113.53	108.82
2	F	506	PNY	CAL-CAO-NAM	-2.71	111.86	116.42
2	C	503	PNY	CAL-CAO-NAM	-2.63	112.00	116.42
2	B	502	PNY	CAK-NAN-CAP	-2.62	117.91	122.59
2	C	503	PNY	CAK-CAL-CAO	2.46	116.46	112.36
2	F	506	PNY	OAE-CAA-CAF	-2.44	108.59	112.96
2	D	504	PNY	CAK-CAL-CAO	2.30	116.19	112.36
2	E	505	PNY	OAC-CAO-CAL	2.21	126.06	122.02
2	E	505	PNY	CAB-CAF-CAA	2.14	112.82	108.90
2	C	503	PNY	CAL-CAK-NAN	-2.09	107.68	111.90

There are no chirality outliers.

All (30) torsion outliers are listed below:

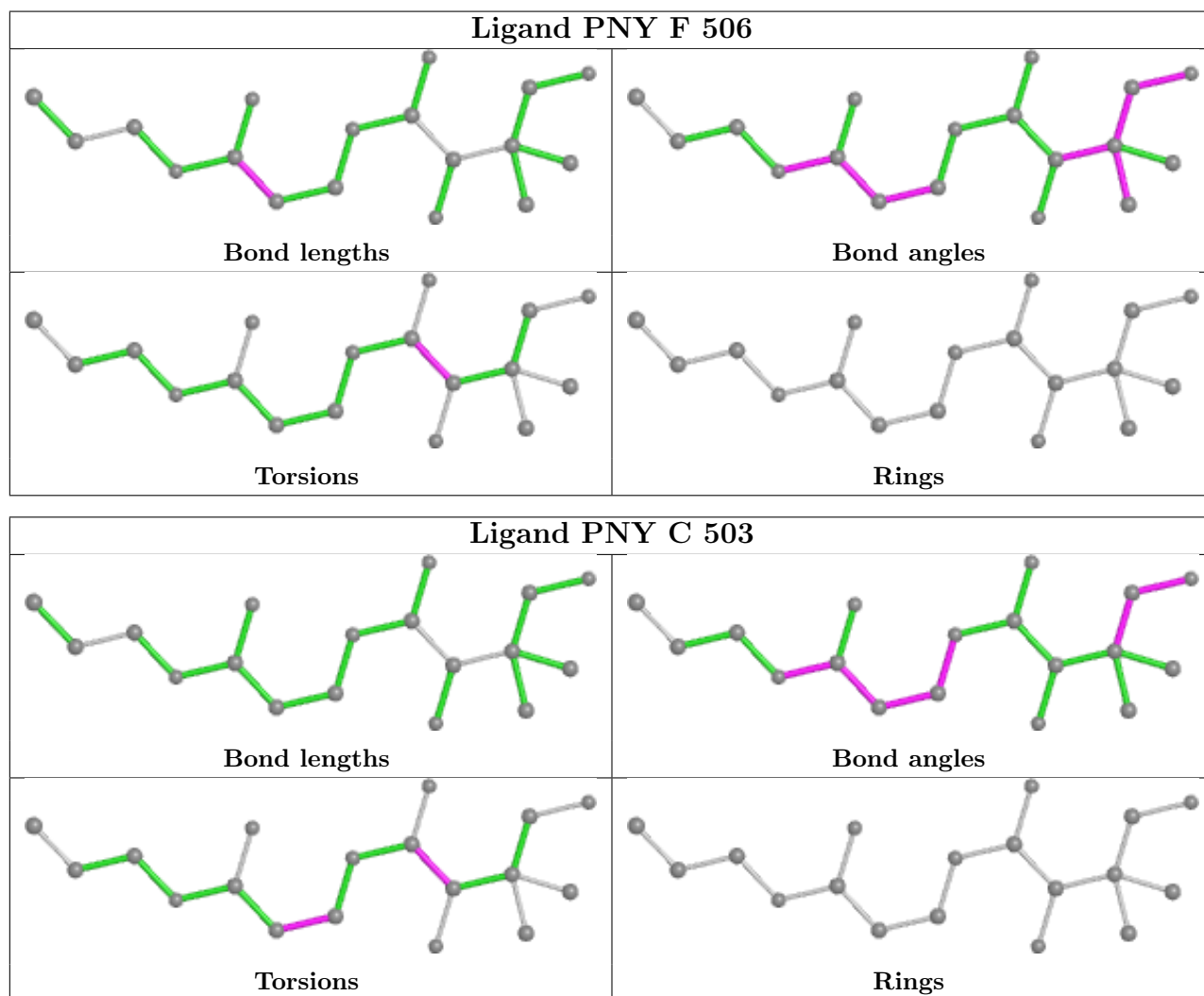
Mol	Chain	Res	Type	Atoms
2	A	501	PNY	CAB-CAF-CAQ-OAR
2	A	501	PNY	CAK-CAL-CAO-NAM
2	A	501	PNY	OAD-CAP-CAQ-CAF
2	A	501	PNY	NAN-CAP-CAQ-CAF
2	B	502	PNY	OAD-CAP-CAQ-CAF
2	B	502	PNY	NAN-CAP-CAQ-CAF
2	B	502	PNY	NAN-CAP-CAQ-OAR
2	C	503	PNY	OAD-CAP-CAQ-CAF
2	C	503	PNY	OAD-CAP-CAQ-OAR
2	C	503	PNY	NAN-CAP-CAQ-CAF
2	C	503	PNY	NAN-CAP-CAQ-OAR
2	E	505	PNY	CAA-CAF-CAQ-CAP
2	E	505	PNY	CAB-CAF-CAQ-CAP
2	E	505	PNY	CAI-CAF-CAQ-CAP
2	E	505	PNY	CAH-CAJ-NAM-CAO
2	A	501	PNY	CAK-CAL-CAO-OAC
2	A	501	PNY	CAL-CAK-NAN-CAP
2	A	501	PNY	NAN-CAK-CAL-CAO
2	C	503	PNY	NAN-CAK-CAL-CAO
2	E	505	PNY	NAN-CAK-CAL-CAO
2	B	502	PNY	OAD-CAP-CAQ-OAR
2	A	501	PNY	CAI-CAF-CAQ-OAR
2	E	505	PNY	CAB-CAF-CAQ-OAR
2	E	505	PNY	CAI-CAF-CAQ-OAR
2	D	504	PNY	OAE-CAA-CAF-CAB
2	D	504	PNY	OAE-CAA-CAF-CAI
2	E	505	PNY	CAA-CAF-CAQ-OAR
2	A	501	PNY	OAD-CAP-CAQ-OAR
2	F	506	PNY	OAD-CAP-CAQ-OAR
2	D	504	PNY	OAE-CAA-CAF-CAQ

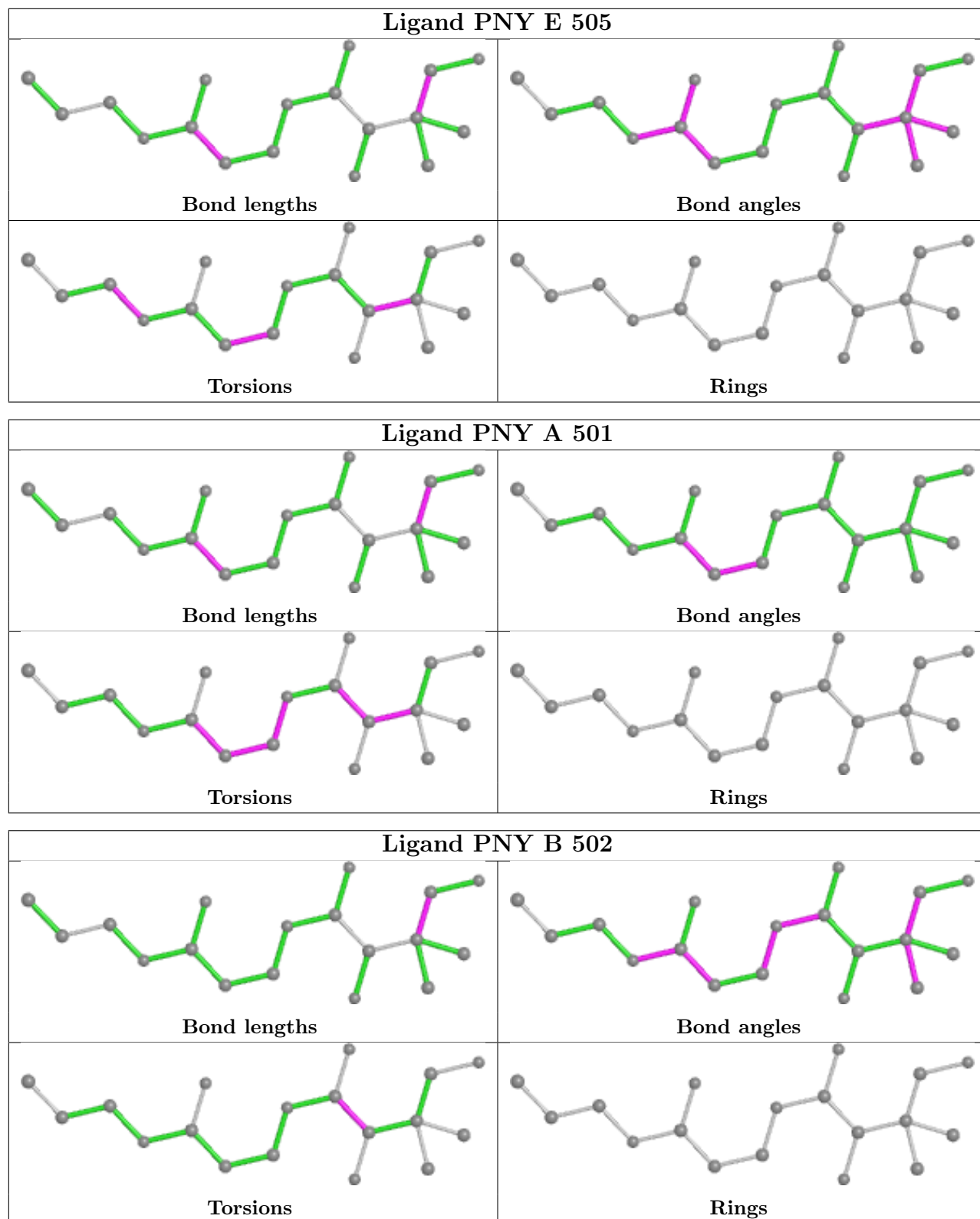
There are no ring outliers.

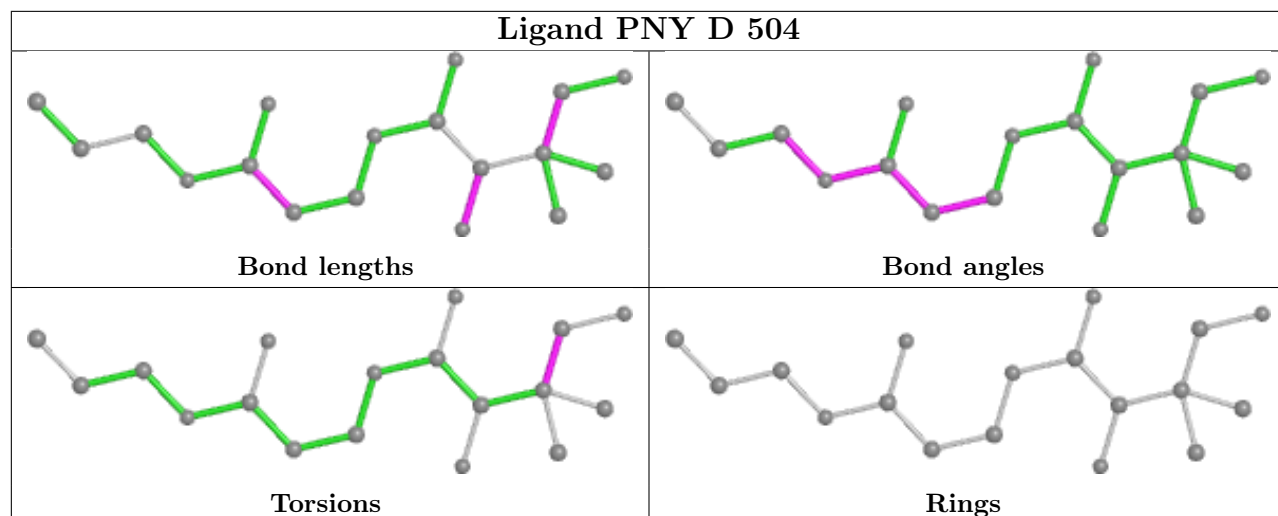
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	PNY	2	0
2	E	505	PNY	1	0
2	A	501	PNY	3	0
2	B	502	PNY	2	0
2	D	504	PNY	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	152/171 (88%)	-0.34	2 (1%) 77 75	24, 40, 67, 80	0
1	B	152/171 (88%)	-0.19	4 (2%) 56 54	21, 42, 76, 90	0
1	C	152/171 (88%)	-0.09	9 (5%) 22 21	26, 48, 89, 103	0
1	D	152/171 (88%)	-0.13	6 (3%) 39 38	27, 46, 86, 102	0
1	E	152/171 (88%)	-0.19	2 (1%) 77 75	23, 43, 69, 92	0
1	F	152/171 (88%)	-0.07	8 (5%) 26 25	27, 46, 84, 102	0
All	All	912/1026 (88%)	-0.17	31 (3%) 45 44	21, 44, 80, 103	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.1
1	F	61	GLU	4.5
1	D	45	LEU	4.0
1	C	47	THR	3.7
1	D	46	PHE	3.6
1	C	61	GLU	3.5
1	C	71	GLU	3.5
1	E	157	GLN	3.2
1	F	72	THR	3.1
1	C	38	ILE	3.0
1	D	48	PRO	3.0
1	F	38	ILE	2.9
1	D	71	GLU	2.9
1	C	45	LEU	2.9
1	F	49	GLU	2.6
1	F	48	PRO	2.5
1	B	45	LEU	2.5
1	E	158	LYS	2.4
1	B	158	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	158	LYS	2.3
1	B	71	GLU	2.3
1	D	47	THR	2.3
1	F	47	THR	2.3
1	F	45	LEU	2.3
1	B	38	ILE	2.2
1	A	158	LYS	2.2
1	A	49	GLU	2.2
1	F	71	GLU	2.2
1	C	46	PHE	2.1
1	C	49	GLU	2.1
1	C	153	HIS	2.1

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](#)

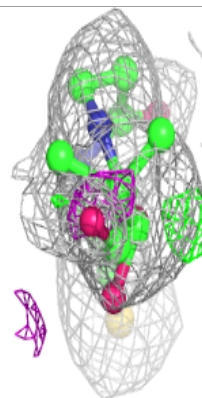
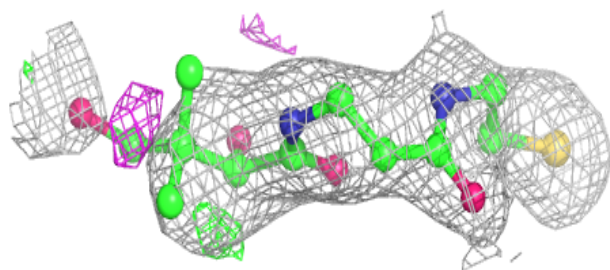
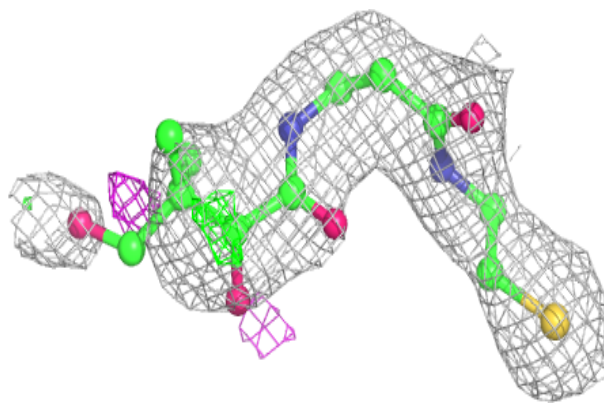
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PNY	A	501	18/18	0.85	0.21	43,65,77,78	0
2	PNY	F	506	18/18	0.86	0.18	44,58,69,69	0
2	PNY	E	505	18/18	0.87	0.17	43,56,62,66	0
2	PNY	B	502	18/18	0.90	0.13	37,60,68,69	0
2	PNY	D	504	18/18	0.92	0.14	44,48,56,57	0
2	PNY	C	503	18/18	0.94	0.13	45,55,60,60	0

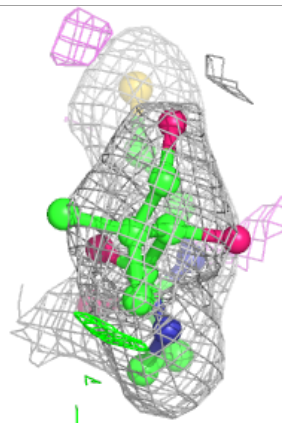
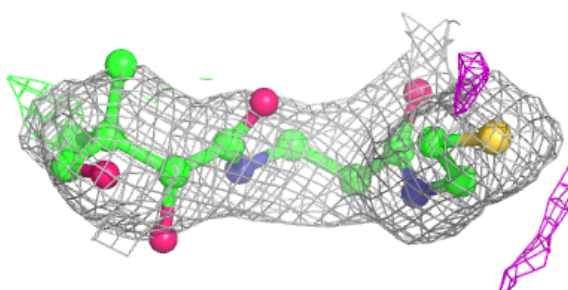
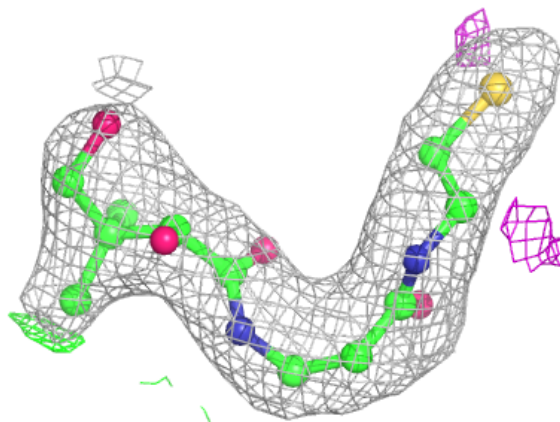
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

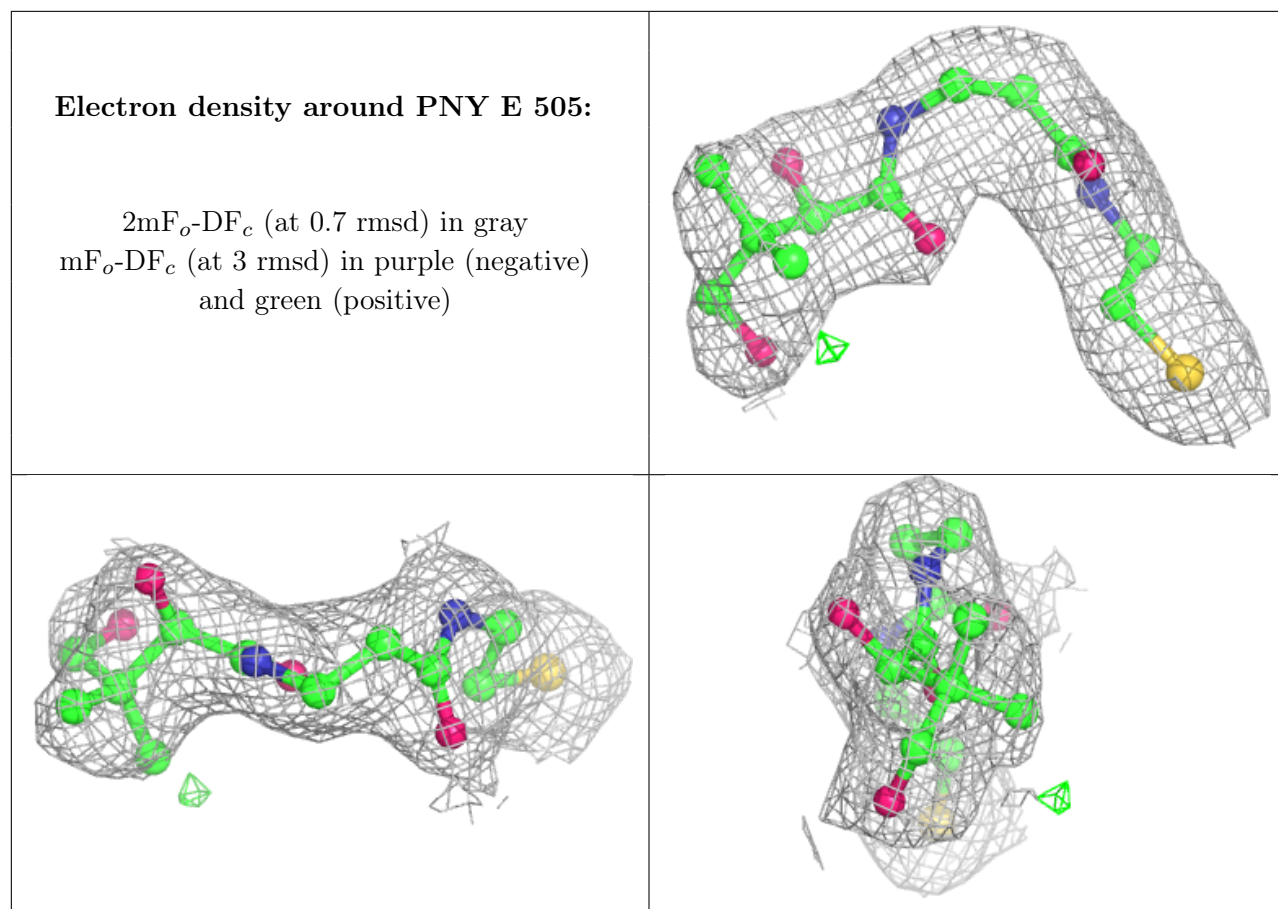
Electron density around PNY A 501:

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

**Electron density around PNY F 506:**

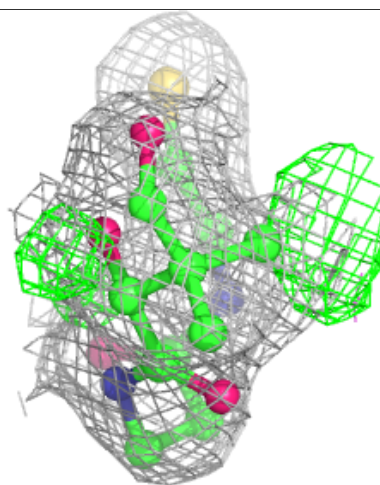
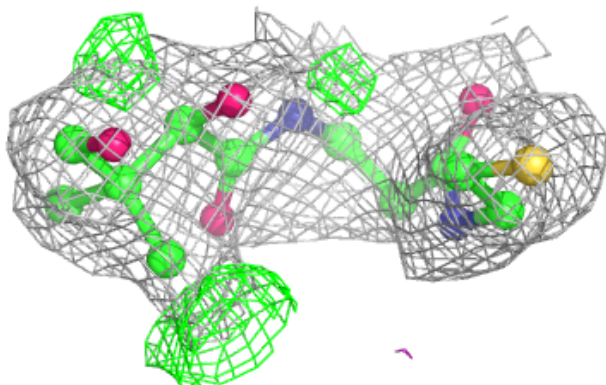
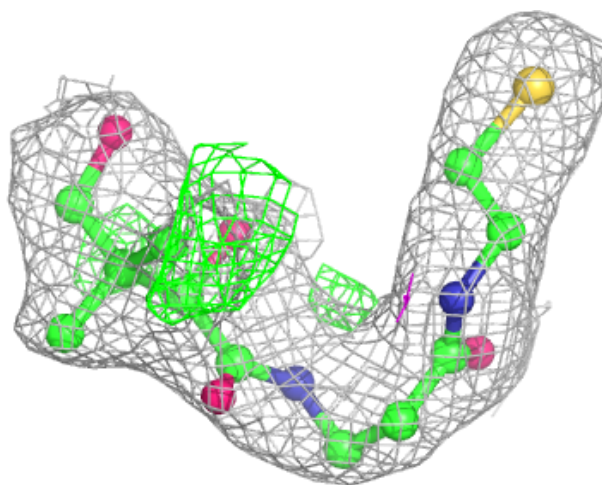
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





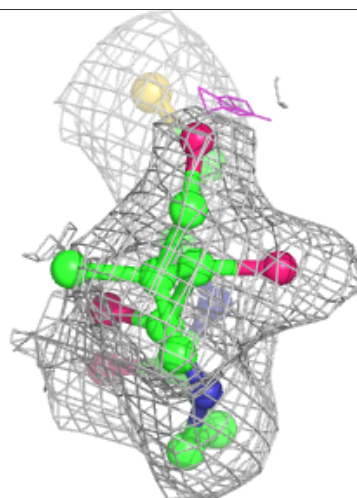
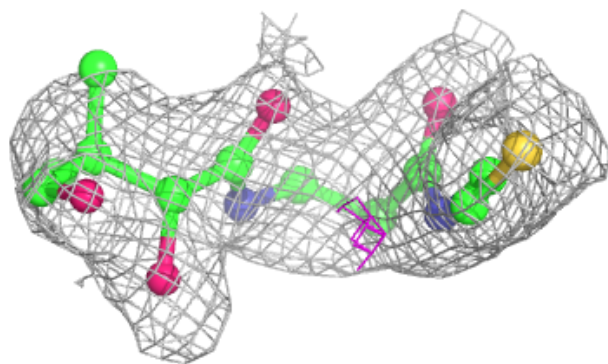
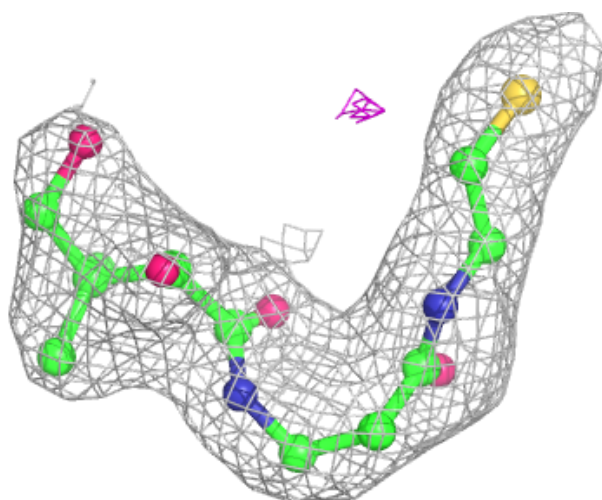
Electron density around PNY B 502:

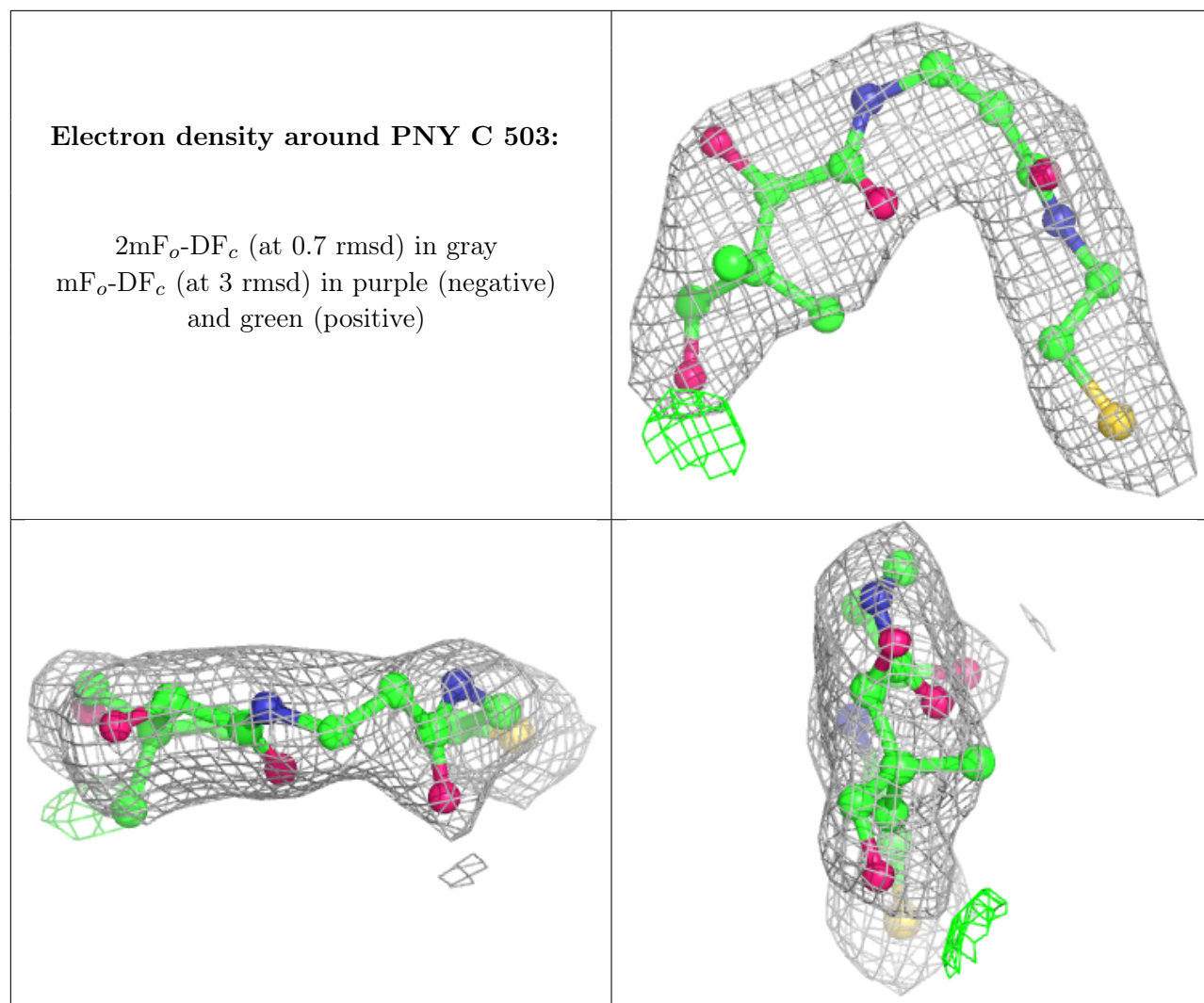
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PNY D 504:

$2mF_o-DF_c$ (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.